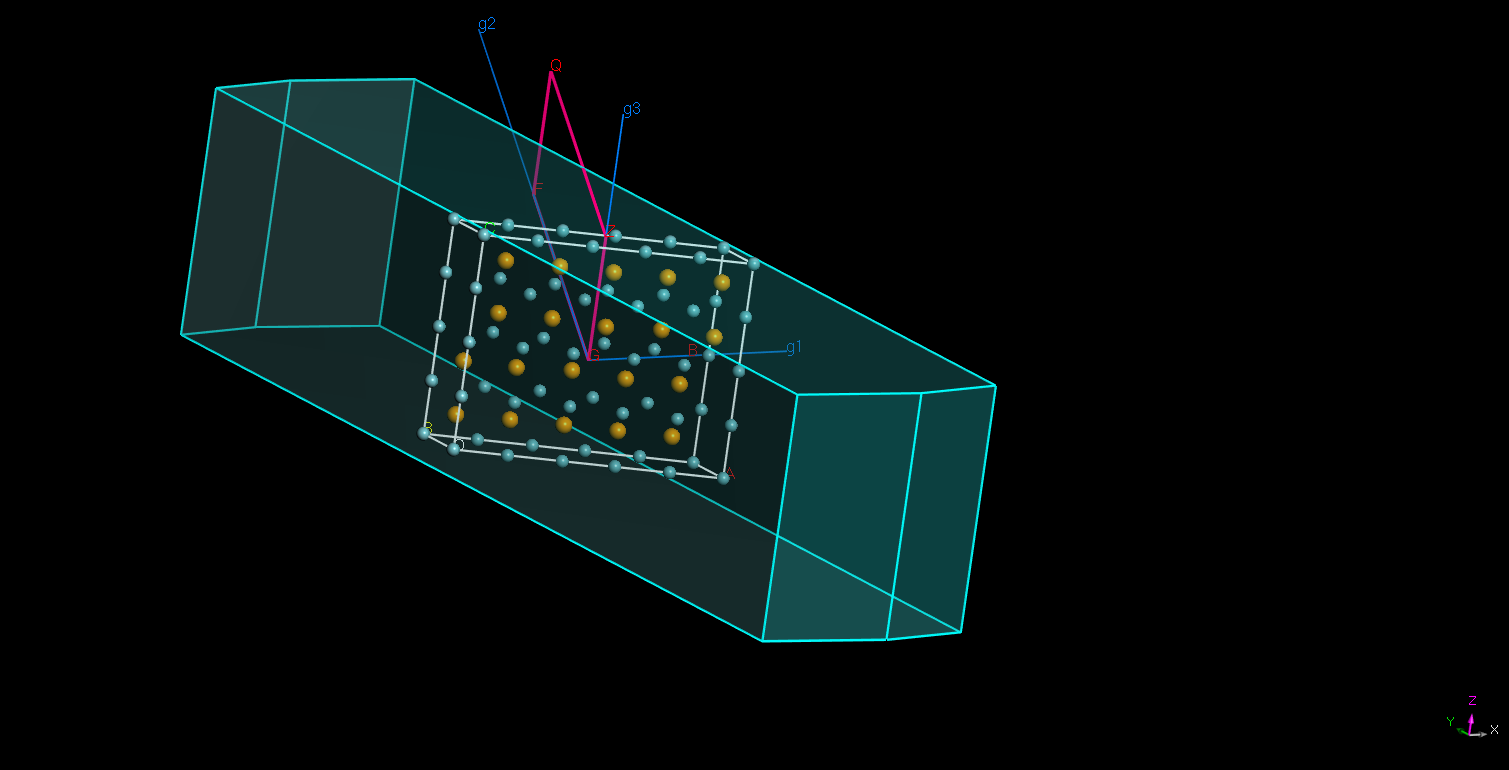
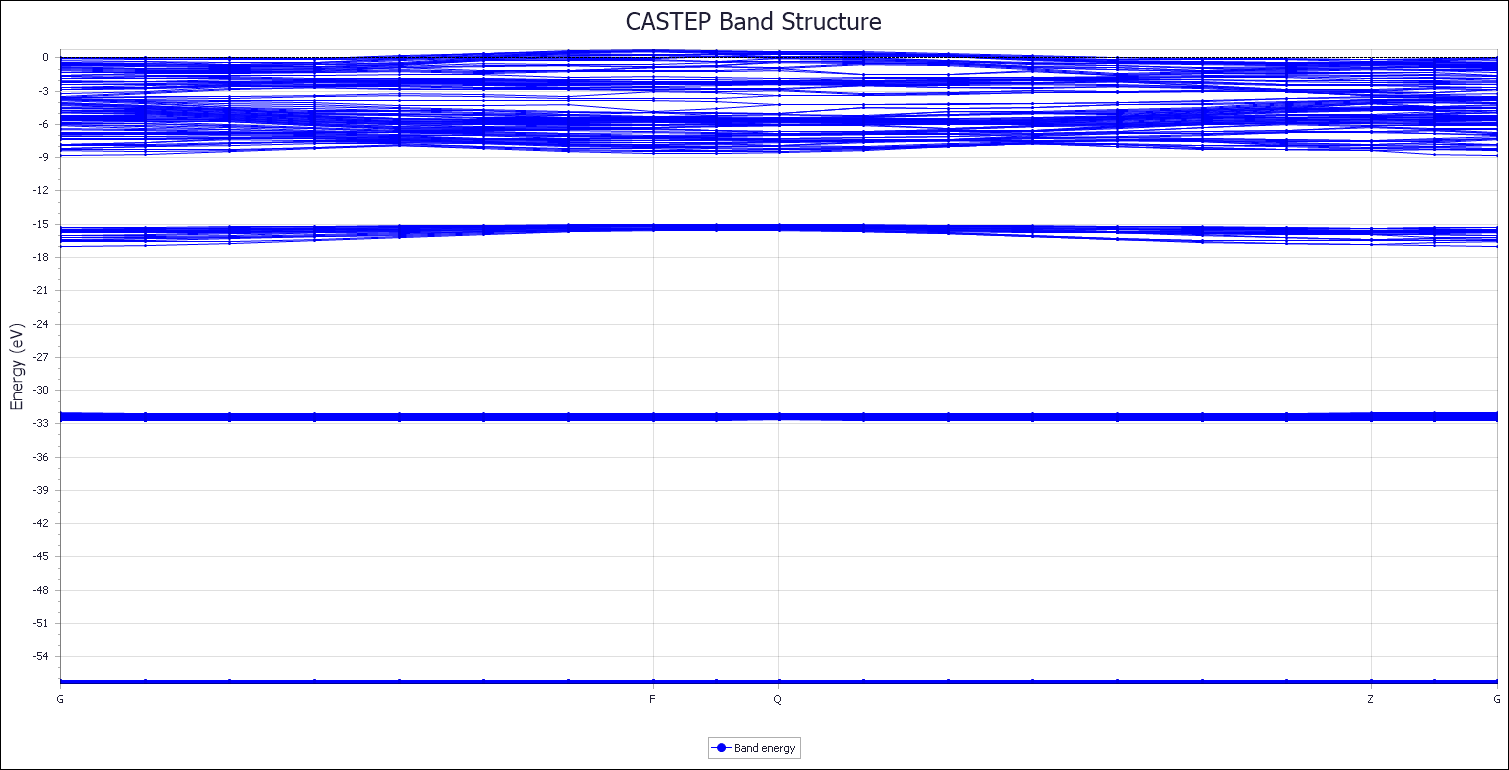
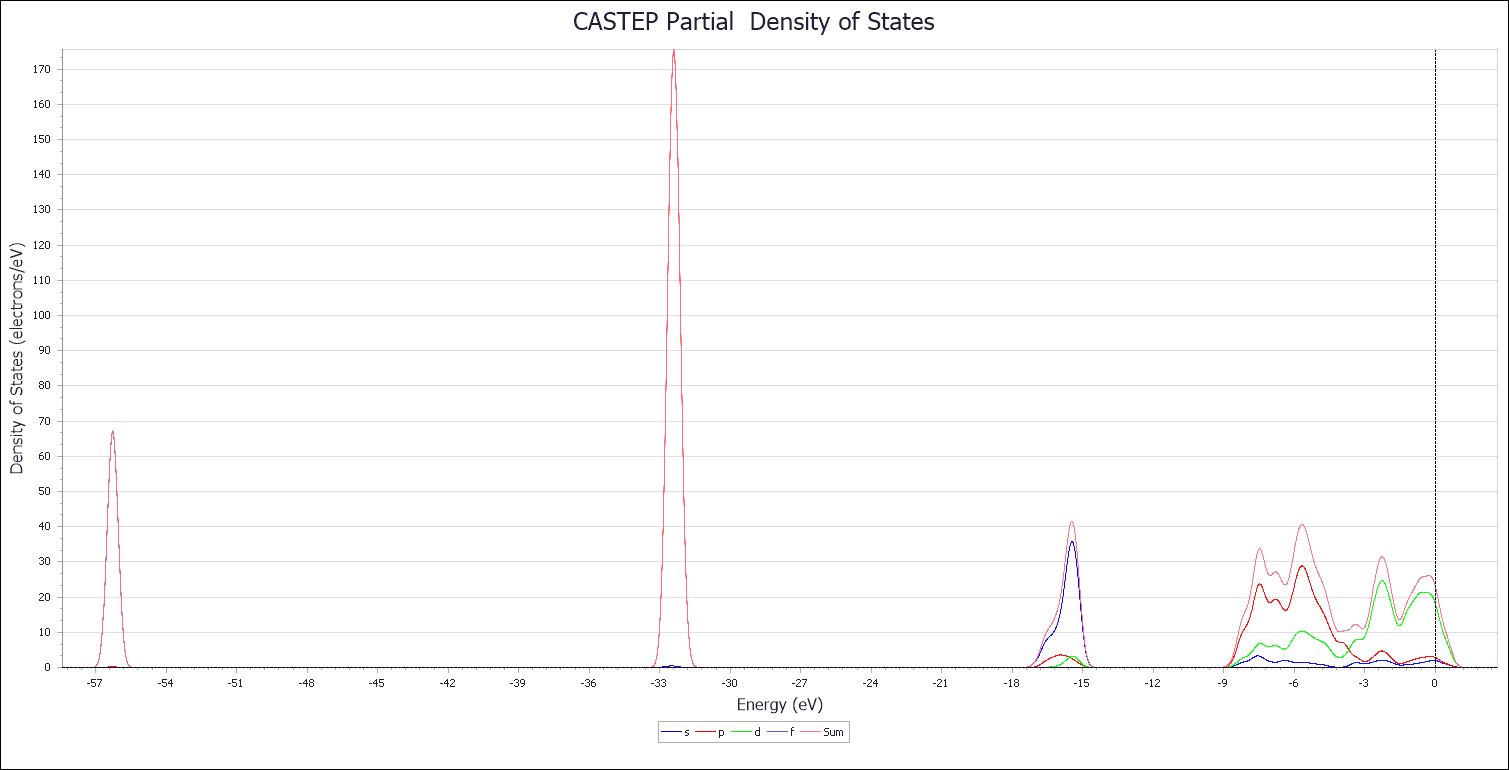
2H-Nb1.1Se2-7-UF CASTEP GeomOpt



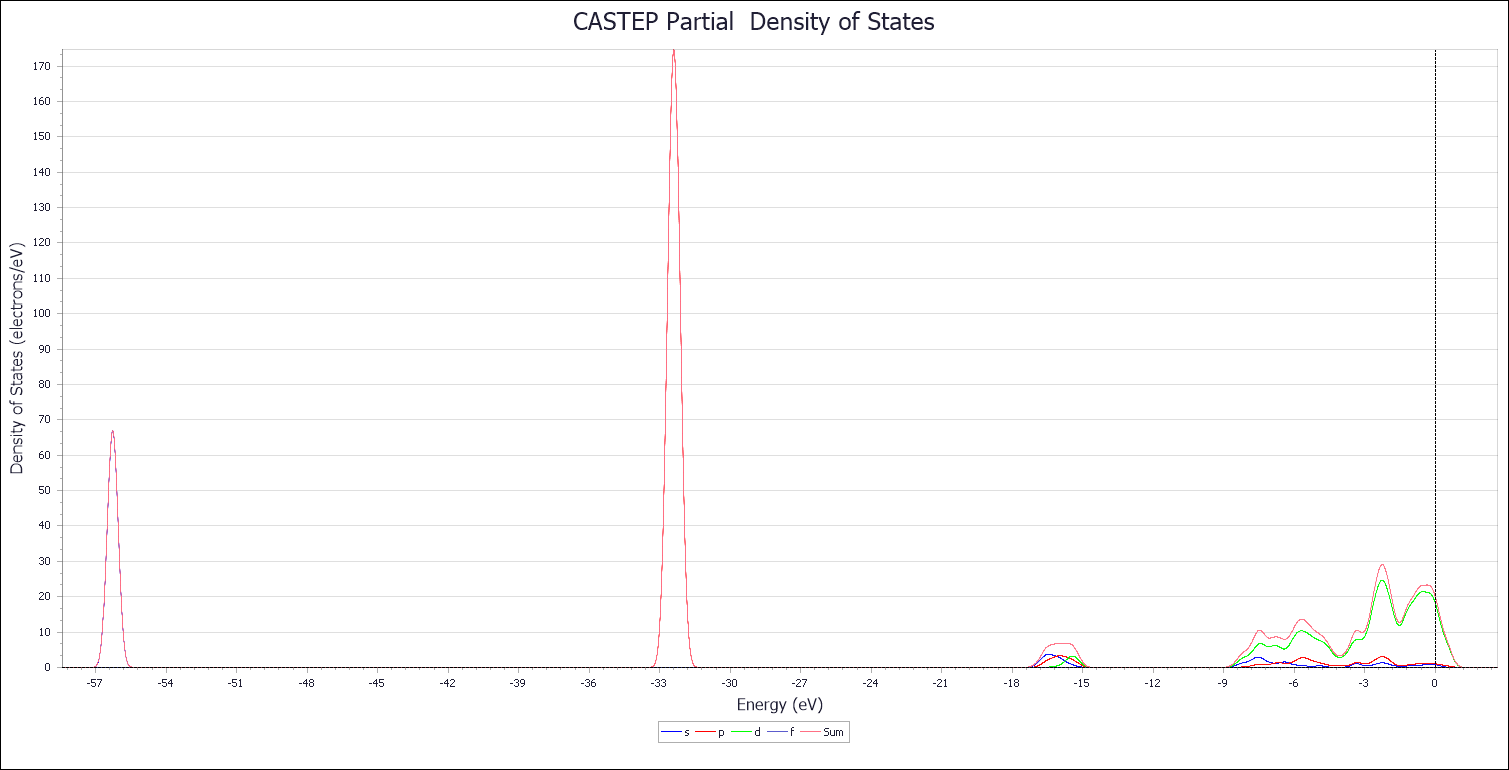
2H-Nb1.1Se2-7-UF Band Structure



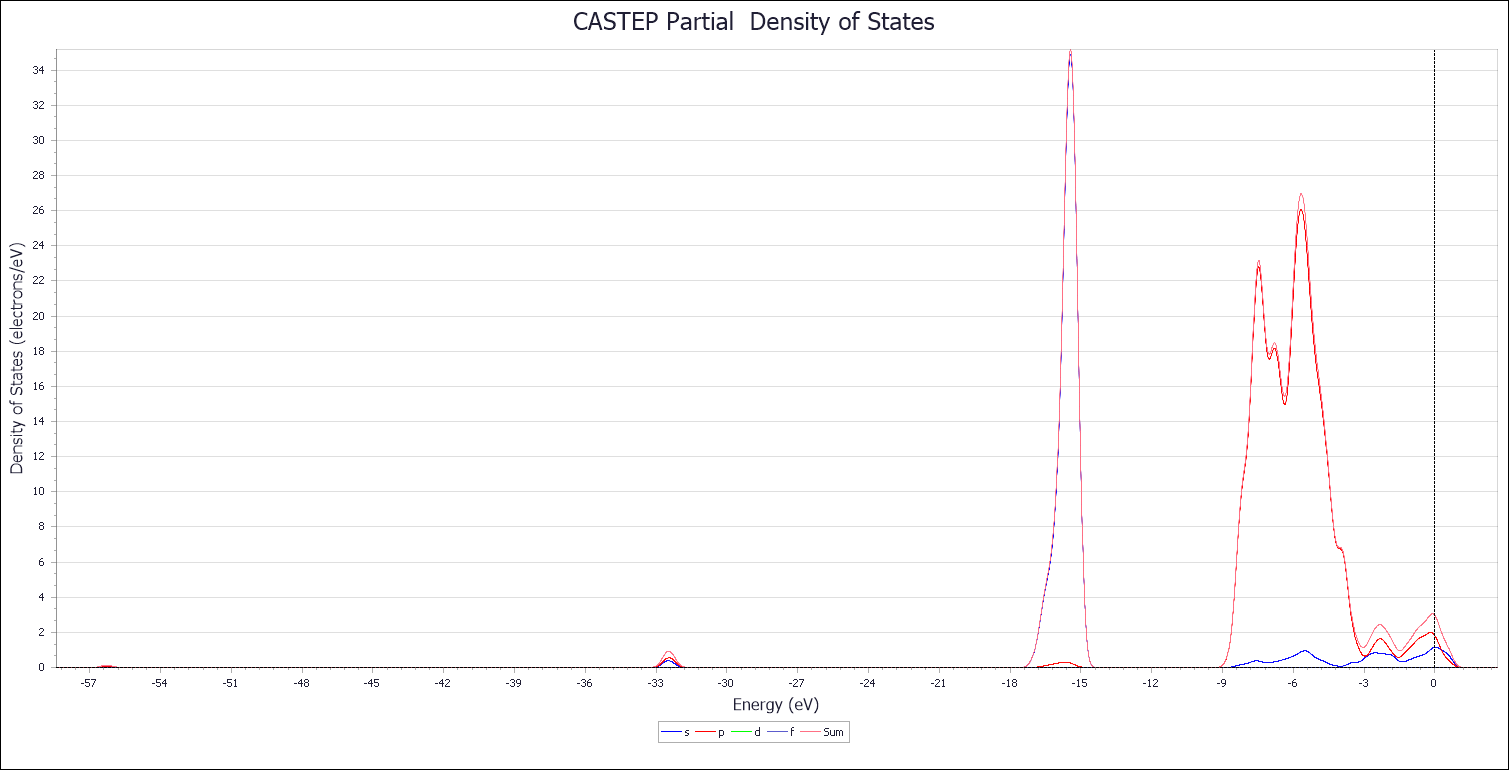
2H-Nb1.1Se2-7-UF PDOS-Total



2H-Nb1.1Se2-7-UF PDOS-Nb



2H-Nb1.1Se2-7-UF PDOS-Se



Job started on host DESKTOP-UVBHK2J

at Wed Mar 4 11:35:50 2020

+-------------------------------------------------+

| |

| CCC AA SSS TTTTT EEEEE PPPP |

| C A A S T E P P |

| C AAAA SS T EEE PPPP |

| C A A S T E P |

| CCC A A SSS T EEEEE P |

| |

+-------------------------------------------------+

| |

| Welcome to Materials Studio CASTEP version 8.0 |

| Ab Initio Total Energy Program |

| |

| Authors: |

| M. Segall, M. Probert, C. Pickard, P. Hasnip, |

| S. Clark, K. Refson, J. R. Yates, M. Payne |

| |

| Contributors: |

| P. Lindan, P. Haynes, J. White, V. Milman, |

| N. Govind, M. Gibson, P. Tulip, V. Cocula, |

| B. Montanari, D. Quigley, M. Glover, |

| L. Bernasconi, A. Perlov, M. Plummer, |

| E. McNellis, J. Meyer, J. Gale, D. Jochym |

| J. Aarons, B. Walker, R. Gillen, D. Jones |

| T. Green |

| |

| Copyright (c) 2000 - 2014 |

| |

| Please cite |

| |

| "First principles methods using CASTEP" |

| |

| Zeitschrift fuer Kristallographie |

| 220(5-6) pp. 567-570 (2005) |

| |

| S. J. Clark, M. D. Segall, C. J. Pickard, |

| P. J. Hasnip, M. J. Probert, K. Refson, |

| M. C. Payne |

| |

| in all publications arising from |

| your use of CASTEP |

| |

+-------------------------------------------------+

This version was compiled for x86\_64-windows-msvc2008 on Dec 04 2014

Code version: 6546

Intel(R) Math Kernel Library Version 11.1.2

Fundamental constants values: CODATA 2010

License checkout of MS\_castep successful

Pseudo atomic calculation performed for Se 4s2 4p4

Converged in 17 iterations to a total energy of -256.4822 eV

Pseudo atomic calculation performed for Nb 4s2 4p6 4d4 5s1

Converged in 18 iterations to a total energy of -1541.3312 eV

Calculation parallelised over 14 processes.

Data is distributed by G-vector(2-way) and k-point(7-way)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Title \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

CASTEP calculation from Materials Studio

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* General Parameters \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

output verbosity : normal (1)

write checkpoint data to : 2H-Nb1.1Se2-7-UF.check

type of calculation : geometry optimization

stress calculation : on

density difference calculation : off

electron localisation func (ELF) calculation : off

Hirshfeld analysis : on

unlimited duration calculation

timing information : on

memory usage estimate : on

write final potential to formatted file : off

write final density to formatted file : off

write BibTeX reference list : on

checkpoint writing : both castep\_bin and check files

output length unit : A

output mass unit : amu

output time unit : ps

output charge unit : e

output spin unit : hbar/2

output energy unit : eV

output force unit : eV/A

output velocity unit : A/ps

output pressure unit : GPa

output inv\_length unit : 1/A

output frequency unit : cm-1

output force constant unit : eV/A\*\*2

output volume unit : A\*\*3

output IR intensity unit : (D/A)\*\*2/amu

output dipole unit : D

output efield unit : eV/A/e

output entropy unit : J/mol/K

wavefunctions paging : none

random number generator seed : randomised (113551346)

data distribution : optimal for this architecture

optimization strategy : balance speed and memory

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Exchange-Correlation Parameters \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

using functional : Perdew Burke Ernzerhof

Divergence correction : off

relativistic treatment : Koelling-Harmon

DFT+D: Semi-empirical dispersion correction : off

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Pseudopotential Parameters \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

pseudopotential representation : reciprocal space

<beta|phi> representation : reciprocal space

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Basis Set Parameters \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

plane wave basis set cut-off : 500.0000 eV

size of standard grid : 1.5000

size of fine gmax : 17.1836 1/A

largest prime factor in FFT : 5

finite basis set correction : automatic

number of sample energies : 3

sample spacing : 5.0000 eV

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Electronic Parameters \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

number of electrons : 380.0

net charge of system : 0.000

net spin of system : 0.000

number of up spins : 190.0

number of down spins : 190.0

treating system as non-spin-polarized

number of bands : 190

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Electronic Minimization Parameters \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Method: Treating system as non-metallic,

and number of SD steps : 1

and number of CG steps : 4

total energy / atom convergence tol. : 0.2000E-05 eV

eigen-energy convergence tolerance : 0.4211E-06 eV

max force / atom convergence tol. : ignored

convergence tolerance window : 3 cycles

max. number of SCF cycles : 100

periodic dipole correction : NONE

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Density Mixing Parameters \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

density-mixing scheme : Pulay

max. length of mixing history : 20

charge density mixing amplitude : 0.5000

cut-off energy for mixing : 500.0 eV

charge density mixing g-vector : 1.500 1/A

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Population Analysis Parameters \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Population analysis with cutoff : 3.000 A

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Geometry Optimization Parameters \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

optimization method : BFGS

variable cell method : fixed basis quality

max. number of steps : 100

estimated bulk modulus : 500.0 GPa

estimated <frequency> : 1668. cm-1

geom line minimiser : on

with line minimiser tolerance : 0.4000

total energy convergence tolerance : 0.5000E-05 eV/atom

max ionic |force| tolerance : 0.1000E-01 eV/A

max ionic |displacement| tolerance : 0.5000E-03 A

max |stress component| tolerance : 0.2000E-01 GPa

convergence tolerance window : 2 steps

backup results every : 5 steps

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.9281129 -8.6187500 0.0000000 0.4208962 0.0000000 0.0000000

0.0000000 3.4475000 0.0000000 1.0522404 1.8225338 0.0000000

0.0000000 0.0000000 12.5702000 0.0000000 0.0000000 0.4998477

Lattice parameters(A) Cell Angles

a = 17.237500 alpha = 90.000000

b = 3.447500 beta = 90.000000

c = 12.570200 gamma = 120.000000

Current cell volume = 646.921185 A\*\*3

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Cell Contents

-------------------------------

Total number of ions in cell = 40

Total number of species in cell = 2

Max number of any one species = 20

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066667 0.666667 0.117300 x

x Se 2 0.133333 0.333333 0.617300 x

x Se 3 0.133333 0.333333 0.882700 x

x Se 4 0.066667 0.666667 0.382700 x

x Se 5 0.266667 0.666667 0.117300 x

x Se 6 0.333333 0.333333 0.617300 x

x Se 7 0.333333 0.333333 0.882700 x

x Se 8 0.266667 0.666667 0.382700 x

x Se 9 0.466667 0.666667 0.117300 x

x Se 10 0.533333 0.333333 0.617300 x

x Se 11 0.533333 0.333333 0.882700 x

x Se 12 0.466667 0.666667 0.382700 x

x Se 13 0.666667 0.666667 0.117300 x

x Se 14 0.733333 0.333333 0.617300 x

x Se 15 0.733333 0.333333 0.882700 x

x Se 16 0.666667 0.666667 0.382700 x

x Se 17 0.866667 0.666667 0.117300 x

x Se 18 0.933333 0.333333 0.617300 x

x Se 19 0.933333 0.333333 0.882700 x

x Se 20 0.866667 0.666667 0.382700 x

x Nb 1 0.000000 0.000000 0.250000 x

x Nb 2 0.000000 0.000000 0.750000 x

x Nb 3 0.000000 0.000000 0.000000 x

x Nb 4 0.000000 0.000000 0.500000 x

x Nb 5 0.200000 0.000000 0.250000 x

x Nb 6 0.200000 0.000000 0.750000 x

x Nb 7 0.200000 0.000000 0.000000 x

x Nb 8 0.200000 0.000000 0.500000 x

x Nb 9 0.400000 0.000000 0.250000 x

x Nb 10 0.400000 0.000000 0.750000 x

x Nb 11 0.400000 0.000000 0.000000 x

x Nb 12 0.400000 0.000000 0.500000 x

x Nb 13 0.600000 0.000000 0.250000 x

x Nb 14 0.600000 0.000000 0.750000 x

x Nb 15 0.600000 0.000000 0.000000 x

x Nb 16 0.600000 0.000000 0.500000 x

x Nb 17 0.800000 0.000000 0.250000 x

x Nb 18 0.800000 0.000000 0.750000 x

x Nb 19 0.800000 0.000000 0.000000 x

x Nb 20 0.800000 0.000000 0.500000 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

No user defined ionic velocities

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Details of Species

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Mass of species in AMU

Se 78.9599991

Nb 92.9059982

Electric Quadrupole Moment (Barn)

Se 1.0000000 No Isotope Defined

Nb -0.3200000 Isotope 93

Files used for pseudopotentials:

Se Se\_00.usp

Nb Nb\_00PBE.usp

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k-Points For BZ Sampling

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MP grid size for SCF calculation is 1 7 2

with an offset of 0.000 0.000 0.000

Number of kpoints used = 7

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Symmetry and Constraints

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Cell is a supercell containing 5 primitive cells

Maximum deviation from symmetry = 0.00000 ANG

There are no symmetry operations specified or generated for this cell

There are no ionic constraints specified or generated for this cell

Point group of crystal = 1: C1, 1, 1

Space group of crystal = 194: P6\_3/mmc, -P 6c 2c

Centre of mass is NOT constrained

Number of cell constraints= 0

Cell constraints are: 1 2 3 4 5 6

External pressure/stress (GPa)

0.00000 0.00000 0.00000

0.00000 0.00000

0.00000

+---------------- MEMORY AND SCRATCH DISK ESTIMATES PER PROCESS --------------+

| Memory Disk |

| Model and support data 156.1 MB 111.0 MB |

| Electronic energy minimisation requirements 80.4 MB 0.0 MB |

| ----------------------------- |

| Approx. total storage required per process 236.5 MB 111.0 MB |

| |

| Requirements will fluctuate during execution and may exceed these estimates |

+-----------------------------------------------------------------------------+

Calculating finite basis set correction with 3 cut-off energies.

Calculating total energy with cut-off of 490.000eV.

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.63678348E+004 5.38 <-- SCF

1 -3.52131684E+004 2.21133340E+002 33.92 <-- SCF

2 -3.62201200E+004 2.51737897E+001 55.92 <-- SCF

3 -3.62583210E+004 9.55022989E-001 77.42 <-- SCF

4 -3.62517267E+004 -1.64856565E-001 102.53 <-- SCF

5 -3.62518734E+004 3.66673397E-003 126.95 <-- SCF

6 -3.62518775E+004 1.04035660E-004 151.77 <-- SCF

7 -3.62519337E+004 1.40366822E-003 176.11 <-- SCF

8 -3.62519645E+004 7.70457788E-004 200.34 <-- SCF

9 -3.62519834E+004 4.73407943E-004 221.84 <-- SCF

10 -3.62519962E+004 3.20245002E-004 239.89 <-- SCF

11 -3.62520050E+004 2.18352504E-004 258.16 <-- SCF

12 -3.62520110E+004 1.51304423E-004 276.64 <-- SCF

13 -3.62520153E+004 1.07785288E-004 293.36 <-- SCF

14 -3.62520184E+004 7.55772050E-005 309.81 <-- SCF

15 -3.62520205E+004 5.33411224E-005 324.92 <-- SCF

16 -3.62520220E+004 3.71542284E-005 340.20 <-- SCF

17 -3.62520229E+004 2.35020778E-005 355.41 <-- SCF

18 -3.62520236E+004 1.67067601E-005 370.72 <-- SCF

19 -3.62520240E+004 1.13048493E-005 385.53 <-- SCF

20 -3.62520243E+004 7.52858921E-006 400.72 <-- SCF

21 -3.62520245E+004 4.55694836E-006 415.78 <-- SCF

22 -3.62520246E+004 2.06818106E-006 431.36 <-- SCF

23 -3.62520246E+004 1.30994241E-006 447.19 <-- SCF

24 -3.62520247E+004 1.85426397E-006 462.27 <-- SCF

25 -3.62520248E+004 9.94963132E-007 477.44 <-- SCF

26 -3.62520248E+004 9.52716635E-007 492.55 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36252.02480124 eV

(energy not corrected for finite basis set)

Calculating total energy with cut-off of 495.000eV.

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62520244E+004 498.89 <-- SCF

1 -3.62520344E+004 2.51613655E-004 526.27 <-- SCF

2 -3.62520347E+004 7.73555550E-006 545.80 <-- SCF

3 -3.62520336E+004 -2.86352909E-005 571.34 <-- SCF

4 -3.62520298E+004 -9.53823668E-005 596.02 <-- SCF

5 -3.62520300E+004 5.70035397E-006 614.83 <-- SCF

6 -3.62520300E+004 -8.18212732E-007 632.56 <-- SCF

7 -3.62520299E+004 -6.60317679E-007 648.98 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36252.02994502 eV

(energy not corrected for finite basis set)

Calculating total energy with cut-off of 500.000eV.

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62520298E+004 655.17 <-- SCF

1 -3.62520401E+004 2.58120005E-004 681.11 <-- SCF

2 -3.62520404E+004 7.99107083E-006 698.84 <-- SCF

3 -3.62520389E+004 -3.78625247E-005 722.52 <-- SCF

4 -3.62520346E+004 -1.06409229E-004 746.91 <-- SCF

5 -3.62520349E+004 6.77515890E-006 766.39 <-- SCF

6 -3.62520349E+004 -1.33452675E-006 782.83 <-- SCF

7 -3.62520348E+004 -5.95016614E-007 800.34 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36252.03482872 eV

(energy not corrected for finite basis set)

For future reference: finite basis dEtot/dlog(Ecut) = -0.495824eV

Total energy corrected for finite basis set = -36252.034869 eV

+---------------- MEMORY AND SCRATCH DISK ESTIMATES PER PROCESS --------------+

| Memory Disk |

| Model and support data 156.1 MB 111.0 MB |

| Electronic energy minimisation requirements 80.4 MB 0.0 MB |

| Geometry minimisation requirements 105.7 MB 0.0 MB |

| ----------------------------- |

| Approx. total storage required per process 342.2 MB 111.0 MB |

| |

| Requirements will fluctuate during execution and may exceed these estimates |

+-----------------------------------------------------------------------------+

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.14682 -0.12229 2.27022 \*

\* Se 2 0.03823 0.25214 2.23537 \*

\* Se 3 0.03802 0.25226 -2.23674 \*

\* Se 4 -0.14668 -0.12236 -2.26911 \*

\* Se 5 -0.27952 0.06111 2.04337 \*

\* Se 6 0.00581 0.20452 2.26846 \*

\* Se 7 0.00628 0.20452 -2.26888 \*

\* Se 8 -0.28025 0.06120 -2.04229 \*

\* Se 9 0.40401 -0.25191 2.16124 \*

\* Se 10 -0.40631 0.25192 2.15990 \*

\* Se 11 -0.40624 0.25196 -2.16010 \*

\* Se 12 0.40399 -0.25204 -2.16117 \*

\* Se 13 -0.00646 -0.20452 2.26962 \*

\* Se 14 0.27990 -0.06127 2.04144 \*

\* Se 15 0.27938 -0.06115 -2.04151 \*

\* Se 16 -0.00698 -0.20438 -2.26967 \*

\* Se 17 -0.03700 -0.25204 2.23715 \*

\* Se 18 0.14879 0.12255 2.26837 \*

\* Se 19 0.14844 0.12229 -2.26895 \*

\* Se 20 -0.03638 -0.25210 -2.23661 \*

\* Nb 1 0.02595 0.00579 0.00240 \*

\* Nb 2 -0.02055 -0.00544 -0.00250 \*

\* Nb 3 0.00131 -0.00006 0.00184 \*

\* Nb 4 0.00382 0.00000 -0.00180 \*

\* Nb 5 0.03330 0.00697 0.00287 \*

\* Nb 6 -0.01500 -0.00538 -0.00263 \*

\* Nb 7 0.00591 0.00158 -0.00068 \*

\* Nb 8 0.00523 0.00151 0.00050 \*

\* Nb 9 0.03035 0.00480 0.00149 \*

\* Nb 10 -0.01982 -0.00735 -0.00139 \*

\* Nb 11 0.00168 0.00098 0.00252 \*

\* Nb 12 -0.00106 0.00074 -0.00274 \*

\* Nb 13 0.01548 0.00729 0.00016 \*

\* Nb 14 -0.03428 -0.00473 0.00005 \*

\* Nb 15 -0.00365 -0.00135 0.00075 \*

\* Nb 16 -0.00449 -0.00099 -0.00092 \*

\* Nb 17 0.01582 0.00557 0.00007 \*

\* Nb 18 -0.03201 -0.00708 -0.00048 \*

\* Nb 19 -0.00486 -0.00149 0.00457 \*

\* Nb 20 -0.00331 -0.00175 -0.00419 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -15.572091 -0.660980 0.001478 \*

\* y -0.660980 -14.193678 0.000441 \*

\* z 0.001478 0.000441 -32.095749 \*

\* \*

\* Pressure: 20.6205 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

BFGS: finished iteration 0 with enthalpy= -3.62520349E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 0.000000E+000 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.278863E+000 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 0.000000E+000 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.209575E+001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 1 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.150021 | -36252.034869 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 1 with trial guess (lambda= 0.983723)

--------------------------------------------------------------------------------

+---------------- MEMORY AND SCRATCH DISK ESTIMATES PER PROCESS --------------+

| Memory Disk |

| Model and support data 160.1 MB 111.0 MB |

| Electronic energy minimisation requirements 83.5 MB 0.0 MB |

| Geometry minimisation requirements 109.9 MB 0.0 MB |

| ----------------------------- |

| Approx. total storage required per process 353.6 MB 111.0 MB |

| |

| Requirements will fluctuate during execution and may exceed these estimates |

+-----------------------------------------------------------------------------+

-------------------------------

Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

15.0768289 -8.6925060 -0.0000120 0.4166413 -0.0001789 0.0000004

0.0014944 3.4795908 -0.0000010 1.0408285 1.8052783 0.0000015

-0.0000122 -0.0000036 12.8347886 0.0000005 0.0000001 0.4895433

Lattice parameters(A) Cell Angles

a = 17.403173 alpha = 90.000033

b = 3.479591 beta = 90.000078

c = 12.834789 gamma = 119.940878

Current cell volume = 673.495078 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066656 0.666599 0.117502 x

x Se 2 0.133336 0.333422 0.617499 x

x Se 3 0.133336 0.333422 0.882501 x

x Se 4 0.066656 0.666599 0.382498 x

x Se 5 0.266646 0.666634 0.117482 x

x Se 6 0.333334 0.333401 0.617502 x

x Se 7 0.333334 0.333401 0.882498 x

x Se 8 0.266646 0.666634 0.382518 x

x Se 9 0.466697 0.666661 0.117492 x

x Se 10 0.533303 0.333339 0.617492 x

x Se 11 0.533303 0.333339 0.882508 x

x Se 12 0.466697 0.666661 0.382508 x

x Se 13 0.666666 0.666599 0.117502 x

x Se 14 0.733354 0.333366 0.617482 x

x Se 15 0.733354 0.333366 0.882518 x

x Se 16 0.666666 0.666599 0.382498 x

x Se 17 0.866664 0.666578 0.117499 x

x Se 18 0.933344 0.333401 0.617502 x

x Se 19 0.933344 0.333401 0.882498 x

x Se 20 0.866664 0.666578 0.382501 x

x Nb 1 0.000002 0.000007 0.250000 x

x Nb 2 -0.000002 -0.000006 0.750000 x

x Nb 3 0.000000 0.000000 0.000000 x

x Nb 4 0.000000 0.000001 0.500000 x

x Nb 5 0.200002 0.000009 0.250000 x

x Nb 6 0.199999 -0.000005 0.750000 x

x Nb 7 0.200000 0.000002 -0.000000 x

x Nb 8 0.200000 0.000001 0.500000 x

x Nb 9 0.400002 0.000007 0.250000 x

x Nb 10 0.399999 -0.000006 0.750000 x

x Nb 11 0.400000 0.000001 0.000000 x

x Nb 12 0.400000 0.000000 0.500000 x

x Nb 13 0.600001 0.000005 0.250000 x

x Nb 14 0.599997 -0.000008 0.750000 x

x Nb 15 0.600000 -0.000001 0.000000 x

x Nb 16 0.600000 -0.000001 0.500000 x

x Nb 17 0.800001 0.000005 0.250000 x

x Nb 18 0.799998 -0.000008 0.750000 x

x Nb 19 0.800000 -0.000001 0.000000 x

x Nb 20 0.800000 -0.000001 0.500000 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62463235E+004 892.09 <-- SCF

1 -3.62606565E+004 3.58324137E-001 915.98 <-- SCF

2 -3.62609162E+004 6.49171644E-003 948.22 <-- SCF

3 -3.62556475E+004 -1.31717263E-001 974.83 <-- SCF

4 -3.62552697E+004 -9.44390839E-003 1001.36 <-- SCF

5 -3.62552265E+004 -1.08088207E-003 1028.27 <-- SCF

6 -3.62552280E+004 3.65581928E-005 1057.84 <-- SCF

7 -3.62552271E+004 -2.11502987E-005 1079.81 <-- SCF

8 -3.62552272E+004 2.15157336E-006 1098.14 <-- SCF

9 -3.62552272E+004 -6.50088923E-007 1116.05 <-- SCF

10 -3.62552272E+004 8.84137926E-008 1132.48 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36255.22718083 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.19331 -0.08186 1.91883 \*

\* Se 2 0.05459 0.28606 1.94014 \*

\* Se 3 0.05423 0.28608 -1.94001 \*

\* Se 4 -0.19315 -0.08186 -1.91927 \*

\* Se 5 -0.27021 0.10535 1.79503 \*

\* Se 6 -0.03972 0.23625 1.91814 \*

\* Se 7 -0.03968 0.23620 -1.91787 \*

\* Se 8 -0.27053 0.10535 -1.79504 \*

\* Se 9 0.43558 -0.30623 1.85835 \*

\* Se 10 -0.43728 0.30611 1.85868 \*

\* Se 11 -0.43709 0.30610 -1.85832 \*

\* Se 12 0.43554 -0.30629 -1.85873 \*

\* Se 13 0.03877 -0.23629 1.91765 \*

\* Se 14 0.26988 -0.10544 1.79527 \*

\* Se 15 0.26994 -0.10539 -1.79477 \*

\* Se 16 0.03866 -0.23625 -1.91805 \*

\* Se 17 -0.05293 -0.28600 1.93971 \*

\* Se 18 0.19490 0.08197 1.91941 \*

\* Se 19 0.19495 0.08189 -1.91870 \*

\* Se 20 -0.05297 -0.28603 -1.94018 \*

\* Nb 1 0.01015 0.00231 -0.00043 \*

\* Nb 2 -0.00834 -0.00226 0.00050 \*

\* Nb 3 0.00111 -0.00011 -0.00105 \*

\* Nb 4 0.00104 -0.00016 0.00087 \*

\* Nb 5 0.02374 0.00276 -0.00039 \*

\* Nb 6 0.00219 -0.00388 0.00044 \*

\* Nb 7 0.00867 0.00151 -0.00429 \*

\* Nb 8 0.00889 0.00151 0.00428 \*

\* Nb 9 0.02389 -0.00108 -0.00034 \*

\* Nb 10 -0.00381 -0.00562 0.00018 \*

\* Nb 11 0.00404 -0.00266 0.00320 \*

\* Nb 12 0.00419 -0.00273 -0.00305 \*

\* Nb 13 0.00201 0.00561 -0.00009 \*

\* Nb 14 -0.02496 0.00132 0.00013 \*

\* Nb 15 -0.00584 0.00277 -0.00356 \*

\* Nb 16 -0.00577 0.00292 0.00346 \*

\* Nb 17 -0.00205 0.00372 -0.00023 \*

\* Nb 18 -0.02288 -0.00260 0.00027 \*

\* Nb 19 -0.00809 -0.00148 0.00284 \*

\* Nb 20 -0.00836 -0.00157 -0.00298 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -7.740805 -0.431154 -0.000213 \*

\* y -0.431154 -6.450616 0.000046 \*

\* z -0.000213 0.000046 -19.963661 \*

\* \*

\* Pressure: 11.3850 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.150021 | -36252.034869 | <-- min BFGS

| trial step | 0.983723 | 0.089940 | -36255.227097 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 1 with line minimization (lambda= 1.475584)

--------------------------------------------------------------------------------

+---------------- MEMORY AND SCRATCH DISK ESTIMATES PER PROCESS --------------+

| Memory Disk |

| Model and support data 161.9 MB 111.0 MB |

| Electronic energy minimisation requirements 85.0 MB 0.0 MB |

| Geometry minimisation requirements 111.9 MB 0.0 MB |

| ----------------------------- |

| Approx. total storage required per process 358.8 MB 111.0 MB |

| |

| Requirements will fluctuate during execution and may exceed these estimates |

+-----------------------------------------------------------------------------+

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

15.1511869 -8.7293840 -0.0000180 0.4145461 -0.0002658 0.0000006

0.0022416 3.4956362 -0.0000015 1.0352140 1.7967730 0.0000022

-0.0000183 -0.0000055 12.9670829 0.0000007 0.0000002 0.4845489

Lattice parameters(A) Cell Angles

a = 17.486012 alpha = 90.000049

b = 3.495637 beta = 90.000117

c = 12.967083 gamma = 119.911732

Current cell volume = 687.029840 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066650 0.666566 0.117603 x

x Se 2 0.133338 0.333467 0.617599 x

x Se 3 0.133338 0.333467 0.882401 x

x Se 4 0.066650 0.666566 0.382397 x

x Se 5 0.266635 0.666618 0.117573 x

x Se 6 0.333334 0.333435 0.617603 x

x Se 7 0.333334 0.333435 0.882397 x

x Se 8 0.266635 0.666618 0.382427 x

x Se 9 0.466712 0.666658 0.117589 x

x Se 10 0.533288 0.333342 0.617588 x

x Se 11 0.533288 0.333342 0.882412 x

x Se 12 0.466712 0.666658 0.382411 x

x Se 13 0.666666 0.666565 0.117603 x

x Se 14 0.733365 0.333382 0.617573 x

x Se 15 0.733365 0.333382 0.882427 x

x Se 16 0.666666 0.666565 0.382397 x

x Se 17 0.866663 0.666534 0.117599 x

x Se 18 0.933350 0.333435 0.617603 x

x Se 19 0.933350 0.333435 0.882397 x

x Se 20 0.866663 0.666534 0.382401 x

x Nb 1 0.000003 0.000010 0.250000 x

x Nb 2 -0.000002 -0.000008 0.750000 x

x Nb 3 0.000000 0.000000 0.000000 x

x Nb 4 0.000000 0.000001 0.500000 x

x Nb 5 0.200004 0.000013 0.250000 x

x Nb 6 0.199998 -0.000007 0.750000 x

x Nb 7 0.200001 0.000002 -0.000000 x

x Nb 8 0.200001 0.000002 0.500000 x

x Nb 9 0.400003 0.000011 0.250000 x

x Nb 10 0.399998 -0.000009 0.750000 x

x Nb 11 0.400000 0.000001 0.000000 x

x Nb 12 0.400000 0.000000 0.500000 x

x Nb 13 0.600002 0.000008 0.250000 x

x Nb 14 0.599996 -0.000012 0.750000 x

x Nb 15 0.600000 -0.000002 0.000000 x

x Nb 16 0.599999 -0.000002 0.500000 x

x Nb 17 0.800002 0.000007 0.250000 x

x Nb 18 0.799996 -0.000012 0.750000 x

x Nb 19 0.799999 -0.000002 0.000001 x

x Nb 20 0.800000 -0.000002 0.499999 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62540698E+004 1225.66 <-- SCF

1 -3.62575822E+004 8.78096653E-002 1250.67 <-- SCF

2 -3.62576457E+004 1.58909491E-003 1279.38 <-- SCF

3 -3.62563518E+004 -3.23488092E-002 1305.12 <-- SCF

4 -3.62562603E+004 -2.28629717E-003 1330.52 <-- SCF

5 -3.62562504E+004 -2.48500929E-004 1357.98 <-- SCF

6 -3.62562506E+004 5.42674787E-006 1382.72 <-- SCF

7 -3.62562503E+004 -7.52943654E-006 1403.53 <-- SCF

8 -3.62562503E+004 6.79095378E-007 1421.55 <-- SCF

9 -3.62562503E+004 -1.80221548E-007 1438.64 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36256.25032761 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.22897 -0.07129 1.76268 \*

\* Se 2 0.08606 0.29618 1.80524 \*

\* Se 3 0.08593 0.29616 -1.80500 \*

\* Se 4 -0.22899 -0.07130 -1.76302 \*

\* Se 5 -0.23588 0.11360 1.71762 \*

\* Se 6 -0.05927 0.27175 1.77937 \*

\* Se 7 -0.05952 0.27178 -1.77931 \*

\* Se 8 -0.23582 0.11360 -1.71782 \*

\* Se 9 0.41724 -0.31110 1.73080 \*

\* Se 10 -0.41859 0.31115 1.73078 \*

\* Se 11 -0.41865 0.31112 -1.73094 \*

\* Se 12 0.41733 -0.31114 -1.73074 \*

\* Se 13 0.05898 -0.27184 1.77921 \*

\* Se 14 0.23539 -0.11354 1.71795 \*

\* Se 15 0.23547 -0.11351 -1.71809 \*

\* Se 16 0.05890 -0.27183 -1.77902 \*

\* Se 17 -0.08480 -0.29623 1.80499 \*

\* Se 18 0.23018 0.07141 1.76309 \*

\* Se 19 0.23038 0.07136 -1.76291 \*

\* Se 20 -0.08498 -0.29629 -1.80497 \*

\* Nb 1 0.00429 0.00006 -0.00025 \*

\* Nb 2 -0.00291 0.00013 0.00028 \*

\* Nb 3 0.00072 0.00005 -0.00030 \*

\* Nb 4 0.00044 0.00002 0.00026 \*

\* Nb 5 0.02205 -0.00031 -0.00027 \*

\* Nb 6 0.01064 -0.00194 0.00033 \*

\* Nb 7 0.01119 0.00127 -0.00355 \*

\* Nb 8 0.01148 0.00131 0.00356 \*

\* Nb 9 0.02217 -0.00523 -0.00010 \*

\* Nb 10 0.00382 -0.00405 0.00008 \*

\* Nb 11 0.00692 -0.00426 0.00439 \*

\* Nb 12 0.00724 -0.00425 -0.00433 \*

\* Nb 13 -0.00536 0.00389 0.00001 \*

\* Nb 14 -0.02274 0.00502 -0.00006 \*

\* Nb 15 -0.00814 0.00416 -0.00452 \*

\* Nb 16 -0.00810 0.00414 0.00458 \*

\* Nb 17 -0.01088 0.00209 -0.00010 \*

\* Nb 18 -0.02107 0.00032 0.00006 \*

\* Nb 19 -0.01088 -0.00120 0.00314 \*

\* Nb 20 -0.01128 -0.00125 -0.00314 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -4.397851 -0.332750 -0.000497 \*

\* y -0.332750 -3.163671 -0.000268 \*

\* z -0.000497 -0.000268 -14.705019 \*

\* \*

\* Pressure: 7.4222 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.150021 | -36252.034869 | <-- min BFGS

| trial step | 0.983723 | 0.089940 | -36255.227097 | <-- min BFGS

| line step | 1.475584 | 0.063267 | -36256.250287 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 1 with enthalpy= -3.62562503E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.053855E-001 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.831398E+000 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.945706E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.470502E+001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 2 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.074199 | -36256.250287 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 2 with trial guess (lambda= 0.817549)

--------------------------------------------------------------------------------

+---------------- MEMORY AND SCRATCH DISK ESTIMATES PER PROCESS --------------+

| Memory Disk |

| Model and support data 163.3 MB 118.8 MB |

| Electronic energy minimisation requirements 88.1 MB 0.0 MB |

| Geometry minimisation requirements 115.9 MB 0.0 MB |

| ----------------------------- |

| Approx. total storage required per process 367.2 MB 118.8 MB |

| |

| Requirements will fluctuate during execution and may exceed these estimates |

+-----------------------------------------------------------------------------+

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

15.2610049 -8.7751910 -0.0000165 0.4114563 -0.0004500 0.0000005

0.0038459 3.5167397 -0.0000009 1.0266918 1.7855279 0.0000017

-0.0000161 -0.0000033 13.2316715 0.0000006 0.0000001 0.4748595

Lattice parameters(A) Cell Angles

a = 17.604041 alpha = 90.000029

b = 3.516742 beta = 90.000107

c = 13.231672 gamma = 119.836563

Current cell volume = 710.576885 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066622 0.666448 0.117901 x

x Se 2 0.133348 0.333659 0.617901 x

x Se 3 0.133348 0.333659 0.882099 x

x Se 4 0.066622 0.666448 0.382099 x

x Se 5 0.266603 0.666597 0.117858 x

x Se 6 0.333328 0.333569 0.617903 x

x Se 7 0.333328 0.333569 0.882097 x

x Se 8 0.266603 0.666596 0.382142 x

x Se 9 0.466767 0.666623 0.117879 x

x Se 10 0.533232 0.333376 0.617879 x

x Se 11 0.533232 0.333376 0.882121 x

x Se 12 0.466767 0.666623 0.382121 x

x Se 13 0.666672 0.666431 0.117903 x

x Se 14 0.733397 0.333403 0.617858 x

x Se 15 0.733397 0.333403 0.882142 x

x Se 16 0.666672 0.666431 0.382097 x

x Se 17 0.866652 0.666342 0.117901 x

x Se 18 0.933379 0.333553 0.617901 x

x Se 19 0.933379 0.333553 0.882099 x

x Se 20 0.866652 0.666342 0.382099 x

x Nb 1 0.000004 0.000013 0.250000 x

x Nb 2 -0.000003 -0.000011 0.750000 x

x Nb 3 0.000000 0.000001 0.000000 x

x Nb 4 0.000001 0.000001 0.500000 x

x Nb 5 0.200007 0.000021 0.250000 x

x Nb 6 0.199999 -0.000006 0.750000 x

x Nb 7 0.200002 0.000007 -0.000001 x

x Nb 8 0.200002 0.000006 0.500001 x

x Nb 9 0.400007 0.000017 0.250000 x

x Nb 10 0.399998 -0.000012 0.750000 x

x Nb 11 0.400001 0.000001 0.000001 x

x Nb 12 0.400001 0.000000 0.499999 x

x Nb 13 0.600002 0.000010 0.250000 x

x Nb 14 0.599993 -0.000018 0.750000 x

x Nb 15 0.599999 -0.000002 -0.000000 x

x Nb 16 0.599999 -0.000002 0.500000 x

x Nb 17 0.800001 0.000007 0.250000 x

x Nb 18 0.799993 -0.000021 0.750000 x

x Nb 19 0.799998 -0.000006 0.000001 x

x Nb 20 0.799998 -0.000006 0.499999 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62503772E+004 1532.56 <-- SCF

1 -3.62612520E+004 2.71871289E-001 1559.03 <-- SCF

2 -3.62615723E+004 8.00653631E-003 1594.31 <-- SCF

3 -3.62579881E+004 -8.96040387E-002 1623.14 <-- SCF

4 -3.62574207E+004 -1.41860227E-002 1650.64 <-- SCF

5 -3.62572269E+004 -4.84416355E-003 1678.53 <-- SCF

6 -3.62572266E+004 -8.40830425E-006 1707.70 <-- SCF

7 -3.62572257E+004 -2.14593182E-005 1732.25 <-- SCF

8 -3.62572258E+004 2.06299066E-006 1756.16 <-- SCF

9 -3.62572256E+004 -4.45284101E-006 1776.48 <-- SCF

10 -3.62572256E+004 -1.11537812E-007 1794.45 <-- SCF

11 -3.62572256E+004 1.32453945E-007 1811.53 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36257.22561082 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.06059 -0.00205 1.54829 \*

\* Se 2 -0.06168 0.00270 1.39965 \*

\* Se 3 -0.06049 0.00187 -1.54915 \*

\* Se 4 0.06166 -0.00310 -1.39867 \*

\* Se 5 0.06089 -0.00269 1.55658 \*

\* Se 6 -0.06131 0.00205 1.39673 \*

\* Se 7 -0.05994 0.00112 -1.54656 \*

\* Se 8 0.06251 -0.00446 -1.41128 \*

\* Se 9 0.05453 -0.00167 1.55313 \*

\* Se 10 -0.05547 0.00231 1.40674 \*

\* Se 11 -0.05455 0.00168 -1.55314 \*

\* Se 12 0.05539 -0.00230 -1.40667 \*

\* Se 13 0.05997 -0.00113 1.54652 \*

\* Se 14 -0.06256 0.00445 1.41124 \*

\* Se 15 -0.06092 0.00268 -1.55652 \*

\* Se 16 0.06130 -0.00204 -1.39669 \*

\* Se 17 0.06052 -0.00187 1.54920 \*

\* Se 18 -0.06158 0.00309 1.39857 \*

\* Se 19 -0.06056 0.00205 -1.54821 \*

\* Se 20 0.06177 -0.00272 -1.39971 \*

\* Nb 1 -0.00635 -0.00591 0.00912 \*

\* Nb 2 0.00606 0.00595 -0.00911 \*

\* Nb 3 -0.00011 0.00000 -0.00009 \*

\* Nb 4 -0.00014 0.00002 0.00008 \*

\* Nb 5 -0.00664 -0.00020 0.00904 \*

\* Nb 6 0.00384 0.01024 -0.00908 \*

\* Nb 7 -0.00490 0.00656 -0.00113 \*

\* Nb 8 -0.00490 0.00653 0.00108 \*

\* Nb 9 -0.00100 -0.00848 0.00902 \*

\* Nb 10 -0.00345 0.00931 -0.00902 \*

\* Nb 11 -0.00627 -0.00056 0.00622 \*

\* Nb 12 -0.00621 -0.00060 -0.00615 \*

\* Nb 13 0.00369 -0.00934 0.00901 \*

\* Nb 14 0.00123 0.00844 -0.00904 \*

\* Nb 15 0.00642 0.00055 -0.00624 \*

\* Nb 16 0.00641 0.00058 0.00617 \*

\* Nb 17 -0.00398 -0.01022 0.00911 \*

\* Nb 18 0.00657 0.00020 -0.00907 \*

\* Nb 19 0.00483 -0.00654 0.00101 \*

\* Nb 20 0.00482 -0.00651 -0.00097 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.633783 -0.195035 -0.000800 \*

\* y -0.195035 1.701546 0.004026 \*

\* z -0.000800 0.004026 -6.511310 \*

\* \*

\* Pressure: 1.3920 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.074199 | -36256.250287 | <-- min BFGS

| trial step | 0.817549 | 0.028197 | -36257.225607 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 2 with line minimization (lambda= 1.226323)

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+---------------- MEMORY AND SCRATCH DISK ESTIMATES PER PROCESS --------------+

| Memory Disk |

| Model and support data 165.1 MB 118.8 MB |

| Electronic energy minimisation requirements 89.5 MB 0.0 MB |

| Geometry minimisation requirements 117.7 MB 0.0 MB |

| ----------------------------- |

| Approx. total storage required per process 372.2 MB 118.8 MB |

| |

| Requirements will fluctuate during execution and may exceed these estimates |

+-----------------------------------------------------------------------------+

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

15.3159140 -8.7980945 -0.0000158 0.4099287 -0.0005402 0.0000005

0.0046480 3.5272914 -0.0000006 1.0224819 1.7799586 0.0000014

-0.0000150 -0.0000023 13.3639658 0.0000005 0.0000001 0.4701587

Lattice parameters(A) Cell Angles

a = 17.663060 alpha = 90.000019

b = 3.527294 beta = 90.000102

c = 13.363966 gamma = 119.799341

Current cell volume = 722.517275 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066607 0.666389 0.118050 x

x Se 2 0.133353 0.333755 0.618052 x

x Se 3 0.133353 0.333755 0.881948 x

x Se 4 0.066607 0.666389 0.381950 x

x Se 5 0.266586 0.666586 0.118001 x

x Se 6 0.333325 0.333636 0.618053 x

x Se 7 0.333325 0.333636 0.881947 x

x Se 8 0.266586 0.666586 0.381999 x

x Se 9 0.466795 0.666605 0.118024 x

x Se 10 0.533204 0.333393 0.618024 x

x Se 11 0.533204 0.333393 0.881976 x

x Se 12 0.466795 0.666605 0.381976 x

x Se 13 0.666675 0.666364 0.118053 x

x Se 14 0.733414 0.333414 0.618001 x

x Se 15 0.733413 0.333414 0.881999 x

x Se 16 0.666675 0.666364 0.381947 x

x Se 17 0.866647 0.666246 0.118052 x

x Se 18 0.933393 0.333613 0.618050 x

x Se 19 0.933393 0.333612 0.881950 x

x Se 20 0.866647 0.666246 0.381948 x

x Nb 1 0.000005 0.000015 0.250000 x

x Nb 2 -0.000004 -0.000012 0.750000 x

x Nb 3 0.000000 0.000001 0.000000 x

x Nb 4 0.000001 0.000002 0.500000 x

x Nb 5 0.200009 0.000026 0.250000 x

x Nb 6 0.200000 -0.000006 0.750000 x

x Nb 7 0.200003 0.000009 -0.000001 x

x Nb 8 0.200003 0.000009 0.500001 x

x Nb 9 0.400008 0.000020 0.250000 x

x Nb 10 0.399998 -0.000013 0.750000 x

x Nb 11 0.400001 0.000001 0.000001 x

x Nb 12 0.400001 0.000000 0.499999 x

x Nb 13 0.600001 0.000011 0.250000 x

x Nb 14 0.599991 -0.000022 0.750000 x

x Nb 15 0.599998 -0.000003 -0.000001 x

x Nb 16 0.599998 -0.000003 0.500001 x

x Nb 17 0.800001 0.000006 0.250000 x

x Nb 18 0.799992 -0.000025 0.750000 x

x Nb 19 0.799997 -0.000008 0.000001 x

x Nb 20 0.799998 -0.000008 0.499999 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62557415E+004 1911.38 <-- SCF

1 -3.62584008E+004 6.64820934E-002 1937.69 <-- SCF

2 -3.62584759E+004 1.87729098E-003 1970.09 <-- SCF

3 -3.62575919E+004 -2.20996303E-002 2000.75 <-- SCF

4 -3.62574684E+004 -3.08696311E-003 2029.22 <-- SCF

5 -3.62574191E+004 -1.23373422E-003 2057.81 <-- SCF

6 -3.62574191E+004 1.59042460E-006 2088.25 <-- SCF

7 -3.62574189E+004 -5.21549590E-006 2110.17 <-- SCF

8 -3.62574190E+004 5.59287199E-007 2132.19 <-- SCF

9 -3.62574189E+004 -8.39037759E-007 2150.33 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36257.41892970 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.05792 -0.00021 1.39907 \*

\* Se 2 -0.06011 0.00556 1.21976 \*

\* Se 3 -0.06065 0.00151 -1.39980 \*

\* Se 4 0.05559 -0.00203 -1.21857 \*

\* Se 5 0.05840 0.00032 1.40577 \*

\* Se 6 -0.06238 0.00389 1.21528 \*

\* Se 7 -0.06152 0.00033 -1.39559 \*

\* Se 8 0.05564 0.00050 -1.23060 \*

\* Se 9 0.05618 -0.00178 1.40281 \*

\* Se 10 -0.06273 0.00513 1.22774 \*

\* Se 11 -0.05634 0.00179 -1.40281 \*

\* Se 12 0.06251 -0.00513 -1.22767 \*

\* Se 13 0.06147 -0.00033 1.39561 \*

\* Se 14 -0.05571 -0.00051 1.23058 \*

\* Se 15 -0.05847 -0.00032 -1.40575 \*

\* Se 16 0.06229 -0.00388 -1.21528 \*

\* Se 17 0.06079 -0.00151 1.39986 \*

\* Se 18 -0.05538 0.00203 1.21849 \*

\* Se 19 -0.05777 0.00021 -1.39902 \*

\* Se 20 0.06030 -0.00558 -1.21981 \*

\* Nb 1 -0.01143 -0.00979 0.01451 \*

\* Nb 2 0.01123 0.00981 -0.01451 \*

\* Nb 3 -0.00002 0.00001 -0.00007 \*

\* Nb 4 -0.00005 0.00002 0.00008 \*

\* Nb 5 -0.01187 -0.00282 0.01451 \*

\* Nb 6 0.00734 0.01540 -0.01458 \*

\* Nb 7 -0.00643 0.00805 -0.00090 \*

\* Nb 8 -0.00633 0.00803 0.00092 \*

\* Nb 9 -0.00536 -0.01314 0.01466 \*

\* Nb 10 -0.00016 0.01450 -0.01464 \*

\* Nb 11 -0.00712 -0.00060 0.00841 \*

\* Nb 12 -0.00697 -0.00061 -0.00847 \*

\* Nb 13 0.00032 -0.01453 0.01465 \*

\* Nb 14 0.00551 0.01313 -0.01471 \*

\* Nb 15 0.00713 0.00060 -0.00843 \*

\* Nb 16 0.00704 0.00058 0.00846 \*

\* Nb 17 -0.00742 -0.01540 0.01463 \*

\* Nb 18 0.01183 0.00283 -0.01457 \*

\* Nb 19 0.00642 -0.00804 0.00080 \*

\* Nb 20 0.00630 -0.00801 -0.00083 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 2.791298 -0.107378 -0.001013 \*

\* y -0.107378 3.797909 0.004194 \*

\* z -0.001013 0.004194 -2.764621 \*

\* \*

\* Pressure: -1.2749 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.074199 | -36256.250287 | <-- min BFGS

| trial step | 0.817549 | 0.028197 | -36257.225607 | <-- min BFGS

| line step | 1.226323 | 0.006958 | -36257.418929 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 2 with enthalpy= -3.62574189E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.921604E-002 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.406982E+000 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.130069E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.797909E+000 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 3 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.006419 | -36257.418929 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 3 with trial guess (lambda= 1.000000)

--------------------------------------------------------------------------------

+---------------- MEMORY AND SCRATCH DISK ESTIMATES PER PROCESS --------------+

| Memory Disk |

| Model and support data 165.3 MB 118.8 MB |

| Electronic energy minimisation requirements 89.7 MB 0.0 MB |

| Geometry minimisation requirements 118.0 MB 0.0 MB |

| ----------------------------- |

| Approx. total storage required per process 373.0 MB 118.8 MB |

| |

| Requirements will fluctuate during execution and may exceed these estimates |

+-----------------------------------------------------------------------------+

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

15.3030623 -8.7798711 0.0000251 0.4102336 -0.0006099 0.0000002

0.0052350 3.5210235 -0.0000122 1.0229406 1.7829561 0.0000061

-0.0000054 -0.0000429 13.4377577 0.0000002 0.0000016 0.4675769

Lattice parameters(A) Cell Angles

a = 17.642841 alpha = 90.000381

b = 3.521027 beta = 89.999848

c = 13.437758 gamma = 119.759128

Current cell volume = 724.676838 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066608 0.666383 0.118247 x

x Se 2 0.133349 0.333774 0.618230 x

x Se 3 0.133349 0.333772 0.881750 x

x Se 4 0.066608 0.666381 0.381772 x

x Se 5 0.266586 0.666594 0.118196 x

x Se 6 0.333318 0.333644 0.618231 x

x Se 7 0.333318 0.333643 0.881750 x

x Se 8 0.266586 0.666594 0.381823 x

x Se 9 0.466809 0.666612 0.118220 x

x Se 10 0.533190 0.333387 0.618201 x

x Se 11 0.533191 0.333387 0.881780 x

x Se 12 0.466809 0.666612 0.381798 x

x Se 13 0.666681 0.666356 0.118250 x

x Se 14 0.733414 0.333406 0.618177 x

x Se 15 0.733414 0.333405 0.881804 x

x Se 16 0.666681 0.666355 0.381769 x

x Se 17 0.866651 0.666229 0.118250 x

x Se 18 0.933393 0.333620 0.618227 x

x Se 19 0.933393 0.333619 0.881753 x

x Se 20 0.866651 0.666227 0.381769 x

x Nb 1 0.000004 0.000010 0.250002 x

x Nb 2 -0.000003 -0.000007 0.749998 x

x Nb 3 0.000000 0.000001 0.000000 x

x Nb 4 0.000001 0.000002 0.500000 x

x Nb 5 0.200008 0.000024 0.250002 x

x Nb 6 0.200000 0.000001 0.749998 x

x Nb 7 0.200002 0.000011 -0.000001 x

x Nb 8 0.200002 0.000011 0.500001 x

x Nb 9 0.400008 0.000015 0.250002 x

x Nb 10 0.399998 -0.000009 0.749998 x

x Nb 11 0.400001 -0.000001 0.000002 x

x Nb 12 0.400001 -0.000002 0.499998 x

x Nb 13 0.600001 0.000006 0.250002 x

x Nb 14 0.599991 -0.000017 0.749998 x

x Nb 15 0.599999 -0.000001 -0.000002 x

x Nb 16 0.599998 -0.000001 0.500002 x

x Nb 17 0.800000 -0.000001 0.250002 x

x Nb 18 0.799992 -0.000023 0.749998 x

x Nb 19 0.799998 -0.000010 0.000002 x

x Nb 20 0.799998 -0.000010 0.499998 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62572391E+004 2251.62 <-- SCF

1 -3.62577048E+004 1.16420203E-002 2279.30 <-- SCF

2 -3.62577289E+004 6.02769648E-004 2311.52 <-- SCF

3 -3.62576900E+004 -9.71630379E-004 2339.70 <-- SCF

4 -3.62575790E+004 -2.77605661E-003 2367.39 <-- SCF

5 -3.62575787E+004 -7.42156895E-006 2394.97 <-- SCF

6 -3.62575780E+004 -1.66010622E-005 2417.97 <-- SCF

7 -3.62575779E+004 -1.55946579E-006 2439.14 <-- SCF

8 -3.62575780E+004 9.03026220E-007 2456.44 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36257.57797012 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.06392 0.00026 1.35090 \*

\* Se 2 -0.06542 0.00846 1.14484 \*

\* Se 3 -0.06647 -0.00006 -1.35197 \*

\* Se 4 0.05953 -0.00289 -1.14307 \*

\* Se 5 0.06367 -0.00016 1.35340 \*

\* Se 6 -0.06878 0.00609 1.14117 \*

\* Se 7 -0.06678 -0.00112 -1.34827 \*

\* Se 8 0.05824 0.00185 -1.15266 \*

\* Se 9 0.05837 -0.00003 1.35256 \*

\* Se 10 -0.07192 0.00644 1.15341 \*

\* Se 11 -0.05859 0.00006 -1.35252 \*

\* Se 12 0.07158 -0.00641 -1.15331 \*

\* Se 13 0.06668 0.00113 1.34827 \*

\* Se 14 -0.05831 -0.00187 1.15273 \*

\* Se 15 -0.06374 0.00015 -1.35338 \*

\* Se 16 0.06860 -0.00607 -1.14120 \*

\* Se 17 0.06667 0.00005 1.35200 \*

\* Se 18 -0.05919 0.00287 1.14302 \*

\* Se 19 -0.06372 -0.00029 -1.35089 \*

\* Se 20 0.06569 -0.00849 -1.14496 \*

\* Nb 1 -0.01478 -0.01276 0.02040 \*

\* Nb 2 0.01458 0.01280 -0.02038 \*

\* Nb 3 0.00001 0.00002 -0.00009 \*

\* Nb 4 0.00000 0.00002 0.00012 \*

\* Nb 5 -0.01388 -0.00573 0.02043 \*

\* Nb 6 0.01210 0.01848 -0.02044 \*

\* Nb 7 -0.00605 0.00794 -0.00040 \*

\* Nb 8 -0.00620 0.00814 0.00038 \*

\* Nb 9 -0.00722 -0.01623 0.02038 \*

\* Nb 10 0.00321 0.01731 -0.02035 \*

\* Nb 11 -0.00697 -0.00068 0.00808 \*

\* Nb 12 -0.00710 -0.00068 -0.00823 \*

\* Nb 13 -0.00307 -0.01733 0.02031 \*

\* Nb 14 0.00739 0.01617 -0.02042 \*

\* Nb 15 0.00694 0.00066 -0.00806 \*

\* Nb 16 0.00708 0.00064 0.00816 \*

\* Nb 17 -0.01215 -0.01845 0.02050 \*

\* Nb 18 0.01382 0.00573 -0.02047 \*

\* Nb 19 0.00604 -0.00794 0.00028 \*

\* Nb 20 0.00621 -0.00809 -0.00027 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 3.167133 -0.061794 -0.001637 \*

\* y -0.061794 4.095674 0.003641 \*

\* z -0.001637 0.003641 -1.476942 \*

\* \*

\* Pressure: -1.9286 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.006419 | -36257.418929 | <-- min BFGS

| trial step | 1.000000 | 0.005276 | -36257.578074 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 3 with line minimization (lambda= 3.585607)

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+---------------- MEMORY AND SCRATCH DISK ESTIMATES PER PROCESS --------------+

| Memory Disk |

| Model and support data 166.2 MB 118.8 MB |

| Electronic energy minimisation requirements 90.3 MB 0.0 MB |

| Geometry minimisation requirements 118.8 MB 0.0 MB |

| ----------------------------- |

| Approx. total storage required per process 375.3 MB 118.8 MB |

| |

| Requirements will fluctuate during execution and may exceed these estimates |

+-----------------------------------------------------------------------------+

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

15.2698331 -8.7327527 0.0001308 0.4110241 -0.0007919 -0.0000006

0.0067526 3.5048172 -0.0000421 1.0241253 1.7907552 0.0000180

0.0000193 -0.0001480 13.6285544 -0.0000008 0.0000055 0.4610309

Lattice parameters(A) Cell Angles

a = 17.590588 alpha = 90.001310

b = 3.504824 beta = 89.999195

c = 13.628554 gamma = 119.654666

Current cell volume = 730.176279 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066610 0.666367 0.118756 x

x Se 2 0.133340 0.333822 0.618692 x

x Se 3 0.133340 0.333816 0.881239 x

x Se 4 0.066609 0.666362 0.381313 x

x Se 5 0.266586 0.666616 0.118700 x

x Se 6 0.333302 0.333667 0.618690 x

x Se 7 0.333303 0.333663 0.881241 x

x Se 8 0.266585 0.666614 0.381366 x

x Se 9 0.466844 0.666629 0.118727 x

x Se 10 0.533154 0.333369 0.618660 x

x Se 11 0.533156 0.333369 0.881273 x

x Se 12 0.466846 0.666629 0.381340 x

x Se 13 0.666697 0.666337 0.118759 x

x Se 14 0.733415 0.333385 0.618633 x

x Se 15 0.733414 0.333384 0.881300 x

x Se 16 0.666697 0.666332 0.381310 x

x Se 17 0.866661 0.666186 0.118761 x

x Se 18 0.933391 0.333640 0.618687 x

x Se 19 0.933391 0.333635 0.881244 x

x Se 20 0.866661 0.666180 0.381308 x

x Nb 1 0.000002 -0.000004 0.250006 x

x Nb 2 -0.000001 0.000007 0.749994 x

x Nb 3 0.000000 0.000001 0.000000 x

x Nb 4 0.000001 0.000002 0.500000 x

x Nb 5 0.200007 0.000018 0.250006 x

x Nb 6 0.200002 0.000020 0.749994 x

x Nb 7 0.200001 0.000017 -0.000001 x

x Nb 8 0.200001 0.000017 0.500001 x

x Nb 9 0.400008 0.000002 0.250006 x

x Nb 10 0.399997 0.000004 0.749994 x

x Nb 11 0.400000 -0.000005 0.000005 x

x Nb 12 0.399999 -0.000006 0.499995 x

x Nb 13 0.600002 -0.000006 0.250006 x

x Nb 14 0.599991 -0.000004 0.749994 x

x Nb 15 0.600000 0.000003 -0.000004 x

x Nb 16 0.600000 0.000003 0.500004 x

x Nb 17 0.799998 -0.000019 0.250006 x

x Nb 18 0.799994 -0.000017 0.749994 x

x Nb 19 0.799999 -0.000016 0.000002 x

x Nb 20 0.799999 -0.000016 0.499998 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62556086E+004 2557.12 <-- SCF

1 -3.62590078E+004 8.49789922E-002 2585.02 <-- SCF

2 -3.62591757E+004 4.19855378E-003 2617.59 <-- SCF

3 -3.62591003E+004 -1.88669113E-003 2645.80 <-- SCF

4 -3.62578427E+004 -3.14390645E-002 2673.53 <-- SCF

5 -3.62578622E+004 4.86996771E-004 2705.72 <-- SCF

6 -3.62578526E+004 -2.38839898E-004 2734.25 <-- SCF

7 -3.62578528E+004 5.21221067E-006 2761.06 <-- SCF

8 -3.62578534E+004 1.32727092E-005 2781.36 <-- SCF

9 -3.62578539E+004 1.30397382E-005 2799.31 <-- SCF

10 -3.62578545E+004 1.47977010E-005 2817.52 <-- SCF

11 -3.62578554E+004 2.19964698E-005 2834.77 <-- SCF

12 -3.62578567E+004 3.33560613E-005 2852.97 <-- SCF

13 -3.62578588E+004 5.31045290E-005 2870.62 <-- SCF

14 -3.62578622E+004 8.48536870E-005 2887.94 <-- SCF

15 -3.62578672E+004 1.24689436E-004 2905.17 <-- SCF

16 -3.62578740E+004 1.71105024E-004 2922.56 <-- SCF

17 -3.62578820E+004 2.00030789E-004 2939.95 <-- SCF

18 -3.62578901E+004 2.01630962E-004 2957.06 <-- SCF

19 -3.62579032E+004 3.26561807E-004 2974.52 <-- SCF

20 -3.62579091E+004 1.47234905E-004 2991.50 <-- SCF

21 -3.62579122E+004 7.82518261E-005 3008.78 <-- SCF

22 -3.62579144E+004 5.41723175E-005 3025.78 <-- SCF

23 -3.62579160E+004 4.13465171E-005 3042.89 <-- SCF

24 -3.62579171E+004 2.70221030E-005 3059.91 <-- SCF

25 -3.62579178E+004 1.79331902E-005 3077.19 <-- SCF

26 -3.62579182E+004 1.02767311E-005 3093.77 <-- SCF

27 -3.62579185E+004 6.65541492E-006 3110.62 <-- SCF

28 -3.62579187E+004 5.36277039E-006 3126.88 <-- SCF

29 -3.62579188E+004 2.44605197E-006 3143.02 <-- SCF

30 -3.62579189E+004 2.49033466E-006 3160.39 <-- SCF

31 -3.62579189E+004 6.87473092E-007 3177.09 <-- SCF

32 -3.62579189E+004 -3.72931863E-007 3194.39 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36257.91890589 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.08935 0.00287 1.21400 \*

\* Se 2 -0.08592 0.03009 1.03663 \*

\* Se 3 -0.09349 -0.01079 -1.21579 \*

\* Se 4 0.06452 -0.00764 -1.03203 \*

\* Se 5 0.09013 -0.00581 1.21634 \*

\* Se 6 -0.09976 0.02365 1.02772 \*

\* Se 7 -0.09143 -0.01059 -1.20789 \*

\* Se 8 0.05675 0.01392 -1.02407 \*

\* Se 9 0.05906 0.01050 1.21162 \*

\* Se 10 -0.12211 0.02285 1.03387 \*

\* Se 11 -0.05916 -0.01052 -1.21165 \*

\* Se 12 0.12122 -0.02287 -1.03348 \*

\* Se 13 0.09156 0.01057 1.20770 \*

\* Se 14 -0.05693 -0.01397 1.02405 \*

\* Se 15 -0.09026 0.00580 -1.21611 \*

\* Se 16 0.09942 -0.02366 -1.02758 \*

\* Se 17 0.09379 0.01074 1.21579 \*

\* Se 18 -0.06377 0.00761 1.03181 \*

\* Se 19 -0.08926 -0.00289 -1.21384 \*

\* Se 20 0.08647 -0.03016 -1.03684 \*

\* Nb 1 -0.03865 -0.00914 0.03166 \*

\* Nb 2 0.03783 0.00920 -0.03169 \*

\* Nb 3 -0.00001 -0.00001 -0.00010 \*

\* Nb 4 -0.00011 0.00005 0.00014 \*

\* Nb 5 -0.02728 -0.00388 0.03305 \*

\* Nb 6 0.04652 0.01428 -0.03362 \*

\* Nb 7 -0.00685 0.00853 0.00013 \*

\* Nb 8 -0.00609 0.00732 -0.00181 \*

\* Nb 9 -0.02702 -0.01421 0.03346 \*

\* Nb 10 0.03768 0.01239 -0.03335 \*

\* Nb 11 -0.00720 -0.00053 0.00836 \*

\* Nb 12 -0.00702 -0.00170 -0.00921 \*

\* Nb 13 -0.03710 -0.01267 0.03320 \*

\* Nb 14 0.02792 0.01415 -0.03346 \*

\* Nb 15 0.00723 0.00062 -0.00854 \*

\* Nb 16 0.00722 0.00181 0.00939 \*

\* Nb 17 -0.04700 -0.01416 0.03350 \*

\* Nb 18 0.02698 0.00396 -0.03301 \*

\* Nb 19 0.00661 -0.00858 -0.00036 \*

\* Nb 20 0.00615 -0.00712 0.00203 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 4.499310 -0.752241 -0.000298 \*

\* y -0.752241 5.676715 0.014847 \*

\* z -0.000298 0.014847 0.451136 \*

\* \*

\* Pressure: -3.5424 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.006419 | -36257.418929 | <-- min BFGS

| trial step | 1.000000 | 0.005276 | -36257.578074 | <-- min BFGS

| line step | 3.585607 | 0.004012 | -36257.918839 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 3 with enthalpy= -3.62579188E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.249775E-002 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.219687E+000 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 9.660978E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 5.676715E+000 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 4 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.062536 | -36257.918839 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 4 with trial guess (lambda= 0.396746)

--------------------------------------------------------------------------------

+---------------- MEMORY AND SCRATCH DISK ESTIMATES PER PROCESS --------------+

| Memory Disk |

| Model and support data 166.4 MB 123.1 MB |

| Electronic energy minimisation requirements 90.3 MB 0.0 MB |

| Geometry minimisation requirements 118.9 MB 0.0 MB |

| ----------------------------- |

| Approx. total storage required per process 375.5 MB 123.1 MB |

| |

| Requirements will fluctuate during execution and may exceed these estimates |

+-----------------------------------------------------------------------------+

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

15.1527632 -8.6100069 0.0003955 0.4139100 -0.0013130 -0.0000018

0.0109856 3.4630544 -0.0001277 1.0290823 1.8110833 0.0000537

0.0000597 -0.0004455 13.8931428 -0.0000023 0.0000167 0.4522508

Lattice parameters(A) Cell Angles

a = 17.428094 alpha = 90.003950

b = 3.463072 beta = 89.997578

c = 13.893143 gamma = 119.424074

Current cell volume = 730.354597 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066622 0.666371 0.119633 x

x Se 2 0.133318 0.333873 0.619477 x

x Se 3 0.133317 0.333844 0.880360 x

x Se 4 0.066619 0.666353 0.380530 x

x Se 5 0.266595 0.666668 0.119572 x

x Se 6 0.333270 0.333679 0.619472 x

x Se 7 0.333271 0.333660 0.880365 x

x Se 8 0.266590 0.666664 0.380588 x

x Se 9 0.466897 0.666673 0.119600 x

x Se 10 0.533092 0.333322 0.619442 x

x Se 11 0.533102 0.333324 0.880400 x

x Se 12 0.466907 0.666675 0.380558 x

x Se 13 0.666728 0.666340 0.119635 x

x Se 14 0.733410 0.333336 0.619412 x

x Se 15 0.733405 0.333332 0.880429 x

x Se 16 0.666729 0.666320 0.380528 x

x Se 17 0.866684 0.666157 0.119640 x

x Se 18 0.933382 0.333649 0.619470 x

x Se 19 0.933379 0.333631 0.880367 x

x Se 20 0.866683 0.666129 0.380522 x

x Nb 1 -0.000004 -0.000037 0.250015 x

x Nb 2 0.000006 0.000040 0.749985 x

x Nb 3 0.000000 0.000001 0.000000 x

x Nb 4 0.000001 0.000002 0.500000 x

x Nb 5 0.200002 0.000002 0.250016 x

x Nb 6 0.200008 0.000063 0.749984 x

x Nb 7 0.199999 0.000027 -0.000002 x

x Nb 8 0.199999 0.000026 0.500002 x

x Nb 9 0.400006 -0.000029 0.250015 x

x Nb 10 0.400000 0.000035 0.749985 x

x Nb 11 0.399997 -0.000014 0.000010 x

x Nb 12 0.399997 -0.000015 0.499990 x

x Nb 13 0.599999 -0.000038 0.250015 x

x Nb 14 0.599993 0.000026 0.749985 x

x Nb 15 0.600002 0.000011 -0.000009 x

x Nb 16 0.600002 0.000012 0.500009 x

x Nb 17 0.799992 -0.000062 0.250015 x

x Nb 18 0.799998 -0.000001 0.749985 x

x Nb 19 0.800001 -0.000026 0.000003 x

x Nb 20 0.800001 -0.000025 0.499998 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62528775E+004 3295.83 <-- SCF

1 -3.62628195E+004 2.48548209E-001 3324.39 <-- SCF

2 -3.62633032E+004 1.20938366E-002 3355.88 <-- SCF

3 -3.62638258E+004 1.30654702E-002 3383.61 <-- SCF

4 -3.62584412E+004 -1.34615685E-001 3411.25 <-- SCF

5 -3.62586279E+004 4.66801051E-003 3441.84 <-- SCF

6 -3.62585746E+004 -1.33303995E-003 3472.42 <-- SCF

7 -3.62585541E+004 -5.13861018E-004 3501.86 <-- SCF

8 -3.62585539E+004 -3.00796314E-006 3530.47 <-- SCF

9 -3.62585541E+004 4.55797775E-006 3556.23 <-- SCF

10 -3.62585540E+004 -2.95665603E-006 3577.16 <-- SCF

11 -3.62585540E+004 -5.89357225E-008 3598.08 <-- SCF

12 -3.62585540E+004 1.09215618E-006 3619.30 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36258.55404822 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.03837 -0.12937 1.02258 \*

\* Se 2 -0.00385 0.25086 1.05733 \*

\* Se 3 0.00239 0.25348 -1.01605 \*

\* Se 4 -0.02718 -0.11894 -1.06517 \*

\* Se 5 -0.20602 0.07730 1.25665 \*

\* Se 6 -0.12252 0.16190 1.03024 \*

\* Se 7 -0.12129 0.18396 -0.98220 \*

\* Se 8 -0.21819 0.09113 -1.27161 \*

\* Se 9 0.44463 -0.25945 1.10792 \*

\* Se 10 -0.46354 0.27693 1.13805 \*

\* Se 11 -0.44426 0.25947 -1.10774 \*

\* Se 12 0.46389 -0.27692 -1.13823 \*

\* Se 13 0.12112 -0.18396 0.98194 \*

\* Se 14 0.21777 -0.09117 1.27147 \*

\* Se 15 0.20562 -0.07734 -1.25652 \*

\* Se 16 0.12243 -0.16193 -1.02998 \*

\* Se 17 -0.00241 -0.25353 1.01630 \*

\* Se 18 0.02725 0.11904 1.06550 \*

\* Se 19 0.03847 0.12947 -1.02291 \*

\* Se 20 0.00376 -0.25093 -1.05756 \*

\* Nb 1 -0.05914 -0.02058 0.00810 \*

\* Nb 2 0.05814 0.02066 -0.00810 \*

\* Nb 3 0.00015 -0.00008 0.00014 \*

\* Nb 4 0.00013 -0.00009 -0.00014 \*

\* Nb 5 -0.08462 -0.01080 0.00787 \*

\* Nb 6 0.05521 0.02859 -0.00751 \*

\* Nb 7 0.00956 0.00598 0.00787 \*

\* Nb 8 0.00955 0.00636 -0.00768 \*

\* Nb 9 -0.00475 -0.02701 0.00781 \*

\* Nb 10 0.09987 0.01873 -0.00793 \*

\* Nb 11 -0.01252 0.00675 -0.00806 \*

\* Nb 12 -0.01218 0.00670 0.00728 \*

\* Nb 13 -0.10021 -0.01869 0.00795 \*

\* Nb 14 0.00469 0.02707 -0.00783 \*

\* Nb 15 0.01264 -0.00678 0.00811 \*

\* Nb 16 0.01235 -0.00672 -0.00733 \*

\* Nb 17 -0.05435 -0.02866 0.00757 \*

\* Nb 18 0.08535 0.01073 -0.00793 \*

\* Nb 19 -0.00977 -0.00586 -0.00826 \*

\* Nb 20 -0.00977 -0.00624 0.00805 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 4.267858 -0.062359 0.005254 \*

\* y -0.062359 4.644625 -0.004999 \*

\* z 0.005254 -0.004999 4.090738 \*

\* \*

\* Pressure: -4.3344 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.062536 | -36257.918839 | <-- min BFGS

| trial step | 0.396746 | 0.027059 | -36258.554041 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 4 with enthalpy= -3.62585540E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.588005E-002 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.293404E+000 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.222446E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.644625E+000 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 5 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.023434 | -36258.554041 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 5 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9695656 -8.4576534 0.0004071 0.4188334 -0.0015880 -0.0000008

0.0129118 3.4054783 -0.0001508 1.0401910 1.8410790 0.0000678

0.0000259 -0.0005324 14.0670959 -0.0000010 0.0000198 0.4466583

Lattice parameters(A) Cell Angles

a = 17.193598 alpha = 90.004705

b = 3.405503 beta = 89.997485

c = 14.067096 gamma = 119.248775

Current cell volume = 718.656059 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066630 0.666296 0.120598 x

x Se 2 0.133297 0.334032 0.620363 x

x Se 3 0.133297 0.334003 0.879395 x

x Se 4 0.066627 0.666284 0.379644 x

x Se 5 0.266577 0.666689 0.120575 x

x Se 6 0.333228 0.333722 0.620351 x

x Se 7 0.333230 0.333714 0.879408 x

x Se 8 0.266571 0.666686 0.379666 x

x Se 9 0.466999 0.666715 0.120579 x

x Se 10 0.532987 0.333284 0.620342 x

x Se 11 0.533000 0.333283 0.879421 x

x Se 12 0.467012 0.666713 0.379658 x

x Se 13 0.666770 0.666285 0.120592 x

x Se 14 0.733429 0.333313 0.620334 x

x Se 15 0.733422 0.333310 0.879425 x

x Se 16 0.666771 0.666277 0.379649 x

x Se 17 0.866704 0.665998 0.120605 x

x Se 18 0.933374 0.333719 0.620356 x

x Se 19 0.933371 0.333707 0.879402 x

x Se 20 0.866704 0.665970 0.379637 x

x Nb 1 -0.000016 -0.000094 0.250023 x

x Nb 2 0.000017 0.000097 0.749977 x

x Nb 3 0.000000 0.000001 0.000000 x

x Nb 4 0.000001 0.000002 0.500000 x

x Nb 5 0.199988 -0.000045 0.250024 x

x Nb 6 0.200018 0.000129 0.749977 x

x Nb 7 0.199999 0.000042 -0.000001 x

x Nb 8 0.199999 0.000042 0.500001 x

x Nb 9 0.400005 -0.000070 0.250023 x

x Nb 10 0.400013 0.000101 0.749977 x

x Nb 11 0.399993 -0.000022 0.000012 x

x Nb 12 0.399992 -0.000023 0.499987 x

x Nb 13 0.599986 -0.000104 0.250023 x

x Nb 14 0.599994 0.000067 0.749977 x

x Nb 15 0.600007 0.000019 -0.000012 x

x Nb 16 0.600006 0.000019 0.500012 x

x Nb 17 0.799982 -0.000129 0.250023 x

x Nb 18 0.800013 0.000047 0.749977 x

x Nb 19 0.800002 -0.000041 0.000002 x

x Nb 20 0.800002 -0.000041 0.499998 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62525759E+004 3724.36 <-- SCF

1 -3.62643969E+004 2.95525788E-001 3754.17 <-- SCF

2 -3.62649668E+004 1.42468944E-002 3788.78 <-- SCF

3 -3.62634087E+004 -3.89525360E-002 3816.05 <-- SCF

4 -3.62589965E+004 -1.10303915E-001 3842.78 <-- SCF

5 -3.62590249E+004 7.10341588E-004 3872.22 <-- SCF

6 -3.62589941E+004 -7.70928567E-004 3900.78 <-- SCF

7 -3.62589919E+004 -5.42270635E-005 3929.70 <-- SCF

8 -3.62589925E+004 1.28757547E-005 3955.55 <-- SCF

9 -3.62589926E+004 3.60948493E-006 3979.11 <-- SCF

10 -3.62589930E+004 8.80852579E-006 3998.02 <-- SCF

11 -3.62589932E+004 5.71572085E-006 4016.42 <-- SCF

12 -3.62589933E+004 3.84335528E-006 4034.61 <-- SCF

13 -3.62589934E+004 2.68833283E-006 4052.12 <-- SCF

14 -3.62589935E+004 1.82115342E-006 4069.38 <-- SCF

15 -3.62589936E+004 1.39056766E-006 4086.58 <-- SCF

16 -3.62589936E+004 1.09090019E-006 4104.45 <-- SCF

17 -3.62589937E+004 8.26738473E-007 4121.77 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36258.99365040 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00792 -0.22774 0.84295 \*

\* Se 2 -0.02810 0.25541 0.88739 \*

\* Se 3 -0.03054 0.24151 -0.82727 \*

\* Se 4 -0.04190 -0.22665 -0.89207 \*

\* Se 5 -0.08983 -0.02514 1.06772 \*

\* Se 6 -0.11203 0.24012 0.79529 \*

\* Se 7 -0.11609 0.23531 -0.71912 \*

\* Se 8 -0.11950 -0.02409 -1.12125 \*

\* Se 9 0.29952 -0.17617 0.89789 \*

\* Se 10 -0.33249 0.18363 0.93857 \*

\* Se 11 -0.29933 0.17616 -0.89772 \*

\* Se 12 0.33274 -0.18361 -0.93876 \*

\* Se 13 0.11603 -0.23522 0.71892 \*

\* Se 14 0.11928 0.02404 1.12117 \*

\* Se 15 0.08963 0.02509 -1.06766 \*

\* Se 16 0.11203 -0.24005 -0.79510 \*

\* Se 17 0.03050 -0.24168 0.82749 \*

\* Se 18 0.04197 0.22684 0.89214 \*

\* Se 19 0.00805 0.22791 -0.84301 \*

\* Se 20 0.02803 -0.25558 -0.88760 \*

\* Nb 1 -0.06516 -0.01813 0.01790 \*

\* Nb 2 0.06437 0.01861 -0.01790 \*

\* Nb 3 0.00015 -0.00034 0.00017 \*

\* Nb 4 0.00013 -0.00034 -0.00016 \*

\* Nb 5 -0.10051 0.00258 0.01797 \*

\* Nb 6 0.07266 0.04527 -0.01755 \*

\* Nb 7 0.00393 -0.00172 0.00758 \*

\* Nb 8 0.00313 -0.00081 -0.00831 \*

\* Nb 9 -0.02399 -0.04048 0.01792 \*

\* Nb 10 0.09086 0.00550 -0.01843 \*

\* Nb 11 -0.02214 0.03000 -0.00309 \*

\* Nb 12 -0.02134 0.02904 0.00289 \*

\* Nb 13 -0.09130 -0.00539 0.01847 \*

\* Nb 14 0.02408 0.04072 -0.01796 \*

\* Nb 15 0.02223 -0.03021 0.00313 \*

\* Nb 16 0.02148 -0.02925 -0.00292 \*

\* Nb 17 -0.07191 -0.04562 0.01761 \*

\* Nb 18 0.10091 -0.00302 -0.01803 \*

\* Nb 19 -0.00418 0.00223 -0.00797 \*

\* Nb 20 -0.00341 0.00131 0.00869 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 2.026669 -0.056777 0.006762 \*

\* y -0.056777 1.826267 -0.033465 \*

\* z 0.006762 -0.033465 4.510709 \*

\* \*

\* Pressure: -2.7879 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.023434 | -36258.554041 | <-- min BFGS

| trial step | 1.000000 | 0.008738 | -36258.993578 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 5 with enthalpy= -3.62589936E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.098843E-002 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.127856E+000 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.412300E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.510709E+000 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 6 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.010377 | -36258.993578 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 6 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8466535 -8.3691723 -0.0000128 0.4222528 -0.0016900 0.0000017

0.0134923 3.3710963 -0.0000275 1.0482960 1.8596447 0.0000227

-0.0000557 -0.0001408 14.0751441 0.0000024 0.0000036 0.4464029

Lattice parameters(A) Cell Angles

a = 17.043068 alpha = 90.001041

b = 3.371123 beta = 89.999959

c = 14.075144 gamma = 119.180972

Current cell volume = 706.043258 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066638 0.666181 0.121137 x

x Se 2 0.133282 0.334163 0.620865 x

x Se 3 0.133282 0.334128 0.878860 x

x Se 4 0.066632 0.666161 0.379141 x

x Se 5 0.266571 0.666671 0.121160 x

x Se 6 0.333199 0.333798 0.620836 x

x Se 7 0.333200 0.333789 0.878892 x

x Se 8 0.266560 0.666659 0.379115 x

x Se 9 0.467061 0.666741 0.121130 x

x Se 10 0.532920 0.333252 0.620857 x

x Se 11 0.532938 0.333257 0.878870 x

x Se 12 0.467079 0.666745 0.379143 x

x Se 13 0.666799 0.666210 0.121108 x

x Se 14 0.733439 0.333340 0.620884 x

x Se 15 0.733429 0.333328 0.878841 x

x Se 16 0.666800 0.666201 0.379164 x

x Se 17 0.866719 0.665874 0.121141 x

x Se 18 0.933369 0.333842 0.620858 x

x Se 19 0.933363 0.333822 0.878864 x

x Se 20 0.866719 0.665839 0.379135 x

x Nb 1 -0.000027 -0.000143 0.250030 x

x Nb 2 0.000028 0.000146 0.749970 x

x Nb 3 0.000001 0.000001 0.000000 x

x Nb 4 0.000001 0.000002 0.500000 x

x Nb 5 0.199971 -0.000090 0.250030 x

x Nb 6 0.200029 0.000198 0.749970 x

x Nb 7 0.199998 0.000048 0.000000 x

x Nb 8 0.199998 0.000048 0.500000 x

x Nb 9 0.400001 -0.000115 0.250030 x

x Nb 10 0.400026 0.000152 0.749970 x

x Nb 11 0.399988 -0.000017 0.000014 x

x Nb 12 0.399988 -0.000019 0.499986 x

x Nb 13 0.599973 -0.000155 0.250030 x

x Nb 14 0.599998 0.000112 0.749971 x

x Nb 15 0.600011 0.000015 -0.000013 x

x Nb 16 0.600011 0.000015 0.500013 x

x Nb 17 0.799971 -0.000197 0.250029 x

x Nb 18 0.800030 0.000091 0.749971 x

x Nb 19 0.800002 -0.000047 0.000000 x

x Nb 20 0.800002 -0.000047 0.500000 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62567189E+004 4225.69 <-- SCF

1 -3.62616900E+004 1.24278298E-001 4253.44 <-- SCF

2 -3.62619374E+004 6.18439374E-003 4283.64 <-- SCF

3 -3.62606104E+004 -3.31751628E-002 4310.86 <-- SCF

4 -3.62591874E+004 -3.55751011E-002 4337.91 <-- SCF

5 -3.62591697E+004 -4.42196643E-004 4364.67 <-- SCF

6 -3.62591669E+004 -7.13520135E-005 4392.95 <-- SCF

7 -3.62591680E+004 2.94694959E-005 4418.94 <-- SCF

8 -3.62591687E+004 1.51929402E-005 4440.41 <-- SCF

9 -3.62591692E+004 1.33479002E-005 4459.78 <-- SCF

10 -3.62591697E+004 1.34068787E-005 4478.11 <-- SCF

11 -3.62591704E+004 1.57990375E-005 4496.89 <-- SCF

12 -3.62591712E+004 2.04710318E-005 4515.38 <-- SCF

13 -3.62591724E+004 3.01179127E-005 4533.61 <-- SCF

14 -3.62591739E+004 3.86977909E-005 4551.88 <-- SCF

15 -3.62591760E+004 5.11251943E-005 4570.44 <-- SCF

16 -3.62591787E+004 6.70180913E-005 4588.31 <-- SCF

17 -3.62591820E+004 8.49093073E-005 4606.66 <-- SCF

18 -3.62591861E+004 1.02197699E-004 4625.03 <-- SCF

19 -3.62591908E+004 1.16772580E-004 4643.80 <-- SCF

20 -3.62591958E+004 1.23957711E-004 4662.08 <-- SCF

21 -3.62592008E+004 1.25913648E-004 4680.69 <-- SCF

22 -3.62592055E+004 1.17305859E-004 4699.59 <-- SCF

23 -3.62592099E+004 1.09298614E-004 4717.39 <-- SCF

24 -3.62592132E+004 8.45106474E-005 4736.20 <-- SCF

25 -3.62592162E+004 7.33851731E-005 4754.33 <-- SCF

26 -3.62592184E+004 5.44181855E-005 4773.22 <-- SCF

27 -3.62592199E+004 3.75424387E-005 4791.62 <-- SCF

28 -3.62592210E+004 2.91886434E-005 4810.16 <-- SCF

29 -3.62592218E+004 1.98721821E-005 4828.11 <-- SCF

30 -3.62592224E+004 1.38300396E-005 4846.77 <-- SCF

31 -3.62592228E+004 9.43070957E-006 4865.33 <-- SCF

32 -3.62592230E+004 5.37167541E-006 4883.91 <-- SCF

33 -3.62592231E+004 2.46501761E-006 4902.05 <-- SCF

34 -3.62592231E+004 1.39713981E-006 4920.28 <-- SCF

35 -3.62592232E+004 1.86100503E-006 4938.47 <-- SCF

36 -3.62592232E+004 -1.08698837E-007 4957.47 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.22319243 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01573 -0.25666 0.79608 \*

\* Se 2 -0.06680 0.23085 0.81126 \*

\* Se 3 -0.05066 0.21788 -0.72216 \*

\* Se 4 0.00042 -0.26018 -0.85171 \*

\* Se 5 0.00909 -0.04130 0.92223 \*

\* Se 6 -0.11172 0.22861 0.69588 \*

\* Se 7 -0.11205 0.22535 -0.61897 \*

\* Se 8 -0.00459 -0.04442 -0.98631 \*

\* Se 9 0.21490 -0.21722 0.78056 \*

\* Se 10 -0.25907 0.19892 0.84037 \*

\* Se 11 -0.21476 0.21759 -0.77997 \*

\* Se 12 0.25890 -0.19873 -0.83976 \*

\* Se 13 0.11248 -0.22503 0.61896 \*

\* Se 14 0.00461 0.04445 0.98678 \*

\* Se 15 -0.00869 0.04117 -0.92194 \*

\* Se 16 0.11222 -0.22837 -0.69569 \*

\* Se 17 0.05023 -0.21850 0.72253 \*

\* Se 18 -0.00092 0.26029 0.85179 \*

\* Se 19 -0.01656 0.25642 -0.79636 \*

\* Se 20 0.06656 -0.23136 -0.81170 \*

\* Nb 1 -0.09777 -0.00629 0.01328 \*

\* Nb 2 0.09728 0.00828 -0.01327 \*

\* Nb 3 0.00004 -0.00086 0.00098 \*

\* Nb 4 -0.00036 -0.00036 -0.00079 \*

\* Nb 5 -0.15500 -0.00016 0.00991 \*

\* Nb 6 0.14757 0.07895 -0.01484 \*

\* Nb 7 0.00826 -0.00782 0.01542 \*

\* Nb 8 0.00372 -0.00746 -0.01677 \*

\* Nb 9 -0.08124 -0.05083 0.01551 \*

\* Nb 10 0.10829 -0.01867 -0.01561 \*

\* Nb 11 -0.03512 0.04875 -0.00743 \*

\* Nb 12 -0.02895 0.04723 0.01158 \*

\* Nb 13 -0.10918 0.01768 0.01472 \*

\* Nb 14 0.08101 0.05112 -0.01630 \*

\* Nb 15 0.03412 -0.04943 0.00740 \*

\* Nb 16 0.02908 -0.04751 -0.01178 \*

\* Nb 17 -0.14554 -0.07853 0.01496 \*

\* Nb 18 0.15538 -0.00170 -0.01004 \*

\* Nb 19 -0.00761 0.00933 -0.01698 \*

\* Nb 20 -0.00333 0.00848 0.01818 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.575895 0.208814 -0.002481 \*

\* y 0.208814 -1.011609 -0.038614 \*

\* z -0.002481 -0.038614 2.790857 \*

\* \*

\* Pressure: -0.4011 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.010377 | -36258.993578 | <-- min BFGS

| trial step | 1.000000 | 0.001812 | -36259.223284 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 6 with enthalpy= -3.62592233E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 5.742643E-003 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 9.877890E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 8.227208E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.790857E+000 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 7 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.002939 | -36259.223284 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 7 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8387145 -8.3730365 -0.0003602 0.4225453 -0.0015713 0.0000014

0.0125358 3.3709962 0.0001166 1.0495375 1.8599927 -0.0000392

-0.0000442 0.0003200 14.0052428 0.0000021 -0.0000155 0.4486309

Lattice parameters(A) Cell Angles

a = 17.038051 alpha = 89.996710

b = 3.371020 beta = 90.002012

c = 14.005243 gamma = 119.221653

Current cell volume = 702.029786 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066642 0.666078 0.121213 x

x Se 2 0.133275 0.334234 0.620945 x

x Se 3 0.133276 0.334197 0.878793 x

x Se 4 0.066634 0.666053 0.379056 x

x Se 5 0.266574 0.666653 0.121259 x

x Se 6 0.333188 0.333860 0.620899 x

x Se 7 0.333189 0.333850 0.878841 x

x Se 8 0.266562 0.666635 0.379006 x

x Se 9 0.467079 0.666708 0.121207 x

x Se 10 0.532898 0.333266 0.620943 x

x Se 11 0.532920 0.333290 0.878793 x

x Se 12 0.467101 0.666731 0.379057 x

x Se 13 0.666811 0.666150 0.121159 x

x Se 14 0.733438 0.333364 0.620994 x

x Se 15 0.733426 0.333346 0.878741 x

x Se 16 0.666811 0.666139 0.379101 x

x Se 17 0.866725 0.665804 0.121208 x

x Se 18 0.933367 0.333950 0.620944 x

x Se 19 0.933359 0.333924 0.878787 x

x Se 20 0.866726 0.665768 0.379055 x

x Nb 1 -0.000037 -0.000172 0.250032 x

x Nb 2 0.000038 0.000176 0.749968 x

x Nb 3 0.000001 0.000001 0.000000 x

x Nb 4 0.000001 0.000002 0.500000 x

x Nb 5 0.199955 -0.000130 0.250031 x

x Nb 6 0.200044 0.000269 0.749968 x

x Nb 7 0.199999 0.000046 0.000002 x

x Nb 8 0.199998 0.000046 0.499998 x

x Nb 9 0.399993 -0.000158 0.250032 x

x Nb 10 0.400037 0.000173 0.749968 x

x Nb 11 0.399984 -0.000005 0.000013 x

x Nb 12 0.399985 -0.000005 0.499988 x

x Nb 13 0.599962 -0.000178 0.250032 x

x Nb 14 0.600006 0.000156 0.749968 x

x Nb 15 0.600015 0.000002 -0.000012 x

x Nb 16 0.600014 0.000001 0.500012 x

x Nb 17 0.799957 -0.000268 0.250031 x

x Nb 18 0.800046 0.000131 0.749969 x

x Nb 19 0.800002 -0.000044 -0.000002 x

x Nb 20 0.800002 -0.000044 0.500002 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62589592E+004 5061.03 <-- SCF

1 -3.62594415E+004 1.20573762E-002 5087.70 <-- SCF

2 -3.62594654E+004 5.98033241E-004 5118.47 <-- SCF

3 -3.62593680E+004 -2.43575253E-003 5146.86 <-- SCF

4 -3.62592694E+004 -2.46445150E-003 5174.45 <-- SCF

5 -3.62592681E+004 -3.27120848E-005 5201.92 <-- SCF

6 -3.62592671E+004 -2.56868977E-005 5227.30 <-- SCF

7 -3.62592671E+004 1.01965281E-006 5249.47 <-- SCF

8 -3.62592673E+004 4.00016990E-006 5268.02 <-- SCF

9 -3.62592674E+004 3.69680190E-006 5285.02 <-- SCF

10 -3.62592676E+004 3.48146826E-006 5301.69 <-- SCF

11 -3.62592677E+004 3.14454887E-006 5318.56 <-- SCF

12 -3.62592678E+004 2.85119663E-006 5335.53 <-- SCF

13 -3.62592679E+004 2.62704970E-006 5352.06 <-- SCF

14 -3.62592680E+004 2.39913247E-006 5369.06 <-- SCF

15 -3.62592681E+004 2.18789736E-006 5385.56 <-- SCF

16 -3.62592682E+004 1.97466704E-006 5402.62 <-- SCF

17 -3.62592682E+004 1.84245332E-006 5419.89 <-- SCF

18 -3.62592683E+004 1.72980754E-006 5436.78 <-- SCF

19 -3.62592684E+004 1.54345669E-006 5453.59 <-- SCF

20 -3.62592684E+004 1.40627731E-006 5470.50 <-- SCF

21 -3.62592685E+004 1.26435408E-006 5487.09 <-- SCF

22 -3.62592685E+004 1.13506811E-006 5503.33 <-- SCF

23 -3.62592686E+004 1.04356275E-006 5519.55 <-- SCF

24 -3.62592686E+004 9.27282024E-007 5535.38 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.26859952 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01755 -0.24173 0.79153 \*

\* Se 2 -0.03760 0.22580 0.79485 \*

\* Se 3 -0.02438 0.21517 -0.70863 \*

\* Se 4 0.00432 -0.24844 -0.84792 \*

\* Se 5 0.00741 -0.03377 0.87476 \*

\* Se 6 -0.11530 0.21994 0.69602 \*

\* Se 7 -0.11644 0.21772 -0.62027 \*

\* Se 8 -0.00528 -0.03916 -0.93837 \*

\* Se 9 0.18843 -0.21155 0.75688 \*

\* Se 10 -0.22521 0.19617 0.80620 \*

\* Se 11 -0.18863 0.21155 -0.75673 \*

\* Se 12 0.22510 -0.19614 -0.80640 \*

\* Se 13 0.11644 -0.21759 0.62029 \*

\* Se 14 0.00548 0.03909 0.93819 \*

\* Se 15 -0.00723 0.03373 -0.87466 \*

\* Se 16 0.11541 -0.21984 -0.69605 \*

\* Se 17 0.02440 -0.21533 0.70861 \*

\* Se 18 -0.00441 0.24858 0.84786 \*

\* Se 19 -0.01758 0.24188 -0.79158 \*

\* Se 20 0.03749 -0.22600 -0.79465 \*

\* Nb 1 -0.10641 -0.02220 0.01870 \*

\* Nb 2 0.10616 0.02276 -0.01870 \*

\* Nb 3 0.00039 -0.00038 0.00006 \*

\* Nb 4 0.00027 -0.00040 -0.00003 \*

\* Nb 5 -0.10208 0.01570 0.02092 \*

\* Nb 6 0.06958 0.05214 -0.02144 \*

\* Nb 7 0.00555 -0.01146 0.00909 \*

\* Nb 8 0.00693 -0.00761 -0.00765 \*

\* Nb 9 -0.05868 -0.05195 0.02033 \*

\* Nb 10 0.08633 -0.00355 -0.01930 \*

\* Nb 11 -0.03944 0.04996 0.00859 \*

\* Nb 12 -0.04002 0.04785 -0.00941 \*

\* Nb 13 -0.08625 0.00386 0.01937 \*

\* Nb 14 0.05821 0.05216 -0.02044 \*

\* Nb 15 0.03933 -0.05035 -0.00847 \*

\* Nb 16 0.04013 -0.04816 0.00939 \*

\* Nb 17 -0.06930 -0.05259 0.02152 \*

\* Nb 18 0.10237 -0.01631 -0.02096 \*

\* Nb 19 -0.00580 0.01216 -0.00927 \*

\* Nb 20 -0.00727 0.00829 0.00778 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.789257 -0.142397 -0.050621 \*

\* y -0.142397 -1.557426 -0.017848 \*

\* z -0.050621 -0.017848 0.663853 \*

\* \*

\* Pressure: 0.5609 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.002939 | -36259.223284 | <-- min BFGS

| trial step | 1.000000 | 0.001143 | -36259.268670 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 7 with line minimization (lambda= 1.636097)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8336646 -8.3754945 -0.0005813 0.4227315 -0.0014957 0.0000012

0.0119273 3.3709326 0.0002083 1.0503282 1.8602145 -0.0000789

-0.0000369 0.0006130 13.9607787 0.0000019 -0.0000278 0.4500598

Lattice parameters(A) Cell Angles

a = 17.034862 alpha = 89.993945

b = 3.370954 beta = 90.003324

c = 13.960779 gamma = 119.247538

Current cell volume = 699.479419 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066645 0.666013 0.121262 x

x Se 2 0.133270 0.334279 0.620995 x

x Se 3 0.133272 0.334242 0.878750 x

x Se 4 0.066636 0.665984 0.379002 x

x Se 5 0.266576 0.666641 0.121322 x

x Se 6 0.333181 0.333900 0.620940 x

x Se 7 0.333182 0.333889 0.878808 x

x Se 8 0.266563 0.666620 0.378937 x

x Se 9 0.467090 0.666688 0.121256 x

x Se 10 0.532884 0.333275 0.620998 x

x Se 11 0.532909 0.333310 0.878744 x

x Se 12 0.467115 0.666722 0.379002 x

x Se 13 0.666818 0.666111 0.121192 x

x Se 14 0.733437 0.333379 0.621063 x

x Se 15 0.733424 0.333358 0.878678 x

x Se 16 0.666819 0.666099 0.379060 x

x Se 17 0.866728 0.665760 0.121250 x

x Se 18 0.933365 0.334019 0.620998 x

x Se 19 0.933356 0.333989 0.878738 x

x Se 20 0.866731 0.665722 0.379004 x

x Nb 1 -0.000044 -0.000191 0.250033 x

x Nb 2 0.000045 0.000195 0.749967 x

x Nb 3 0.000001 0.000000 0.000001 x

x Nb 4 0.000001 0.000002 0.500000 x

x Nb 5 0.199944 -0.000157 0.250032 x

x Nb 6 0.200053 0.000314 0.749967 x

x Nb 7 0.199999 0.000045 0.000004 x

x Nb 8 0.199998 0.000044 0.499996 x

x Nb 9 0.399988 -0.000185 0.250033 x

x Nb 10 0.400044 0.000187 0.749967 x

x Nb 11 0.399982 0.000003 0.000012 x

x Nb 12 0.399983 0.000003 0.499989 x

x Nb 13 0.599954 -0.000192 0.250033 x

x Nb 14 0.600011 0.000184 0.749967 x

x Nb 15 0.600017 -0.000006 -0.000011 x

x Nb 16 0.600016 -0.000007 0.500011 x

x Nb 17 0.799947 -0.000313 0.250033 x

x Nb 18 0.800056 0.000157 0.749968 x

x Nb 19 0.800001 -0.000043 -0.000003 x

x Nb 20 0.800002 -0.000042 0.500004 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62591572E+004 5638.64 <-- SCF

1 -3.62593453E+004 4.70072254E-003 5664.77 <-- SCF

2 -3.62593560E+004 2.68616870E-004 5695.14 <-- SCF

3 -3.62593095E+004 -1.16207829E-003 5722.16 <-- SCF

4 -3.62592824E+004 -6.77857795E-004 5749.45 <-- SCF

5 -3.62592812E+004 -3.08024493E-005 5776.06 <-- SCF

6 -3.62592809E+004 -6.14462092E-006 5797.53 <-- SCF

7 -3.62592810E+004 2.96683482E-006 5816.52 <-- SCF

8 -3.62592812E+004 2.74562957E-006 5832.67 <-- SCF

9 -3.62592812E+004 2.18349969E-006 5848.89 <-- SCF

10 -3.62592813E+004 1.83593670E-006 5865.16 <-- SCF

11 -3.62592814E+004 1.53847232E-006 5881.44 <-- SCF

12 -3.62592814E+004 1.33498043E-006 5898.09 <-- SCF

13 -3.62592815E+004 1.07500215E-006 5914.42 <-- SCF

14 -3.62592815E+004 9.52293124E-007 5930.53 <-- SCF

15 -3.62592815E+004 7.31487258E-007 5947.09 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.28153648 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02619 -0.23062 0.79014 \*

\* Se 2 -0.01457 0.22125 0.78760 \*

\* Se 3 -0.00618 0.21020 -0.70301 \*

\* Se 4 0.01094 -0.23970 -0.84870 \*

\* Se 5 0.01142 -0.03364 0.84378 \*

\* Se 6 -0.12306 0.21656 0.69497 \*

\* Se 7 -0.13019 0.21601 -0.61854 \*

\* Se 8 -0.00443 -0.03901 -0.90511 \*

\* Se 9 0.17130 -0.20781 0.75136 \*

\* Se 10 -0.20153 0.19489 0.79572 \*

\* Se 11 -0.17114 0.20781 -0.75128 \*

\* Se 12 0.20179 -0.19484 -0.79588 \*

\* Se 13 0.13016 -0.21594 0.61839 \*

\* Se 14 0.00432 0.03897 0.90504 \*

\* Se 15 -0.01153 0.03362 -0.84373 \*

\* Se 16 0.12307 -0.21651 -0.69484 \*

\* Se 17 0.00608 -0.21027 0.70304 \*

\* Se 18 -0.01090 0.23979 0.84870 \*

\* Se 19 -0.02615 0.23073 -0.79022 \*

\* Se 20 0.01437 -0.22136 -0.78752 \*

\* Nb 1 -0.07980 -0.02485 0.01873 \*

\* Nb 2 0.07929 0.02530 -0.01875 \*

\* Nb 3 0.00014 -0.00030 0.00010 \*

\* Nb 4 0.00012 -0.00029 -0.00008 \*

\* Nb 5 -0.10700 0.00938 0.02034 \*

\* Nb 6 0.06211 0.04796 -0.02010 \*

\* Nb 7 0.00019 -0.00128 0.01077 \*

\* Nb 8 0.00010 0.00078 -0.01054 \*

\* Nb 9 -0.03166 -0.04613 0.02084 \*

\* Nb 10 0.08008 0.00829 -0.01951 \*

\* Nb 11 -0.02727 0.03722 0.00749 \*

\* Nb 12 -0.02870 0.03564 -0.00984 \*

\* Nb 13 -0.08025 -0.00807 0.01961 \*

\* Nb 14 0.03151 0.04630 -0.02087 \*

\* Nb 15 0.02730 -0.03750 -0.00749 \*

\* Nb 16 0.02880 -0.03591 0.00986 \*

\* Nb 17 -0.06156 -0.04832 0.02015 \*

\* Nb 18 0.10731 -0.00979 -0.02034 \*

\* Nb 19 -0.00034 0.00176 -0.01097 \*

\* Nb 20 -0.00030 -0.00032 0.01072 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -1.278844 -0.166542 -0.014357 \*

\* y -0.166542 -1.846788 -0.001063 \*

\* z -0.014357 -0.001063 -0.284083 \*

\* \*

\* Pressure: 1.1366 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.002939 | -36259.223284 | <-- min BFGS

| trial step | 1.000000 | 0.001143 | -36259.268670 | <-- min BFGS

| line step | 1.636097 | 0.000309 | -36259.281654 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 7 with enthalpy= -3.62592817E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.459257E-003 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 9.059638E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.502912E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.846788E+000 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 8 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.002381 | -36259.281654 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 8 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8198460 -8.3672056 -0.0007118 0.4230937 -0.0015538 -0.0000028

0.0123706 3.3683705 0.0003301 1.0509866 1.8614888 -0.0001405

0.0000963 0.0009989 13.9556420 -0.0000033 -0.0000441 0.4502255

Lattice parameters(A) Cell Angles

a = 17.018753 alpha = 89.990283

b = 3.368393 beta = 90.004068

c = 13.955642 gamma = 119.238417

Current cell volume = 698.092464 A\*\*3

-------------------------------

Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066651 0.665828 0.121602 x

x Se 2 0.133260 0.334455 0.621323 x

x Se 3 0.133263 0.334410 0.878428 x

x Se 4 0.066638 0.665786 0.378663 x

x Se 5 0.266576 0.666618 0.121691 x

x Se 6 0.333153 0.334024 0.621242 x

x Se 7 0.333154 0.334009 0.878511 x

x Se 8 0.266559 0.666586 0.378567 x

x Se 9 0.467139 0.666628 0.121593 x

x Se 10 0.532827 0.333308 0.621333 x

x Se 11 0.532860 0.333370 0.878407 x

x Se 12 0.467172 0.666689 0.378667 x

x Se 13 0.666846 0.665991 0.121490 x

x Se 14 0.733441 0.333413 0.621433 x

x Se 15 0.733424 0.333381 0.878309 x

x Se 16 0.666846 0.665975 0.378758 x

x Se 17 0.866737 0.665591 0.121572 x

x Se 18 0.933363 0.334218 0.621337 x

x Se 19 0.933350 0.334174 0.878399 x

x Se 20 0.866741 0.665546 0.378676 x

x Nb 1 -0.000061 -0.000251 0.250038 x

x Nb 2 0.000062 0.000256 0.749962 x

x Nb 3 0.000001 0.000000 0.000001 x

x Nb 4 0.000001 0.000001 0.499999 x

x Nb 5 0.199919 -0.000217 0.250038 x

x Nb 6 0.200073 0.000417 0.749961 x

x Nb 7 0.200000 0.000046 0.000007 x

x Nb 8 0.199999 0.000045 0.499993 x

x Nb 9 0.399978 -0.000253 0.250039 x

x Nb 10 0.400063 0.000237 0.749961 x

x Nb 11 0.399976 0.000020 0.000013 x

x Nb 12 0.399977 0.000020 0.499988 x

x Nb 13 0.599936 -0.000241 0.250039 x

x Nb 14 0.600021 0.000251 0.749961 x

x Nb 15 0.600023 -0.000024 -0.000012 x

x Nb 16 0.600022 -0.000024 0.500011 x

x Nb 17 0.799928 -0.000415 0.250038 x

x Nb 18 0.800082 0.000217 0.749963 x

x Nb 19 0.800001 -0.000042 -0.000007 x

x Nb 20 0.800002 -0.000042 0.500007 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62592162E+004 6049.84 <-- SCF

1 -3.62599140E+004 1.74449345E-002 6077.72 <-- SCF

2 -3.62599463E+004 8.09867384E-004 6105.97 <-- SCF

3 -3.62598850E+004 -1.53396734E-003 6133.09 <-- SCF

4 -3.62593279E+004 -1.39272681E-002 6159.22 <-- SCF

5 -3.62593438E+004 3.96823333E-004 6188.48 <-- SCF

6 -3.62593400E+004 -9.52246297E-005 6213.31 <-- SCF

7 -3.62593402E+004 6.78540669E-006 6236.41 <-- SCF

8 -3.62593404E+004 4.85699309E-006 6254.47 <-- SCF

9 -3.62593405E+004 1.33947508E-006 6270.81 <-- SCF

10 -3.62593405E+004 1.61569726E-006 6288.17 <-- SCF

11 -3.62593406E+004 1.34837870E-006 6304.62 <-- SCF

12 -3.62593406E+004 9.28575912E-007 6320.81 <-- SCF

13 -3.62593407E+004 7.09047384E-007 6337.14 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.34066764 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02030 -0.20352 0.70319 \*

\* Se 2 0.00084 0.19928 0.66593 \*

\* Se 3 0.00131 0.18124 -0.60419 \*

\* Se 4 0.02451 -0.21234 -0.76042 \*

\* Se 5 0.02964 -0.03341 0.74560 \*

\* Se 6 -0.12423 0.20422 0.59351 \*

\* Se 7 -0.13001 0.20280 -0.53550 \*

\* Se 8 0.02163 -0.03344 -0.80022 \*

\* Se 9 0.12723 -0.22842 0.66570 \*

\* Se 10 -0.15077 0.21283 0.71554 \*

\* Se 11 -0.12709 0.22839 -0.66565 \*

\* Se 12 0.15098 -0.21282 -0.71571 \*

\* Se 13 0.12995 -0.20276 0.53539 \*

\* Se 14 -0.02174 0.03337 0.80015 \*

\* Se 15 -0.02977 0.03337 -0.74558 \*

\* Se 16 0.12423 -0.20419 -0.59344 \*

\* Se 17 -0.00137 -0.18125 0.60426 \*

\* Se 18 -0.02445 0.21242 0.76051 \*

\* Se 19 -0.02022 0.20363 -0.70332 \*

\* Se 20 -0.00099 -0.19932 -0.66588 \*

\* Nb 1 -0.07682 -0.02913 0.01867 \*

\* Nb 2 0.07621 0.02948 -0.01869 \*

\* Nb 3 0.00012 -0.00027 0.00006 \*

\* Nb 4 0.00012 -0.00026 -0.00005 \*

\* Nb 5 -0.10805 0.00727 0.02016 \*

\* Nb 6 0.06171 0.04949 -0.01964 \*

\* Nb 7 -0.00131 0.00269 0.01275 \*

\* Nb 8 -0.00131 0.00483 -0.01227 \*

\* Nb 9 -0.02628 -0.04582 0.02078 \*

\* Nb 10 0.07195 0.01629 -0.01900 \*

\* Nb 11 -0.02674 0.03360 0.01075 \*

\* Nb 12 -0.02890 0.03245 -0.01327 \*

\* Nb 13 -0.07213 -0.01612 0.01911 \*

\* Nb 14 0.02621 0.04599 -0.02077 \*

\* Nb 15 0.02683 -0.03379 -0.01073 \*

\* Nb 16 0.02900 -0.03265 0.01327 \*

\* Nb 17 -0.06117 -0.04984 0.01967 \*

\* Nb 18 0.10835 -0.00759 -0.02018 \*

\* Nb 19 0.00112 -0.00228 -0.01296 \*

\* Nb 20 0.00110 -0.00443 0.01248 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -1.564601 -0.147510 -0.004549 \*

\* y -0.147510 -2.060275 0.009145 \*

\* z -0.004549 0.009145 -0.586896 \*

\* \*

\* Pressure: 1.4039 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.002381 | -36259.281654 | <-- min BFGS

| trial step | 1.000000 | 0.001960 | -36259.340776 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 8 with line minimization (lambda= 5.658613)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.7554709 -8.3285911 -0.0013197 0.4247895 -0.0018270 -0.0000215

0.0144359 3.3564345 0.0008977 1.0540644 1.8674487 -0.0004291

0.0007170 0.0027964 13.9317121 -0.0000277 -0.0001205 0.4509988

Lattice parameters(A) Cell Angles

a = 16.943711 alpha = 89.973163

b = 3.356466 beta = 90.007548

c = 13.931712 gamma = 119.195735

Current cell volume = 691.653770 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066677 0.664966 0.123184 x

x Se 2 0.133210 0.335274 0.622852 x

x Se 3 0.133222 0.335196 0.876929 x

x Se 4 0.066647 0.664861 0.377083 x

x Se 5 0.266575 0.666511 0.123410 x

x Se 6 0.333025 0.334602 0.622649 x

x Se 7 0.333023 0.334567 0.877125 x

x Se 8 0.266541 0.666428 0.376844 x

x Se 9 0.467368 0.666350 0.123161 x

x Se 10 0.532562 0.333461 0.622893 x

x Se 11 0.532631 0.333648 0.876840 x

x Se 12 0.467437 0.666537 0.377107 x

x Se 13 0.666977 0.665434 0.122875 x

x Se 14 0.733458 0.333570 0.623156 x

x Se 15 0.733425 0.333488 0.876591 x

x Se 16 0.666974 0.665398 0.377351 x

x Se 17 0.866778 0.664803 0.123072 x

x Se 18 0.933354 0.335143 0.622917 x

x Se 19 0.933324 0.335036 0.876816 x

x Se 20 0.866791 0.664726 0.377147 x

x Nb 1 -0.000142 -0.000532 0.250064 x

x Nb 2 0.000142 0.000540 0.749936 x

x Nb 3 0.000001 -0.000002 0.000001 x

x Nb 4 0.000001 0.000000 0.499999 x

x Nb 5 0.199802 -0.000500 0.250062 x

x Nb 6 0.200165 0.000897 0.749934 x

x Nb 7 0.200002 0.000048 0.000021 x

x Nb 8 0.199999 0.000048 0.499978 x

x Nb 9 0.399932 -0.000567 0.250067 x

x Nb 10 0.400149 0.000465 0.749933 x

x Nb 11 0.399948 0.000100 0.000015 x

x Nb 12 0.399951 0.000099 0.499986 x

x Nb 13 0.599849 -0.000472 0.250066 x

x Nb 14 0.600067 0.000566 0.749932 x

x Nb 15 0.600051 -0.000107 -0.000015 x

x Nb 16 0.600048 -0.000104 0.500013 x

x Nb 17 0.799837 -0.000892 0.250066 x

x Nb 18 0.800199 0.000497 0.749938 x

x Nb 19 0.799999 -0.000042 -0.000022 x

x Nb 20 0.800001 -0.000042 0.500023 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62567683E+004 6440.28 <-- SCF

1 -3.62718740E+004 3.77642883E-001 6467.77 <-- SCF

2 -3.62727019E+004 2.06979343E-002 6496.56 <-- SCF

3 -3.62702898E+004 -6.03034638E-002 6523.39 <-- SCF

4 -3.62592887E+004 -2.75027850E-001 6550.17 <-- SCF

5 -3.62595404E+004 6.29273490E-003 6579.28 <-- SCF

6 -3.62594773E+004 -1.57723043E-003 6606.34 <-- SCF

7 -3.62594864E+004 2.29239272E-004 6633.77 <-- SCF

8 -3.62594888E+004 5.88834452E-005 6658.89 <-- SCF

9 -3.62594891E+004 6.69621780E-006 6682.20 <-- SCF

10 -3.62594899E+004 2.18030416E-005 6701.95 <-- SCF

11 -3.62594904E+004 1.14325965E-005 6719.81 <-- SCF

12 -3.62594907E+004 6.46152085E-006 6736.42 <-- SCF

13 -3.62594908E+004 3.62294152E-006 6753.47 <-- SCF

14 -3.62594909E+004 1.99526933E-006 6770.72 <-- SCF

15 -3.62594909E+004 1.19906198E-006 6787.45 <-- SCF

16 -3.62594910E+004 7.17473822E-007 6804.27 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.49095494 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.07212 -0.05235 0.39833 \*

\* Se 2 -0.04539 0.12710 0.35981 \*

\* Se 3 -0.06594 0.12266 -0.35834 \*

\* Se 4 0.04553 -0.06923 -0.40354 \*

\* Se 5 0.10533 -0.02794 0.42988 \*

\* Se 6 -0.14221 0.14341 0.34635 \*

\* Se 7 -0.12989 0.14121 -0.32497 \*

\* Se 8 0.11179 -0.01867 -0.47310 \*

\* Se 9 0.03700 -0.07831 0.44420 \*

\* Se 10 -0.03910 0.10572 0.43768 \*

\* Se 11 -0.03696 0.07834 -0.44408 \*

\* Se 12 0.03919 -0.10578 -0.43777 \*

\* Se 13 0.12979 -0.14122 0.32485 \*

\* Se 14 -0.11190 0.01863 0.47307 \*

\* Se 15 -0.10558 0.02792 -0.42995 \*

\* Se 16 0.14209 -0.14342 -0.34635 \*

\* Se 17 0.06603 -0.12259 0.35852 \*

\* Se 18 -0.04533 0.06934 0.40344 \*

\* Se 19 -0.07191 0.05247 -0.39834 \*

\* Se 20 0.04548 -0.12704 -0.35995 \*

\* Nb 1 -0.07027 -0.05002 0.01336 \*

\* Nb 2 0.06978 0.05011 -0.01336 \*

\* Nb 3 0.00004 -0.00017 -0.00003 \*

\* Nb 4 0.00007 -0.00017 0.00000 \*

\* Nb 5 -0.11311 0.00052 0.01613 \*

\* Nb 6 0.05983 0.06534 -0.01545 \*

\* Nb 7 -0.00499 0.01161 0.02054 \*

\* Nb 8 -0.00628 0.01513 -0.01828 \*

\* Nb 9 -0.00240 -0.05296 0.01821 \*

\* Nb 10 0.03190 0.04823 -0.01325 \*

\* Nb 11 -0.02965 0.02945 0.02420 \*

\* Nb 12 -0.03466 0.02855 -0.02894 \*

\* Nb 13 -0.03216 -0.04810 0.01343 \*

\* Nb 14 0.00250 0.05314 -0.01822 \*

\* Nb 15 0.02974 -0.02956 -0.02417 \*

\* Nb 16 0.03475 -0.02867 0.02897 \*

\* Nb 17 -0.05942 -0.06557 0.01549 \*

\* Nb 18 0.11326 -0.00064 -0.01613 \*

\* Nb 19 0.00484 -0.01147 -0.02062 \*

\* Nb 20 0.00609 -0.01501 0.01835 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -2.899786 -0.121044 0.007094 \*

\* y -0.121044 -3.297090 0.041067 \*

\* z 0.007094 0.041067 -1.865399 \*

\* \*

\* Pressure: 2.6874 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.002381 | -36259.281654 | <-- min BFGS

| trial step | 1.000000 | 0.001960 | -36259.340776 | <-- min BFGS

| line step | 5.658613 | 0.000532 | -36259.491081 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 8 with enthalpy= -3.62594911E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 5.235653E-003 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 4.864851E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.915907E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.297090E+000 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 9 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.009842 | -36259.491081 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 9 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8012720 -8.3636091 -0.0014680 0.4232847 -0.0021562 -0.0000371

0.0171926 3.3751145 0.0012329 1.0489090 1.8562785 -0.0006064

0.0012410 0.0038480 13.9269336 -0.0000482 -0.0001646 0.4511536

Lattice parameters(A) Cell Angles

a = 17.000812 alpha = 89.963214

b = 3.375159 beta = 90.008291

c = 13.926934 gamma = 119.177203

Current cell volume = 697.736235 A\*\*3

-------------------------------

Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066700 0.664188 0.124441 x

x Se 2 0.133169 0.336054 0.624080 x

x Se 3 0.133187 0.335937 0.875752 x

x Se 4 0.066653 0.664011 0.375803 x

x Se 5 0.266582 0.666422 0.124780 x

x Se 6 0.332905 0.335156 0.623768 x

x Se 7 0.332901 0.335102 0.876052 x

x Se 8 0.266533 0.666300 0.375442 x

x Se 9 0.467563 0.666056 0.124405 x

x Se 10 0.532334 0.333655 0.624153 x

x Se 11 0.532436 0.333944 0.875596 x

x Se 12 0.467665 0.666343 0.375848 x

x Se 13 0.667099 0.664899 0.123948 x

x Se 14 0.733466 0.333698 0.624558 x

x Se 15 0.733418 0.333577 0.875221 x

x Se 16 0.667095 0.664844 0.376232 x

x Se 17 0.866814 0.664061 0.124249 x

x Se 18 0.933348 0.335993 0.624197 x

x Se 19 0.933300 0.335813 0.875559 x

x Se 20 0.866832 0.663945 0.375919 x

x Nb 1 -0.000219 -0.000810 0.250087 x

x Nb 2 0.000219 0.000821 0.749913 x

x Nb 3 0.000001 -0.000003 0.000002 x

x Nb 4 0.000001 -0.000001 0.499999 x

x Nb 5 0.199691 -0.000768 0.250085 x

x Nb 6 0.200250 0.001349 0.749909 x

x Nb 7 0.200004 0.000052 0.000036 x

x Nb 8 0.199999 0.000053 0.499962 x

x Nb 9 0.399891 -0.000859 0.250093 x

x Nb 10 0.400228 0.000686 0.749909 x

x Nb 11 0.399921 0.000179 0.000020 x

x Nb 12 0.399924 0.000174 0.499981 x

x Nb 13 0.599769 -0.000695 0.250090 x

x Nb 14 0.600108 0.000859 0.749906 x

x Nb 15 0.600078 -0.000187 -0.000020 x

x Nb 16 0.600074 -0.000180 0.500018 x

x Nb 17 0.799752 -0.001342 0.250090 x

x Nb 18 0.800311 0.000762 0.749915 x

x Nb 19 0.799997 -0.000042 -0.000038 x

x Nb 20 0.800001 -0.000045 0.500039 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62576723E+004 6906.66 <-- SCF

1 -3.62678746E+004 2.55055931E-001 6935.23 <-- SCF

2 -3.62683910E+004 1.29107342E-002 6964.72 <-- SCF

3 -3.62676912E+004 -1.74956822E-002 6991.62 <-- SCF

4 -3.62595407E+004 -2.03760500E-001 7017.78 <-- SCF

5 -3.62597324E+004 4.79253476E-003 7047.08 <-- SCF

6 -3.62596852E+004 -1.18002835E-003 7074.45 <-- SCF

7 -3.62596866E+004 3.45841452E-005 7102.98 <-- SCF

8 -3.62596891E+004 6.05541466E-005 7127.22 <-- SCF

9 -3.62596893E+004 6.99351033E-006 7151.03 <-- SCF

10 -3.62596901E+004 1.82022911E-005 7170.08 <-- SCF

11 -3.62596905E+004 1.05752422E-005 7188.20 <-- SCF

12 -3.62596908E+004 6.84748564E-006 7207.44 <-- SCF

13 -3.62596909E+004 4.19318663E-006 7224.48 <-- SCF

14 -3.62596910E+004 2.59272925E-006 7241.75 <-- SCF

15 -3.62596911E+004 1.96323458E-006 7258.94 <-- SCF

16 -3.62596912E+004 1.39766695E-006 7275.97 <-- SCF

17 -3.62596912E+004 1.01875722E-006 7293.41 <-- SCF

18 -3.62596912E+004 8.10086061E-007 7310.97 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.69123809 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.09266 0.04827 0.19855 \*

\* Se 2 -0.13803 -0.01781 0.20926 \*

\* Se 3 -0.14779 -0.02656 -0.20545 \*

\* Se 4 0.10351 0.03364 -0.19925 \*

\* Se 5 0.06775 0.00967 0.22576 \*

\* Se 6 -0.12335 0.06781 0.14539 \*

\* Se 7 -0.13038 0.05113 -0.15550 \*

\* Se 8 0.07325 0.00025 -0.23444 \*

\* Se 9 -0.09214 0.03808 0.27359 \*

\* Se 10 0.10187 -0.03117 0.28803 \*

\* Se 11 0.09235 -0.03811 -0.27363 \*

\* Se 12 -0.10164 0.03107 -0.28820 \*

\* Se 13 0.13033 -0.05120 0.15534 \*

\* Se 14 -0.07338 -0.00045 0.23446 \*

\* Se 15 -0.06802 -0.00978 -0.22583 \*

\* Se 16 0.12323 -0.06790 -0.14536 \*

\* Se 17 0.14777 0.02678 0.20551 \*

\* Se 18 -0.10343 -0.03349 0.19924 \*

\* Se 19 -0.09245 -0.04817 -0.19864 \*

\* Se 20 0.13800 0.01806 -0.20927 \*

\* Nb 1 -0.05149 -0.06376 0.00403 \*

\* Nb 2 0.05098 0.06396 -0.00398 \*

\* Nb 3 0.00007 -0.00027 -0.00001 \*

\* Nb 4 0.00010 -0.00025 -0.00002 \*

\* Nb 5 -0.10095 -0.00095 0.01045 \*

\* Nb 6 0.04948 0.07849 -0.01052 \*

\* Nb 7 -0.00277 0.00998 0.02614 \*

\* Nb 8 -0.00222 0.01505 -0.02248 \*

\* Nb 9 0.03300 -0.06250 0.01446 \*

\* Nb 10 -0.01460 0.06726 -0.00593 \*

\* Nb 11 -0.03126 0.03563 0.03079 \*

\* Nb 12 -0.03821 0.03329 -0.03766 \*

\* Nb 13 0.01417 -0.06710 0.00620 \*

\* Nb 14 -0.03269 0.06279 -0.01453 \*

\* Nb 15 0.03138 -0.03576 -0.03070 \*

\* Nb 16 0.03836 -0.03343 0.03768 \*

\* Nb 17 -0.04894 -0.07888 0.01061 \*

\* Nb 18 0.10097 0.00068 -0.01039 \*

\* Nb 19 0.00258 -0.00961 -0.02621 \*

\* Nb 20 0.00194 -0.01472 0.02254 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -1.582801 -0.044740 0.018869 \*

\* y -0.044740 -1.425835 0.069756 \*

\* z 0.018869 0.069756 -0.563523 \*

\* \*

\* Pressure: 1.1907 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.009842 | -36259.491081 | <-- min BFGS

| trial step | 1.000000 | 0.004898 | -36259.691370 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 9 with line minimization (lambda= 1.990689)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8466466 -8.3983010 -0.0016149 0.4218049 -0.0024764 -0.0000525

0.0199236 3.3936206 0.0015649 1.0438541 1.8453415 -0.0007801

0.0017601 0.0048899 13.9221995 -0.0000684 -0.0002077 0.4513070

Lattice parameters(A) Cell Angles

a = 17.057385 alpha = 89.953413

b = 3.393679 beta = 90.009028

c = 13.922201 gamma = 119.159159

Current cell volume = 703.783919 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066723 0.663418 0.125686 x

x Se 2 0.133128 0.336827 0.625296 x

x Se 3 0.133152 0.336671 0.874586 x

x Se 4 0.066659 0.663169 0.374535 x

x Se 5 0.266588 0.666333 0.126137 x

x Se 6 0.332786 0.335705 0.624877 x

x Se 7 0.332780 0.335632 0.874989 x

x Se 8 0.266525 0.666172 0.374054 x

x Se 9 0.467757 0.665763 0.125638 x

x Se 10 0.532108 0.333847 0.625401 x

x Se 11 0.532242 0.334237 0.874364 x

x Se 12 0.467891 0.666151 0.374600 x

x Se 13 0.667220 0.664370 0.125011 x

x Se 14 0.733474 0.333826 0.625947 x

x Se 15 0.733412 0.333666 0.873864 x

x Se 16 0.667214 0.664296 0.375123 x

x Se 17 0.866849 0.663326 0.125415 x

x Se 18 0.933342 0.336835 0.625465 x

x Se 19 0.933277 0.336583 0.874314 x

x Se 20 0.866873 0.663170 0.374703 x

x Nb 1 -0.000296 -0.001086 0.250110 x

x Nb 2 0.000295 0.001099 0.749890 x

x Nb 3 0.000001 -0.000005 0.000002 x

x Nb 4 0.000001 -0.000002 0.499998 x

x Nb 5 0.199580 -0.001033 0.250108 x

x Nb 6 0.200335 0.001797 0.749885 x

x Nb 7 0.200006 0.000056 0.000051 x

x Nb 8 0.200000 0.000058 0.499947 x

x Nb 9 0.399851 -0.001149 0.250118 x

x Nb 10 0.400307 0.000905 0.749885 x

x Nb 11 0.399894 0.000256 0.000025 x

x Nb 12 0.399899 0.000248 0.499975 x

x Nb 13 0.599691 -0.000916 0.250114 x

x Nb 14 0.600148 0.001148 0.749881 x

x Nb 15 0.600104 -0.000267 -0.000025 x

x Nb 16 0.600100 -0.000255 0.500023 x

x Nb 17 0.799668 -0.001789 0.250115 x

x Nb 18 0.800421 0.001025 0.749892 x

x Nb 19 0.799995 -0.000042 -0.000054 x

x Nb 20 0.800001 -0.000047 0.500055 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62577952E+004 7413.83 <-- SCF

1 -3.62676740E+004 2.46970424E-001 7442.30 <-- SCF

2 -3.62681844E+004 1.27598965E-002 7472.42 <-- SCF

3 -3.62676887E+004 -1.23934790E-002 7499.77 <-- SCF

4 -3.62596234E+004 -2.01631775E-001 7527.25 <-- SCF

5 -3.62598046E+004 4.53077110E-003 7556.34 <-- SCF

6 -3.62597615E+004 -1.07721441E-003 7583.25 <-- SCF

7 -3.62597614E+004 -4.68706697E-006 7611.89 <-- SCF

8 -3.62597637E+004 5.94306952E-005 7636.17 <-- SCF

9 -3.62597643E+004 1.43583349E-005 7660.16 <-- SCF

10 -3.62597652E+004 2.18418276E-005 7679.70 <-- SCF

11 -3.62597658E+004 1.43607036E-005 7698.53 <-- SCF

12 -3.62597662E+004 1.11455624E-005 7717.48 <-- SCF

13 -3.62597666E+004 8.77223195E-006 7735.62 <-- SCF

14 -3.62597669E+004 7.52176927E-006 7754.27 <-- SCF

15 -3.62597671E+004 6.97432041E-006 7772.72 <-- SCF

16 -3.62597674E+004 7.17006212E-006 7791.25 <-- SCF

17 -3.62597677E+004 6.91920649E-006 7809.77 <-- SCF

18 -3.62597680E+004 7.18519419E-006 7828.44 <-- SCF

19 -3.62597683E+004 7.51262543E-006 7846.78 <-- SCF

20 -3.62597686E+004 8.03494686E-006 7864.22 <-- SCF

21 -3.62597690E+004 8.60519863E-006 7881.50 <-- SCF

22 -3.62597693E+004 8.86684403E-006 7899.27 <-- SCF

23 -3.62597697E+004 9.53099883E-006 7916.72 <-- SCF

24 -3.62597701E+004 1.09881203E-005 7934.38 <-- SCF

25 -3.62597706E+004 1.09968142E-005 7951.64 <-- SCF

26 -3.62597710E+004 1.07498913E-005 7969.22 <-- SCF

27 -3.62597715E+004 1.22643385E-005 7987.05 <-- SCF

28 -3.62597719E+004 1.14441104E-005 8004.33 <-- SCF

29 -3.62597724E+004 1.11857777E-005 8022.09 <-- SCF

30 -3.62597729E+004 1.18043811E-005 8039.88 <-- SCF

31 -3.62597733E+004 1.16880033E-005 8057.30 <-- SCF

32 -3.62597738E+004 1.17840072E-005 8074.81 <-- SCF

33 -3.62597743E+004 1.17942723E-005 8092.27 <-- SCF

34 -3.62597748E+004 1.29264463E-005 8109.91 <-- SCF

35 -3.62597753E+004 1.20054511E-005 8127.58 <-- SCF

36 -3.62597758E+004 1.20338323E-005 8145.28 <-- SCF

37 -3.62597762E+004 1.07990321E-005 8162.73 <-- SCF

38 -3.62597765E+004 9.07698943E-006 8180.45 <-- SCF

39 -3.62597769E+004 9.63209504E-006 8198.19 <-- SCF

40 -3.62597773E+004 8.27759230E-006 8215.66 <-- SCF

41 -3.62597776E+004 7.24849959E-006 8233.70 <-- SCF

42 -3.62597778E+004 6.87316433E-006 8250.98 <-- SCF

43 -3.62597782E+004 9.54651822E-006 8268.25 <-- SCF

44 -3.62597785E+004 7.23931461E-006 8285.69 <-- SCF

45 -3.62597788E+004 6.77370817E-006 8303.34 <-- SCF

46 -3.62597790E+004 4.95744152E-006 8320.72 <-- SCF

47 -3.62597792E+004 6.81700447E-006 8339.02 <-- SCF

48 -3.62597795E+004 6.34690462E-006 8356.95 <-- SCF

49 -3.62597796E+004 2.48236236E-006 8374.53 <-- SCF

50 -3.62597797E+004 3.10640074E-006 8393.14 <-- SCF

51 -3.62597797E+004 -5.13831117E-007 8411.81 <-- SCF

52 -3.62597797E+004 9.29113112E-007 8430.25 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.77973847 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.10770 0.02141 0.15189 \*

\* Se 2 -0.17060 -0.10294 0.11021 \*

\* Se 3 -0.17350 -0.08273 -0.11440 \*

\* Se 4 0.13798 0.03980 -0.13761 \*

\* Se 5 0.06489 -0.05675 0.07300 \*

\* Se 6 -0.12669 -0.08484 0.09966 \*

\* Se 7 -0.11730 -0.08865 -0.10367 \*

\* Se 8 0.07075 -0.05292 -0.07298 \*

\* Se 9 -0.14657 0.03494 0.06752 \*

\* Se 10 0.15547 -0.05519 0.06269 \*

\* Se 11 0.14662 -0.03488 -0.06732 \*

\* Se 12 -0.15549 0.05514 -0.06294 \*

\* Se 13 0.11724 0.08858 0.10292 \*

\* Se 14 -0.07112 0.05247 0.07295 \*

\* Se 15 -0.06505 0.05651 -0.07311 \*

\* Se 16 0.12726 0.08477 -0.09905 \*

\* Se 17 0.17265 0.08261 0.11484 \*

\* Se 18 -0.13823 -0.03958 0.13730 \*

\* Se 19 -0.10734 -0.02092 -0.15253 \*

\* Se 20 0.17011 0.10319 -0.11046 \*

\* Nb 1 -0.03156 -0.08843 -0.01532 \*

\* Nb 2 0.03078 0.08945 0.01554 \*

\* Nb 3 0.00012 -0.00068 0.00018 \*

\* Nb 4 0.00024 -0.00032 -0.00012 \*

\* Nb 5 -0.12693 0.00780 0.00835 \*

\* Nb 6 0.05708 0.09511 -0.01525 \*

\* Nb 7 0.00326 -0.01655 0.01616 \*

\* Nb 8 0.02252 -0.01402 -0.01673 \*

\* Nb 9 0.06691 -0.09639 0.00594 \*

\* Nb 10 -0.03050 0.08479 0.00792 \*

\* Nb 11 -0.05228 0.07633 0.03911 \*

\* Nb 12 -0.06858 0.06048 -0.04985 \*

\* Nb 13 0.02940 -0.08347 -0.00784 \*

\* Nb 14 -0.06594 0.09634 -0.00688 \*

\* Nb 15 0.05311 -0.07675 -0.03849 \*

\* Nb 16 0.06975 -0.06087 0.05026 \*

\* Nb 17 -0.05538 -0.09634 0.01525 \*

\* Nb 18 0.12676 -0.00894 -0.00771 \*

\* Nb 19 -0.00409 0.01765 -0.01632 \*

\* Nb 20 -0.02344 0.01478 0.01688 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.746245 0.514546 0.058840 \*

\* y 0.514546 0.297225 0.083432 \*

\* z 0.058840 0.083432 -0.628111 \*

\* \*

\* Pressure: -0.1385 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.009842 | -36259.491081 | <-- min BFGS

| trial step | 1.000000 | 0.004898 | -36259.691370 | <-- min BFGS

| line step | 1.990689 | 0.000314 | -36259.779816 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 9 with enthalpy= -3.62597798E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.218376E-003 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.277032E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.886353E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 7.462446E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 10 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.001242 | -36259.779816 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 10 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8211188 -8.3837521 -0.0018908 0.4225402 -0.0024651 -0.0000422

0.0197631 3.3875200 0.0014966 1.0457422 1.8487033 -0.0007226

0.0014222 0.0046527 13.9616005 -0.0000549 -0.0001985 0.4500334

Lattice parameters(A) Cell Angles

a = 17.028002 alpha = 89.955560

b = 3.387578 beta = 90.010683

c = 13.961601 gamma = 119.160952

Current cell volume = 703.280954 A\*\*3

-------------------------------

Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066742 0.663151 0.126357 x

x Se 2 0.133094 0.337062 0.625934 x

x Se 3 0.133120 0.336897 0.873946 x

x Se 4 0.066674 0.662889 0.373876 x

x Se 5 0.266594 0.666298 0.126848 x

x Se 6 0.332725 0.335860 0.625474 x

x Se 7 0.332720 0.335782 0.874390 x

x Se 8 0.266526 0.666125 0.373349 x

x Se 9 0.467834 0.665653 0.126298 x

x Se 10 0.532019 0.333915 0.626048 x

x Se 11 0.532165 0.334348 0.873703 x

x Se 12 0.467980 0.666083 0.373952 x

x Se 13 0.667280 0.664221 0.125609 x

x Se 14 0.733474 0.333872 0.626652 x

x Se 15 0.733406 0.333700 0.873153 x

x Se 16 0.667275 0.664141 0.374527 x

x Se 17 0.866880 0.663099 0.126055 x

x Se 18 0.933327 0.337115 0.626124 x

x Se 19 0.933258 0.336850 0.873642 x

x Se 20 0.866906 0.662936 0.374064 x

x Nb 1 -0.000328 -0.001231 0.250118 x

x Nb 2 0.000327 0.001245 0.749882 x

x Nb 3 0.000001 -0.000005 0.000002 x

x Nb 4 0.000001 -0.000003 0.499998 x

x Nb 5 0.199527 -0.001162 0.250119 x

x Nb 6 0.200374 0.002022 0.749873 x

x Nb 7 0.200006 0.000054 0.000058 x

x Nb 8 0.200001 0.000061 0.499939 x

x Nb 9 0.399840 -0.001283 0.250130 x

x Nb 10 0.400335 0.001017 0.749875 x

x Nb 11 0.399879 0.000299 0.000032 x

x Nb 12 0.399883 0.000282 0.499968 x

x Nb 13 0.599662 -0.001028 0.250123 x

x Nb 14 0.600158 0.001284 0.749869 x

x Nb 15 0.600119 -0.000310 -0.000031 x

x Nb 16 0.600116 -0.000288 0.500031 x

x Nb 17 0.799630 -0.002012 0.250127 x

x Nb 18 0.800475 0.001153 0.749881 x

x Nb 19 0.799994 -0.000040 -0.000061 x

x Nb 20 0.799999 -0.000050 0.500063 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62592737E+004 8537.11 <-- SCF

1 -3.62618174E+004 6.35923278E-002 8567.83 <-- SCF

2 -3.62619348E+004 2.93561715E-003 8598.59 <-- SCF

3 -3.62616320E+004 -7.57037466E-003 8625.59 <-- SCF

4 -3.62597584E+004 -4.68401053E-002 8652.72 <-- SCF

5 -3.62597958E+004 9.36583662E-004 8679.94 <-- SCF

6 -3.62597853E+004 -2.63691263E-004 8707.88 <-- SCF

7 -3.62597855E+004 5.93186531E-006 8733.34 <-- SCF

8 -3.62597861E+004 1.43266809E-005 8754.19 <-- SCF

9 -3.62597862E+004 2.95831882E-006 8773.38 <-- SCF

10 -3.62597864E+004 3.62313704E-006 8791.48 <-- SCF

11 -3.62597865E+004 3.89481120E-006 8810.61 <-- SCF

12 -3.62597866E+004 2.76958855E-006 8828.78 <-- SCF

13 -3.62597867E+004 2.20750120E-006 8847.17 <-- SCF

14 -3.62597868E+004 1.79431711E-006 8864.95 <-- SCF

15 -3.62597868E+004 1.50144206E-006 8883.28 <-- SCF

16 -3.62597869E+004 1.22863503E-006 8901.91 <-- SCF

17 -3.62597869E+004 1.04362663E-006 8919.88 <-- SCF

18 -3.62597870E+004 8.47102713E-007 8937.12 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.78696455 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.06056 0.04734 0.02591 \*

\* Se 2 -0.13525 -0.05636 0.07413 \*

\* Se 3 -0.13420 -0.02541 -0.07891 \*

\* Se 4 0.08749 0.03823 -0.03928 \*

\* Se 5 0.05177 -0.08720 -0.07474 \*

\* Se 6 -0.13023 -0.05248 0.07061 \*

\* Se 7 -0.12936 -0.03006 -0.08794 \*

\* Se 8 0.07761 -0.08733 0.05194 \*

\* Se 9 -0.10668 -0.01032 0.03754 \*

\* Se 10 0.13851 -0.01770 0.02767 \*

\* Se 11 0.10687 0.01023 -0.03760 \*

\* Se 12 -0.13856 0.01778 -0.02768 \*

\* Se 13 0.12944 0.02999 0.08757 \*

\* Se 14 -0.07759 0.08710 -0.05190 \*

\* Se 15 -0.05209 0.08703 0.07450 \*

\* Se 16 0.13020 0.05245 -0.07043 \*

\* Se 17 0.13409 0.02542 0.07927 \*

\* Se 18 -0.08735 -0.03801 0.03937 \*

\* Se 19 -0.06022 -0.04714 -0.02603 \*

\* Se 20 0.13511 0.05632 -0.07449 \*

\* Nb 1 -0.06800 -0.05260 0.00066 \*

\* Nb 2 0.06734 0.05325 -0.00063 \*

\* Nb 3 -0.00011 -0.00042 0.00007 \*

\* Nb 4 -0.00002 -0.00046 -0.00015 \*

\* Nb 5 -0.11369 0.04264 0.00135 \*

\* Nb 6 0.05898 0.06125 0.00278 \*

\* Nb 7 -0.00353 0.01221 0.03148 \*

\* Nb 8 0.00303 0.01396 -0.02637 \*

\* Nb 9 0.04234 -0.03192 0.01347 \*

\* Nb 10 -0.04468 0.05955 0.00491 \*

\* Nb 11 -0.02657 0.03660 0.03577 \*

\* Nb 12 -0.04319 0.03686 -0.04799 \*

\* Nb 13 0.04459 -0.05914 -0.00466 \*

\* Nb 14 -0.04223 0.03242 -0.01330 \*

\* Nb 15 0.02669 -0.03679 -0.03554 \*

\* Nb 16 0.04322 -0.03699 0.04782 \*

\* Nb 17 -0.05874 -0.06222 -0.00268 \*

\* Nb 18 0.11406 -0.04321 -0.00137 \*

\* Nb 19 0.00354 -0.01157 -0.03171 \*

\* Nb 20 -0.00314 -0.01330 0.02660 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.602899 -0.148479 0.020368 \*

\* y -0.148479 0.176094 0.078374 \*

\* z 0.020368 0.078374 0.401692 \*

\* \*

\* Pressure: 0.0084 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.001242 | -36259.779816 | <-- min BFGS

| trial step | 1.000000 | -0.000101 | -36259.787073 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 10 with enthalpy= -3.62597871E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.814234E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.642407E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 9.937857E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 6.028987E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 11 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000175 | -36259.787073 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 11 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8271831 -8.3847622 -0.0017176 0.4223360 -0.0025203 -0.0000377

0.0202223 3.3887174 0.0013491 1.0449934 1.8479128 -0.0006474

0.0012701 0.0041698 13.9514146 -0.0000491 -0.0001790 0.4503619

Lattice parameters(A) Cell Angles

a = 17.033778 alpha = 89.960034

b = 3.388778 beta = 90.009666

c = 13.951415 gamma = 119.146220

Current cell volume = 703.356174 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066752 0.663038 0.126594 x

x Se 2 0.133075 0.337148 0.626169 x

x Se 3 0.133101 0.336987 0.873720 x

x Se 4 0.066684 0.662768 0.373634 x

x Se 5 0.266600 0.666262 0.127096 x

x Se 6 0.332692 0.335911 0.625688 x

x Se 7 0.332687 0.335836 0.874182 x

x Se 8 0.266530 0.666087 0.373094 x

x Se 9 0.467860 0.665576 0.126532 x

x Se 10 0.531989 0.333969 0.626284 x

x Se 11 0.532139 0.334425 0.873470 x

x Se 12 0.468010 0.666030 0.373717 x

x Se 13 0.667313 0.664167 0.125817 x

x Se 14 0.733469 0.333910 0.626907 x

x Se 15 0.733400 0.333736 0.872905 x

x Se 16 0.667308 0.664091 0.374313 x

x Se 17 0.866899 0.663009 0.126281 x

x Se 18 0.933317 0.337237 0.626366 x

x Se 19 0.933248 0.336963 0.873405 x

x Se 20 0.866926 0.662850 0.373829 x

x Nb 1 -0.000347 -0.001315 0.250122 x

x Nb 2 0.000346 0.001330 0.749878 x

x Nb 3 0.000001 -0.000006 0.000002 x

x Nb 4 0.000001 -0.000003 0.499998 x

x Nb 5 0.199497 -0.001223 0.250123 x

x Nb 6 0.200395 0.002141 0.749868 x

x Nb 7 0.200007 0.000057 0.000064 x

x Nb 8 0.200002 0.000066 0.499934 x

x Nb 9 0.399837 -0.001343 0.250136 x

x Nb 10 0.400346 0.001070 0.749871 x

x Nb 11 0.399872 0.000322 0.000036 x

x Nb 12 0.399874 0.000300 0.499962 x

x Nb 13 0.599651 -0.001082 0.250127 x

x Nb 14 0.600162 0.001343 0.749863 x

x Nb 15 0.600126 -0.000334 -0.000036 x

x Nb 16 0.600125 -0.000307 0.500037 x

x Nb 17 0.799610 -0.002131 0.250132 x

x Nb 18 0.800505 0.001212 0.749877 x

x Nb 19 0.799994 -0.000041 -0.000067 x

x Nb 20 0.799998 -0.000055 0.500069 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597309E+004 9040.28 <-- SCF

1 -3.62600611E+004 8.25502649E-003 9067.50 <-- SCF

2 -3.62600770E+004 3.99368092E-004 9096.55 <-- SCF

3 -3.62600310E+004 -1.14999972E-003 9123.89 <-- SCF

4 -3.62597859E+004 -6.12787481E-003 9150.47 <-- SCF

5 -3.62597913E+004 1.35338348E-004 9177.91 <-- SCF

6 -3.62597906E+004 -1.68792995E-005 9202.27 <-- SCF

7 -3.62597905E+004 -4.01845232E-006 9224.45 <-- SCF

8 -3.62597906E+004 1.92177725E-006 9243.83 <-- SCF

9 -3.62597906E+004 8.66082113E-007 9262.39 <-- SCF

10 -3.62597906E+004 4.36834632E-007 9280.33 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.79061780 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.04030 0.05935 0.00022 \*

\* Se 2 -0.13243 -0.01978 0.05859 \*

\* Se 3 -0.12959 0.00786 -0.06040 \*

\* Se 4 0.07197 0.05683 0.00928 \*

\* Se 5 0.03603 -0.08458 -0.11350 \*

\* Se 6 -0.13503 -0.02843 0.07078 \*

\* Se 7 -0.12840 -0.00665 -0.08928 \*

\* Se 8 0.06983 -0.08400 0.10827 \*

\* Se 9 -0.07680 -0.02699 0.02123 \*

\* Se 10 0.11266 -0.00271 0.02133 \*

\* Se 11 0.07703 0.02686 -0.02136 \*

\* Se 12 -0.11267 0.00277 -0.02132 \*

\* Se 13 0.12852 0.00658 0.08892 \*

\* Se 14 -0.06977 0.08379 -0.10828 \*

\* Se 15 -0.03636 0.08444 0.11337 \*

\* Se 16 0.13503 0.02841 -0.07061 \*

\* Se 17 0.12944 -0.00787 0.06070 \*

\* Se 18 -0.07184 -0.05661 -0.00921 \*

\* Se 19 -0.03996 -0.05914 -0.00036 \*

\* Se 20 0.13226 0.01974 -0.05887 \*

\* Nb 1 -0.06658 -0.05240 -0.00258 \*

\* Nb 2 0.06598 0.05293 0.00258 \*

\* Nb 3 -0.00013 -0.00035 0.00006 \*

\* Nb 4 -0.00003 -0.00039 -0.00013 \*

\* Nb 5 -0.10795 0.04177 0.00089 \*

\* Nb 6 0.05780 0.06229 0.00321 \*

\* Nb 7 -0.00330 0.01369 0.03156 \*

\* Nb 8 0.00199 0.01626 -0.02655 \*

\* Nb 9 0.04531 -0.03076 0.01148 \*

\* Nb 10 -0.05336 0.06288 0.00744 \*

\* Nb 11 -0.02375 0.03450 0.03382 \*

\* Nb 12 -0.03880 0.03339 -0.04543 \*

\* Nb 13 0.05315 -0.06254 -0.00715 \*

\* Nb 14 -0.04515 0.03126 -0.01132 \*

\* Nb 15 0.02385 -0.03466 -0.03361 \*

\* Nb 16 0.03889 -0.03359 0.04528 \*

\* Nb 17 -0.05757 -0.06313 -0.00311 \*

\* Nb 18 0.10822 -0.04221 -0.00090 \*

\* Nb 19 0.00332 -0.01314 -0.03181 \*

\* Nb 20 -0.00211 -0.01569 0.02677 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.559840 -0.143786 0.017334 \*

\* y -0.143786 0.236399 0.066865 \*

\* z 0.017334 0.066865 0.263827 \*

\* \*

\* Pressure: 0.0199 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000175 | -36259.787073 | <-- min BFGS

| trial step | 1.000000 | 0.000100 | -36259.790758 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 11 with line minimization (lambda= 2.333841)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8352719 -8.3861096 -0.0014865 0.4220640 -0.0025937 -0.0000317

0.0208348 3.3903145 0.0011525 1.0439961 1.8468595 -0.0005471

0.0010674 0.0035257 13.9378283 -0.0000413 -0.0001530 0.4508009

Lattice parameters(A) Cell Angles

a = 17.041483 alpha = 89.966004

b = 3.390379 beta = 90.008310

c = 13.937829 gamma = 119.126587

Current cell volume = 703.455500 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066766 0.662887 0.126910 x

x Se 2 0.133048 0.337262 0.626483 x

x Se 3 0.133076 0.337107 0.873418 x

x Se 4 0.066697 0.662606 0.373312 x

x Se 5 0.266607 0.666214 0.127427 x

x Se 6 0.332649 0.335979 0.625973 x

x Se 7 0.332643 0.335908 0.873905 x

x Se 8 0.266537 0.666035 0.372753 x

x Se 9 0.467895 0.665473 0.126844 x

x Se 10 0.531949 0.334040 0.626598 x

x Se 11 0.532104 0.334528 0.873157 x

x Se 12 0.468049 0.665958 0.373403 x

x Se 13 0.667357 0.664095 0.126095 x

x Se 14 0.733463 0.333962 0.627247 x

x Se 15 0.733393 0.333783 0.872574 x

x Se 16 0.667352 0.664024 0.374027 x

x Se 17 0.866924 0.662889 0.126584 x

x Se 18 0.933304 0.337399 0.626688 x

x Se 19 0.933234 0.337115 0.873089 x

x Se 20 0.866952 0.662735 0.373516 x

x Nb 1 -0.000373 -0.001428 0.250127 x

x Nb 2 0.000372 0.001443 0.749873 x

x Nb 3 0.000001 -0.000006 0.000003 x

x Nb 4 0.000001 -0.000003 0.499998 x

x Nb 5 0.199457 -0.001303 0.250129 x

x Nb 6 0.200422 0.002301 0.749862 x

x Nb 7 0.200007 0.000060 0.000072 x

x Nb 8 0.200003 0.000073 0.499927 x

x Nb 9 0.399832 -0.001422 0.250144 x

x Nb 10 0.400361 0.001142 0.749866 x

x Nb 11 0.399861 0.000354 0.000043 x

x Nb 12 0.399863 0.000325 0.499954 x

x Nb 13 0.599636 -0.001154 0.250132 x

x Nb 14 0.600167 0.001423 0.749855 x

x Nb 15 0.600136 -0.000366 -0.000042 x

x Nb 16 0.600136 -0.000332 0.500045 x

x Nb 17 0.799582 -0.002291 0.250138 x

x Nb 18 0.800545 0.001292 0.749871 x

x Nb 19 0.799994 -0.000043 -0.000075 x

x Nb 20 0.799997 -0.000061 0.500076 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62596843E+004 9380.28 <-- SCF

1 -3.62602972E+004 1.53205310E-002 9406.75 <-- SCF

2 -3.62603305E+004 8.34062725E-004 9435.06 <-- SCF

3 -3.62602455E+004 -2.12500527E-003 9460.67 <-- SCF

4 -3.62597838E+004 -1.15433035E-002 9485.97 <-- SCF

5 -3.62597943E+004 2.62412195E-004 9511.59 <-- SCF

6 -3.62597926E+004 -4.18693838E-005 9535.55 <-- SCF

7 -3.62597923E+004 -8.25468297E-006 9558.11 <-- SCF

8 -3.62597925E+004 4.28128906E-006 9577.45 <-- SCF

9 -3.62597925E+004 1.01029428E-006 9595.16 <-- SCF

10 -3.62597925E+004 9.04527997E-007 9612.34 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.79253149 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00472 0.05736 -0.01438 \*

\* Se 2 -0.12210 0.03129 0.03051 \*

\* Se 3 -0.11642 0.05441 -0.03662 \*

\* Se 4 0.04046 0.06883 0.03173 \*

\* Se 5 0.00836 -0.08252 -0.15512 \*

\* Se 6 -0.12540 0.00154 0.06684 \*

\* Se 7 -0.11229 0.02006 -0.08208 \*

\* Se 8 0.04504 -0.08058 0.15316 \*

\* Se 9 -0.04791 -0.05808 0.00250 \*

\* Se 10 0.07856 0.01833 -0.00044 \*

\* Se 11 0.04805 0.05788 -0.00261 \*

\* Se 12 -0.07852 -0.01827 0.00041 \*

\* Se 13 0.11248 -0.02014 0.08173 \*

\* Se 14 -0.04496 0.08038 -0.15319 \*

\* Se 15 -0.00868 0.08239 0.15498 \*

\* Se 16 0.12548 -0.00158 -0.06672 \*

\* Se 17 0.11618 -0.05444 0.03697 \*

\* Se 18 -0.04029 -0.06861 -0.03162 \*

\* Se 19 -0.00434 -0.05713 0.01422 \*

\* Se 20 0.12186 -0.03134 -0.03078 \*

\* Nb 1 -0.06155 -0.05339 -0.00584 \*

\* Nb 2 0.06097 0.05388 0.00583 \*

\* Nb 3 -0.00015 -0.00032 0.00008 \*

\* Nb 4 -0.00002 -0.00035 -0.00014 \*

\* Nb 5 -0.10273 0.04146 -0.00078 \*

\* Nb 6 0.05447 0.06307 0.00495 \*

\* Nb 7 -0.00316 0.01468 0.03147 \*

\* Nb 8 0.00071 0.01764 -0.02669 \*

\* Nb 9 0.05022 -0.02964 0.00934 \*

\* Nb 10 -0.06606 0.06620 0.00986 \*

\* Nb 11 -0.02139 0.03231 0.03254 \*

\* Nb 12 -0.03557 0.03080 -0.04374 \*

\* Nb 13 0.06571 -0.06590 -0.00954 \*

\* Nb 14 -0.04997 0.03020 -0.00917 \*

\* Nb 15 0.02146 -0.03245 -0.03231 \*

\* Nb 16 0.03564 -0.03098 0.04356 \*

\* Nb 17 -0.05420 -0.06386 -0.00485 \*

\* Nb 18 0.10295 -0.04187 0.00080 \*

\* Nb 19 0.00321 -0.01416 -0.03177 \*

\* Nb 20 -0.00083 -0.01712 0.02693 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.522599 -0.129751 0.012156 \*

\* y -0.129751 0.295060 0.052278 \*

\* z 0.012156 0.052278 0.058182 \*

\* \*

\* Pressure: 0.0565 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000175 | -36259.787073 | <-- min BFGS

| trial step | 1.000000 | 0.000100 | -36259.790758 | <-- min BFGS

| line step | 2.333841 | 0.000018 | -36259.792677 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 11 with enthalpy= -3.62597927E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.401002E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.788308E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 8.311731E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 5.225993E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 12 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000106 | -36259.792677 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 12 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8458664 -8.3841485 -0.0011263 0.4217359 -0.0026419 -0.0000244

0.0212377 3.3902487 0.0008820 1.0429609 1.8467777 -0.0004129

0.0008215 0.0026508 13.9311836 -0.0000319 -0.0001171 0.4510159

Lattice parameters(A) Cell Angles

a = 17.049742 alpha = 89.974172

b = 3.390315 beta = 90.006204

c = 13.931184 gamma = 119.096514

Current cell volume = 703.653444 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066770 0.662909 0.126923 x

x Se 2 0.133030 0.337231 0.626503 x

x Se 3 0.133059 0.337091 0.873399 x

x Se 4 0.066705 0.662642 0.373299 x

x Se 5 0.266610 0.666173 0.127420 x

x Se 6 0.332629 0.335935 0.625996 x

x Se 7 0.332625 0.335878 0.873883 x

x Se 8 0.266544 0.666004 0.372757 x

x Se 9 0.467888 0.665419 0.126858 x

x Se 10 0.531959 0.334081 0.626613 x

x Se 11 0.532111 0.334581 0.873144 x

x Se 12 0.468039 0.665917 0.373388 x

x Se 13 0.667375 0.664125 0.126117 x

x Se 14 0.733455 0.333993 0.627244 x

x Se 15 0.733389 0.333825 0.872581 x

x Se 16 0.667371 0.664067 0.374005 x

x Se 17 0.866941 0.662904 0.126603 x

x Se 18 0.933296 0.337363 0.626701 x

x Se 19 0.933230 0.337093 0.873077 x

x Se 20 0.866970 0.662766 0.373495 x

x Nb 1 -0.000383 -0.001486 0.250127 x

x Nb 2 0.000381 0.001501 0.749873 x

x Nb 3 0.000001 -0.000007 0.000003 x

x Nb 4 0.000001 -0.000004 0.499998 x

x Nb 5 0.199440 -0.001322 0.250130 x

x Nb 6 0.200432 0.002366 0.749862 x

x Nb 7 0.200007 0.000066 0.000078 x

x Nb 8 0.200003 0.000083 0.499922 x

x Nb 9 0.399838 -0.001431 0.250146 x

x Nb 10 0.400355 0.001164 0.749867 x

x Nb 11 0.399858 0.000368 0.000049 x

x Nb 12 0.399857 0.000333 0.499946 x

x Nb 13 0.599642 -0.001177 0.250131 x

x Nb 14 0.600161 0.001432 0.749852 x

x Nb 15 0.600140 -0.000381 -0.000048 x

x Nb 16 0.600142 -0.000340 0.500053 x

x Nb 17 0.799573 -0.002356 0.250138 x

x Nb 18 0.800562 0.001311 0.749871 x

x Nb 19 0.799994 -0.000049 -0.000081 x

x Nb 20 0.799997 -0.000070 0.500081 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597857E+004 9711.91 <-- SCF

1 -3.62598037E+004 4.48577369E-004 9738.80 <-- SCF

2 -3.62598046E+004 2.39047079E-005 9764.27 <-- SCF

3 -3.62598035E+004 -2.83475614E-005 9791.23 <-- SCF

4 -3.62597948E+004 -2.16819449E-004 9817.42 <-- SCF

5 -3.62597954E+004 1.43919161E-005 9839.75 <-- SCF

6 -3.62597953E+004 -2.94524181E-006 9857.98 <-- SCF

7 -3.62597952E+004 -1.00111718E-006 9876.78 <-- SCF

8 -3.62597953E+004 2.87876766E-007 9893.77 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.79525803 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00954 0.05545 -0.01689 \*

\* Se 2 -0.12957 0.03425 0.02593 \*

\* Se 3 -0.12457 0.05644 -0.03293 \*

\* Se 4 0.04367 0.06747 0.03494 \*

\* Se 5 0.00978 -0.08141 -0.15576 \*

\* Se 6 -0.13018 0.00742 0.06604 \*

\* Se 7 -0.11724 0.02440 -0.08100 \*

\* Se 8 0.04509 -0.08026 0.15424 \*

\* Se 9 -0.04217 -0.06027 0.00361 \*

\* Se 10 0.07104 0.02071 -0.00246 \*

\* Se 11 0.04228 0.06008 -0.00366 \*

\* Se 12 -0.07101 -0.02063 0.00239 \*

\* Se 13 0.11747 -0.02448 0.08057 \*

\* Se 14 -0.04500 0.08008 -0.15427 \*

\* Se 15 -0.01009 0.08128 0.15563 \*

\* Se 16 0.13031 -0.00748 -0.06586 \*

\* Se 17 0.12427 -0.05647 0.03337 \*

\* Se 18 -0.04347 -0.06728 -0.03477 \*

\* Se 19 -0.00915 -0.05522 0.01666 \*

\* Se 20 0.12927 -0.03428 -0.02627 \*

\* Nb 1 -0.05913 -0.05323 -0.00627 \*

\* Nb 2 0.05843 0.05388 0.00624 \*

\* Nb 3 -0.00020 -0.00035 0.00018 \*

\* Nb 4 -0.00005 -0.00037 -0.00023 \*

\* Nb 5 -0.11117 0.04180 -0.00063 \*

\* Nb 6 0.05267 0.06155 0.00413 \*

\* Nb 7 -0.01045 0.01694 0.03243 \*

\* Nb 8 -0.00506 0.01968 -0.02705 \*

\* Nb 9 0.04316 -0.02844 0.00936 \*

\* Nb 10 -0.06339 0.06638 0.00993 \*

\* Nb 11 -0.02569 0.02981 0.03199 \*

\* Nb 12 -0.03971 0.02770 -0.04342 \*

\* Nb 13 0.06291 -0.06611 -0.00961 \*

\* Nb 14 -0.04281 0.02912 -0.00923 \*

\* Nb 15 0.02575 -0.02996 -0.03170 \*

\* Nb 16 0.03979 -0.02789 0.04320 \*

\* Nb 17 -0.05226 -0.06243 -0.00402 \*

\* Nb 18 0.11141 -0.04237 0.00066 \*

\* Nb 19 0.01057 -0.01637 -0.03288 \*

\* Nb 20 0.00498 -0.01912 0.02741 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.404636 -0.105635 0.008982 \*

\* y -0.105635 0.280680 0.034566 \*

\* z 0.008982 0.034566 -0.000457 \*

\* \*

\* Pressure: 0.0415 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000106 | -36259.792677 | <-- min BFGS

| trial step | 1.000000 | 0.000085 | -36259.795380 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 12 with line minimization (lambda= 5.154105)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8898774 -8.3760020 0.0003697 0.4203787 -0.0028412 0.0000058

0.0229115 3.3899754 -0.0002415 1.0386780 1.8464404 0.0001456

-0.0001996 -0.0009840 13.9035806 0.0000069 0.0000321 0.4519113

Lattice parameters(A) Cell Angles

a = 17.084082 alpha = 90.008142

b = 3.390053 beta = 89.997489

c = 13.903581 gamma = 118.971823

Current cell volume = 704.469752 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066788 0.663002 0.126975 x

x Se 2 0.132956 0.337102 0.626589 x

x Se 3 0.132988 0.337026 0.873320 x

x Se 4 0.066739 0.662789 0.373243 x

x Se 5 0.266624 0.665999 0.127390 x

x Se 6 0.332550 0.335754 0.626087 x

x Se 7 0.332551 0.335752 0.873791 x

x Se 8 0.266574 0.665874 0.372771 x

x Se 9 0.467860 0.665196 0.126915 x

x Se 10 0.532001 0.334251 0.626674 x

x Se 11 0.532140 0.334804 0.873087 x

x Se 12 0.467997 0.665747 0.373327 x

x Se 13 0.667449 0.664251 0.126208 x

x Se 14 0.733425 0.334122 0.627229 x

x Se 15 0.733375 0.333998 0.872611 x

x Se 16 0.667450 0.664248 0.373914 x

x Se 17 0.867012 0.662969 0.126681 x

x Se 18 0.933262 0.337217 0.626757 x

x Se 19 0.933213 0.337001 0.873024 x

x Se 20 0.867044 0.662894 0.373409 x

x Nb 1 -0.000424 -0.001727 0.250125 x

x Nb 2 0.000422 0.001744 0.749875 x

x Nb 3 0.000001 -0.000008 0.000003 x

x Nb 4 0.000001 -0.000005 0.499998 x

x Nb 5 0.199371 -0.001401 0.250131 x

x Nb 6 0.200470 0.002636 0.749863 x

x Nb 7 0.200005 0.000089 0.000102 x

x Nb 8 0.200005 0.000120 0.499901 x

x Nb 9 0.399861 -0.001469 0.250155 x

x Nb 10 0.400330 0.001257 0.749872 x

x Nb 11 0.399842 0.000428 0.000074 x

x Nb 12 0.399832 0.000367 0.499912 x

x Nb 13 0.599667 -0.001269 0.250127 x

x Nb 14 0.600138 0.001472 0.749843 x

x Nb 15 0.600156 -0.000442 -0.000073 x

x Nb 16 0.600167 -0.000375 0.500087 x

x Nb 17 0.799535 -0.002627 0.250137 x

x Nb 18 0.800632 0.001389 0.749869 x

x Nb 19 0.799995 -0.000070 -0.000105 x

x Nb 20 0.799995 -0.000106 0.500102 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62596463E+004 9993.89 <-- SCF

1 -3.62598390E+004 4.81787244E-003 10018.91 <-- SCF

2 -3.62598496E+004 2.63418193E-004 10047.48 <-- SCF

3 -3.62598184E+004 -7.80032549E-004 10073.56 <-- SCF

4 -3.62598016E+004 -4.19264091E-004 10099.05 <-- SCF

5 -3.62598001E+004 -3.68288205E-005 10124.44 <-- SCF

6 -3.62597999E+004 -5.00052436E-006 10145.28 <-- SCF

7 -3.62598000E+004 1.01635475E-006 10163.86 <-- SCF

8 -3.62598000E+004 9.84142730E-007 10180.98 <-- SCF

9 -3.62598000E+004 6.84797458E-007 10198.81 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.80004188 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.03474 0.04517 -0.02770 \*

\* Se 2 -0.15044 0.05169 0.00785 \*

\* Se 3 -0.14775 0.07156 -0.01831 \*

\* Se 4 0.06510 0.05881 0.04707 \*

\* Se 5 0.02399 -0.07682 -0.16355 \*

\* Se 6 -0.13560 0.02956 0.06379 \*

\* Se 7 -0.12190 0.04176 -0.07573 \*

\* Se 8 0.05338 -0.07785 0.16232 \*

\* Se 9 -0.01791 -0.07691 0.00034 \*

\* Se 10 0.03911 0.03793 -0.01564 \*

\* Se 11 0.01787 0.07676 -0.00021 \*

\* Se 12 -0.03919 -0.03783 0.01549 \*

\* Se 13 0.12230 -0.04183 0.07515 \*

\* Se 14 -0.05324 0.07769 -0.16233 \*

\* Se 15 -0.02417 0.07671 0.16343 \*

\* Se 16 0.13588 -0.02964 -0.06350 \*

\* Se 17 0.14729 -0.07165 0.01898 \*

\* Se 18 -0.06487 -0.05866 -0.04681 \*

\* Se 19 -0.03435 -0.04496 0.02734 \*

\* Se 20 0.14997 -0.05175 -0.00836 \*

\* Nb 1 -0.05504 -0.03833 -0.00794 \*

\* Nb 2 0.05419 0.03939 0.00787 \*

\* Nb 3 -0.00028 -0.00040 0.00037 \*

\* Nb 4 -0.00010 -0.00041 -0.00040 \*

\* Nb 5 -0.11481 0.04133 -0.00238 \*

\* Nb 6 0.06622 0.04781 0.00347 \*

\* Nb 7 -0.00841 0.01677 0.02610 \*

\* Nb 8 -0.00222 0.01908 -0.01980 \*

\* Nb 9 0.01835 -0.02111 0.00573 \*

\* Nb 10 -0.03629 0.05432 0.01139 \*

\* Nb 11 -0.02104 0.02446 0.02097 \*

\* Nb 12 -0.03678 0.02178 -0.03178 \*

\* Nb 13 0.03555 -0.05414 -0.01111 \*

\* Nb 14 -0.01785 0.02208 -0.00566 \*

\* Nb 15 0.02101 -0.02466 -0.02055 \*

\* Nb 16 0.03682 -0.02199 0.03147 \*

\* Nb 17 -0.06562 -0.04887 -0.00336 \*

\* Nb 18 0.11512 -0.04233 0.00244 \*

\* Nb 19 0.00872 -0.01609 -0.02687 \*

\* Nb 20 0.00224 -0.01844 0.02043 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.135597 -0.046396 -0.006121 \*

\* y -0.046396 0.263380 -0.042805 \*

\* z -0.006121 -0.042805 -0.217149 \*

\* \*

\* Pressure: -0.0606 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000106 | -36259.792677 | <-- min BFGS

| trial step | 1.000000 | 0.000085 | -36259.795380 | <-- min BFGS

| line step | 5.154105 | -4.457E-006 | -36259.800087 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 12 with enthalpy= -3.62598001E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.852612E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.877734E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.159465E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.633801E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 13 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000142 | -36259.800087 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 13 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8911132 -8.3675782 0.0004479 0.4203338 -0.0028619 0.0000093

0.0230600 3.3868899 -0.0003331 1.0384677 1.8480784 0.0001927

-0.0003152 -0.0012733 13.9109733 0.0000113 0.0000443 0.4516712

Lattice parameters(A) Cell Angles

a = 17.081031 alpha = 90.010888

b = 3.386968 beta = 89.997060

c = 13.910973 gamma = 118.942298

Current cell volume = 704.278046 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066787 0.663179 0.126747 x

x Se 2 0.132944 0.336942 0.626375 x

x Se 3 0.132976 0.336888 0.873525 x

x Se 4 0.066746 0.662996 0.373477 x

x Se 5 0.266626 0.665974 0.127115 x

x Se 6 0.332553 0.335620 0.625901 x

x Se 7 0.332556 0.335636 0.873967 x

x Se 8 0.266583 0.665868 0.373050 x

x Se 9 0.467821 0.665194 0.126694 x

x Se 10 0.532050 0.334259 0.626448 x

x Se 11 0.532179 0.334806 0.873308 x

x Se 12 0.467949 0.665740 0.373552 x

x Se 13 0.667445 0.664367 0.126032 x

x Se 14 0.733416 0.334128 0.626951 x

x Se 15 0.733374 0.334023 0.872886 x

x Se 16 0.667447 0.664382 0.374100 x

x Se 17 0.867024 0.663107 0.126477 x

x Se 18 0.933255 0.337010 0.626523 x

x Se 19 0.933214 0.336824 0.873252 x

x Se 20 0.867056 0.663054 0.373623 x

x Nb 1 -0.000419 -0.001727 0.250120 x

x Nb 2 0.000417 0.001743 0.749880 x

x Nb 3 0.000001 -0.000008 0.000003 x

x Nb 4 0.000001 -0.000005 0.499998 x

x Nb 5 0.199375 -0.001367 0.250127 x

x Nb 6 0.200463 0.002609 0.749868 x

x Nb 7 0.200004 0.000097 0.000104 x

x Nb 8 0.200005 0.000131 0.499899 x

x Nb 9 0.399873 -0.001419 0.250152 x

x Nb 10 0.400309 0.001236 0.749878 x

x Nb 11 0.399843 0.000423 0.000078 x

x Nb 12 0.399832 0.000356 0.499906 x

x Nb 13 0.599688 -0.001248 0.250121 x

x Nb 14 0.600126 0.001423 0.749846 x

x Nb 15 0.600155 -0.000436 -0.000077 x

x Nb 16 0.600167 -0.000364 0.500093 x

x Nb 17 0.799541 -0.002602 0.250132 x

x Nb 18 0.800627 0.001355 0.749873 x

x Nb 19 0.799997 -0.000078 -0.000108 x

x Nb 20 0.799995 -0.000117 0.500104 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597453E+004 10297.98 <-- SCF

1 -3.62600388E+004 7.33856309E-003 10324.84 <-- SCF

2 -3.62600524E+004 3.40358158E-004 10354.53 <-- SCF

3 -3.62600037E+004 -1.21878478E-003 10383.62 <-- SCF

4 -3.62597993E+004 -5.10851314E-003 10411.09 <-- SCF

5 -3.62598037E+004 1.08970411E-004 10439.62 <-- SCF

6 -3.62598031E+004 -1.58650068E-005 10462.70 <-- SCF

7 -3.62598029E+004 -2.86042817E-006 10485.97 <-- SCF

8 -3.62598030E+004 8.64999052E-007 10503.84 <-- SCF

9 -3.62598030E+004 2.25320631E-007 10520.88 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.80298296 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.06659 0.04834 -0.01745 \*

\* Se 2 -0.16805 0.01959 0.02798 \*

\* Se 3 -0.16949 0.03982 -0.03168 \*

\* Se 4 0.09337 0.05250 0.03708 \*

\* Se 5 0.05271 -0.07612 -0.12796 \*

\* Se 6 -0.15436 0.02103 0.07675 \*

\* Se 7 -0.14270 0.03366 -0.08769 \*

\* Se 8 0.07839 -0.07805 0.11987 \*

\* Se 9 -0.02739 -0.05768 0.00908 \*

\* Se 10 0.05655 0.02516 -0.00159 \*

\* Se 11 0.02727 0.05761 -0.00876 \*

\* Se 12 -0.05685 -0.02503 0.00132 \*

\* Se 13 0.14329 -0.03377 0.08678 \*

\* Se 14 -0.07825 0.07787 -0.11983 \*

\* Se 15 -0.05286 0.07598 0.12784 \*

\* Se 16 0.15481 -0.02115 -0.07616 \*

\* Se 17 0.16897 -0.03985 0.03258 \*

\* Se 18 -0.09310 -0.05237 -0.03671 \*

\* Se 19 -0.06617 -0.04817 0.01689 \*

\* Se 20 0.16751 -0.01958 -0.02870 \*

\* Nb 1 -0.05057 -0.03101 -0.00881 \*

\* Nb 2 0.04934 0.03290 0.00873 \*

\* Nb 3 -0.00043 -0.00060 0.00071 \*

\* Nb 4 -0.00020 -0.00061 -0.00071 \*

\* Nb 5 -0.12532 0.04080 -0.00212 \*

\* Nb 6 0.08022 0.04595 0.00027 \*

\* Nb 7 -0.00890 0.01660 0.02526 \*

\* Nb 8 0.00074 0.01932 -0.01773 \*

\* Nb 9 0.01135 -0.01837 0.00703 \*

\* Nb 10 -0.02272 0.04785 0.01230 \*

\* Nb 11 -0.02115 0.02437 0.01504 \*

\* Nb 12 -0.04056 0.02023 -0.02787 \*

\* Nb 13 0.02148 -0.04777 -0.01206 \*

\* Nb 14 -0.01053 0.01989 -0.00703 \*

\* Nb 15 0.02099 -0.02469 -0.01438 \*

\* Nb 16 0.04056 -0.02053 0.02738 \*

\* Nb 17 -0.07919 -0.04752 -0.00012 \*

\* Nb 18 0.12575 -0.04263 0.00222 \*

\* Nb 19 0.00950 -0.01560 -0.02661 \*

\* Nb 20 -0.00057 -0.01839 0.01887 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.185371 -0.034471 -0.005790 \*

\* y -0.034471 0.106038 -0.045459 \*

\* z -0.005790 -0.045459 -0.108575 \*

\* \*

\* Pressure: -0.0609 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000142 | -36259.800087 | <-- min BFGS

| trial step | 1.000000 | 0.000069 | -36259.803041 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 13 with line minimization (lambda= 1.948254)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8922852 -8.3595903 0.0005221 0.4202912 -0.0028816 0.0000125

0.0232009 3.3839641 -0.0004199 1.0382682 1.8496345 0.0002374

-0.0004248 -0.0015477 13.9179834 0.0000156 0.0000559 0.4514437

Lattice parameters(A) Cell Angles

a = 17.078141 alpha = 90.013493

b = 3.384044 beta = 89.996655

c = 13.917983 gamma = 118.914288

Current cell volume = 704.095572 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066785 0.663347 0.126531 x

x Se 2 0.132934 0.336791 0.626172 x

x Se 3 0.132964 0.336756 0.873719 x

x Se 4 0.066752 0.663192 0.373699 x

x Se 5 0.266627 0.665950 0.126855 x

x Se 6 0.332555 0.335493 0.625724 x

x Se 7 0.332560 0.335525 0.874135 x

x Se 8 0.266591 0.665862 0.373314 x

x Se 9 0.467783 0.665193 0.126484 x

x Se 10 0.532097 0.334265 0.626235 x

x Se 11 0.532216 0.334808 0.873518 x

x Se 12 0.467902 0.665733 0.373766 x

x Se 13 0.667440 0.664478 0.125864 x

x Se 14 0.733408 0.334134 0.626686 x

x Se 15 0.733372 0.334047 0.873146 x

x Se 16 0.667445 0.664509 0.374277 x

x Se 17 0.867036 0.663239 0.126283 x

x Se 18 0.933250 0.336814 0.626300 x

x Se 19 0.933215 0.336656 0.873468 x

x Se 20 0.867067 0.663205 0.373826 x

x Nb 1 -0.000414 -0.001727 0.250115 x

x Nb 2 0.000412 0.001742 0.749885 x

x Nb 3 0.000001 -0.000008 0.000003 x

x Nb 4 0.000001 -0.000005 0.499998 x

x Nb 5 0.199379 -0.001334 0.250123 x

x Nb 6 0.200457 0.002585 0.749873 x

x Nb 7 0.200003 0.000104 0.000107 x

x Nb 8 0.200005 0.000141 0.499898 x

x Nb 9 0.399884 -0.001372 0.250150 x

x Nb 10 0.400289 0.001216 0.749884 x

x Nb 11 0.399845 0.000419 0.000082 x

x Nb 12 0.399832 0.000346 0.499900 x

x Nb 13 0.599708 -0.001228 0.250115 x

x Nb 14 0.600115 0.001376 0.749849 x

x Nb 15 0.600153 -0.000431 -0.000081 x

x Nb 16 0.600168 -0.000354 0.500099 x

x Nb 17 0.799548 -0.002578 0.250127 x

x Nb 18 0.800623 0.001322 0.749877 x

x Nb 19 0.799998 -0.000085 -0.000111 x

x Nb 20 0.799996 -0.000127 0.500105 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597489E+004 10619.66 <-- SCF

1 -3.62600531E+004 7.60458099E-003 10647.08 <-- SCF

2 -3.62600669E+004 3.45933956E-004 10675.66 <-- SCF

3 -3.62600221E+004 -1.12045576E-003 10702.09 <-- SCF

4 -3.62597994E+004 -5.56696485E-003 10728.72 <-- SCF

5 -3.62598046E+004 1.27930766E-004 10755.14 <-- SCF

6 -3.62598039E+004 -1.67997041E-005 10777.95 <-- SCF

7 -3.62598038E+004 -3.54871843E-006 10799.53 <-- SCF

8 -3.62598038E+004 9.18078789E-007 10817.66 <-- SCF

9 -3.62598038E+004 2.14602936E-007 10834.83 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.80379683 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.09188 0.04142 -0.00168 \*

\* Se 2 -0.17845 -0.00680 0.05446 \*

\* Se 3 -0.18294 0.01301 -0.05416 \*

\* Se 4 0.11293 0.03584 0.00602 \*

\* Se 5 0.07601 -0.07524 -0.08545 \*

\* Se 6 -0.16294 0.01098 0.08625 \*

\* Se 7 -0.15761 0.02491 -0.09770 \*

\* Se 8 0.09257 -0.07800 0.06159 \*

\* Se 9 -0.04589 -0.04444 0.01930 \*

\* Se 10 0.07748 0.01436 0.00645 \*

\* Se 11 0.04564 0.04444 -0.01881 \*

\* Se 12 -0.07797 -0.01421 -0.00687 \*

\* Se 13 0.15838 -0.02504 0.09645 \*

\* Se 14 -0.09244 0.07781 -0.06152 \*

\* Se 15 -0.07609 0.07507 0.08526 \*

\* Se 16 0.16353 -0.01112 -0.08535 \*

\* Se 17 0.18235 -0.01298 0.05534 \*

\* Se 18 -0.11262 -0.03575 -0.00551 \*

\* Se 19 -0.09147 -0.04129 0.00100 \*

\* Se 20 0.17785 0.00688 -0.05548 \*

\* Nb 1 -0.04532 -0.02070 -0.00928 \*

\* Nb 2 0.04373 0.02347 0.00920 \*

\* Nb 3 -0.00058 -0.00084 0.00105 \*

\* Nb 4 -0.00034 -0.00084 -0.00104 \*

\* Nb 5 -0.13509 0.03948 -0.00144 \*

\* Nb 6 0.09184 0.04381 -0.00350 \*

\* Nb 7 -0.01012 0.01497 0.02419 \*

\* Nb 8 0.00243 0.01839 -0.01487 \*

\* Nb 9 0.00307 -0.01501 0.00843 \*

\* Nb 10 -0.01014 0.03947 0.01321 \*

\* Nb 11 -0.02028 0.02579 0.00863 \*

\* Nb 12 -0.04440 0.02037 -0.02402 \*

\* Nb 13 0.00848 -0.03948 -0.01299 \*

\* Nb 14 -0.00199 0.01710 -0.00848 \*

\* Nb 15 0.02000 -0.02625 -0.00772 \*

\* Nb 16 0.04439 -0.02076 0.02336 \*

\* Nb 17 -0.09045 -0.04591 0.00370 \*

\* Nb 18 0.13568 -0.04216 0.00157 \*

\* Nb 19 0.01101 -0.01361 -0.02611 \*

\* Nb 20 -0.00210 -0.01713 0.01653 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.228495 -0.028151 -0.006938 \*

\* y -0.028151 -0.045541 -0.050193 \*

\* z -0.006938 -0.050193 -0.024327 \*

\* \*

\* Pressure: -0.0529 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000142 | -36259.800087 | <-- min BFGS

| trial step | 1.000000 | 0.000069 | -36259.803041 | <-- min BFGS

| line step | 1.948254 | -0.000016 | -36259.803862 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 13 with enthalpy= -3.62598039E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 9.437247E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.912269E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.560348E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.284952E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 14 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000067 | -36259.803862 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 14 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8909188 -8.3542701 0.0003973 0.4202946 -0.0029462 0.0000142

0.0237122 3.3827199 -0.0003989 1.0379973 1.8501597 0.0002328

-0.0004793 -0.0014823 13.9201089 0.0000178 0.0000531 0.4513747

Lattice parameters(A) Cell Angles

a = 17.074346 alpha = 90.012872

b = 3.382803 beta = 89.997402

c = 13.920109 gamma = 118.892159

Current cell volume = 703.938581 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066798 0.663343 0.126657 x

x Se 2 0.132903 0.336786 0.626303 x

x Se 3 0.132934 0.336765 0.873588 x

x Se 4 0.066767 0.663195 0.373576 x

x Se 5 0.266636 0.665906 0.126967 x

x Se 6 0.332520 0.335473 0.625853 x

x Se 7 0.332526 0.335518 0.874004 x

x Se 8 0.266603 0.665825 0.373199 x

x Se 9 0.467791 0.665115 0.126613 x

x Se 10 0.532091 0.334323 0.626360 x

x Se 11 0.532208 0.334885 0.873389 x

x Se 12 0.467908 0.665676 0.373640 x

x Se 13 0.667474 0.664485 0.125995 x

x Se 14 0.733396 0.334171 0.626802 x

x Se 15 0.733364 0.334090 0.873034 x

x Se 16 0.667480 0.664530 0.374148 x

x Se 17 0.867065 0.663229 0.126415 x

x Se 18 0.933234 0.336811 0.626424 x

x Se 19 0.933203 0.336661 0.873342 x

x Se 20 0.867097 0.663210 0.373695 x

x Nb 1 -0.000429 -0.001802 0.250115 x

x Nb 2 0.000427 0.001819 0.749885 x

x Nb 3 0.000001 -0.000009 0.000003 x

x Nb 4 0.000001 -0.000005 0.499998 x

x Nb 5 0.199349 -0.001380 0.250125 x

x Nb 6 0.200477 0.002694 0.749871 x

x Nb 7 0.200002 0.000112 0.000115 x

x Nb 8 0.200005 0.000154 0.499892 x

x Nb 9 0.399885 -0.001404 0.250154 x

x Nb 10 0.400289 0.001259 0.749884 x

x Nb 11 0.399839 0.000437 0.000088 x

x Nb 12 0.399822 0.000354 0.499891 x

x Nb 13 0.599707 -0.001271 0.250115 x

x Nb 14 0.600114 0.001409 0.749845 x

x Nb 15 0.600159 -0.000450 -0.000086 x

x Nb 16 0.600177 -0.000362 0.500107 x

x Nb 17 0.799528 -0.002687 0.250129 x

x Nb 18 0.800653 0.001367 0.749876 x

x Nb 19 0.799999 -0.000092 -0.000118 x

x Nb 20 0.799995 -0.000139 0.500111 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597888E+004 10935.23 <-- SCF

1 -3.62598749E+004 2.15258793E-003 10963.50 <-- SCF

2 -3.62598796E+004 1.17622380E-004 10989.75 <-- SCF

3 -3.62598647E+004 -3.72239966E-004 11016.11 <-- SCF

4 -3.62598042E+004 -1.51326574E-003 11041.81 <-- SCF

5 -3.62598059E+004 4.32827006E-005 11066.25 <-- SCF

6 -3.62598055E+004 -1.14714273E-005 11088.36 <-- SCF

7 -3.62598054E+004 -2.13708274E-006 11108.09 <-- SCF

8 -3.62598054E+004 3.41977074E-007 11126.25 <-- SCF

9 -3.62598054E+004 6.07618761E-007 11143.33 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.80544070 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.07852 0.04130 -0.00991 \*

\* Se 2 -0.17481 0.01505 0.04005 \*

\* Se 3 -0.17876 0.03500 -0.04195 \*

\* Se 4 0.10232 0.04137 0.02376 \*

\* Se 5 0.06781 -0.07074 -0.10761 \*

\* Se 6 -0.16083 0.02607 0.08182 \*

\* Se 7 -0.14972 0.03852 -0.08964 \*

\* Se 8 0.08654 -0.07383 0.09010 \*

\* Se 9 -0.02911 -0.05725 0.01615 \*

\* Se 10 0.05880 0.02604 0.00205 \*

\* Se 11 0.02876 0.05725 -0.01559 \*

\* Se 12 -0.05937 -0.02587 -0.00252 \*

\* Se 13 0.15064 -0.03863 0.08830 \*

\* Se 14 -0.08635 0.07361 -0.09001 \*

\* Se 15 -0.06783 0.07055 0.10748 \*

\* Se 16 0.16155 -0.02622 -0.08090 \*

\* Se 17 0.17807 -0.03503 0.04329 \*

\* Se 18 -0.10201 -0.04125 -0.02318 \*

\* Se 19 -0.07813 -0.04113 0.00909 \*

\* Se 20 0.17410 -0.01501 -0.04115 \*

\* Nb 1 -0.03982 -0.01561 -0.01017 \*

\* Nb 2 0.03815 0.01873 0.01003 \*

\* Nb 3 -0.00065 -0.00097 0.00121 \*

\* Nb 4 -0.00038 -0.00096 -0.00117 \*

\* Nb 5 -0.13724 0.03953 -0.00205 \*

\* Nb 6 0.08948 0.04396 -0.00351 \*

\* Nb 7 -0.01214 0.01288 0.02381 \*

\* Nb 8 0.00075 0.01650 -0.01414 \*

\* Nb 9 -0.00076 -0.01633 0.00791 \*

\* Nb 10 -0.01362 0.03445 0.01417 \*

\* Nb 11 -0.02124 0.02844 0.00460 \*

\* Nb 12 -0.04584 0.02248 -0.02033 \*

\* Nb 13 0.01183 -0.03447 -0.01394 \*

\* Nb 14 0.00193 0.01863 -0.00801 \*

\* Nb 15 0.02092 -0.02897 -0.00360 \*

\* Nb 16 0.04584 -0.02291 0.01962 \*

\* Nb 17 -0.08801 -0.04626 0.00373 \*

\* Nb 18 0.13785 -0.04254 0.00223 \*

\* Nb 19 0.01313 -0.01132 -0.02596 \*

\* Nb 20 -0.00040 -0.01508 0.01596 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.193351 -0.020650 -0.008382 \*

\* y -0.020650 -0.093613 -0.050483 \*

\* z -0.008382 -0.050483 -0.041366 \*

\* \*

\* Pressure: -0.0195 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000067 | -36259.803862 | <-- min BFGS

| trial step | 1.000000 | 0.000049 | -36259.805493 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 14 with line minimization (lambda= 3.785436)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8871129 -8.3394513 0.0000496 0.4203040 -0.0031264 0.0000188

0.0251366 3.3792543 -0.0003404 1.0372420 1.8516253 0.0002199

-0.0006312 -0.0013003 13.9260292 0.0000239 0.0000453 0.4511828

Lattice parameters(A) Cell Angles

a = 17.063780 alpha = 90.011141

b = 3.379348 beta = 89.999485

c = 13.926029 gamma = 118.830456

Current cell volume = 703.500716 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066832 0.663332 0.127008 x

x Se 2 0.132818 0.336773 0.626670 x

x Se 3 0.132851 0.336791 0.873223 x

x Se 4 0.066811 0.663205 0.373231 x

x Se 5 0.266659 0.665784 0.127279 x

x Se 6 0.332423 0.335415 0.626213 x

x Se 7 0.332432 0.335499 0.873639 x

x Se 8 0.266635 0.665722 0.372878 x

x Se 9 0.467813 0.664898 0.126972 x

x Se 10 0.532075 0.334484 0.626710 x

x Se 11 0.532186 0.335102 0.873030 x

x Se 12 0.467923 0.665514 0.373291 x

x Se 13 0.667568 0.664505 0.126360 x

x Se 14 0.733365 0.334274 0.627122 x

x Se 15 0.733340 0.334212 0.872722 x

x Se 16 0.667578 0.664587 0.373789 x

x Se 17 0.867149 0.663204 0.126780 x

x Se 18 0.933191 0.336802 0.626769 x

x Se 19 0.933169 0.336673 0.872991 x

x Se 20 0.867182 0.663222 0.373328 x

x Nb 1 -0.000473 -0.002011 0.250117 x

x Nb 2 0.000471 0.002030 0.749883 x

x Nb 3 0.000001 -0.000011 0.000003 x

x Nb 4 0.000001 -0.000007 0.499997 x

x Nb 5 0.199266 -0.001507 0.250130 x

x Nb 6 0.200532 0.002997 0.749865 x

x Nb 7 0.199999 0.000133 0.000135 x

x Nb 8 0.200006 0.000192 0.499876 x

x Nb 9 0.399888 -0.001493 0.250166 x

x Nb 10 0.400292 0.001379 0.749885 x

x Nb 11 0.399822 0.000490 0.000103 x

x Nb 12 0.399796 0.000376 0.499868 x

x Nb 13 0.599704 -0.001392 0.250114 x

x Nb 14 0.600111 0.001501 0.749833 x

x Nb 15 0.600176 -0.000504 -0.000101 x

x Nb 16 0.600203 -0.000384 0.500130 x

x Nb 17 0.799474 -0.002992 0.250135 x

x Nb 18 0.800737 0.001491 0.749871 x

x Nb 19 0.800002 -0.000110 -0.000140 x

x Nb 20 0.799994 -0.000175 0.500128 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62596693E+004 11246.48 <-- SCF

1 -3.62604594E+004 1.97532790E-002 11274.30 <-- SCF

2 -3.62605046E+004 1.12916588E-003 11302.48 <-- SCF

3 -3.62603822E+004 -3.05957367E-003 11328.95 <-- SCF

4 -3.62597964E+004 -1.46447736E-002 11355.19 <-- SCF

5 -3.62598100E+004 3.39024688E-004 11381.73 <-- SCF

6 -3.62598070E+004 -7.45718045E-005 11408.08 <-- SCF

7 -3.62598066E+004 -1.00326717E-005 11431.48 <-- SCF

8 -3.62598068E+004 5.18797776E-006 11453.03 <-- SCF

9 -3.62598068E+004 1.24864381E-006 11471.19 <-- SCF

10 -3.62598069E+004 1.09329261E-006 11488.89 <-- SCF

11 -3.62598069E+004 8.09725814E-007 11506.44 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.80690681 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.03989 0.02489 -0.03377 \*

\* Se 2 -0.14749 0.07703 0.00598 \*

\* Se 3 -0.14774 0.09743 -0.01629 \*

\* Se 4 0.06850 0.04277 0.04950 \*

\* Se 5 0.04378 -0.06060 -0.15065 \*

\* Se 6 -0.12530 0.06001 0.05159 \*

\* Se 7 -0.10801 0.07226 -0.06311 \*

\* Se 8 0.06305 -0.06270 0.14770 \*

\* Se 9 -0.00011 -0.10061 0.00945 \*

\* Se 10 0.01142 0.05935 -0.01877 \*

\* Se 11 -0.00043 0.10056 -0.00894 \*

\* Se 12 -0.01196 -0.05915 0.01834 \*

\* Se 13 0.10894 -0.07227 0.06179 \*

\* Se 14 -0.06274 0.06243 -0.14759 \*

\* Se 15 -0.04363 0.06040 0.15058 \*

\* Se 16 0.12610 -0.06009 -0.05077 \*

\* Se 17 0.14693 -0.09764 0.01768 \*

\* Se 18 -0.06821 -0.04262 -0.04892 \*

\* Se 19 -0.03951 -0.02464 0.03297 \*

\* Se 20 0.14669 -0.07717 -0.00704 \*

\* Nb 1 -0.02491 -0.00406 -0.01053 \*

\* Nb 2 0.02356 0.00704 0.01031 \*

\* Nb 3 -0.00063 -0.00094 0.00114 \*

\* Nb 4 -0.00032 -0.00091 -0.00105 \*

\* Nb 5 -0.13117 0.04188 -0.00430 \*

\* Nb 6 0.08116 0.04145 -0.00178 \*

\* Nb 7 -0.01088 0.00896 0.02101 \*

\* Nb 8 0.00100 0.01236 -0.01197 \*

\* Nb 9 -0.00567 -0.01765 0.00409 \*

\* Nb 10 -0.01794 0.02343 0.01425 \*

\* Nb 11 -0.02007 0.03094 -0.00333 \*

\* Nb 12 -0.04370 0.02597 -0.01020 \*

\* Nb 13 0.01638 -0.02340 -0.01398 \*

\* Nb 14 0.00668 0.01978 -0.00425 \*

\* Nb 15 0.01977 -0.03145 0.00425 \*

\* Nb 16 0.04370 -0.02639 0.00955 \*

\* Nb 17 -0.07994 -0.04363 0.00198 \*

\* Nb 18 0.13168 -0.04474 0.00456 \*

\* Nb 19 0.01185 -0.00738 -0.02305 \*

\* Nb 20 -0.00071 -0.01092 0.01360 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.077657 0.027553 -0.012942 \*

\* y 0.027553 -0.263546 -0.046494 \*

\* z -0.012942 -0.046494 -0.112027 \*

\* \*

\* Pressure: 0.0993 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000067 | -36259.803862 | <-- min BFGS

| trial step | 1.000000 | 0.000049 | -36259.805493 | <-- min BFGS

| line step | 3.785436 | -9.305E-007 | -36259.807020 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 14 with enthalpy= -3.62598070E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.896182E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.777193E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.233579E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.635459E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 15 ...

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Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000075 | -36259.807020 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 15 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8908834 -8.3336828 -0.0001370 0.4201586 -0.0031983 0.0000209

0.0257130 3.3779524 -0.0003044 1.0365653 1.8521671 0.0002094

-0.0007025 -0.0011814 13.9298300 0.0000268 0.0000404 0.4510597

Lattice parameters(A) Cell Angles

a = 17.064251 alpha = 90.010043

b = 3.378050 beta = 90.000608

c = 13.929830 gamma = 118.797430

Current cell volume = 703.665056 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066849 0.663474 0.126959 x

x Se 2 0.132765 0.336638 0.626644 x

x Se 3 0.132797 0.336693 0.873244 x

x Se 4 0.066839 0.663387 0.373286 x

x Se 5 0.266674 0.665706 0.127169 x

x Se 6 0.332376 0.335284 0.626208 x

x Se 7 0.332389 0.335403 0.873635 x

x Se 8 0.266659 0.665668 0.372984 x

x Se 9 0.467791 0.664776 0.126935 x

x Se 10 0.532109 0.334578 0.626665 x

x Se 11 0.532209 0.335224 0.873067 x

x Se 12 0.467890 0.665421 0.373335 x

x Se 13 0.667612 0.664601 0.126363 x

x Se 14 0.733340 0.334327 0.627016 x

x Se 15 0.733325 0.334290 0.872832 x

x Se 16 0.667625 0.664719 0.373794 x

x Se 17 0.867202 0.663300 0.126759 x

x Se 18 0.933163 0.336620 0.626715 x

x Se 19 0.933153 0.336531 0.873039 x

x Se 20 0.867235 0.663357 0.373353 x

x Nb 1 -0.000489 -0.002101 0.250112 x

x Nb 2 0.000486 0.002122 0.749888 x

x Nb 3 0.000000 -0.000012 0.000003 x

x Nb 4 0.000001 -0.000008 0.499997 x

x Nb 5 0.199225 -0.001546 0.250128 x

x Nb 6 0.200555 0.003131 0.749867 x

x Nb 7 0.199997 0.000147 0.000148 x

x Nb 8 0.200007 0.000219 0.499867 x

x Nb 9 0.399898 -0.001499 0.250169 x

x Nb 10 0.400276 0.001416 0.749891 x

x Nb 11 0.399815 0.000514 0.000111 x

x Nb 12 0.399782 0.000377 0.499853 x

x Nb 13 0.599720 -0.001429 0.250108 x

x Nb 14 0.600102 0.001510 0.749830 x

x Nb 15 0.600183 -0.000529 -0.000109 x

x Nb 16 0.600217 -0.000386 0.500145 x

x Nb 17 0.799451 -0.003127 0.250134 x

x Nb 18 0.800778 0.001528 0.749872 x

x Nb 19 0.800005 -0.000122 -0.000153 x

x Nb 20 0.799994 -0.000200 0.500138 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597987E+004 11610.03 <-- SCF

1 -3.62598343E+004 8.89788931E-004 11637.34 <-- SCF

2 -3.62598364E+004 5.08903127E-005 11663.08 <-- SCF

3 -3.62598338E+004 -6.33105622E-005 11689.67 <-- SCF

4 -3.62598077E+004 -6.53101513E-004 11715.59 <-- SCF

5 -3.62598096E+004 4.79083982E-005 11739.66 <-- SCF

6 -3.62598092E+004 -1.05835874E-005 11760.17 <-- SCF

7 -3.62598089E+004 -7.11239585E-006 11779.67 <-- SCF

8 -3.62598089E+004 3.89025266E-007 11797.36 <-- SCF

9 -3.62598090E+004 6.99157220E-007 11814.05 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.80895394 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.04386 0.02206 -0.03222 \*

\* Se 2 -0.14469 0.07249 0.00624 \*

\* Se 3 -0.14756 0.09263 -0.01630 \*

\* Se 4 0.07101 0.03878 0.04949 \*

\* Se 5 0.04835 -0.05427 -0.14531 \*

\* Se 6 -0.12528 0.06110 0.04822 \*

\* Se 7 -0.10674 0.07383 -0.05988 \*

\* Se 8 0.06250 -0.05686 0.13977 \*

\* Se 9 0.00213 -0.10012 0.01487 \*

\* Se 10 0.00993 0.06039 -0.01876 \*

\* Se 11 -0.00282 0.10011 -0.01416 \*

\* Se 12 -0.01062 -0.06015 0.01822 \*

\* Se 13 0.10791 -0.07381 0.05818 \*

\* Se 14 -0.06221 0.05656 -0.13959 \*

\* Se 15 -0.04817 0.05405 0.14526 \*

\* Se 16 0.12628 -0.06120 -0.04715 \*

\* Se 17 0.14664 -0.09291 0.01800 \*

\* Se 18 -0.07067 -0.03860 -0.04879 \*

\* Se 19 -0.04347 -0.02178 0.03119 \*

\* Se 20 0.14379 -0.07264 -0.00754 \*

\* Nb 1 -0.00746 0.00901 -0.01109 \*

\* Nb 2 0.00580 -0.00531 0.01080 \*

\* Nb 3 -0.00082 -0.00116 0.00146 \*

\* Nb 4 -0.00046 -0.00114 -0.00134 \*

\* Nb 5 -0.13797 0.03660 -0.00411 \*

\* Nb 6 0.07882 0.04223 -0.00460 \*

\* Nb 7 -0.01815 0.00714 0.01739 \*

\* Nb 8 -0.00406 0.01072 -0.00768 \*

\* Nb 9 -0.01190 -0.01821 0.00436 \*

\* Nb 10 -0.01649 0.01577 0.01453 \*

\* Nb 11 -0.02000 0.03150 -0.01481 \*

\* Nb 12 -0.04678 0.02584 0.00019 \*

\* Nb 13 0.01456 -0.01582 -0.01428 \*

\* Nb 14 0.01327 0.02084 -0.00466 \*

\* Nb 15 0.01959 -0.03214 0.01597 \*

\* Nb 16 0.04680 -0.02634 -0.00096 \*

\* Nb 17 -0.07734 -0.04481 0.00486 \*

\* Nb 18 0.13856 -0.04017 0.00448 \*

\* Nb 19 0.01941 -0.00522 -0.01997 \*

\* Nb 20 0.00446 -0.00900 0.00974 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.151851 0.052812 -0.013764 \*

\* y 0.052812 -0.293928 -0.044014 \*

\* z -0.013764 -0.044014 -0.026371 \*

\* \*

\* Pressure: 0.0561 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000075 | -36259.807020 | <-- min BFGS

| trial step | 1.000000 | 0.000061 | -36259.809094 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 15 with line minimization (lambda= 5.209139)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9067539 -8.3094028 -0.0009224 0.4195479 -0.0035006 0.0000300

0.0281394 3.3724725 -0.0001524 1.0337201 1.8544546 0.0001649

-0.0010029 -0.0006811 13.9458280 0.0000390 0.0000200 0.4505423

Lattice parameters(A) Cell Angles

a = 17.066268 alpha = 90.005422

b = 3.372590 beta = 90.005333

c = 13.945828 gamma = 118.658348

Current cell volume = 704.354101 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066919 0.664073 0.126754 x

x Se 2 0.132538 0.336071 0.626535 x

x Se 3 0.132572 0.336284 0.873332 x

x Se 4 0.066957 0.664153 0.373515 x

x Se 5 0.266737 0.665378 0.126708 x

x Se 6 0.332179 0.334733 0.626187 x

x Se 7 0.332209 0.334999 0.873621 x

x Se 8 0.266764 0.665442 0.373429 x

x Se 9 0.467695 0.664259 0.126779 x

x Se 10 0.532249 0.334973 0.626479 x

x Se 11 0.532304 0.335739 0.873224 x

x Se 12 0.467749 0.665025 0.373521 x

x Se 13 0.667793 0.665006 0.126375 x

x Se 14 0.733236 0.334553 0.626571 x

x Se 15 0.733262 0.334616 0.873293 x

x Se 16 0.667823 0.665271 0.373815 x

x Se 17 0.867427 0.663708 0.126673 x

x Se 18 0.933045 0.335857 0.626486 x

x Se 19 0.933083 0.335934 0.873244 x

x Se 20 0.867461 0.663922 0.373460 x

x Nb 1 -0.000555 -0.002479 0.250094 x

x Nb 2 0.000550 0.002506 0.749906 x

x Nb 3 -0.000000 -0.000017 0.000005 x

x Nb 4 0.000000 -0.000013 0.499996 x

x Nb 5 0.199054 -0.001709 0.250122 x

x Nb 6 0.200655 0.003692 0.749872 x

x Nb 7 0.199985 0.000206 0.000200 x

x Nb 8 0.200009 0.000332 0.499829 x

x Nb 9 0.399938 -0.001526 0.250181 x

x Nb 10 0.400210 0.001571 0.749918 x

x Nb 11 0.399785 0.000619 0.000148 x

x Nb 12 0.399722 0.000383 0.499790 x

x Nb 13 0.599784 -0.001587 0.250082 x

x Nb 14 0.600063 0.001548 0.749818 x

x Nb 15 0.600213 -0.000636 -0.000145 x

x Nb 16 0.600278 -0.000393 0.500207 x

x Nb 17 0.799352 -0.003696 0.250129 x

x Nb 18 0.800949 0.001682 0.749879 x

x Nb 19 0.800017 -0.000174 -0.000207 x

x Nb 20 0.799991 -0.000307 0.500178 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62596357E+004 11917.52 <-- SCF

1 -3.62601909E+004 1.38785941E-002 11944.86 <-- SCF

2 -3.62602217E+004 7.71928145E-004 11973.55 <-- SCF

3 -3.62601017E+004 -2.99998212E-003 11999.80 <-- SCF

4 -3.62598070E+004 -7.36822532E-003 12025.73 <-- SCF

5 -3.62598195E+004 3.12795247E-004 12052.50 <-- SCF

6 -3.62598135E+004 -1.50955205E-004 12078.20 <-- SCF

7 -3.62598118E+004 -4.30471939E-005 12101.83 <-- SCF

8 -3.62598118E+004 9.12014606E-007 12122.36 <-- SCF

9 -3.62598119E+004 2.93919016E-006 12140.22 <-- SCF

10 -3.62598120E+004 2.03635357E-006 12157.59 <-- SCF

11 -3.62598120E+004 1.37913581E-006 12174.95 <-- SCF

12 -3.62598121E+004 1.16265198E-006 12191.28 <-- SCF

13 -3.62598121E+004 1.01423982E-006 12207.48 <-- SCF

14 -3.62598122E+004 1.00121788E-006 12224.38 <-- SCF

15 -3.62598122E+004 8.25355026E-007 12240.91 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.81220697 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.06918 0.00163 -0.01826 \*

\* Se 2 -0.10176 0.05058 0.02167 \*

\* Se 3 -0.10481 0.06715 -0.03250 \*

\* Se 4 0.08171 0.00719 0.02582 \*

\* Se 5 0.07037 -0.03044 -0.07866 \*

\* Se 6 -0.10359 0.06464 0.03646 \*

\* Se 7 -0.07641 0.07866 -0.05120 \*

\* Se 8 0.05934 -0.03235 0.04465 \*

\* Se 9 0.00843 -0.10266 0.02961 \*

\* Se 10 0.00641 0.07004 -0.01853 \*

\* Se 11 -0.00924 0.10276 -0.02871 \*

\* Se 12 -0.00726 -0.06972 0.01811 \*

\* Se 13 0.07792 -0.07835 0.04895 \*

\* Se 14 -0.05920 0.03201 -0.04448 \*

\* Se 15 -0.07006 0.03016 0.07865 \*

\* Se 16 0.10480 -0.06458 -0.03519 \*

\* Se 17 0.10404 -0.06785 0.03438 \*

\* Se 18 -0.08150 -0.00692 -0.02526 \*

\* Se 19 -0.06895 -0.00119 0.01716 \*

\* Se 20 0.10099 -0.05099 -0.02302 \*

\* Nb 1 0.04662 0.05288 -0.00800 \*

\* Nb 2 -0.04855 -0.04824 0.00761 \*

\* Nb 3 -0.00091 -0.00171 0.00175 \*

\* Nb 4 -0.00054 -0.00163 -0.00152 \*

\* Nb 5 -0.13060 0.02336 -0.00158 \*

\* Nb 6 0.07952 0.03577 -0.01258 \*

\* Nb 7 -0.02137 0.00139 0.00601 \*

\* Nb 8 -0.00201 0.00466 0.00467 \*

\* Nb 9 -0.04394 -0.01488 0.00361 \*

\* Nb 10 0.00778 -0.01591 0.01019 \*

\* Nb 11 -0.01723 0.03281 -0.04480 \*

\* Nb 12 -0.04954 0.02647 0.03193 \*

\* Nb 13 -0.00994 0.01591 -0.01001 \*

\* Nb 14 0.04542 0.01786 -0.00414 \*

\* Nb 15 0.01676 -0.03372 0.04616 \*

\* Nb 16 0.04974 -0.02711 -0.03266 \*

\* Nb 17 -0.07798 -0.03891 0.01299 \*

\* Nb 18 0.13133 -0.02767 0.00210 \*

\* Nb 19 0.02276 0.00126 -0.00904 \*

\* Nb 20 0.00227 -0.00233 -0.00235 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.459784 0.136250 -0.015759 \*

\* y 0.136250 -0.396334 -0.038285 \*

\* z -0.015759 -0.038285 0.293732 \*

\* \*

\* Pressure: -0.1191 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000075 | -36259.807020 | <-- min BFGS

| trial step | 1.000000 | 0.000061 | -36259.809094 | <-- min BFGS

| line step | 5.209139 | -0.000017 | -36259.812380 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 15 with enthalpy= -3.62598124E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.339998E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.342312E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 8.292443E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.597838E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 16 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000169 | -36259.812380 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 16 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8986341 -8.3199319 -0.0015815 0.4198110 -0.0034344 0.0000180

0.0276164 3.3757330 0.0003225 1.0346788 1.8528157 -0.0000697

-0.0005905 0.0008542 13.9402480 0.0000237 -0.0000433 0.4507226

Lattice parameters(A) Cell Angles

a = 17.064307 alpha = 89.991035

b = 3.375846 beta = 90.009141

c = 13.940248 gamma = 118.711840

Current cell volume = 704.311199 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066931 0.664097 0.126755 x

x Se 2 0.132515 0.336068 0.626546 x

x Se 3 0.132547 0.336290 0.873322 x

x Se 4 0.066972 0.664188 0.373515 x

x Se 5 0.266749 0.665375 0.126694 x

x Se 6 0.332156 0.334740 0.626204 x

x Se 7 0.332190 0.335021 0.873605 x

x Se 8 0.266776 0.665436 0.373436 x

x Se 9 0.467699 0.664189 0.126789 x

x Se 10 0.532247 0.335022 0.626483 x

x Se 11 0.532300 0.335809 0.873213 x

x Se 12 0.467751 0.664976 0.373517 x

x Se 13 0.667812 0.664984 0.126391 x

x Se 14 0.733224 0.334559 0.626565 x

x Se 15 0.733251 0.334619 0.873306 x

x Se 16 0.667845 0.665264 0.373799 x

x Se 17 0.867451 0.663701 0.126683 x

x Se 18 0.933030 0.335822 0.626487 x

x Se 19 0.933070 0.335911 0.873243 x

x Se 20 0.867484 0.663925 0.373449 x

x Nb 1 -0.000554 -0.002458 0.250092 x

x Nb 2 0.000550 0.002488 0.749908 x

x Nb 3 -0.000000 -0.000018 0.000005 x

x Nb 4 0.000000 -0.000014 0.499995 x

x Nb 5 0.199030 -0.001747 0.250121 x

x Nb 6 0.200671 0.003758 0.749870 x

x Nb 7 0.199982 0.000204 0.000203 x

x Nb 8 0.200009 0.000339 0.499828 x

x Nb 9 0.399931 -0.001553 0.250182 x

x Nb 10 0.400213 0.001578 0.749921 x

x Nb 11 0.399782 0.000632 0.000142 x

x Nb 12 0.399714 0.000379 0.499793 x

x Nb 13 0.599781 -0.001594 0.250079 x

x Nb 14 0.600070 0.001578 0.749816 x

x Nb 15 0.600216 -0.000650 -0.000139 x

x Nb 16 0.600286 -0.000390 0.500204 x

x Nb 17 0.799336 -0.003763 0.250131 x

x Nb 18 0.800974 0.001718 0.749880 x

x Nb 19 0.800020 -0.000169 -0.000211 x

x Nb 20 0.799991 -0.000312 0.500179 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597994E+004 12344.22 <-- SCF

1 -3.62598195E+004 5.03629924E-004 12368.27 <-- SCF

2 -3.62598204E+004 2.13212714E-005 12393.91 <-- SCF

3 -3.62598172E+004 -8.05249519E-005 12419.62 <-- SCF

4 -3.62598165E+004 -1.55215774E-005 12442.17 <-- SCF

5 -3.62598163E+004 -6.31102253E-006 12463.22 <-- SCF

6 -3.62598163E+004 6.58831525E-007 12480.53 <-- SCF

7 -3.62598163E+004 7.39616403E-007 12496.97 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.81634453 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.05089 0.00442 -0.02029 \*

\* Se 2 -0.08276 0.04703 0.01826 \*

\* Se 3 -0.08616 0.06261 -0.03031 \*

\* Se 4 0.06277 0.01091 0.02998 \*

\* Se 5 0.05478 -0.02489 -0.08203 \*

\* Se 6 -0.08836 0.05711 0.03307 \*

\* Se 7 -0.06249 0.07163 -0.04944 \*

\* Se 8 0.04260 -0.02728 0.04653 \*

\* Se 9 0.00000 -0.09968 0.03379 \*

\* Se 10 0.01458 0.06624 -0.01913 \*

\* Se 11 -0.00092 0.09980 -0.03278 \*

\* Se 12 -0.01552 -0.06589 0.01865 \*

\* Se 13 0.06411 -0.07126 0.04692 \*

\* Se 14 -0.04247 0.02687 -0.04632 \*

\* Se 15 -0.05447 0.02455 0.08200 \*

\* Se 16 0.08965 -0.05703 -0.03164 \*

\* Se 17 0.08535 -0.06338 0.03237 \*

\* Se 18 -0.06253 -0.01066 -0.02939 \*

\* Se 19 -0.05066 -0.00400 0.01913 \*

\* Se 20 0.08197 -0.04750 -0.01975 \*

\* Nb 1 0.06870 0.05407 -0.00965 \*

\* Nb 2 -0.07075 -0.04912 0.00925 \*

\* Nb 3 -0.00100 -0.00178 0.00186 \*

\* Nb 4 -0.00063 -0.00171 -0.00162 \*

\* Nb 5 -0.12984 0.01652 -0.00198 \*

\* Nb 6 0.07298 0.04412 -0.01450 \*

\* Nb 7 -0.02660 0.00144 0.00719 \*

\* Nb 8 -0.00402 0.00558 0.00498 \*

\* Nb 9 -0.03154 -0.02225 0.00473 \*

\* Nb 10 -0.00520 -0.01444 0.01219 \*

\* Nb 11 -0.01521 0.03440 -0.05199 \*

\* Nb 12 -0.05212 0.02705 0.03670 \*

\* Nb 13 0.00282 0.01434 -0.01203 \*

\* Nb 14 0.03326 0.02543 -0.00534 \*

\* Nb 15 0.01466 -0.03532 0.05349 \*

\* Nb 16 0.05242 -0.02764 -0.03746 \*

\* Nb 17 -0.07137 -0.04743 0.01499 \*

\* Nb 18 0.13065 -0.02108 0.00254 \*

\* Nb 19 0.02816 0.00137 -0.01048 \*

\* Nb 20 0.00429 -0.00316 -0.00251 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.313205 0.109719 -0.010989 \*

\* y 0.109719 -0.259974 -0.004327 \*

\* z -0.010989 -0.004327 0.239953 \*

\* \*

\* Pressure: -0.0977 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000169 | -36259.812380 | <-- min BFGS

| trial step | 1.000000 | 0.000123 | -36259.816540 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 16 with line minimization (lambda= 3.670792)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8769480 -8.3480529 -0.0033419 0.4205156 -0.0032578 -0.0000143

0.0262196 3.3844413 0.0015911 1.0372427 1.8484559 -0.0006957

0.0005112 0.0049544 13.9253449 -0.0000176 -0.0002120 0.4512051

Lattice parameters(A) Cell Angles

a = 17.059120 alpha = 89.952665

b = 3.384543 beta = 90.019366

c = 13.925346 gamma = 118.854667

Current cell volume = 704.191197 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066965 0.664159 0.126757 x

x Se 2 0.132451 0.336060 0.626576 x

x Se 3 0.132482 0.336305 0.873295 x

x Se 4 0.067012 0.664281 0.373513 x

x Se 5 0.266781 0.665367 0.126659 x

x Se 6 0.332097 0.334761 0.626248 x

x Se 7 0.332139 0.335080 0.873561 x

x Se 8 0.266808 0.665420 0.373454 x

x Se 9 0.467710 0.664002 0.126817 x

x Se 10 0.532239 0.335154 0.626494 x

x Se 11 0.532288 0.335996 0.873186 x

x Se 12 0.467759 0.664843 0.373505 x

x Se 13 0.667864 0.664927 0.126434 x

x Se 14 0.733192 0.334574 0.626547 x

x Se 15 0.733219 0.334627 0.873341 x

x Se 16 0.667904 0.665245 0.373755 x

x Se 17 0.867516 0.663685 0.126711 x

x Se 18 0.932990 0.335729 0.626488 x

x Se 19 0.933037 0.335850 0.873240 x

x Se 20 0.867547 0.663931 0.373419 x

x Nb 1 -0.000554 -0.002403 0.250086 x

x Nb 2 0.000548 0.002439 0.749914 x

x Nb 3 -0.000001 -0.000022 0.000006 x

x Nb 4 0.000000 -0.000017 0.499995 x

x Nb 5 0.198965 -0.001850 0.250120 x

x Nb 6 0.200715 0.003935 0.749864 x

x Nb 7 0.199975 0.000196 0.000210 x

x Nb 8 0.200009 0.000357 0.499827 x

x Nb 9 0.399912 -0.001624 0.250185 x

x Nb 10 0.400222 0.001595 0.749928 x

x Nb 11 0.399773 0.000667 0.000126 x

x Nb 12 0.399692 0.000369 0.499801 x

x Nb 13 0.599771 -0.001615 0.250072 x

x Nb 14 0.600089 0.001657 0.749814 x

x Nb 15 0.600224 -0.000687 -0.000121 x

x Nb 16 0.600307 -0.000381 0.500195 x

x Nb 17 0.799293 -0.003943 0.250137 x

x Nb 18 0.801039 0.001813 0.749881 x

x Nb 19 0.800028 -0.000156 -0.000220 x

x Nb 20 0.799992 -0.000326 0.500181 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597016E+004 12599.91 <-- SCF

1 -3.62598476E+004 3.64974250E-003 12623.91 <-- SCF

2 -3.62598573E+004 2.43659108E-004 12653.00 <-- SCF

3 -3.62598383E+004 -4.75877401E-004 12679.70 <-- SCF

4 -3.62598221E+004 -4.04209966E-004 12705.78 <-- SCF

5 -3.62598219E+004 -5.47497735E-006 12732.58 <-- SCF

6 -3.62598209E+004 -2.41442396E-005 12755.31 <-- SCF

7 -3.62598209E+004 -3.57209071E-008 12774.61 <-- SCF

8 -3.62598210E+004 2.50268731E-006 12792.02 <-- SCF

9 -3.62598211E+004 2.23292282E-006 12808.20 <-- SCF

10 -3.62598212E+004 1.95923814E-006 12824.36 <-- SCF

11 -3.62598213E+004 1.76063023E-006 12840.61 <-- SCF

12 -3.62598213E+004 1.76617562E-006 12856.69 <-- SCF

13 -3.62598214E+004 1.66496943E-006 12873.02 <-- SCF

14 -3.62598215E+004 1.65972628E-006 12889.41 <-- SCF

15 -3.62598215E+004 1.63865903E-006 12905.61 <-- SCF

16 -3.62598216E+004 1.59414478E-006 12921.69 <-- SCF

17 -3.62598217E+004 1.51286926E-006 12938.22 <-- SCF

18 -3.62598217E+004 1.52437365E-006 12954.48 <-- SCF

19 -3.62598218E+004 1.46972980E-006 12970.69 <-- SCF

20 -3.62598218E+004 1.43508299E-006 12986.89 <-- SCF

21 -3.62598219E+004 1.48140558E-006 13003.19 <-- SCF

22 -3.62598220E+004 1.40419997E-006 13019.52 <-- SCF

23 -3.62598220E+004 1.39298111E-006 13035.56 <-- SCF

24 -3.62598221E+004 1.26730288E-006 13051.62 <-- SCF

25 -3.62598221E+004 1.32064541E-006 13067.70 <-- SCF

26 -3.62598222E+004 1.08662224E-006 13084.06 <-- SCF

27 -3.62598222E+004 1.49882040E-006 13100.22 <-- SCF

28 -3.62598223E+004 7.23089900E-007 13116.50 <-- SCF

29 -3.62598223E+004 9.95406751E-007 13132.62 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.82229384 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00389 0.01120 -0.02309 \*

\* Se 2 -0.02823 0.03723 0.01018 \*

\* Se 3 -0.02987 0.05139 -0.02621 \*

\* Se 4 0.01302 0.02029 0.03735 \*

\* Se 5 0.02040 -0.01265 -0.08336 \*

\* Se 6 -0.04257 0.03795 0.02406 \*

\* Se 7 -0.02270 0.05295 -0.04638 \*

\* Se 8 0.00316 -0.01598 0.04650 \*

\* Se 9 -0.02644 -0.09134 0.04873 \*

\* Se 10 0.03891 0.05502 -0.01580 \*

\* Se 11 0.02536 0.09162 -0.04755 \*

\* Se 12 -0.04025 -0.05462 0.01530 \*

\* Se 13 0.02477 -0.05257 0.04303 \*

\* Se 14 -0.00345 0.01534 -0.04619 \*

\* Se 15 -0.02053 0.01214 0.08329 \*

\* Se 16 0.04427 -0.03778 -0.02209 \*

\* Se 17 0.02892 -0.05223 0.02878 \*

\* Se 18 -0.01233 -0.02008 -0.03653 \*

\* Se 19 -0.00337 -0.01079 0.02191 \*

\* Se 20 0.02744 -0.03766 -0.01228 \*

\* Nb 1 0.13686 0.05410 -0.01156 \*

\* Nb 2 -0.13934 -0.04851 0.01139 \*

\* Nb 3 -0.00127 -0.00194 0.00196 \*

\* Nb 4 -0.00108 -0.00172 -0.00202 \*

\* Nb 5 -0.09438 0.00137 -0.00187 \*

\* Nb 6 0.04299 0.06478 -0.01664 \*

\* Nb 7 -0.02900 0.00541 0.01255 \*

\* Nb 8 -0.00204 0.01186 0.00236 \*

\* Nb 9 0.01589 -0.03519 0.00564 \*

\* Nb 10 -0.04226 -0.00572 0.01446 \*

\* Nb 11 -0.00629 0.03229 -0.06273 \*

\* Nb 12 -0.05138 0.02339 0.04739 \*

\* Nb 13 0.03927 0.00550 -0.01448 \*

\* Nb 14 -0.01345 0.03895 -0.00628 \*

\* Nb 15 0.00564 -0.03315 0.06483 \*

\* Nb 16 0.05193 -0.02392 -0.04839 \*

\* Nb 17 -0.04115 -0.06844 0.01733 \*

\* Nb 18 0.09527 -0.00662 0.00225 \*

\* Nb 19 0.03087 -0.00245 -0.01645 \*

\* Nb 20 0.00254 -0.00943 0.00062 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.101849 0.024035 0.012068 \*

\* y 0.024035 0.140236 0.084253 \*

\* z 0.012068 0.084253 0.125467 \*

\* \*

\* Pressure: -0.0546 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000169 | -36259.812380 | <-- min BFGS

| trial step | 1.000000 | 0.000123 | -36259.816540 | <-- min BFGS

| line step | 3.670792 | -8.487E-006 | -36259.822369 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 16 with enthalpy= -3.62598224E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.497272E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.479788E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.667837E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.402359E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 17 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000158 | -36259.822369 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 17 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8874334 -8.3386994 -0.0037590 0.4201235 -0.0034328 -0.0000098

0.0276433 3.3831674 0.0016793 1.0355041 1.8487296 -0.0007237

0.0003668 0.0052426 13.9172810 -0.0000115 -0.0002240 0.4514665

Lattice parameters(A) Cell Angles

a = 17.063692 alpha = 89.949966

b = 3.383281 beta = 90.021852

c = 13.917282 gamma = 118.785773

Current cell volume = 704.175170 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067031 0.664556 0.126719 x

x Se 2 0.132258 0.335697 0.626619 x

x Se 3 0.132289 0.336070 0.873242 x

x Se 4 0.067115 0.664808 0.373567 x

x Se 5 0.266840 0.665105 0.126424 x

x Se 6 0.331917 0.334394 0.626349 x

x Se 7 0.331975 0.334845 0.873437 x

x Se 8 0.266895 0.665225 0.373662 x

x Se 9 0.467654 0.663495 0.126827 x

x Se 10 0.532329 0.335535 0.626473 x

x Se 11 0.532345 0.336501 0.873176 x

x Se 12 0.467668 0.664462 0.373526 x

x Se 13 0.668028 0.665165 0.126556 x

x Se 14 0.733105 0.334769 0.626338 x

x Se 15 0.733159 0.334887 0.873576 x

x Se 16 0.668085 0.665613 0.373656 x

x Se 17 0.867708 0.663917 0.126766 x

x Se 18 0.932887 0.335204 0.626435 x

x Se 19 0.932971 0.335455 0.873277 x

x Se 20 0.867740 0.664292 0.373375 x

x Nb 1 -0.000600 -0.002659 0.250072 x

x Nb 2 0.000593 0.002703 0.749928 x

x Nb 3 -0.000001 -0.000028 0.000007 x

x Nb 4 -0.000000 -0.000022 0.499993 x

x Nb 5 0.198799 -0.002049 0.250117 x

x Nb 6 0.200814 0.004488 0.749862 x

x Nb 7 0.199962 0.000234 0.000255 x

x Nb 8 0.200011 0.000450 0.499796 x

x Nb 9 0.399936 -0.001705 0.250198 x

x Nb 10 0.400178 0.001730 0.749949 x

x Nb 11 0.399745 0.000777 0.000144 x

x Nb 12 0.399634 0.000380 0.499760 x

x Nb 13 0.599813 -0.001752 0.250052 x

x Nb 14 0.600067 0.001749 0.749800 x

x Nb 15 0.600253 -0.000799 -0.000138 x

x Nb 16 0.600366 -0.000393 0.500236 x

x Nb 17 0.799196 -0.004503 0.250139 x

x Nb 18 0.801205 0.002002 0.749884 x

x Nb 19 0.800041 -0.000184 -0.000267 x

x Nb 20 0.799990 -0.000412 0.500214 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597568E+004 13235.58 <-- SCF

1 -3.62599558E+004 4.97672511E-003 13262.44 <-- SCF

2 -3.62599659E+004 2.51571752E-004 13290.19 <-- SCF

3 -3.62599311E+004 -8.69861918E-004 13316.70 <-- SCF

4 -3.62598235E+004 -2.68951694E-003 13342.91 <-- SCF

5 -3.62598290E+004 1.37550617E-004 13369.38 <-- SCF

6 -3.62598263E+004 -6.81069605E-005 13394.20 <-- SCF

7 -3.62598255E+004 -1.95940458E-005 13415.53 <-- SCF

8 -3.62598255E+004 -3.23016081E-007 13435.00 <-- SCF

9 -3.62598256E+004 1.40640724E-006 13452.41 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.82557174 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00411 -0.00763 -0.02172 \*

\* Se 2 0.02729 0.03701 0.00215 \*

\* Se 3 0.03346 0.04863 -0.02762 \*

\* Se 4 -0.01057 -0.00415 0.02910 \*

\* Se 5 0.00455 0.00883 -0.02261 \*

\* Se 6 -0.00928 0.04327 0.00438 \*

\* Se 7 0.01408 0.05532 -0.04059 \*

\* Se 8 -0.02310 0.00256 -0.00487 \*

\* Se 9 -0.01633 -0.10281 0.05868 \*

\* Se 10 0.02565 0.06878 -0.02335 \*

\* Se 11 0.01531 0.10324 -0.05748 \*

\* Se 12 -0.02699 -0.06832 0.02291 \*

\* Se 13 -0.01173 -0.05481 0.03665 \*

\* Se 14 0.02286 -0.00333 0.00535 \*

\* Se 15 -0.00473 -0.00951 0.02251 \*

\* Se 16 0.01112 -0.04287 -0.00192 \*

\* Se 17 -0.03460 -0.04983 0.03053 \*

\* Se 18 0.01097 0.00423 -0.02842 \*

\* Se 19 0.00442 0.00810 0.02084 \*

\* Se 20 -0.02815 -0.03763 -0.00469 \*

\* Nb 1 0.18429 0.08560 -0.00859 \*

\* Nb 2 -0.18684 -0.07946 0.00863 \*

\* Nb 3 -0.00122 -0.00208 0.00205 \*

\* Nb 4 -0.00176 -0.00221 -0.00236 \*

\* Nb 5 -0.08007 -0.01662 -0.00611 \*

\* Nb 6 0.02523 0.06300 -0.01891 \*

\* Nb 7 -0.03953 0.00574 -0.00087 \*

\* Nb 8 -0.00405 0.01289 0.01759 \*

\* Nb 9 -0.00666 -0.04755 0.00188 \*

\* Nb 10 -0.01839 -0.01992 0.00525 \*

\* Nb 11 0.00641 0.03092 -0.08962 \*

\* Nb 12 -0.03721 0.02515 0.07991 \*

\* Nb 13 0.01536 0.01923 -0.00557 \*

\* Nb 14 0.00938 0.05130 -0.00245 \*

\* Nb 15 -0.00726 -0.03166 0.09154 \*

\* Nb 16 0.03832 -0.02517 -0.08046 \*

\* Nb 17 -0.02388 -0.06695 0.01972 \*

\* Nb 18 0.08138 0.01163 0.00623 \*

\* Nb 19 0.04173 -0.00264 -0.00310 \*

\* Nb 20 0.00466 -0.01029 -0.01458 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.054244 0.094096 0.006657 \*

\* y 0.094096 0.022964 0.085377 \*

\* z 0.006657 0.085377 0.146617 \*

\* \*

\* Pressure: -0.0384 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000158 | -36259.822369 | <-- min BFGS

| trial step | 1.000000 | 0.000040 | -36259.825632 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 17 with enthalpy= -3.62598256E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 8.156086E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.033801E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.653155E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.466173E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 18 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000076 | -36259.825632 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 18 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8997633 -8.3407298 -0.0033090 0.4197479 -0.0034817 -0.0000052

0.0280758 3.3847374 0.0014191 1.0343503 1.8477493 -0.0006005

0.0002092 0.0043993 13.8975110 -0.0000057 -0.0001895 0.4521087

Lattice parameters(A) Cell Angles

a = 17.075442 alpha = 89.957835

b = 3.384854 beta = 90.019210

c = 13.897512 gamma = 118.764395

Current cell volume = 704.130621 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067072 0.664712 0.126783 x

x Se 2 0.132144 0.335572 0.626732 x

x Se 3 0.132178 0.336025 0.873127 x

x Se 4 0.067175 0.665035 0.373509 x

x Se 5 0.266876 0.664949 0.126383 x

x Se 6 0.331801 0.334243 0.626485 x

x Se 7 0.331872 0.334782 0.873289 x

x Se 8 0.266944 0.665093 0.373679 x

x Se 9 0.467634 0.663120 0.126928 x

x Se 10 0.532366 0.335814 0.626547 x

x Se 11 0.532365 0.336875 0.873076 x

x Se 12 0.467630 0.664183 0.373451 x

x Se 13 0.668133 0.665230 0.126702 x

x Se 14 0.733056 0.334899 0.626321 x

x Se 15 0.733123 0.335041 0.873617 x

x Se 16 0.668202 0.665766 0.373521 x

x Se 17 0.867819 0.663959 0.126883 x

x Se 18 0.932827 0.334978 0.626493 x

x Se 19 0.932931 0.335301 0.873212 x

x Se 20 0.867853 0.664415 0.373260 x

x Nb 1 -0.000615 -0.002746 0.250064 x

x Nb 2 0.000607 0.002797 0.749935 x

x Nb 3 -0.000002 -0.000033 0.000008 x

x Nb 4 -0.000001 -0.000027 0.499992 x

x Nb 5 0.198683 -0.002218 0.250116 x

x Nb 6 0.200882 0.004887 0.749856 x

x Nb 7 0.199951 0.000246 0.000282 x

x Nb 8 0.200012 0.000506 0.499780 x

x Nb 9 0.399945 -0.001804 0.250209 x

x Nb 10 0.400158 0.001813 0.749959 x

x Nb 11 0.399726 0.000866 0.000142 x

x Nb 12 0.399593 0.000397 0.499746 x

x Nb 13 0.599832 -0.001839 0.250041 x

x Nb 14 0.600059 0.001858 0.749789 x

x Nb 15 0.600271 -0.000891 -0.000136 x

x Nb 16 0.600407 -0.000411 0.500249 x

x Nb 17 0.799128 -0.004908 0.250146 x

x Nb 18 0.801322 0.002163 0.749885 x

x Nb 19 0.800053 -0.000188 -0.000296 x

x Nb 20 0.799989 -0.000463 0.500232 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597739E+004 13555.48 <-- SCF

1 -3.62598998E+004 3.14845732E-003 13582.50 <-- SCF

2 -3.62599068E+004 1.72732871E-004 13610.53 <-- SCF

3 -3.62598837E+004 -5.76789430E-004 13637.06 <-- SCF

4 -3.62598251E+004 -1.46539898E-003 13662.66 <-- SCF

5 -3.62598285E+004 8.68005999E-005 13688.61 <-- SCF

6 -3.62598274E+004 -2.78302765E-005 13712.38 <-- SCF

7 -3.62598272E+004 -5.26544617E-006 13732.92 <-- SCF

8 -3.62598274E+004 3.91223592E-006 13751.50 <-- SCF

9 -3.62598275E+004 4.31488514E-006 13769.14 <-- SCF

10 -3.62598277E+004 3.87357271E-006 13786.03 <-- SCF

11 -3.62598278E+004 3.54499809E-006 13803.06 <-- SCF

12 -3.62598280E+004 3.16555936E-006 13819.20 <-- SCF

13 -3.62598281E+004 3.10245597E-006 13835.34 <-- SCF

14 -3.62598282E+004 2.48088317E-006 13851.41 <-- SCF

15 -3.62598283E+004 2.54163513E-006 13867.56 <-- SCF

16 -3.62598284E+004 2.35328691E-006 13884.06 <-- SCF

17 -3.62598285E+004 2.23273426E-006 13900.22 <-- SCF

18 -3.62598286E+004 2.05530111E-006 13916.56 <-- SCF

19 -3.62598286E+004 1.92892249E-006 13932.72 <-- SCF

20 -3.62598287E+004 1.79457929E-006 13948.86 <-- SCF

21 -3.62598288E+004 1.68302075E-006 13964.83 <-- SCF

22 -3.62598288E+004 1.56238814E-006 13980.95 <-- SCF

23 -3.62598289E+004 1.47157249E-006 13997.02 <-- SCF

24 -3.62598289E+004 1.38164996E-006 14013.16 <-- SCF

25 -3.62598290E+004 1.29813686E-006 14029.31 <-- SCF

26 -3.62598291E+004 1.21734734E-006 14045.48 <-- SCF

27 -3.62598291E+004 1.13806609E-006 14061.56 <-- SCF

28 -3.62598291E+004 1.13326053E-006 14077.70 <-- SCF

29 -3.62598292E+004 8.11540970E-007 14093.84 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.82917383 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.01466 -0.01863 -0.03790 \*

\* Se 2 0.06677 0.05209 -0.01018 \*

\* Se 3 0.07663 0.06403 -0.02384 \*

\* Se 4 -0.02975 -0.01403 0.04766 \*

\* Se 5 -0.00666 0.02184 -0.01361 \*

\* Se 6 0.02100 0.04344 -0.00081 \*

\* Se 7 0.04765 0.04964 -0.03819 \*

\* Se 8 -0.03910 0.01460 -0.00484 \*

\* Se 9 -0.00544 -0.11563 0.06061 \*

\* Se 10 0.00751 0.08305 -0.03046 \*

\* Se 11 0.00461 0.11615 -0.05987 \*

\* Se 12 -0.00887 -0.08266 0.03043 \*

\* Se 13 -0.04540 -0.04906 0.03457 \*

\* Se 14 0.03851 -0.01549 0.00543 \*

\* Se 15 0.00612 -0.02264 0.01352 \*

\* Se 16 -0.01934 -0.04270 0.00315 \*

\* Se 17 -0.07742 -0.06540 0.02650 \*

\* Se 18 0.03020 0.01402 -0.04717 \*

\* Se 19 0.01486 0.01909 0.03751 \*

\* Se 20 -0.06711 -0.05291 0.00760 \*

\* Nb 1 0.20082 0.09230 -0.00599 \*

\* Nb 2 -0.20323 -0.08732 0.00617 \*

\* Nb 3 -0.00107 -0.00193 0.00147 \*

\* Nb 4 -0.00202 -0.00191 -0.00210 \*

\* Nb 5 -0.04627 -0.01895 -0.00880 \*

\* Nb 6 0.00127 0.06017 -0.01412 \*

\* Nb 7 -0.03699 0.00941 -0.00705 \*

\* Nb 8 0.00059 0.01573 0.02269 \*

\* Nb 9 -0.01202 -0.05477 -0.00380 \*

\* Nb 10 -0.01146 -0.02254 -0.00117 \*

\* Nb 11 0.01109 0.02982 -0.08596 \*

\* Nb 12 -0.02836 0.02531 0.08549 \*

\* Nb 13 0.00890 0.02169 0.00059 \*

\* Nb 14 0.01516 0.05797 0.00325 \*

\* Nb 15 -0.01207 -0.03021 0.08787 \*

\* Nb 16 0.02986 -0.02499 -0.08560 \*

\* Nb 17 -0.00098 -0.06336 0.01493 \*

\* Nb 18 0.04764 0.01517 0.00885 \*

\* Nb 19 0.03917 -0.00674 0.00358 \*

\* Nb 20 -0.00015 -0.01366 -0.02038 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.019353 0.082999 0.011663 \*

\* y 0.082999 0.017116 0.063088 \*

\* z 0.011663 0.063088 -0.026713 \*

\* \*

\* Pressure: 0.0097 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000076 | -36259.825632 | <-- min BFGS

| trial step | 1.000000 | -2.439E-006 | -36259.829229 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 18 with enthalpy= -3.62598292E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 8.992521E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.212806E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.651039E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 8.299918E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 19 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000022 | -36259.829229 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 19 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9010214 -8.3435475 -0.0027667 0.4197430 -0.0034261 -0.0000017

0.0276309 3.3851071 0.0011409 1.0345745 1.8476815 -0.0004714

0.0000851 0.0034978 13.8953936 -0.0000014 -0.0001524 0.4521776

Lattice parameters(A) Cell Angles

a = 17.077916 alpha = 89.966265

b = 3.385220 beta = 90.016022

c = 13.895394 gamma = 118.778163

Current cell volume = 704.108616 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067063 0.664653 0.126783 x

x Se 2 0.132172 0.335652 0.626727 x

x Se 3 0.132206 0.336097 0.873130 x

x Se 4 0.067161 0.664960 0.373508 x

x Se 5 0.266869 0.664985 0.126407 x

x Se 6 0.331823 0.334309 0.626474 x

x Se 7 0.331894 0.334843 0.873299 x

x Se 8 0.266930 0.665111 0.373654 x

x Se 9 0.467639 0.663125 0.126935 x

x Se 10 0.532357 0.335809 0.626547 x

x Se 11 0.532359 0.336871 0.873070 x

x Se 12 0.467640 0.664188 0.373452 x

x Se 13 0.668110 0.665169 0.126692 x

x Se 14 0.733070 0.334881 0.626347 x

x Se 15 0.733130 0.335005 0.873593 x

x Se 16 0.668180 0.665700 0.373532 x

x Se 17 0.867791 0.663886 0.126880 x

x Se 18 0.932841 0.335053 0.626495 x

x Se 19 0.932940 0.335361 0.873212 x

x Se 20 0.867826 0.664335 0.373265 x

x Nb 1 -0.000590 -0.002630 0.250065 x

x Nb 2 0.000582 0.002681 0.749934 x

x Nb 3 -0.000002 -0.000034 0.000008 x

x Nb 4 -0.000001 -0.000027 0.499992 x

x Nb 5 0.198696 -0.002219 0.250116 x

x Nb 6 0.200872 0.004855 0.749854 x

x Nb 7 0.199949 0.000235 0.000276 x

x Nb 8 0.200012 0.000502 0.499786 x

x Nb 9 0.399941 -0.001821 0.250207 x

x Nb 10 0.400161 0.001784 0.749957 x

x Nb 11 0.399730 0.000870 0.000129 x

x Nb 12 0.399596 0.000399 0.499761 x

x Nb 13 0.599829 -0.001810 0.250043 x

x Nb 14 0.600063 0.001875 0.749791 x

x Nb 15 0.600267 -0.000895 -0.000122 x

x Nb 16 0.600404 -0.000412 0.500234 x

x Nb 17 0.799138 -0.004876 0.250148 x

x Nb 18 0.801309 0.002163 0.749886 x

x Nb 19 0.800056 -0.000177 -0.000291 x

x Nb 20 0.799990 -0.000458 0.500227 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598273E+004 14196.34 <-- SCF

1 -3.62598396E+004 3.08976433E-004 14224.02 <-- SCF

2 -3.62598404E+004 1.92299417E-005 14246.50 <-- SCF

3 -3.62598395E+004 -2.40366945E-005 14272.70 <-- SCF

4 -3.62598296E+004 -2.45555236E-004 14298.45 <-- SCF

5 -3.62598300E+004 8.00593948E-006 14319.61 <-- SCF

6 -3.62598299E+004 -5.32277803E-007 14337.06 <-- SCF

7 -3.62598299E+004 2.05261264E-007 14353.81 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.82994056 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00815 -0.01454 -0.03671 \*

\* Se 2 0.05768 0.05108 -0.00437 \*

\* Se 3 0.06958 0.06464 -0.03039 \*

\* Se 4 -0.02016 -0.01045 0.04492 \*

\* Se 5 -0.00345 0.01926 -0.00885 \*

\* Se 6 0.02060 0.04415 0.00647 \*

\* Se 7 0.04355 0.05107 -0.04722 \*

\* Se 8 -0.03584 0.01313 -0.00733 \*

\* Se 9 -0.00488 -0.11433 0.06369 \*

\* Se 10 0.00667 0.08131 -0.02278 \*

\* Se 11 0.00432 0.11494 -0.06331 \*

\* Se 12 -0.00780 -0.08093 0.02306 \*

\* Se 13 -0.04140 -0.05039 0.04390 \*

\* Se 14 0.03537 -0.01401 0.00779 \*

\* Se 15 0.00285 -0.02008 0.00878 \*

\* Se 16 -0.01903 -0.04326 -0.00448 \*

\* Se 17 -0.07048 -0.06617 0.03291 \*

\* Se 18 0.02047 0.01047 -0.04437 \*

\* Se 19 0.00837 0.01508 0.03653 \*

\* Se 20 -0.05811 -0.05205 0.00200 \*

\* Nb 1 0.17539 0.08405 -0.00324 \*

\* Nb 2 -0.17818 -0.07982 0.00348 \*

\* Nb 3 -0.00070 -0.00162 0.00125 \*

\* Nb 4 -0.00213 -0.00190 -0.00214 \*

\* Nb 5 -0.03065 -0.02096 -0.00835 \*

\* Nb 6 -0.01094 0.05714 -0.01070 \*

\* Nb 7 -0.03398 0.00823 -0.01319 \*

\* Nb 8 0.00303 0.01627 0.02604 \*

\* Nb 9 -0.02105 -0.06530 -0.00571 \*

\* Nb 10 0.00566 -0.01690 -0.00669 \*

\* Nb 11 0.00764 0.03092 -0.08643 \*

\* Nb 12 -0.01848 0.03162 0.09503 \*

\* Nb 13 -0.00794 0.01568 0.00605 \*

\* Nb 14 0.02450 0.06790 0.00523 \*

\* Nb 15 -0.00855 -0.03127 0.08805 \*

\* Nb 16 0.02049 -0.03088 -0.09479 \*

\* Nb 17 0.01109 -0.05977 0.01163 \*

\* Nb 18 0.03200 0.01833 0.00821 \*

\* Nb 19 0.03568 -0.00596 0.01024 \*

\* Nb 20 -0.00302 -0.01469 -0.02423 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.083542 0.082349 0.004381 \*

\* y 0.082349 -0.031258 0.050170 \*

\* z 0.004381 0.050170 0.053557 \*

\* \*

\* Pressure: 0.0204 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000022 | -36259.829229 | <-- min BFGS

| trial step | 1.000000 | 0.000023 | -36259.829972 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 19 with line minimization (lambda=-15.574494)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8801689 -8.2968460 -0.0117548 0.4198272 -0.0043492 -0.0000588

0.0350053 3.3789791 0.0057524 1.0308567 1.8488172 -0.0026059

0.0021427 0.0184400 13.9304884 -0.0000714 -0.0007671 0.4510394

Lattice parameters(A) Cell Angles

a = 17.036937 alpha = 89.826534

b = 3.379165 beta = 90.068769

c = 13.930501 gamma = 118.549527

Current cell volume = 704.466174 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067211 0.665642 0.126778 x

x Se 2 0.131714 0.334326 0.626810 x

x Se 3 0.131736 0.334896 0.873080 x

x Se 4 0.067397 0.666202 0.373533 x

x Se 5 0.266983 0.664390 0.126001 x

x Se 6 0.331466 0.333209 0.626663 x

x Se 7 0.331524 0.333821 0.873132 x

x Se 8 0.267152 0.664822 0.374075 x

x Se 9 0.467545 0.663045 0.126818 x

x Se 10 0.532512 0.335889 0.626552 x

x Se 11 0.532455 0.336949 0.873185 x

x Se 12 0.467486 0.664110 0.373445 x

x Se 13 0.668478 0.666182 0.126863 x

x Se 14 0.732849 0.335177 0.625925 x

x Se 15 0.733016 0.335605 0.873998 x

x Se 16 0.668536 0.666791 0.373340 x

x Se 17 0.868261 0.665096 0.126927 x

x Se 18 0.932605 0.333812 0.626469 x

x Se 19 0.932793 0.334372 0.873217 x

x Se 20 0.868282 0.665665 0.373185 x

x Nb 1 -0.001003 -0.004562 0.250052 x

x Nb 2 0.000995 0.004601 0.749946 x

x Nb 3 -0.000001 -0.000026 0.000007 x

x Nb 4 0.000002 -0.000015 0.499994 x

x Nb 5 0.198486 -0.002212 0.250125 x

x Nb 6 0.201037 0.005381 0.749886 x

x Nb 7 0.199986 0.000413 0.000368 x

x Nb 8 0.200015 0.000582 0.499686 x

x Nb 9 0.400000 -0.001548 0.250235 x

x Nb 10 0.400104 0.002261 0.749994 x

x Nb 11 0.399664 0.000808 0.000351 x

x Nb 12 0.399544 0.000366 0.499503 x

x Nb 13 0.599887 -0.002277 0.250008 x

x Nb 14 0.600001 0.001588 0.749764 x

x Nb 15 0.600334 -0.000830 -0.000346 x

x Nb 16 0.600454 -0.000389 0.500491 x

x Nb 17 0.798974 -0.005394 0.250114 x

x Nb 18 0.801518 0.002163 0.749877 x

x Nb 19 0.800017 -0.000366 -0.000379 x

x Nb 20 0.799986 -0.000544 0.500324 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62592909E+004 14456.64 <-- SCF

1 -3.62606063E+004 3.28836881E-002 14483.64 <-- SCF

2 -3.62606676E+004 1.53261162E-003 14512.81 <-- SCF

3 -3.62604014E+004 -6.65568169E-003 14539.69 <-- SCF

4 -3.62598013E+004 -1.50008702E-002 14565.95 <-- SCF

5 -3.62598240E+004 5.67944121E-004 14592.72 <-- SCF

6 -3.62598100E+004 -3.49859762E-004 14619.08 <-- SCF

7 -3.62598056E+004 -1.11177227E-004 14643.02 <-- SCF

8 -3.62598057E+004 1.63250637E-006 14665.28 <-- SCF

9 -3.62598059E+004 5.77064204E-006 14684.89 <-- SCF

10 -3.62598060E+004 2.53663730E-006 14702.78 <-- SCF

11 -3.62598060E+004 1.10840767E-006 14720.58 <-- SCF

12 -3.62598061E+004 1.61829324E-006 14738.73 <-- SCF

13 -3.62598062E+004 1.24323501E-006 14755.58 <-- SCF

14 -3.62598062E+004 1.04119555E-006 14772.58 <-- SCF

15 -3.62598062E+004 8.98792661E-007 14788.72 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.80623626 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.06097 -0.09968 -0.03485 \*

\* Se 2 0.14489 0.09349 -0.05536 \*

\* Se 3 0.16671 0.09146 0.01931 \*

\* Se 4 -0.11209 -0.08731 0.02187 \*

\* Se 5 -0.02366 0.00614 0.04327 \*

\* Se 6 0.07480 0.07034 -0.02752 \*

\* Se 7 0.10331 0.05804 -0.01279 \*

\* Se 8 -0.05918 -0.00233 -0.04322 \*

\* Se 9 0.02307 -0.13292 0.05233 \*

\* Se 10 -0.03982 0.11004 -0.04287 \*

\* Se 11 -0.02357 0.13308 -0.05213 \*

\* Se 12 0.03889 -0.10987 0.04329 \*

\* Se 13 -0.10129 -0.05751 0.01063 \*

\* Se 14 0.05816 0.00082 0.04345 \*

\* Se 15 0.02302 -0.00742 -0.04286 \*

\* Se 16 -0.07341 -0.06946 0.02896 \*

\* Se 17 -0.16763 -0.09299 -0.01751 \*

\* Se 18 0.11246 0.08768 -0.02165 \*

\* Se 19 0.06068 0.10058 0.03487 \*

\* Se 20 -0.14485 -0.09412 0.05362 \*

\* Nb 1 0.27097 0.16924 0.00199 \*

\* Nb 2 -0.27454 -0.16252 -0.00199 \*

\* Nb 3 -0.00007 -0.00373 0.00186 \*

\* Nb 4 -0.00138 -0.00385 -0.00236 \*

\* Nb 5 0.02693 -0.02265 -0.00415 \*

\* Nb 6 -0.08283 0.02416 -0.01591 \*

\* Nb 7 -0.04681 0.00396 -0.03665 \*

\* Nb 8 -0.01120 0.00748 0.05134 \*

\* Nb 9 -0.06623 -0.03520 -0.01588 \*

\* Nb 10 0.01138 -0.07850 -0.01046 \*

\* Nb 11 -0.00013 0.03599 -0.12749 \*

\* Nb 12 -0.01687 0.03545 0.14196 \*

\* Nb 13 -0.01438 0.07795 0.00989 \*

\* Nb 14 0.06910 0.03836 0.01513 \*

\* Nb 15 -0.00001 -0.03718 0.12950 \*

\* Nb 16 0.01929 -0.03567 -0.14246 \*

\* Nb 17 0.08398 -0.02869 0.01680 \*

\* Nb 18 -0.02419 0.01832 0.00418 \*

\* Nb 19 0.04724 0.00169 0.03280 \*

\* Nb 20 0.01024 -0.00268 -0.04892 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.173049 0.425019 0.016464 \*

\* y 0.425019 -0.052217 0.333857 \*

\* z 0.016464 0.333857 0.474077 \*

\* \*

\* Pressure: -0.0829 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000022 | -36259.829229 | <-- min BFGS

| trial step | 1.000000 | 0.000023 | -36259.829972 | <-- min BFGS

| line step | -15.574494 | 0.000080 | -36259.806425 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 19 with quad minimization (lambda= 6.884290)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9084245 -8.3601275 0.0004243 0.4197140 -0.0030993 0.0000191

0.0250128 3.3872826 -0.0004963 1.0358931 1.8472845 0.0002886

-0.0006454 -0.0018069 13.8829342 0.0000242 0.0000661 0.4525834

Lattice parameters(A) Cell Angles

a = 17.092479 alpha = 90.015872

b = 3.387375 beta = 89.997254

c = 13.882934 gamma = 118.859113

Current cell volume = 703.978005 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067011 0.664301 0.126785 x

x Se 2 0.132334 0.336123 0.626697 x

x Se 3 0.132373 0.336524 0.873147 x

x Se 4 0.067077 0.664519 0.373499 x

x Se 5 0.266828 0.665197 0.126552 x

x Se 6 0.331950 0.334700 0.626407 x

x Se 7 0.332025 0.335206 0.873359 x

x Se 8 0.266851 0.665213 0.373505 x

x Se 9 0.467673 0.663154 0.126976 x

x Se 10 0.532302 0.335781 0.626545 x

x Se 11 0.532325 0.336843 0.873028 x

x Se 12 0.467694 0.664216 0.373454 x

x Se 13 0.667980 0.664810 0.126631 x

x Se 14 0.733148 0.334777 0.626497 x

x Se 15 0.733170 0.334792 0.873448 x

x Se 16 0.668054 0.665312 0.373600 x

x Se 17 0.867624 0.663457 0.126863 x

x Se 18 0.932925 0.335494 0.626504 x

x Se 19 0.932992 0.335712 0.873210 x

x Se 20 0.867663 0.663863 0.373294 x

x Nb 1 -0.000444 -0.001944 0.250070 x

x Nb 2 0.000435 0.002000 0.749930 x

x Nb 3 -0.000002 -0.000036 0.000009 x

x Nb 4 -0.000002 -0.000032 0.499991 x

x Nb 5 0.198771 -0.002221 0.250113 x

x Nb 6 0.200813 0.004668 0.749842 x

x Nb 7 0.199936 0.000172 0.000244 x

x Nb 8 0.200010 0.000473 0.499821 x

x Nb 9 0.399920 -0.001918 0.250197 x

x Nb 10 0.400181 0.001615 0.749944 x

x Nb 11 0.399753 0.000892 0.000050 x

x Nb 12 0.399615 0.000410 0.499853 x

x Nb 13 0.599808 -0.001645 0.250056 x

x Nb 14 0.600085 0.001977 0.749800 x

x Nb 15 0.600244 -0.000918 -0.000043 x

x Nb 16 0.600386 -0.000420 0.500142 x

x Nb 17 0.799197 -0.004693 0.250160 x

x Nb 18 0.801235 0.002164 0.749889 x

x Nb 19 0.800069 -0.000110 -0.000260 x

x Nb 20 0.799991 -0.000427 0.500192 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62588945E+004 14891.97 <-- SCF

1 -3.62610350E+004 5.35135802E-002 14918.70 <-- SCF

2 -3.62611329E+004 2.44862002E-003 14947.44 <-- SCF

3 -3.62606596E+004 -1.18324735E-002 14974.16 <-- SCF

4 -3.62598285E+004 -2.07788016E-002 15000.47 <-- SCF

5 -3.62598616E+004 8.26502113E-004 15026.83 <-- SCF

6 -3.62598379E+004 -5.92013050E-004 15052.73 <-- SCF

7 -3.62598309E+004 -1.75219018E-004 15076.64 <-- SCF

8 -3.62598307E+004 -4.11080980E-006 15099.83 <-- SCF

9 -3.62598309E+004 6.06331647E-006 15120.11 <-- SCF

10 -3.62598312E+004 5.21396117E-006 15138.23 <-- SCF

11 -3.62598313E+004 3.11487374E-006 15155.55 <-- SCF

12 -3.62598314E+004 3.00206106E-006 15173.72 <-- SCF

13 -3.62598315E+004 2.81156235E-006 15190.84 <-- SCF

14 -3.62598316E+004 2.71170743E-006 15207.88 <-- SCF

15 -3.62598317E+004 2.50103225E-006 15224.12 <-- SCF

16 -3.62598318E+004 2.54305400E-006 15240.06 <-- SCF

17 -3.62598319E+004 2.55390642E-006 15256.02 <-- SCF

18 -3.62598320E+004 2.88300710E-006 15272.22 <-- SCF

19 -3.62598321E+004 1.41964434E-006 15288.27 <-- SCF

20 -3.62598321E+004 5.01831598E-007 15304.41 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.83211459 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00134 0.01023 -0.03092 \*

\* Se 2 0.00510 0.04382 0.01277 \*

\* Se 3 0.01357 0.06427 -0.04828 \*

\* Se 4 0.00847 0.01513 0.05281 \*

\* Se 5 0.00097 0.00926 -0.03695 \*

\* Se 6 -0.00537 0.03316 0.02761 \*

\* Se 7 0.01988 0.04762 -0.06466 \*

\* Se 8 -0.01875 0.00590 0.02255 \*

\* Se 9 -0.01221 -0.10835 0.06629 \*

\* Se 10 0.02280 0.07109 -0.01826 \*

\* Se 11 0.01410 0.10889 -0.06641 \*

\* Se 12 -0.02127 -0.07050 0.01891 \*

\* Se 13 -0.01949 -0.04627 0.06074 \*

\* Se 14 0.01592 -0.00681 -0.02316 \*

\* Se 15 -0.00390 -0.00993 0.03777 \*

\* Se 16 0.00544 -0.03184 -0.02558 \*

\* Se 17 -0.01449 -0.06617 0.05153 \*

\* Se 18 -0.00628 -0.01436 -0.05129 \*

\* Se 19 0.00071 -0.00901 0.02958 \*

\* Se 20 -0.00582 -0.04525 -0.01524 \*

\* Nb 1 0.11093 0.04495 -0.00284 \*

\* Nb 2 -0.11778 -0.03926 0.00249 \*

\* Nb 3 0.00014 -0.00376 0.00224 \*

\* Nb 4 -0.00097 -0.00380 -0.00294 \*

\* Nb 5 -0.04353 -0.01661 -0.00395 \*

\* Nb 6 0.00712 0.06252 -0.01763 \*

\* Nb 7 -0.03399 0.01563 -0.00781 \*

\* Nb 8 0.00449 0.02831 0.02129 \*

\* Nb 9 -0.01963 -0.07507 0.00540 \*

\* Nb 10 -0.00902 0.01270 -0.00813 \*

\* Nb 11 0.00502 0.02411 -0.05464 \*

\* Nb 12 -0.01865 0.02617 0.05800 \*

\* Nb 13 0.00369 -0.01315 0.00843 \*

\* Nb 14 0.02257 0.07829 -0.00643 \*

\* Nb 15 -0.00602 -0.02627 0.05702 \*

\* Nb 16 0.02050 -0.02690 -0.05841 \*

\* Nb 17 -0.00247 -0.06638 0.01809 \*

\* Nb 18 0.04749 0.01269 0.00467 \*

\* Nb 19 0.03487 -0.01056 0.00333 \*

\* Nb 20 -0.00549 -0.02446 -0.01802 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.061068 -0.028169 0.050003 \*

\* y -0.028169 -0.042722 -0.055688 \*

\* z 0.050003 -0.055688 -0.050451 \*

\* \*

\* Pressure: 0.0514 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000022 | -36259.829229 | <-- min BFGS

| trial step | 1.000000 | 0.000023 | -36259.829972 | <-- min BFGS

| line step | -15.574494 | 0.000080 | -36259.806425 | <-- min BFGS

| quad step | 6.884290 | 1.563E-006 | -36259.832119 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 19 with enthalpy= -3.62598321E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.225597E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.283220E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.029112E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 6.106764E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 20 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000084 | -36259.832119 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 20 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9204272 -8.3709641 0.0015689 0.4194493 -0.0029653 0.0000489

0.0239646 3.3898454 -0.0014691 1.0357981 1.8462093 0.0007845

-0.0016531 -0.0049650 13.8675216 0.0000623 0.0001959 0.4530865

Lattice parameters(A) Cell Angles

a = 17.108249 alpha = 90.045391

b = 3.389930 beta = 89.990665

c = 13.867523 gamma = 118.889143

Current cell volume = 704.172493 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067023 0.664226 0.126909 x

x Se 2 0.132317 0.336344 0.626857 x

x Se 3 0.132361 0.336811 0.872970 x

x Se 4 0.067089 0.664461 0.373381 x

x Se 5 0.266842 0.665175 0.126661 x

x Se 6 0.331904 0.334825 0.626568 x

x Se 7 0.331998 0.335416 0.873172 x

x Se 8 0.266850 0.665138 0.373367 x

x Se 9 0.467681 0.662716 0.127180 x

x Se 10 0.532298 0.336099 0.626678 x

x Se 11 0.532316 0.337281 0.872825 x

x Se 12 0.467698 0.663897 0.373321 x

x Se 13 0.668009 0.664605 0.126813 x

x Se 14 0.733149 0.334848 0.626634 x

x Se 15 0.733156 0.334811 0.873339 x

x Se 16 0.668101 0.665192 0.373441 x

x Se 17 0.867635 0.663164 0.127043 x

x Se 18 0.932914 0.335554 0.626622 x

x Se 19 0.932980 0.335790 0.873085 x

x Se 20 0.867680 0.663638 0.373131 x

x Nb 1 -0.000354 -0.001544 0.250065 x

x Nb 2 0.000343 0.001611 0.749935 x

x Nb 3 -0.000003 -0.000045 0.000011 x

x Nb 4 -0.000003 -0.000041 0.499989 x

x Nb 5 0.198688 -0.002425 0.250110 x

x Nb 6 0.200851 0.005010 0.749826 x

x Nb 7 0.199912 0.000145 0.000251 x

x Nb 8 0.200011 0.000530 0.499829 x

x Nb 9 0.399912 -0.002132 0.250203 x

x Nb 10 0.400176 0.001604 0.749945 x

x Nb 11 0.399748 0.001013 -0.000010 x

x Nb 12 0.399581 0.000442 0.499906 x

x Nb 13 0.599811 -0.001641 0.250054 x

x Nb 14 0.600095 0.002207 0.749794 x

x Nb 15 0.600248 -0.001043 0.000019 x

x Nb 16 0.600421 -0.000450 0.500089 x

x Nb 17 0.799160 -0.005042 0.250177 x

x Nb 18 0.801318 0.002357 0.749892 x

x Nb 19 0.800095 -0.000069 -0.000270 x

x Nb 20 0.799990 -0.000476 0.500187 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597721E+004 15407.94 <-- SCF

1 -3.62600089E+004 5.92076912E-003 15435.05 <-- SCF

2 -3.62600229E+004 3.49904823E-004 15462.88 <-- SCF

3 -3.62599863E+004 -9.15984388E-004 15489.45 <-- SCF

4 -3.62598298E+004 -3.91321538E-003 15515.36 <-- SCF

5 -3.62598354E+004 1.40869740E-004 15541.31 <-- SCF

6 -3.62598338E+004 -3.86758401E-005 15565.56 <-- SCF

7 -3.62598335E+004 -8.18739042E-006 15587.05 <-- SCF

8 -3.62598336E+004 2.61832767E-006 15606.28 <-- SCF

9 -3.62598337E+004 2.61295103E-006 15623.88 <-- SCF

10 -3.62598338E+004 2.19794669E-006 15640.64 <-- SCF

11 -3.62598339E+004 1.77545264E-006 15656.69 <-- SCF

12 -3.62598339E+004 1.62701558E-006 15672.77 <-- SCF

13 -3.62598340E+004 1.63497659E-006 15689.38 <-- SCF

14 -3.62598341E+004 1.48194556E-006 15705.39 <-- SCF

15 -3.62598341E+004 1.38059072E-006 15721.58 <-- SCF

16 -3.62598342E+004 1.26970488E-006 15737.72 <-- SCF

17 -3.62598342E+004 1.20600830E-006 15753.95 <-- SCF

18 -3.62598343E+004 1.08768117E-006 15770.05 <-- SCF

19 -3.62598343E+004 1.03553183E-006 15786.28 <-- SCF

20 -3.62598343E+004 9.62938894E-007 15802.66 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.83434759 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00259 0.01563 -0.05048 \*

\* Se 2 0.02653 0.06392 0.02063 \*

\* Se 3 0.03343 0.08099 -0.04587 \*

\* Se 4 0.00391 0.02453 0.07074 \*

\* Se 5 -0.01086 0.01661 -0.06241 \*

\* Se 6 0.03023 0.02940 0.03316 \*

\* Se 7 0.04460 0.03862 -0.05674 \*

\* Se 8 -0.02833 0.01575 0.05276 \*

\* Se 9 -0.02517 -0.11196 0.05190 \*

\* Se 10 0.01711 0.08322 -0.00936 \*

\* Se 11 0.02646 0.11285 -0.05285 \*

\* Se 12 -0.01598 -0.08267 0.01010 \*

\* Se 13 -0.04453 -0.03766 0.05477 \*

\* Se 14 0.02686 -0.01641 -0.05322 \*

\* Se 15 0.00897 -0.01730 0.06286 \*

\* Se 16 -0.03002 -0.02828 -0.03130 \*

\* Se 17 -0.03425 -0.08277 0.04750 \*

\* Se 18 -0.00256 -0.02375 -0.06964 \*

\* Se 19 0.00415 -0.01450 0.04971 \*

\* Se 20 -0.02725 -0.06592 -0.02251 \*

\* Nb 1 0.09425 0.01892 0.00085 \*

\* Nb 2 -0.09854 -0.01607 -0.00071 \*

\* Nb 3 -0.00006 -0.00208 0.00116 \*

\* Nb 4 -0.00101 -0.00236 -0.00198 \*

\* Nb 5 -0.02954 -0.02134 -0.00688 \*

\* Nb 6 -0.01528 0.06545 -0.00512 \*

\* Nb 7 -0.02138 0.01745 -0.01635 \*

\* Nb 8 0.00311 0.02426 0.01856 \*

\* Nb 9 -0.01571 -0.08624 0.00057 \*

\* Nb 10 -0.00818 0.03448 -0.01423 \*

\* Nb 11 0.00134 0.02153 -0.04358 \*

\* Nb 12 -0.01345 0.02386 0.05364 \*

\* Nb 13 0.00458 -0.03493 0.01403 \*

\* Nb 14 0.01798 0.08776 -0.00074 \*

\* Nb 15 -0.00228 -0.02257 0.04497 \*

\* Nb 16 0.01456 -0.02400 -0.05346 \*

\* Nb 17 0.01796 -0.06741 0.00539 \*

\* Nb 18 0.03203 0.01972 0.00693 \*

\* Nb 19 0.02232 -0.01464 0.01395 \*

\* Nb 20 -0.00343 -0.02205 -0.01677 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.018259 -0.073006 -0.001803 \*

\* y -0.073006 0.027213 -0.119649 \*

\* z -0.001803 -0.119649 -0.170606 \*

\* \*

\* Pressure: 0.0539 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000084 | -36259.832119 | <-- min BFGS

| trial step | 1.000000 | 0.000018 | -36259.834438 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 20 with enthalpy= -3.62598344E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 5.797545E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.273873E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.227973E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.706061E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 21 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000081 | -36259.834438 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 21 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9235256 -8.3710976 0.0009350 0.4193589 -0.0029711 0.0000637

0.0240180 3.3900004 -0.0014706 1.0355441 1.8461103 0.0008216

-0.0021412 -0.0049717 13.8701135 0.0000815 0.0001959 0.4530018

Lattice parameters(A) Cell Angles

a = 17.111017 alpha = 90.045454

b = 3.390086 beta = 89.994536

c = 13.870115 gamma = 118.883570

Current cell volume = 704.488107 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067058 0.664346 0.126993 x

x Se 2 0.132231 0.336383 0.627003 x

x Se 3 0.132280 0.336951 0.872801 x

x Se 4 0.067139 0.664645 0.373315 x

x Se 5 0.266874 0.665071 0.126658 x

x Se 6 0.331804 0.334789 0.626742 x

x Se 7 0.331918 0.335494 0.872966 x

x Se 8 0.266882 0.665017 0.373344 x

x Se 9 0.467666 0.662178 0.127350 x

x Se 10 0.532328 0.336496 0.626777 x

x Se 11 0.532331 0.337819 0.872656 x

x Se 12 0.467667 0.663499 0.373222 x

x Se 13 0.668089 0.664532 0.127016 x

x Se 14 0.733117 0.334966 0.626658 x

x Se 15 0.733124 0.334911 0.873342 x

x Se 16 0.668202 0.665232 0.373269 x

x Se 17 0.867716 0.663019 0.127215 x

x Se 18 0.932865 0.335372 0.626689 x

x Se 19 0.932945 0.335674 0.873001 x

x Se 20 0.867765 0.663595 0.372983 x

x Nb 1 -0.000302 -0.001332 0.250056 x

x Nb 2 0.000289 0.001410 0.749943 x

x Nb 3 -0.000004 -0.000054 0.000012 x

x Nb 4 -0.000004 -0.000051 0.499987 x

x Nb 5 0.198566 -0.002656 0.250106 x

x Nb 6 0.200914 0.005472 0.749813 x

x Nb 7 0.199889 0.000144 0.000270 x

x Nb 8 0.200012 0.000617 0.499826 x

x Nb 9 0.399911 -0.002348 0.250211 x

x Nb 10 0.400156 0.001662 0.749952 x

x Nb 11 0.399734 0.001143 -0.000050 x

x Nb 12 0.399534 0.000470 0.499934 x

x Nb 13 0.599828 -0.001706 0.250047 x

x Nb 14 0.600098 0.002439 0.749785 x

x Nb 15 0.600261 -0.001178 0.000061 x

x Nb 16 0.600468 -0.000478 0.500061 x

x Nb 17 0.799098 -0.005513 0.250190 x

x Nb 18 0.801442 0.002577 0.749896 x

x Nb 19 0.800119 -0.000054 -0.000293 x

x Nb 20 0.799989 -0.000554 0.500192 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597994E+004 15905.39 <-- SCF

1 -3.62599694E+004 4.24910846E-003 15932.61 <-- SCF

2 -3.62599804E+004 2.76113757E-004 15959.80 <-- SCF

3 -3.62599530E+004 -6.86132341E-004 15986.41 <-- SCF

4 -3.62598320E+004 -3.02388436E-003 16012.22 <-- SCF

5 -3.62598384E+004 1.60287061E-004 16038.23 <-- SCF

6 -3.62598368E+004 -4.22042387E-005 16062.94 <-- SCF

7 -3.62598361E+004 -1.76681192E-005 16084.88 <-- SCF

8 -3.62598360E+004 -6.01012738E-007 16103.92 <-- SCF

9 -3.62598361E+004 1.81561298E-006 16121.52 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.83610130 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02041 0.00922 -0.06251 \*

\* Se 2 0.05741 0.08028 0.02390 \*

\* Se 3 0.06269 0.08724 -0.03517 \*

\* Se 4 -0.01745 0.02212 0.08151 \*

\* Se 5 -0.02594 0.02794 -0.06515 \*

\* Se 6 0.07037 0.02188 0.03150 \*

\* Se 7 0.08004 0.02861 -0.03932 \*

\* Se 8 -0.04577 0.02948 0.06064 \*

\* Se 9 -0.03189 -0.10662 0.02575 \*

\* Se 10 0.01168 0.09520 -0.00131 \*

\* Se 11 0.03312 0.10781 -0.02731 \*

\* Se 12 -0.01053 -0.09453 0.00200 \*

\* Se 13 -0.08032 -0.02761 0.03892 \*

\* Se 14 0.04494 -0.03013 -0.06119 \*

\* Se 15 0.02457 -0.02862 0.06568 \*

\* Se 16 -0.06994 -0.02101 -0.02963 \*

\* Se 17 -0.06340 -0.08861 0.03481 \*

\* Se 18 0.01823 -0.02121 -0.08066 \*

\* Se 19 0.02169 -0.00797 0.06192 \*

\* Se 20 -0.05829 -0.08252 -0.02476 \*

\* Nb 1 0.10465 0.01526 0.00470 \*

\* Nb 2 -0.10785 -0.01335 -0.00449 \*

\* Nb 3 -0.00015 -0.00175 0.00082 \*

\* Nb 4 -0.00095 -0.00194 -0.00152 \*

\* Nb 5 -0.01228 -0.02787 -0.00607 \*

\* Nb 6 -0.03947 0.06866 -0.00442 \*

\* Nb 7 -0.02103 0.01829 -0.02529 \*

\* Nb 8 -0.00395 0.02146 0.02152 \*

\* Nb 9 -0.02139 -0.09153 0.00292 \*

\* Nb 10 -0.01232 0.04165 -0.01949 \*

\* Nb 11 0.00090 0.01858 -0.04569 \*

\* Nb 12 -0.01205 0.01975 0.05673 \*

\* Nb 13 0.00971 -0.04171 0.01933 \*

\* Nb 14 0.02284 0.09228 -0.00282 \*

\* Nb 15 -0.00159 -0.01956 0.04661 \*

\* Nb 16 0.01282 -0.02015 -0.05648 \*

\* Nb 17 0.04138 -0.07008 0.00450 \*

\* Nb 18 0.01431 0.02671 0.00597 \*

\* Nb 19 0.02180 -0.01602 0.02374 \*

\* Nb 20 0.00382 -0.01956 -0.02019 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.011060 -0.078831 -0.032289 \*

\* y -0.078831 0.096103 -0.116053 \*

\* z -0.032289 -0.116053 -0.114708 \*

\* \*

\* Pressure: 0.0025 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000081 | -36259.834438 | <-- min BFGS

| trial step | 1.000000 | 0.000046 | -36259.836168 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 21 with line minimization (lambda= 2.334888)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9276616 -8.3712757 0.0000888 0.4192383 -0.0029789 0.0000833

0.0240894 3.3902073 -0.0014726 1.0352052 1.8459783 0.0008711

-0.0027929 -0.0049807 13.8735734 0.0001072 0.0001960 0.4528888

Lattice parameters(A) Cell Angles

a = 17.114711 alpha = 90.045538

b = 3.390293 beta = 89.999702

c = 13.873575 gamma = 118.876135

Current cell volume = 704.909542 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067106 0.664506 0.127104 x

x Se 2 0.132116 0.336435 0.627198 x

x Se 3 0.132171 0.337138 0.872576 x

x Se 4 0.067206 0.664891 0.373226 x

x Se 5 0.266917 0.664932 0.126655 x

x Se 6 0.331671 0.334741 0.626974 x

x Se 7 0.331813 0.335598 0.872691 x

x Se 8 0.266923 0.664856 0.373312 x

x Se 9 0.467646 0.661460 0.127577 x

x Se 10 0.532368 0.337027 0.626908 x

x Se 11 0.532351 0.338538 0.872429 x

x Se 12 0.467626 0.662969 0.373090 x

x Se 13 0.668197 0.664434 0.127288 x

x Se 14 0.733075 0.335123 0.626690 x

x Se 15 0.733080 0.335045 0.873345 x

x Se 16 0.668336 0.665285 0.373040 x

x Se 17 0.867823 0.662824 0.127444 x

x Se 18 0.932799 0.335129 0.626779 x

x Se 19 0.932898 0.335518 0.872888 x

x Se 20 0.867880 0.663537 0.372785 x

x Nb 1 -0.000233 -0.001050 0.250044 x

x Nb 2 0.000216 0.001143 0.749955 x

x Nb 3 -0.000004 -0.000066 0.000015 x

x Nb 4 -0.000005 -0.000064 0.499984 x

x Nb 5 0.198402 -0.002965 0.250100 x

x Nb 6 0.200999 0.006089 0.749797 x

x Nb 7 0.199857 0.000143 0.000295 x

x Nb 8 0.200014 0.000733 0.499821 x

x Nb 9 0.399910 -0.002635 0.250223 x

x Nb 10 0.400131 0.001739 0.749962 x

x Nb 11 0.399716 0.001317 -0.000104 x

x Nb 12 0.399473 0.000508 0.499971 x

x Nb 13 0.599850 -0.001794 0.250038 x

x Nb 14 0.600102 0.002749 0.749773 x

x Nb 15 0.600279 -0.001358 0.000117 x

x Nb 16 0.600530 -0.000515 0.500023 x

x Nb 17 0.799016 -0.006141 0.250207 x

x Nb 18 0.801607 0.002871 0.749902 x

x Nb 19 0.800152 -0.000034 -0.000323 x

x Nb 20 0.799988 -0.000658 0.500200 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597715E+004 16224.61 <-- SCF

1 -3.62600725E+004 7.52500630E-003 16251.75 <-- SCF

2 -3.62600918E+004 4.83500576E-004 16278.88 <-- SCF

3 -3.62600422E+004 -1.24121930E-003 16305.45 <-- SCF

4 -3.62598296E+004 -5.31308338E-003 16331.03 <-- SCF

5 -3.62598407E+004 2.75876425E-004 16357.31 <-- SCF

6 -3.62598377E+004 -7.32946574E-005 16382.83 <-- SCF

7 -3.62598365E+004 -3.18195466E-005 16406.16 <-- SCF

8 -3.62598364E+004 -1.41720970E-006 16426.12 <-- SCF

9 -3.62598365E+004 2.62320810E-006 16443.91 <-- SCF

10 -3.62598366E+004 1.84975292E-006 16461.34 <-- SCF

11 -3.62598366E+004 1.41745517E-006 16478.17 <-- SCF

12 -3.62598367E+004 9.47821978E-007 16494.92 <-- SCF

13 -3.62598367E+004 7.61915675E-007 16511.62 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.83671192 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.04165 -0.00117 -0.08425 \*

\* Se 2 0.09337 0.09838 0.00951 \*

\* Se 3 0.09678 0.08720 0.00860 \*

\* Se 4 -0.04247 0.01745 0.09850 \*

\* Se 5 -0.03973 0.04259 -0.07504 \*

\* Se 6 0.12543 0.00432 0.01368 \*

\* Se 7 0.13176 0.01865 0.01128 \*

\* Se 8 -0.06390 0.04615 0.07427 \*

\* Se 9 -0.03349 -0.09175 -0.03232 \*

\* Se 10 0.00650 0.10936 0.00693 \*

\* Se 11 0.03479 0.09305 0.03032 \*

\* Se 12 -0.00534 -0.10862 -0.00623 \*

\* Se 13 -0.13236 -0.01705 -0.00920 \*

\* Se 14 0.06362 -0.04698 -0.07482 \*

\* Se 15 0.03885 -0.04343 0.07555 \*

\* Se 16 -0.12486 -0.00375 -0.01282 \*

\* Se 17 -0.09738 -0.08791 -0.01167 \*

\* Se 18 0.04284 -0.01644 -0.09780 \*

\* Se 19 0.04271 0.00250 0.08376 \*

\* Se 20 -0.09440 -0.10059 -0.00837 \*

\* Nb 1 0.12784 0.01286 0.00795 \*

\* Nb 2 -0.13010 -0.01196 -0.00774 \*

\* Nb 3 -0.00026 -0.00144 0.00052 \*

\* Nb 4 -0.00075 -0.00164 -0.00112 \*

\* Nb 5 0.01374 -0.03821 -0.00708 \*

\* Nb 6 -0.06169 0.07067 -0.00340 \*

\* Nb 7 -0.01644 0.01764 -0.03364 \*

\* Nb 8 -0.00346 0.01786 0.02513 \*

\* Nb 9 -0.02399 -0.09904 0.00352 \*

\* Nb 10 -0.01289 0.04700 -0.02461 \*

\* Nb 11 0.00449 0.01402 -0.04986 \*

\* Nb 12 -0.00917 0.01479 0.06149 \*

\* Nb 13 0.01103 -0.04688 0.02441 \*

\* Nb 14 0.02465 0.09916 -0.00329 \*

\* Nb 15 -0.00535 -0.01496 0.05044 \*

\* Nb 16 0.00935 -0.01532 -0.06118 \*

\* Nb 17 0.06296 -0.07169 0.00327 \*

\* Nb 18 -0.01208 0.03733 0.00689 \*

\* Nb 19 0.01736 -0.01584 0.03262 \*

\* Nb 20 0.00366 -0.01628 -0.02420 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.049497 -0.089375 -0.044278 \*

\* y -0.089375 0.182814 -0.110147 \*

\* z -0.044278 -0.110147 -0.042676 \*

\* \*

\* Pressure: -0.0632 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000081 | -36259.834438 | <-- min BFGS

| trial step | 1.000000 | 0.000046 | -36259.836168 | <-- min BFGS

| line step | 2.334888 | -0.000022 | -36259.836771 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 21 with enthalpy= -3.62598368E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 5.831351E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.382017E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.550702E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.828141E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 22 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000123 | -36259.836771 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 22 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9281234 -8.3722093 -0.0005099 0.4192692 -0.0029005 0.0000950

0.0234489 3.3894956 -0.0014352 1.0356142 1.8465587 0.0008829

-0.0031782 -0.0048529 13.8777124 0.0001225 0.0001909 0.4527538

Lattice parameters(A) Cell Angles

a = 17.115571 alpha = 90.044385

b = 3.389577 beta = 90.003351

c = 13.877714 gamma = 118.888845

Current cell volume = 704.920018 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067106 0.664623 0.126905 x

x Se 2 0.132120 0.336493 0.627043 x

x Se 3 0.132178 0.337249 0.872706 x

x Se 4 0.067209 0.665041 0.373439 x

x Se 5 0.266921 0.664950 0.126421 x

x Se 6 0.331675 0.334754 0.626848 x

x Se 7 0.331831 0.335682 0.872789 x

x Se 8 0.266919 0.664839 0.373533 x

x Se 9 0.467611 0.661167 0.127449 x

x Se 10 0.532411 0.337254 0.626727 x

x Se 11 0.532386 0.338832 0.872558 x

x Se 12 0.467583 0.662742 0.373271 x

x Se 13 0.668180 0.664354 0.127187 x

x Se 14 0.733079 0.335136 0.626469 x

x Se 15 0.733075 0.335025 0.873579 x

x Se 16 0.668333 0.665276 0.373168 x

x Se 17 0.867815 0.662708 0.127315 x

x Se 18 0.932796 0.334981 0.626567 x

x Se 19 0.932899 0.335404 0.873086 x

x Se 20 0.867875 0.663476 0.372938 x

x Nb 1 -0.000143 -0.000674 0.250037 x

x Nb 2 0.000125 0.000774 0.749962 x

x Nb 3 -0.000005 -0.000072 0.000016 x

x Nb 4 -0.000006 -0.000072 0.499982 x

x Nb 5 0.198371 -0.003061 0.250092 x

x Nb 6 0.201001 0.006238 0.749790 x

x Nb 7 0.199838 0.000129 0.000292 x

x Nb 8 0.200014 0.000785 0.499835 x

x Nb 9 0.399907 -0.002773 0.250221 x

x Nb 10 0.400111 0.001704 0.749964 x

x Nb 11 0.399720 0.001388 -0.000154 x

x Nb 12 0.399456 0.000518 0.500018 x

x Nb 13 0.599868 -0.001765 0.250035 x

x Nb 14 0.600106 0.002898 0.749775 x

x Nb 15 0.600274 -0.001432 0.000169 x

x Nb 16 0.600548 -0.000523 0.499975 x

x Nb 17 0.799014 -0.006296 0.250214 x

x Nb 18 0.801640 0.002960 0.749911 x

x Nb 19 0.800173 -0.000010 -0.000322 x

x Nb 20 0.799988 -0.000703 0.500189 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598033E+004 16614.80 <-- SCF

1 -3.62599913E+004 4.70117716E-003 16642.14 <-- SCF

2 -3.62600018E+004 2.60314961E-004 16669.56 <-- SCF

3 -3.62599697E+004 -8.02480920E-004 16695.61 <-- SCF

4 -3.62598369E+004 -3.31875881E-003 16721.64 <-- SCF

5 -3.62598400E+004 7.72570157E-005 16747.47 <-- SCF

6 -3.62598392E+004 -1.90455145E-005 16770.02 <-- SCF

7 -3.62598392E+004 -1.89316368E-006 16790.94 <-- SCF

8 -3.62598392E+004 1.42118138E-006 16808.69 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.83921059 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02153 0.01643 -0.07384 \*

\* Se 2 0.07982 0.07076 0.04323 \*

\* Se 3 0.08571 0.06488 -0.03831 \*

\* Se 4 -0.02937 0.01994 0.07618 \*

\* Se 5 -0.03373 0.04244 -0.01861 \*

\* Se 6 0.10795 0.00100 0.02376 \*

\* Se 7 0.12025 0.01290 -0.01315 \*

\* Se 8 -0.05635 0.04774 0.01507 \*

\* Se 9 -0.02701 -0.07916 0.00568 \*

\* Se 10 0.01136 0.08977 0.00191 \*

\* Se 11 0.02812 0.08051 -0.00786 \*

\* Se 12 -0.01010 -0.08880 -0.00093 \*

\* Se 13 -0.12057 -0.01154 0.01484 \*

\* Se 14 0.05636 -0.04851 -0.01521 \*

\* Se 15 0.03315 -0.04316 0.01890 \*

\* Se 16 -0.10677 -0.00047 -0.02181 \*

\* Se 17 -0.08638 -0.06591 0.03555 \*

\* Se 18 0.02922 -0.01917 -0.07621 \*

\* Se 19 0.02226 -0.01519 0.07349 \*

\* Se 20 -0.08125 -0.07341 -0.04323 \*

\* Nb 1 0.11896 0.00356 0.00944 \*

\* Nb 2 -0.12037 -0.00326 -0.00925 \*

\* Nb 3 -0.00030 -0.00115 0.00028 \*

\* Nb 4 -0.00078 -0.00131 -0.00081 \*

\* Nb 5 0.01432 -0.04072 -0.00491 \*

\* Nb 6 -0.06209 0.07268 -0.00517 \*

\* Nb 7 -0.01568 0.01705 -0.03955 \*

\* Nb 8 -0.00352 0.01697 0.02860 \*

\* Nb 9 -0.03107 -0.10333 0.00723 \*

\* Nb 10 -0.00317 0.05337 -0.02840 \*

\* Nb 11 0.00300 0.01426 -0.04878 \*

\* Nb 12 -0.01109 0.01287 0.05945 \*

\* Nb 13 0.00184 -0.05304 0.02830 \*

\* Nb 14 0.03134 0.10308 -0.00695 \*

\* Nb 15 -0.00390 -0.01492 0.04912 \*

\* Nb 16 0.01115 -0.01312 -0.05890 \*

\* Nb 17 0.06286 -0.07329 0.00502 \*

\* Nb 18 -0.01308 0.04037 0.00476 \*

\* Nb 19 0.01664 -0.01550 0.03908 \*

\* Nb 20 0.00381 -0.01563 -0.02802 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.088980 -0.116861 -0.052127 \*

\* y -0.116861 0.167282 -0.106140 \*

\* z -0.052127 -0.106140 0.039535 \*

\* \*

\* Pressure: -0.0986 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000123 | -36259.836771 | <-- min BFGS

| trial step | 1.000000 | 0.000061 | -36259.839274 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 22 with line minimization (lambda= 1.980133)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9285759 -8.3731244 -0.0010967 0.4192994 -0.0028236 0.0001064

0.0228211 3.3887980 -0.0013985 1.0360153 1.8471279 0.0008944

-0.0035558 -0.0047276 13.8817691 0.0001375 0.0001859 0.4526215

Lattice parameters(A) Cell Angles

a = 17.116413 alpha = 90.043255

b = 3.388875 beta = 90.006926

c = 13.881770 gamma = 118.901306

Current cell volume = 704.930143 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067106 0.664738 0.126710 x

x Se 2 0.132125 0.336549 0.626891 x

x Se 3 0.132186 0.337358 0.872834 x

x Se 4 0.067213 0.665188 0.373647 x

x Se 5 0.266925 0.664966 0.126192 x

x Se 6 0.331678 0.334767 0.626725 x

x Se 7 0.331848 0.335765 0.872886 x

x Se 8 0.266914 0.664823 0.373751 x

x Se 9 0.467576 0.660880 0.127324 x

x Se 10 0.532454 0.337477 0.626549 x

x Se 11 0.532421 0.339120 0.872683 x

x Se 12 0.467540 0.662520 0.373449 x

x Se 13 0.668163 0.664276 0.127088 x

x Se 14 0.733083 0.335149 0.626252 x

x Se 15 0.733071 0.335005 0.873808 x

x Se 16 0.668330 0.665266 0.373292 x

x Se 17 0.867807 0.662595 0.127188 x

x Se 18 0.932793 0.334836 0.626360 x

x Se 19 0.932899 0.335292 0.873281 x

x Se 20 0.867870 0.663416 0.373089 x

x Nb 1 -0.000056 -0.000306 0.250030 x

x Nb 2 0.000035 0.000412 0.749970 x

x Nb 3 -0.000005 -0.000079 0.000017 x

x Nb 4 -0.000007 -0.000079 0.499981 x

x Nb 5 0.198340 -0.003156 0.250083 x

x Nb 6 0.201004 0.006383 0.749784 x

x Nb 7 0.199819 0.000115 0.000288 x

x Nb 8 0.200014 0.000837 0.499848 x

x Nb 9 0.399905 -0.002908 0.250219 x

x Nb 10 0.400091 0.001670 0.749967 x

x Nb 11 0.399724 0.001457 -0.000203 x

x Nb 12 0.399439 0.000527 0.500065 x

x Nb 13 0.599886 -0.001736 0.250032 x

x Nb 14 0.600110 0.003045 0.749776 x

x Nb 15 0.600270 -0.001504 0.000219 x

x Nb 16 0.600566 -0.000531 0.499929 x

x Nb 17 0.799012 -0.006447 0.250221 x

x Nb 18 0.801671 0.003048 0.749919 x

x Nb 19 0.800193 0.000013 -0.000321 x

x Nb 20 0.799988 -0.000748 0.500178 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598042E+004 16911.95 <-- SCF

1 -3.62600136E+004 5.23462867E-003 16939.23 <-- SCF

2 -3.62600258E+004 3.04167830E-004 16966.08 <-- SCF

3 -3.62599934E+004 -8.10481074E-004 16991.89 <-- SCF

4 -3.62598372E+004 -3.90460990E-003 17017.58 <-- SCF

5 -3.62598412E+004 9.97789545E-005 17043.33 <-- SCF

6 -3.62598402E+004 -2.45337858E-005 17067.33 <-- SCF

7 -3.62598400E+004 -3.73657152E-006 17088.22 <-- SCF

8 -3.62598401E+004 2.04015713E-006 17106.67 <-- SCF

9 -3.62598402E+004 1.29086309E-006 17124.09 <-- SCF

10 -3.62598402E+004 7.03429449E-007 17140.98 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.84019365 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00535 0.02710 -0.06033 \*

\* Se 2 0.06358 0.04313 0.06514 \*

\* Se 3 0.07410 0.04214 -0.07721 \*

\* Se 4 -0.02029 0.01245 0.03867 \*

\* Se 5 -0.03078 0.03770 0.00877 \*

\* Se 6 0.09047 -0.00268 0.02774 \*

\* Se 7 0.11206 0.00847 -0.03184 \*

\* Se 8 -0.05310 0.04499 -0.02148 \*

\* Se 9 -0.02010 -0.06458 0.04593 \*

\* Se 10 0.02147 0.06758 -0.00137 \*

\* Se 11 0.02099 0.06600 -0.04802 \*

\* Se 12 -0.02020 -0.06636 0.00246 \*

\* Se 13 -0.11191 -0.00736 0.03266 \*

\* Se 14 0.05347 -0.04585 0.02184 \*

\* Se 15 0.03055 -0.03846 -0.00861 \*

\* Se 16 -0.08862 0.00333 -0.02468 \*

\* Se 17 -0.07508 -0.04350 0.07549 \*

\* Se 18 0.01977 -0.01189 -0.03938 \*

\* Se 19 0.00561 -0.02619 0.06050 \*

\* Se 20 -0.06561 -0.04606 -0.06667 \*

\* Nb 1 0.11611 -0.00228 0.01008 \*

\* Nb 2 -0.11683 0.00238 -0.00991 \*

\* Nb 3 -0.00036 -0.00084 0.00006 \*

\* Nb 4 -0.00072 -0.00099 -0.00054 \*

\* Nb 5 0.01072 -0.04268 -0.00377 \*

\* Nb 6 -0.05299 0.07513 -0.00656 \*

\* Nb 7 -0.01209 0.01556 -0.04144 \*

\* Nb 8 -0.00152 0.01512 0.02811 \*

\* Nb 9 -0.03262 -0.10620 0.00933 \*

\* Nb 10 0.00818 0.05585 -0.02949 \*

\* Nb 11 0.00551 0.01342 -0.04519 \*

\* Nb 12 -0.01131 0.01128 0.05657 \*

\* Nb 13 -0.00925 -0.05530 0.02937 \*

\* Nb 14 0.03247 0.10578 -0.00904 \*

\* Nb 15 -0.00647 -0.01391 0.04532 \*

\* Nb 16 0.01117 -0.01144 -0.05592 \*

\* Nb 17 0.05349 -0.07541 0.00631 \*

\* Nb 18 -0.00970 0.04254 0.00362 \*

\* Nb 19 0.01322 -0.01411 0.04130 \*

\* Nb 20 0.00199 -0.01385 -0.02784 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.112377 -0.154394 -0.058860 \*

\* y -0.154394 0.148257 -0.101642 \*

\* z -0.058860 -0.101642 0.108188 \*

\* \*

\* Pressure: -0.1229 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000123 | -36259.836771 | <-- min BFGS

| trial step | 1.000000 | 0.000061 | -36259.839274 | <-- min BFGS

| line step | 1.980133 | 0.000010 | -36259.840262 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 22 with enthalpy= -3.62598403E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 8.728543E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.172779E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.423715E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.543939E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 23 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000157 | -36259.840262 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 23 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9299210 -8.3741509 -0.0008504 0.4193740 -0.0026229 0.0001400

0.0211803 3.3864500 -0.0020762 1.0370455 1.8489046 0.0012701

-0.0046803 -0.0069145 13.8866771 0.0001807 0.0002763 0.4524616

Lattice parameters(A) Cell Angles

a = 17.118088 alpha = 90.063776

b = 3.386517 beta = 90.005732

c = 13.886680 gamma = 118.929589

Current cell volume = 704.565232 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067099 0.664673 0.126687 x

x Se 2 0.132179 0.337117 0.626968 x

x Se 3 0.132253 0.338052 0.872695 x

x Se 4 0.067197 0.665141 0.373698 x

x Se 5 0.266924 0.665051 0.126177 x

x Se 6 0.331689 0.335109 0.626820 x

x Se 7 0.331900 0.336288 0.872720 x

x Se 8 0.266869 0.664764 0.373724 x

x Se 9 0.467558 0.659986 0.127513 x

x Se 10 0.532476 0.338157 0.626565 x

x Se 11 0.532438 0.340018 0.872495 x

x Se 12 0.467517 0.661842 0.373433 x

x Se 13 0.668114 0.663765 0.127247 x

x Se 14 0.733127 0.335199 0.626278 x

x Se 15 0.733070 0.334911 0.873824 x

x Se 16 0.668322 0.664935 0.373202 x

x Se 17 0.867739 0.661886 0.127332 x

x Se 18 0.932809 0.334889 0.626310 x

x Se 19 0.932907 0.335366 0.873302 x

x Se 20 0.867815 0.662837 0.373006 x

x Nb 1 0.000218 0.000864 0.250020 x

x Nb 2 -0.000244 -0.000736 0.749979 x

x Nb 3 -0.000007 -0.000098 0.000021 x

x Nb 4 -0.000010 -0.000102 0.499976 x

x Nb 5 0.198240 -0.003527 0.250069 x

x Nb 6 0.201019 0.006909 0.749752 x

x Nb 7 0.199763 0.000058 0.000272 x

x Nb 8 0.200015 0.000972 0.499891 x

x Nb 9 0.399880 -0.003443 0.250222 x

x Nb 10 0.400070 0.001609 0.749959 x

x Nb 11 0.399732 0.001693 -0.000365 x

x Nb 12 0.399387 0.000586 0.500225 x

x Nb 13 0.599902 -0.001693 0.250040 x

x Nb 14 0.600140 0.003613 0.749772 x

x Nb 15 0.600260 -0.001751 0.000386 x

x Nb 16 0.600619 -0.000585 0.499768 x

x Nb 17 0.798999 -0.006990 0.250254 x

x Nb 18 0.801775 0.003400 0.749934 x

x Nb 19 0.800252 0.000101 -0.000313 x

x Nb 20 0.799988 -0.000865 0.500140 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597482E+004 17243.88 <-- SCF

1 -3.62600216E+004 6.83652522E-003 17271.28 <-- SCF

2 -3.62600370E+004 3.83858214E-004 17299.59 <-- SCF

3 -3.62599854E+004 -1.29062485E-003 17326.53 <-- SCF

4 -3.62598402E+004 -3.62896283E-003 17352.47 <-- SCF

5 -3.62598484E+004 2.04467219E-004 17379.14 <-- SCF

6 -3.62598450E+004 -8.43526573E-005 17404.66 <-- SCF

7 -3.62598438E+004 -3.01427784E-005 17426.75 <-- SCF

8 -3.62598438E+004 -9.18766646E-007 17446.91 <-- SCF

9 -3.62598438E+004 3.67813696E-007 17465.38 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.84378208 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00106 0.04581 -0.06437 \*

\* Se 2 0.03801 0.03503 0.08745 \*

\* Se 3 0.03877 0.01823 -0.06826 \*

\* Se 4 -0.00957 0.02410 0.03955 \*

\* Se 5 -0.03083 0.03816 0.00096 \*

\* Se 6 0.10614 -0.01223 0.03412 \*

\* Se 7 0.11010 0.00689 -0.01056 \*

\* Se 8 -0.04511 0.04883 -0.01263 \*

\* Se 9 -0.01128 -0.01871 0.00875 \*

\* Se 10 0.02222 0.04944 0.01175 \*

\* Se 11 0.01226 0.02010 -0.01133 \*

\* Se 12 -0.02078 -0.04806 -0.01060 \*

\* Se 13 -0.11163 -0.00524 0.01416 \*

\* Se 14 0.04654 -0.04971 0.01310 \*

\* Se 15 0.03133 -0.03900 -0.00093 \*

\* Se 16 -0.10398 0.01262 -0.03130 \*

\* Se 17 -0.03915 -0.01875 0.06320 \*

\* Se 18 0.00836 -0.02369 -0.04069 \*

\* Se 19 0.00090 -0.04511 0.06467 \*

\* Se 20 -0.04000 -0.03765 -0.08750 \*

\* Nb 1 0.11008 -0.02061 0.01302 \*

\* Nb 2 -0.11006 0.02022 -0.01289 \*

\* Nb 3 -0.00053 -0.00058 -0.00018 \*

\* Nb 4 -0.00080 -0.00086 -0.00026 \*

\* Nb 5 -0.00590 -0.04481 -0.00174 \*

\* Nb 6 -0.02803 0.08942 -0.01083 \*

\* Nb 7 -0.01010 0.02066 -0.03948 \*

\* Nb 8 0.00113 0.01971 0.02103 \*

\* Nb 9 -0.03279 -0.11918 0.02147 \*

\* Nb 10 0.01110 0.07632 -0.03707 \*

\* Nb 11 0.00649 0.00930 -0.03609 \*

\* Nb 12 -0.01609 0.00601 0.04528 \*

\* Nb 13 -0.01105 -0.07546 0.03718 \*

\* Nb 14 0.03173 0.11829 -0.02098 \*

\* Nb 15 -0.00752 -0.00982 0.03580 \*

\* Nb 16 0.01576 -0.00633 -0.04454 \*

\* Nb 17 0.02760 -0.08967 0.01033 \*

\* Nb 18 0.00661 0.04451 0.00148 \*

\* Nb 19 0.01143 -0.01961 0.03980 \*

\* Nb 20 -0.00034 -0.01857 -0.02089 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.095445 -0.258429 -0.071606 \*

\* y -0.258429 0.009262 -0.141290 \*

\* z -0.071606 -0.141290 0.071515 \*

\* \*

\* Pressure: -0.0587 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000157 | -36259.840262 | <-- min BFGS

| trial step | 1.000000 | 0.000090 | -36259.843827 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 23 with line minimization (lambda= 2.350446)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9317376 -8.3755371 -0.0005178 0.4194752 -0.0023511 0.0001855

0.0189644 3.3832792 -0.0029915 1.0384400 1.8513096 0.0017782

-0.0061989 -0.0098679 13.8933050 0.0002392 0.0003985 0.4522459

Lattice parameters(A) Cell Angles

a = 17.120351 alpha = 90.091498

b = 3.383334 beta = 90.004120

c = 13.893310 gamma = 118.967844

Current cell volume = 704.071449 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067090 0.664585 0.126657 x

x Se 2 0.132251 0.337884 0.627072 x

x Se 3 0.132344 0.338990 0.872507 x

x Se 4 0.067177 0.665078 0.373767 x

x Se 5 0.266923 0.665166 0.126156 x

x Se 6 0.331703 0.335571 0.626950 x

x Se 7 0.331970 0.336995 0.872495 x

x Se 8 0.266808 0.664683 0.373689 x

x Se 9 0.467534 0.658779 0.127768 x

x Se 10 0.532506 0.339074 0.626587 x

x Se 11 0.532462 0.341230 0.872241 x

x Se 12 0.467486 0.660927 0.373411 x

x Se 13 0.668048 0.663075 0.127463 x

x Se 14 0.733186 0.335266 0.626314 x

x Se 15 0.733070 0.334783 0.873845 x

x Se 16 0.668311 0.664489 0.373079 x

x Se 17 0.867646 0.660930 0.127527 x

x Se 18 0.932832 0.334959 0.626243 x

x Se 19 0.932918 0.335465 0.873330 x

x Se 20 0.867740 0.662054 0.372896 x

x Nb 1 0.000588 0.002444 0.250007 x

x Nb 2 -0.000621 -0.002287 0.749992 x

x Nb 3 -0.000009 -0.000125 0.000026 x

x Nb 4 -0.000013 -0.000133 0.499969 x

x Nb 5 0.198104 -0.004028 0.250049 x

x Nb 6 0.201041 0.007620 0.749710 x

x Nb 7 0.199686 -0.000020 0.000250 x

x Nb 8 0.200015 0.001156 0.499949 x

x Nb 9 0.399845 -0.004165 0.250225 x

x Nb 10 0.400043 0.001528 0.749948 x

x Nb 11 0.399743 0.002012 -0.000584 x

x Nb 12 0.399317 0.000666 0.500441 x

x Nb 13 0.599922 -0.001635 0.250050 x

x Nb 14 0.600180 0.004379 0.749767 x

x Nb 15 0.600246 -0.002084 0.000610 x

x Nb 16 0.600692 -0.000659 0.499551 x

x Nb 17 0.798981 -0.007723 0.250298 x

x Nb 18 0.801914 0.003875 0.749954 x

x Nb 19 0.800333 0.000220 -0.000301 x

x Nb 20 0.799988 -0.001024 0.500090 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62596728E+004 17568.47 <-- SCF

1 -3.62600903E+004 1.04377853E-002 17595.64 <-- SCF

2 -3.62601116E+004 5.31596296E-004 17624.70 <-- SCF

3 -3.62599839E+004 -3.19384566E-003 17651.48 <-- SCF

4 -3.62598483E+004 -3.38792421E-003 17677.88 <-- SCF

5 -3.62598496E+004 3.04422195E-005 17704.77 <-- SCF

6 -3.62598459E+004 -9.14598559E-005 17730.30 <-- SCF

7 -3.62598453E+004 -1.43933059E-005 17752.70 <-- SCF

8 -3.62598454E+004 2.18138322E-006 17773.23 <-- SCF

9 -3.62598454E+004 9.12700297E-007 17791.11 <-- SCF

10 -3.62598455E+004 1.19493964E-006 17808.59 <-- SCF

11 -3.62598455E+004 9.28727497E-007 17825.83 <-- SCF

12 -3.62598456E+004 8.02392182E-007 17842.75 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.84556393 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01046 0.07131 -0.07727 \*

\* Se 2 0.00136 0.01299 0.10504 \*

\* Se 3 -0.00685 -0.01361 -0.03348 \*

\* Se 4 0.01011 0.04002 0.03963 \*

\* Se 5 -0.02062 0.04205 -0.01768 \*

\* Se 6 0.13090 -0.02147 0.03811 \*

\* Se 7 0.10237 0.01189 0.03760 \*

\* Se 8 -0.02553 0.05511 -0.00417 \*

\* Se 9 0.01419 0.03577 -0.03872 \*

\* Se 10 0.01719 0.01180 0.03523 \*

\* Se 11 -0.01339 -0.03415 0.03577 \*

\* Se 12 -0.01596 -0.01020 -0.03390 \*

\* Se 13 -0.10634 -0.00942 -0.03060 \*

\* Se 14 0.02821 -0.05597 0.00456 \*

\* Se 15 0.02184 -0.04311 0.01759 \*

\* Se 16 -0.12905 0.02168 -0.03665 \*

\* Se 17 0.00606 0.01279 0.02559 \*

\* Se 18 -0.01148 -0.03976 -0.04150 \*

\* Se 19 -0.01060 -0.07082 0.07776 \*

\* Se 20 -0.00226 -0.01463 -0.10155 \*

\* Nb 1 0.09570 -0.05464 0.01001 \*

\* Nb 2 -0.09450 0.05308 -0.01009 \*

\* Nb 3 -0.00076 -0.00015 -0.00068 \*

\* Nb 4 -0.00059 -0.00043 0.00008 \*

\* Nb 5 -0.02158 -0.04745 -0.00370 \*

\* Nb 6 0.01008 0.10401 -0.01169 \*

\* Nb 7 -0.00240 0.02426 -0.03706 \*

\* Nb 8 0.01124 0.02199 0.01519 \*

\* Nb 9 -0.02786 -0.13451 0.02903 \*

\* Nb 10 0.02057 0.10469 -0.03937 \*

\* Nb 11 0.01611 0.00476 -0.02681 \*

\* Nb 12 -0.02083 -0.00286 0.02713 \*

\* Nb 13 -0.01989 -0.10367 0.03936 \*

\* Nb 14 0.02644 0.13301 -0.02863 \*

\* Nb 15 -0.01727 -0.00521 0.02613 \*

\* Nb 16 0.01998 0.00260 -0.02619 \*

\* Nb 17 -0.01126 -0.10398 0.01071 \*

\* Nb 18 0.02199 0.04742 0.00332 \*

\* Nb 19 0.00428 -0.02375 0.03782 \*

\* Nb 20 -0.01006 -0.02143 -0.01587 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.062521 -0.404260 -0.089616 \*

\* y -0.404260 -0.195938 -0.194892 \*

\* z -0.089616 -0.194892 0.003404 \*

\* \*

\* Pressure: 0.0433 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000157 | -36259.840262 | <-- min BFGS

| trial step | 1.000000 | 0.000090 | -36259.843827 | <-- min BFGS

| line step | 2.350446 | -0.000016 | -36259.845652 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 23 with enthalpy= -3.62598457E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.347492E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.404010E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.050426E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.042600E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 24 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000088 | -36259.845652 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 24 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9237548 -8.3703966 -0.0019363 0.4196179 -0.0024983 0.0001608

0.0201432 3.3832071 -0.0020000 1.0381775 1.8509880 0.0012860

-0.0053653 -0.0066470 13.8991250 0.0002078 0.0002660 0.4520564

Lattice parameters(A) Cell Angles

a = 17.110874 alpha = 90.061402

b = 3.383268 beta = 90.012370

c = 13.899128 gamma = 118.945944

Current cell volume = 704.112117 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067104 0.664693 0.126624 x

x Se 2 0.132223 0.337913 0.627094 x

x Se 3 0.132316 0.339052 0.872480 x

x Se 4 0.067196 0.665206 0.373805 x

x Se 5 0.266932 0.665149 0.126093 x

x Se 6 0.331684 0.335579 0.626982 x

x Se 7 0.331959 0.337062 0.872455 x

x Se 8 0.266815 0.664660 0.373740 x

x Se 9 0.467522 0.658555 0.127784 x

x Se 10 0.532527 0.339264 0.626579 x

x Se 11 0.532474 0.341455 0.872224 x

x Se 12 0.467464 0.660738 0.373420 x

x Se 13 0.668059 0.663010 0.127502 x

x Se 14 0.733179 0.335287 0.626263 x

x Se 15 0.733060 0.334798 0.873907 x

x Se 16 0.668330 0.664483 0.373048 x

x Se 17 0.867673 0.660865 0.127554 x

x Se 18 0.932812 0.334832 0.626205 x

x Se 19 0.932905 0.335359 0.873363 x

x Se 20 0.867769 0.662021 0.372873 x

x Nb 1 0.000628 0.002570 0.250004 x

x Nb 2 -0.000662 -0.002410 0.749995 x

x Nb 3 -0.000009 -0.000129 0.000027 x

x Nb 4 -0.000014 -0.000138 0.499968 x

x Nb 5 0.198059 -0.004139 0.250045 x

x Nb 6 0.201060 0.007830 0.749704 x

x Nb 7 0.199675 -0.000011 0.000249 x

x Nb 8 0.200017 0.001207 0.499953 x

x Nb 9 0.399840 -0.004329 0.250231 x

x Nb 10 0.400035 0.001594 0.749945 x

x Nb 11 0.399741 0.002069 -0.000609 x

x Nb 12 0.399298 0.000671 0.500462 x

x Nb 13 0.599929 -0.001705 0.250052 x

x Nb 14 0.600187 0.004550 0.749762 x

x Nb 15 0.600248 -0.002143 0.000636 x

x Nb 16 0.600712 -0.000664 0.499530 x

x Nb 17 0.798963 -0.007936 0.250305 x

x Nb 18 0.801961 0.003982 0.749958 x

x Nb 19 0.800345 0.000218 -0.000302 x

x Nb 20 0.799987 -0.001070 0.500086 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598362E+004 17945.95 <-- SCF

1 -3.62598653E+004 7.27470690E-004 17973.27 <-- SCF

2 -3.62598668E+004 3.81248553E-005 17999.30 <-- SCF

3 -3.62598663E+004 -1.23615443E-005 18026.11 <-- SCF

4 -3.62598472E+004 -4.77760473E-004 18051.92 <-- SCF

5 -3.62598482E+004 2.67350105E-005 18076.47 <-- SCF

6 -3.62598479E+004 -7.50224524E-006 18097.16 <-- SCF

7 -3.62598478E+004 -2.78984451E-006 18115.89 <-- SCF

8 -3.62598478E+004 1.84000197E-007 18133.55 <-- SCF

9 -3.62598479E+004 1.43578987E-006 18151.83 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.84789738 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00367 0.06357 -0.07447 \*

\* Se 2 0.00820 0.01307 0.10457 \*

\* Se 3 0.00059 -0.01542 -0.02919 \*

\* Se 4 -0.00069 0.03040 0.03354 \*

\* Se 5 -0.02765 0.03761 -0.01444 \*

\* Se 6 0.14123 -0.01892 0.03596 \*

\* Se 7 0.10866 0.01589 0.04511 \*

\* Se 8 -0.03525 0.05191 -0.01095 \*

\* Se 9 0.02156 0.03872 -0.03836 \*

\* Se 10 0.01220 0.00646 0.03311 \*

\* Se 11 -0.02089 -0.03703 0.03538 \*

\* Se 12 -0.01106 -0.00484 -0.03170 \*

\* Se 13 -0.11265 -0.01336 -0.03785 \*

\* Se 14 0.03807 -0.05285 0.01151 \*

\* Se 15 0.02893 -0.03876 0.01428 \*

\* Se 16 -0.13921 0.01923 -0.03481 \*

\* Se 17 -0.00127 0.01458 0.02124 \*

\* Se 18 -0.00090 -0.03016 -0.03564 \*

\* Se 19 -0.00407 -0.06335 0.07523 \*

\* Se 20 -0.00919 -0.01456 -0.10076 \*

\* Nb 1 0.10397 -0.04662 0.01126 \*

\* Nb 2 -0.10255 0.04506 -0.01133 \*

\* Nb 3 -0.00067 -0.00010 -0.00082 \*

\* Nb 4 -0.00063 -0.00049 0.00003 \*

\* Nb 5 -0.01775 -0.04464 -0.00228 \*

\* Nb 6 0.00503 0.09878 -0.01359 \*

\* Nb 7 -0.00513 0.02398 -0.03913 \*

\* Nb 8 0.01066 0.02237 0.01738 \*

\* Nb 9 -0.02910 -0.12874 0.03105 \*

\* Nb 10 0.01883 0.10013 -0.04080 \*

\* Nb 11 0.01629 0.00363 -0.02804 \*

\* Nb 12 -0.02401 -0.00491 0.02796 \*

\* Nb 13 -0.01774 -0.09909 0.04076 \*

\* Nb 14 0.02773 0.12728 -0.03076 \*

\* Nb 15 -0.01737 -0.00404 0.02728 \*

\* Nb 16 0.02337 0.00472 -0.02698 \*

\* Nb 17 -0.00655 -0.09876 0.01260 \*

\* Nb 18 0.01789 0.04456 0.00180 \*

\* Nb 19 0.00700 -0.02352 0.03998 \*

\* Nb 20 -0.00954 -0.02178 -0.01813 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.017828 -0.348122 -0.073157 \*

\* y -0.348122 -0.154537 -0.125393 \*

\* z -0.073157 -0.125393 0.066507 \*

\* \*

\* Pressure: 0.0234 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000088 | -36259.845652 | <-- min BFGS

| trial step | 1.000000 | 0.000065 | -36259.847941 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 24 with line minimization (lambda= 3.899183)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9006114 -8.3554936 -0.0060486 0.4200327 -0.0029253 0.0000896

0.0235605 3.3829981 0.0008746 1.0374171 1.8500582 -0.0001379

-0.0029485 0.0026909 13.9159985 0.0001174 -0.0001175 0.4515081

Lattice parameters(A) Cell Angles

a = 17.083399 alpha = 89.974193

b = 3.383080 beta = 90.036294

c = 13.915999 gamma = 118.882438

Current cell volume = 704.227381 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067143 0.665007 0.126530 x

x Se 2 0.132139 0.337998 0.627157 x

x Se 3 0.132237 0.339232 0.872400 x

x Se 4 0.067253 0.665578 0.373916 x

x Se 5 0.266959 0.665099 0.125913 x

x Se 6 0.331630 0.335603 0.627074 x

x Se 7 0.331927 0.337258 0.872339 x

x Se 8 0.266837 0.664593 0.373889 x

x Se 9 0.467485 0.657906 0.127832 x

x Se 10 0.532589 0.339817 0.626555 x

x Se 11 0.532511 0.342109 0.872175 x

x Se 12 0.467403 0.660189 0.373445 x

x Se 13 0.668091 0.662822 0.127617 x

x Se 14 0.733157 0.335350 0.626115 x

x Se 15 0.733032 0.334842 0.874088 x

x Se 16 0.668386 0.664466 0.372959 x

x Se 17 0.867751 0.660675 0.127635 x

x Se 18 0.932756 0.334465 0.626095 x

x Se 19 0.932867 0.335051 0.873456 x

x Se 20 0.867851 0.661926 0.372808 x

x Nb 1 0.000743 0.002937 0.249996 x

x Nb 2 -0.000781 -0.002765 0.750003 x

x Nb 3 -0.000010 -0.000142 0.000029 x

x Nb 4 -0.000015 -0.000153 0.499965 x

x Nb 5 0.197927 -0.004462 0.250034 x

x Nb 6 0.201115 0.008439 0.749686 x

x Nb 7 0.199642 0.000016 0.000247 x

x Nb 8 0.200020 0.001356 0.499966 x

x Nb 9 0.399825 -0.004804 0.250247 x

x Nb 10 0.400011 0.001788 0.749938 x

x Nb 11 0.399734 0.002233 -0.000681 x

x Nb 12 0.399242 0.000685 0.500523 x

x Nb 13 0.599949 -0.001908 0.250060 x

x Nb 14 0.600204 0.005043 0.749745 x

x Nb 15 0.600254 -0.002315 0.000710 x

x Nb 16 0.600768 -0.000678 0.499468 x

x Nb 17 0.798910 -0.008556 0.250322 x

x Nb 18 0.802094 0.004292 0.749969 x

x Nb 19 0.800380 0.000212 -0.000304 x

x Nb 20 0.799984 -0.001205 0.500077 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597530E+004 18255.05 <-- SCF

1 -3.62600512E+004 7.45506482E-003 18282.06 <-- SCF

2 -3.62600681E+004 4.21866851E-004 18311.50 <-- SCF

3 -3.62600847E+004 4.16957695E-004 18338.20 <-- SCF

4 -3.62598405E+004 -6.10603087E-003 18364.22 <-- SCF

5 -3.62598542E+004 3.43336492E-004 18390.78 <-- SCF

6 -3.62598513E+004 -7.38694904E-005 18416.72 <-- SCF

7 -3.62598498E+004 -3.59218002E-005 18438.97 <-- SCF

8 -3.62598499E+004 1.77129611E-006 18458.83 <-- SCF

9 -3.62598501E+004 3.55341819E-006 18477.08 <-- SCF

10 -3.62598502E+004 4.24402291E-006 18494.33 <-- SCF

11 -3.62598504E+004 3.40151864E-006 18511.67 <-- SCF

12 -3.62598505E+004 2.83212612E-006 18528.78 <-- SCF

13 -3.62598506E+004 2.75640373E-006 18545.92 <-- SCF

14 -3.62598506E+004 1.60607856E-006 18563.17 <-- SCF

15 -3.62598507E+004 1.53618910E-006 18579.83 <-- SCF

16 -3.62598508E+004 1.52417149E-006 18596.45 <-- SCF

17 -3.62598508E+004 1.27986542E-006 18612.48 <-- SCF

18 -3.62598509E+004 1.21046568E-006 18628.67 <-- SCF

19 -3.62598509E+004 1.30962362E-006 18645.39 <-- SCF

20 -3.62598510E+004 1.48125446E-006 18662.50 <-- SCF

21 -3.62598510E+004 7.32374032E-007 18678.56 <-- SCF

22 -3.62598510E+004 5.67687342E-007 18694.62 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.85103068 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00895 0.03866 -0.07008 \*

\* Se 2 0.03035 0.01450 0.09657 \*

\* Se 3 0.02509 -0.01806 -0.00978 \*

\* Se 4 -0.02121 0.00680 0.01803 \*

\* Se 5 -0.03456 0.02011 -0.02019 \*

\* Se 6 0.17605 -0.01096 0.03023 \*

\* Se 7 0.13575 0.03227 0.07255 \*

\* Se 8 -0.05401 0.04034 -0.02787 \*

\* Se 9 0.03862 0.03907 -0.04052 \*

\* Se 10 0.00065 -0.00691 0.03297 \*

\* Se 11 -0.03847 -0.03711 0.03734 \*

\* Se 12 0.00023 0.00872 -0.03123 \*

\* Se 13 -0.13990 -0.02983 -0.06484 \*

\* Se 14 0.05689 -0.04176 0.02827 \*

\* Se 15 0.03604 -0.02170 0.02053 \*

\* Se 16 -0.17358 0.01180 -0.03053 \*

\* Se 17 -0.02570 0.01718 0.00178 \*

\* Se 18 0.01972 -0.00609 -0.02025 \*

\* Se 19 0.00802 -0.03899 0.07171 \*

\* Se 20 -0.03181 -0.01578 -0.09164 \*

\* Nb 1 0.13762 -0.02338 0.01366 \*

\* Nb 2 -0.13660 0.02207 -0.01419 \*

\* Nb 3 -0.00071 -0.00066 -0.00085 \*

\* Nb 4 -0.00044 -0.00100 0.00000 \*

\* Nb 5 -0.00034 -0.03945 -0.00079 \*

\* Nb 6 -0.00109 0.07805 -0.01914 \*

\* Nb 7 -0.00708 0.02658 -0.04456 \*

\* Nb 8 0.01379 0.02266 0.02237 \*

\* Nb 9 -0.03699 -0.10946 0.03046 \*

\* Nb 10 0.01536 0.09062 -0.03897 \*

\* Nb 11 0.02106 -0.00602 -0.02506 \*

\* Nb 12 -0.03397 -0.01441 0.02405 \*

\* Nb 13 -0.01414 -0.08946 0.03905 \*

\* Nb 14 0.03587 0.10801 -0.03029 \*

\* Nb 15 -0.02192 0.00546 0.02390 \*

\* Nb 16 0.03363 0.01383 -0.02309 \*

\* Nb 17 -0.00013 -0.07814 0.01816 \*

\* Nb 18 0.00053 0.03929 0.00013 \*

\* Nb 19 0.00907 -0.02547 0.04507 \*

\* Nb 20 -0.01273 -0.02138 -0.02296 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.113768 -0.192536 -0.010318 \*

\* y -0.192536 -0.024461 0.057038 \*

\* z -0.010318 0.057038 0.244690 \*

\* \*

\* Pressure: -0.0355 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000088 | -36259.845652 | <-- min BFGS

| trial step | 1.000000 | 0.000065 | -36259.847941 | <-- min BFGS

| line step | 3.899183 | 3.683E-006 | -36259.851099 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 24 with enthalpy= -3.62598511E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.361856E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.789596E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.468588E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.446899E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 25 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000180 | -36259.851099 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 25 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9002624 -8.3530210 -0.0064594 0.4199489 -0.0030931 0.0000578

0.0249269 3.3843231 0.0015911 1.0364972 1.8489220 -0.0005304

-0.0018766 0.0050415 13.9075763 0.0000765 -0.0002130 0.4517816

Lattice parameters(A) Cell Angles

a = 17.081886 alpha = 89.952352

b = 3.384415 beta = 90.038566

c = 13.907577 gamma = 118.852804

Current cell volume = 704.217191 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067129 0.665012 0.126388 x

x Se 2 0.132213 0.338547 0.627168 x

x Se 3 0.132320 0.339848 0.872365 x

x Se 4 0.067228 0.665559 0.374064 x

x Se 5 0.266944 0.665220 0.125807 x

x Se 6 0.331705 0.336002 0.627077 x

x Se 7 0.332029 0.337827 0.872309 x

x Se 8 0.266778 0.664596 0.373947 x

x Se 9 0.467468 0.657208 0.127887 x

x Se 10 0.532616 0.340408 0.626492 x

x Se 11 0.532528 0.342814 0.872120 x

x Se 12 0.467376 0.659603 0.373508 x

x Se 13 0.667991 0.662263 0.127643 x

x Se 14 0.733215 0.335339 0.626058 x

x Se 15 0.733047 0.334712 0.874194 x

x Se 16 0.668314 0.664079 0.372961 x

x Se 17 0.867666 0.660046 0.127671 x

x Se 18 0.932782 0.334488 0.625948 x

x Se 19 0.932882 0.335054 0.873597 x

x Se 20 0.867776 0.661364 0.372795 x

x Nb 1 0.001017 0.004003 0.249992 x

x Nb 2 -0.001060 -0.003815 0.750007 x

x Nb 3 -0.000012 -0.000159 0.000032 x

x Nb 4 -0.000018 -0.000174 0.499961 x

x Nb 5 0.197857 -0.004818 0.250019 x

x Nb 6 0.201114 0.008941 0.749656 x

x Nb 7 0.199593 -0.000010 0.000212 x

x Nb 8 0.200023 0.001500 0.500014 x

x Nb 9 0.399793 -0.005436 0.250257 x

x Nb 10 0.399998 0.001851 0.749915 x

x Nb 11 0.399749 0.002441 -0.000833 x

x Nb 12 0.399197 0.000715 0.500677 x

x Nb 13 0.599958 -0.001984 0.250082 x

x Nb 14 0.600240 0.005700 0.749734 x

x Nb 15 0.600238 -0.002534 0.000866 x

x Nb 16 0.600814 -0.000705 0.499314 x

x Nb 17 0.798913 -0.009072 0.250353 x

x Nb 18 0.802167 0.004633 0.749984 x

x Nb 19 0.800432 0.000265 -0.000276 x

x Nb 20 0.799981 -0.001332 0.500033 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597720E+004 18798.50 <-- SCF

1 -3.62599646E+004 4.81492662E-003 18824.70 <-- SCF

2 -3.62599752E+004 2.63894444E-004 18853.33 <-- SCF

3 -3.62599276E+004 -1.19124975E-003 18879.70 <-- SCF

4 -3.62598554E+004 -1.80445629E-003 18905.56 <-- SCF

5 -3.62598569E+004 3.82829446E-005 18931.70 <-- SCF

6 -3.62598553E+004 -3.89746878E-005 18956.11 <-- SCF

7 -3.62598550E+004 -8.62033441E-006 18976.80 <-- SCF

8 -3.62598551E+004 1.26071866E-006 18996.48 <-- SCF

9 -3.62598551E+004 6.19835139E-007 19013.73 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.85507593 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00325 0.03085 -0.05905 \*

\* Se 2 -0.00352 0.00119 0.11300 \*

\* Se 3 -0.00833 -0.02556 -0.02313 \*

\* Se 4 -0.00371 0.00343 0.00922 \*

\* Se 5 -0.03243 0.00266 -0.03209 \*

\* Se 6 0.16700 -0.00541 0.03915 \*

\* Se 7 0.09764 0.03598 0.07029 \*

\* Se 8 -0.04547 0.02389 -0.02643 \*

\* Se 9 0.05128 0.04324 -0.03588 \*

\* Se 10 -0.00276 -0.03221 0.02934 \*

\* Se 11 -0.05150 -0.04093 0.03211 \*

\* Se 12 0.00348 0.03433 -0.02735 \*

\* Se 13 -0.10263 -0.03402 -0.06132 \*

\* Se 14 0.04913 -0.02509 0.02733 \*

\* Se 15 0.03486 -0.00438 0.03198 \*

\* Se 16 -0.16552 0.00647 -0.04025 \*

\* Se 17 0.00701 0.02450 0.01551 \*

\* Se 18 0.00234 -0.00258 -0.01150 \*

\* Se 19 -0.00455 -0.03195 0.06169 \*

\* Se 20 0.00295 -0.00250 -0.10712 \*

\* Nb 1 0.10609 -0.03455 0.01277 \*

\* Nb 2 -0.10313 0.03160 -0.01362 \*

\* Nb 3 -0.00052 0.00038 -0.00181 \*

\* Nb 4 -0.00011 0.00007 0.00090 \*

\* Nb 5 0.00518 -0.02444 -0.00151 \*

\* Nb 6 0.02147 0.06856 -0.01583 \*

\* Nb 7 0.00315 0.03195 -0.04615 \*

\* Nb 8 0.02254 0.02979 0.02063 \*

\* Nb 9 -0.03318 -0.09580 0.03810 \*

\* Nb 10 0.02770 0.10032 -0.04107 \*

\* Nb 11 0.02399 -0.00741 -0.00780 \*

\* Nb 12 -0.03440 -0.01919 0.00443 \*

\* Nb 13 -0.02516 -0.09898 0.04113 \*

\* Nb 14 0.03127 0.09342 -0.03813 \*

\* Nb 15 -0.02521 0.00759 0.00532 \*

\* Nb 16 0.03388 0.01911 -0.00334 \*

\* Nb 17 -0.02422 -0.06769 0.01438 \*

\* Nb 18 -0.00546 0.02525 0.00089 \*

\* Nb 19 -0.00103 -0.03226 0.04793 \*

\* Nb 20 -0.02136 -0.02963 -0.02275 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.069295 -0.133134 -0.011436 \*

\* y -0.133134 -0.003087 0.108454 \*

\* z -0.011436 0.108454 0.147152 \*

\* \*

\* Pressure: -0.0249 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000180 | -36259.851099 | <-- min BFGS

| trial step | 1.000000 | 0.000116 | -36259.855132 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 25 with line minimization (lambda= 2.810042)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8996308 -8.3485456 -0.0072030 0.4197977 -0.0033964 0.0000004

0.0274001 3.3867214 0.0028879 1.0348357 1.8468700 -0.0012406

0.0000636 0.0092963 13.8923319 0.0000025 -0.0003857 0.4522775

Lattice parameters(A) Cell Angles

a = 17.079147 alpha = 89.912803

b = 3.386833 beta = 90.042677

c = 13.892335 gamma = 118.799207

Current cell volume = 704.197040 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067103 0.665021 0.126131 x

x Se 2 0.132345 0.339541 0.627187 x

x Se 3 0.132471 0.340962 0.872302 x

x Se 4 0.067184 0.665525 0.374331 x

x Se 5 0.266916 0.665440 0.125617 x

x Se 6 0.331839 0.336724 0.627083 x

x Se 7 0.332213 0.338858 0.872255 x

x Se 8 0.266672 0.664601 0.374052 x

x Se 9 0.467437 0.655944 0.127986 x

x Se 10 0.532664 0.341478 0.626379 x

x Se 11 0.532560 0.344089 0.872019 x

x Se 12 0.467327 0.658541 0.373623 x

x Se 13 0.667809 0.661252 0.127691 x

x Se 14 0.733321 0.335320 0.625953 x

x Se 15 0.733073 0.334477 0.874385 x

x Se 16 0.668184 0.663377 0.372964 x

x Se 17 0.867513 0.658906 0.127737 x

x Se 18 0.932827 0.334529 0.625682 x

x Se 19 0.932909 0.335058 0.873852 x

x Se 20 0.867641 0.660346 0.372770 x

x Nb 1 0.001515 0.005933 0.249986 x

x Nb 2 -0.001565 -0.005716 0.750014 x

x Nb 3 -0.000014 -0.000191 0.000037 x

x Nb 4 -0.000022 -0.000211 0.499954 x

x Nb 5 0.197730 -0.005461 0.249992 x

x Nb 6 0.201111 0.009849 0.749601 x

x Nb 7 0.199505 -0.000057 0.000149 x

x Nb 8 0.200029 0.001761 0.500101 x

x Nb 9 0.399735 -0.006582 0.250275 x

x Nb 10 0.399975 0.001966 0.749873 x

x Nb 11 0.399776 0.002819 -0.001109 x

x Nb 12 0.399116 0.000769 0.500956 x

x Nb 13 0.599973 -0.002122 0.250123 x

x Nb 14 0.600304 0.006890 0.749715 x

x Nb 15 0.600207 -0.002930 0.001147 x

x Nb 16 0.600899 -0.000753 0.499035 x

x Nb 17 0.798918 -0.010006 0.250410 x

x Nb 18 0.802299 0.005249 0.750012 x

x Nb 19 0.800526 0.000363 -0.000223 x

x Nb 20 0.799976 -0.001561 0.499954 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62595895E+004 19116.73 <-- SCF

1 -3.62601893E+004 1.49944022E-002 19143.28 <-- SCF

2 -3.62602203E+004 7.75869262E-004 19173.14 <-- SCF

3 -3.62600296E+004 -4.76911504E-003 19200.08 <-- SCF

4 -3.62598643E+004 -4.13080133E-003 19226.16 <-- SCF

5 -3.62598630E+004 -3.27852233E-005 19252.69 <-- SCF

6 -3.62598592E+004 -9.62182278E-005 19278.72 <-- SCF

7 -3.62598582E+004 -2.42286559E-005 19302.23 <-- SCF

8 -3.62598584E+004 3.66340225E-006 19322.44 <-- SCF

9 -3.62598584E+004 -3.67346720E-008 19340.75 <-- SCF

10 -3.62598584E+004 5.95115299E-007 19358.28 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.85838891 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02717 0.01601 -0.03144 \*

\* Se 2 -0.06225 -0.01665 0.14526 \*

\* Se 3 -0.05585 -0.03359 -0.05253 \*

\* Se 4 0.03370 0.00900 0.00610 \*

\* Se 5 -0.02320 -0.02240 -0.04678 \*

\* Se 6 0.14403 0.00786 0.05795 \*

\* Se 7 0.03074 0.04178 0.06558 \*

\* Se 8 -0.02553 -0.00394 -0.02552 \*

\* Se 9 0.06543 0.04007 -0.03022 \*

\* Se 10 -0.00091 -0.05940 0.02395 \*

\* Se 11 -0.06537 -0.03751 0.02628 \*

\* Se 12 0.00147 0.06249 -0.02160 \*

\* Se 13 -0.03537 -0.04122 -0.05444 \*

\* Se 14 0.03031 0.00276 0.02624 \*

\* Se 15 0.02625 0.02016 0.04660 \*

\* Se 16 -0.14559 -0.00647 -0.06113 \*

\* Se 17 0.05243 0.03323 0.04587 \*

\* Se 18 -0.03486 -0.00743 -0.00797 \*

\* Se 19 -0.02886 -0.01738 0.03455 \*

\* Se 20 0.06225 0.01450 -0.13815 \*

\* Nb 1 0.05689 -0.05172 0.01054 \*

\* Nb 2 -0.05203 0.04647 -0.01188 \*

\* Nb 3 -0.00034 0.00159 -0.00307 \*

\* Nb 4 0.00029 0.00121 0.00184 \*

\* Nb 5 0.00375 0.00079 -0.00449 \*

\* Nb 6 0.05703 0.05117 -0.01151 \*

\* Nb 7 0.01807 0.04195 -0.05023 \*

\* Nb 8 0.03808 0.03828 0.01791 \*

\* Nb 9 -0.03266 -0.07740 0.04594 \*

\* Nb 10 0.05048 0.11543 -0.04268 \*

\* Nb 11 0.03117 -0.01651 0.02564 \*

\* Nb 12 -0.03546 -0.03109 -0.03250 \*

\* Nb 13 -0.04545 -0.11363 0.04277 \*

\* Nb 14 0.02975 0.07380 -0.04631 \*

\* Nb 15 -0.03193 0.01714 -0.02860 \*

\* Nb 16 0.03468 0.03135 0.03377 \*

\* Nb 17 -0.06139 -0.04900 0.00938 \*

\* Nb 18 -0.00443 0.00163 0.00345 \*

\* Nb 19 -0.01604 -0.04383 0.05326 \*

\* Nb 20 -0.03646 -0.03948 -0.02183 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.003872 -0.028125 0.028360 \*

\* y -0.028125 0.039821 0.202864 \*

\* z 0.028360 0.202864 -0.012083 \*

\* \*

\* Pressure: -0.0080 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000180 | -36259.851099 | <-- min BFGS

| trial step | 1.000000 | 0.000116 | -36259.855132 | <-- min BFGS

| line step | 2.810042 | 0.000012 | -36259.858451 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 25 with enthalpy= -3.62598585E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.837952E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.589114E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.225933E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.028636E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 26 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000048 | -36259.858451 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 26 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9020015 -8.3421867 -0.0063506 0.4196730 -0.0035025 0.0000036

0.0282556 3.3856576 0.0024913 1.0340650 1.8471950 -0.0010627

-0.0000531 0.0080225 13.8929301 0.0000064 -0.0003328 0.4522579

Lattice parameters(A) Cell Angles

a = 17.078108 alpha = 89.924759

b = 3.385776 beta = 90.037658

c = 13.892932 gamma = 118.762084

Current cell volume = 704.215488 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067110 0.665051 0.126142 x

x Se 2 0.132347 0.339848 0.627313 x

x Se 3 0.132481 0.341341 0.872161 x

x Se 4 0.067191 0.665567 0.374330 x

x Se 5 0.266916 0.665443 0.125614 x

x Se 6 0.331847 0.336954 0.627204 x

x Se 7 0.332234 0.339208 0.872117 x

x Se 8 0.266649 0.664540 0.374014 x

x Se 9 0.467431 0.655385 0.128132 x

x Se 10 0.532685 0.341928 0.626439 x

x Se 11 0.532566 0.344653 0.871874 x

x Se 12 0.467306 0.658095 0.373563 x

x Se 13 0.667789 0.660909 0.127828 x

x Se 14 0.733343 0.335376 0.625992 x

x Se 15 0.733072 0.334468 0.874387 x

x Se 16 0.668178 0.663155 0.372845 x

x Se 17 0.867501 0.658518 0.127878 x

x Se 18 0.932821 0.334491 0.625684 x

x Se 19 0.932903 0.335033 0.873841 x

x Se 20 0.867638 0.660031 0.372642 x

x Nb 1 0.001681 0.006559 0.249982 x

x Nb 2 -0.001734 -0.006330 0.750017 x

x Nb 3 -0.000015 -0.000203 0.000038 x

x Nb 4 -0.000024 -0.000225 0.499951 x

x Nb 5 0.197645 -0.005738 0.249983 x

x Nb 6 0.201140 0.010327 0.749579 x

x Nb 7 0.199471 -0.000054 0.000134 x

x Nb 8 0.200035 0.001891 0.500126 x

x Nb 9 0.399717 -0.007028 0.250289 x

x Nb 10 0.399965 0.002070 0.749859 x

x Nb 11 0.399780 0.002983 -0.001201 x

x Nb 12 0.399072 0.000784 0.501044 x

x Nb 13 0.599980 -0.002236 0.250136 x

x Nb 14 0.600324 0.007354 0.749700 x

x Nb 15 0.600202 -0.003100 0.001241 x

x Nb 16 0.600944 -0.000766 0.498948 x

x Nb 17 0.798891 -0.010495 0.250433 x

x Nb 18 0.802386 0.005514 0.750021 x

x Nb 19 0.800562 0.000379 -0.000213 x

x Nb 20 0.799971 -0.001678 0.499932 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598169E+004 19460.88 <-- SCF

1 -3.62599692E+004 3.80621700E-003 19488.23 <-- SCF

2 -3.62599778E+004 2.15255377E-004 19516.23 <-- SCF

3 -3.62599527E+004 -6.26507865E-004 19543.02 <-- SCF

4 -3.62598561E+004 -2.41585203E-003 19569.02 <-- SCF

5 -3.62598617E+004 1.41129546E-004 19595.78 <-- SCF

6 -3.62598600E+004 -4.32751722E-005 19620.47 <-- SCF

7 -3.62598593E+004 -1.70064271E-005 19641.89 <-- SCF

8 -3.62598594E+004 7.05799747E-007 19661.14 <-- SCF

9 -3.62598594E+004 9.97391589E-007 19679.23 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.85939397 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02755 0.01560 -0.04085 \*

\* Se 2 -0.07374 -0.01017 0.12262 \*

\* Se 3 -0.05786 -0.03444 -0.03424 \*

\* Se 4 0.03568 0.00886 0.01696 \*

\* Se 5 -0.02423 -0.02488 -0.05200 \*

\* Se 6 0.14534 0.01647 0.04567 \*

\* Se 7 0.02361 0.04382 0.09956 \*

\* Se 8 -0.02340 -0.00482 -0.02227 \*

\* Se 9 0.06758 0.03765 -0.05791 \*

\* Se 10 -0.01972 -0.05436 0.02342 \*

\* Se 11 -0.06727 -0.03542 0.05393 \*

\* Se 12 0.02028 0.05803 -0.02087 \*

\* Se 13 -0.02770 -0.04540 -0.08760 \*

\* Se 14 0.02862 0.00394 0.02290 \*

\* Se 15 0.02774 0.02264 0.05163 \*

\* Se 16 -0.14856 -0.01447 -0.05151 \*

\* Se 17 0.05431 0.03560 0.02860 \*

\* Se 18 -0.03708 -0.00716 -0.01928 \*

\* Se 19 -0.02952 -0.01706 0.04410 \*

\* Se 20 0.07368 0.00774 -0.11266 \*

\* Nb 1 0.04265 -0.05397 0.01327 \*

\* Nb 2 -0.03751 0.04774 -0.01488 \*

\* Nb 3 -0.00026 0.00187 -0.00347 \*

\* Nb 4 0.00034 0.00147 0.00209 \*

\* Nb 5 0.00354 0.00618 -0.00312 \*

\* Nb 6 0.06370 0.04338 -0.01207 \*

\* Nb 7 0.02009 0.04402 -0.05272 \*

\* Nb 8 0.03795 0.03951 0.01949 \*

\* Nb 9 -0.04001 -0.07139 0.04948 \*

\* Nb 10 0.05425 0.12116 -0.04319 \*

\* Nb 11 0.03235 -0.02008 0.03181 \*

\* Nb 12 -0.03743 -0.03688 -0.04150 \*

\* Nb 13 -0.04827 -0.11909 0.04326 \*

\* Nb 14 0.03669 0.06723 -0.04978 \*

\* Nb 15 -0.03279 0.02094 -0.03535 \*

\* Nb 16 0.03687 0.03713 0.04275 \*

\* Nb 17 -0.06837 -0.04071 0.00966 \*

\* Nb 18 -0.00456 -0.00315 0.00195 \*

\* Nb 19 -0.01820 -0.04634 0.05618 \*

\* Nb 20 -0.03632 -0.04116 -0.02404 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.047183 -0.003595 0.026779 \*

\* y -0.003595 -0.010763 0.178414 \*

\* z 0.026779 0.178414 -0.030583 \*

\* \*

\* Pressure: -0.0019 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000048 | -36259.858451 | <-- min BFGS

| trial step | 1.000000 | 0.000020 | -36259.859476 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 26 with line minimization (lambda= 1.718794)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9037055 -8.3376159 -0.0057378 0.4195834 -0.0035787 0.0000060

0.0288705 3.3848930 0.0022062 1.0335113 1.8474290 -0.0009348

-0.0001370 0.0071070 13.8933600 0.0000092 -0.0002948 0.4522439

Lattice parameters(A) Cell Angles

a = 17.077362 alpha = 89.933355

b = 3.385017 beta = 90.034053

c = 13.893362 gamma = 118.735394

Current cell volume = 704.228602 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067115 0.665072 0.126149 x

x Se 2 0.132348 0.340068 0.627404 x

x Se 3 0.132488 0.341613 0.872061 x

x Se 4 0.067196 0.665597 0.374329 x

x Se 5 0.266917 0.665445 0.125613 x

x Se 6 0.331853 0.337119 0.627292 x

x Se 7 0.332249 0.339460 0.872017 x

x Se 8 0.266633 0.664495 0.373987 x

x Se 9 0.467426 0.654983 0.128236 x

x Se 10 0.532700 0.342251 0.626482 x

x Se 11 0.532570 0.345058 0.871769 x

x Se 12 0.467290 0.657774 0.373521 x

x Se 13 0.667774 0.660662 0.127926 x

x Se 14 0.733359 0.335417 0.626019 x

x Se 15 0.733071 0.334461 0.874389 x

x Se 16 0.668173 0.662995 0.372760 x

x Se 17 0.867493 0.658238 0.127980 x

x Se 18 0.932816 0.334464 0.625685 x

x Se 19 0.932898 0.335016 0.873832 x

x Se 20 0.867636 0.659803 0.372550 x

x Nb 1 0.001800 0.007008 0.249980 x

x Nb 2 -0.001855 -0.006771 0.750019 x

x Nb 3 -0.000016 -0.000211 0.000040 x

x Nb 4 -0.000025 -0.000235 0.499949 x

x Nb 5 0.197584 -0.005936 0.249977 x

x Nb 6 0.201160 0.010670 0.749563 x

x Nb 7 0.199447 -0.000051 0.000123 x

x Nb 8 0.200038 0.001984 0.500144 x

x Nb 9 0.399704 -0.007349 0.250299 x

x Nb 10 0.399958 0.002146 0.749849 x

x Nb 11 0.399783 0.003100 -0.001267 x

x Nb 12 0.399040 0.000796 0.501106 x

x Nb 13 0.599986 -0.002317 0.250146 x

x Nb 14 0.600339 0.007687 0.749690 x

x Nb 15 0.600198 -0.003223 0.001308 x

x Nb 16 0.600977 -0.000776 0.498885 x

x Nb 17 0.798871 -0.010846 0.250449 x

x Nb 18 0.802448 0.005705 0.750027 x

x Nb 19 0.800588 0.000390 -0.000206 x

x Nb 20 0.799968 -0.001762 0.499917 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598382E+004 19782.31 <-- SCF

1 -3.62598949E+004 1.41544819E-003 19808.91 <-- SCF

2 -3.62598977E+004 7.16157205E-005 19836.17 <-- SCF

3 -3.62598798E+004 -4.47079361E-004 19862.34 <-- SCF

4 -3.62598599E+004 -4.97440619E-004 19887.84 <-- SCF

5 -3.62598599E+004 7.43745245E-008 19912.80 <-- SCF

6 -3.62598597E+004 -7.10279555E-006 19932.45 <-- SCF

7 -3.62598597E+004 -1.04262803E-008 19951.25 <-- SCF

8 -3.62598597E+004 7.38566289E-007 19968.67 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.85968232 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.03094 0.01555 -0.04853 \*

\* Se 2 -0.07838 -0.00554 0.10143 \*

\* Se 3 -0.05782 -0.03848 -0.01981 \*

\* Se 4 0.04011 0.00875 0.02379 \*

\* Se 5 -0.02140 -0.02619 -0.05762 \*

\* Se 6 0.14825 0.02381 0.03391 \*

\* Se 7 0.02229 0.04051 0.12765 \*

\* Se 8 -0.01787 -0.00560 -0.01923 \*

\* Se 9 0.06955 0.04539 -0.08539 \*

\* Se 10 -0.03553 -0.05037 0.02283 \*

\* Se 11 -0.06923 -0.04370 0.08156 \*

\* Se 12 0.03591 0.05433 -0.02022 \*

\* Se 13 -0.02623 -0.04404 -0.11506 \*

\* Se 14 0.02324 0.00499 0.01972 \*

\* Se 15 0.02502 0.02393 0.05732 \*

\* Se 16 -0.15266 -0.02137 -0.04172 \*

\* Se 17 0.05486 0.04096 0.01431 \*

\* Se 18 -0.04143 -0.00691 -0.02626 \*

\* Se 19 -0.03280 -0.01706 0.05192 \*

\* Se 20 0.07805 0.00315 -0.09006 \*

\* Nb 1 0.03193 -0.05673 0.01177 \*

\* Nb 2 -0.02640 0.05006 -0.01342 \*

\* Nb 3 -0.00020 0.00194 -0.00367 \*

\* Nb 4 0.00041 0.00158 0.00212 \*

\* Nb 5 0.00622 0.00971 -0.00490 \*

\* Nb 6 0.07150 0.03798 -0.01014 \*

\* Nb 7 0.02362 0.04500 -0.05466 \*

\* Nb 8 0.04348 0.04121 0.02197 \*

\* Nb 9 -0.04210 -0.06902 0.04988 \*

\* Nb 10 0.05860 0.12326 -0.04198 \*

\* Nb 11 0.03605 -0.02089 0.03647 \*

\* Nb 12 -0.03830 -0.03949 -0.04583 \*

\* Nb 13 -0.05251 -0.12114 0.04217 \*

\* Nb 14 0.03896 0.06476 -0.05029 \*

\* Nb 15 -0.03650 0.02184 -0.04012 \*

\* Nb 16 0.03763 0.03982 0.04721 \*

\* Nb 17 -0.07644 -0.03493 0.00764 \*

\* Nb 18 -0.00727 -0.00643 0.00365 \*

\* Nb 19 -0.02165 -0.04754 0.05825 \*

\* Nb 20 -0.04188 -0.04307 -0.02666 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.081463 0.014273 0.025019 \*

\* y 0.014273 -0.049087 0.163558 \*

\* z 0.025019 0.163558 -0.041522 \*

\* \*

\* Pressure: 0.0030 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000048 | -36259.858451 | <-- min BFGS

| trial step | 1.000000 | 0.000020 | -36259.859476 | <-- min BFGS

| line step | 1.718794 | -4.679E-006 | -36259.859762 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 26 with enthalpy= -3.62598598E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 3.277221E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.596980E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.719845E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.635583E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 27 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000039 | -36259.859762 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 27 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9016267 -8.3358473 -0.0042276 0.4196082 -0.0036397 0.0000055

0.0293618 3.3850132 0.0016100 1.0333165 1.8472147 -0.0006778

-0.0001383 0.0051751 13.8930673 0.0000079 -0.0002152 0.4522534

Lattice parameters(A) Cell Angles

a = 17.074684 alpha = 89.951414

b = 3.385141 beta = 90.025103

c = 13.893068 gamma = 118.725319

Current cell volume = 704.197208 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067113 0.665082 0.126124 x

x Se 2 0.132353 0.340014 0.627399 x

x Se 3 0.132493 0.341523 0.872089 x

x Se 4 0.067192 0.665588 0.374345 x

x Se 5 0.266907 0.665442 0.125603 x

x Se 6 0.331894 0.337178 0.627266 x

x Se 7 0.332269 0.339469 0.872079 x

x Se 8 0.266625 0.664513 0.373989 x

x Se 9 0.467438 0.655162 0.128186 x

x Se 10 0.532692 0.342123 0.626468 x

x Se 11 0.532559 0.344880 0.871818 x

x Se 12 0.467298 0.657905 0.373535 x

x Se 13 0.667753 0.660649 0.127867 x

x Se 14 0.733368 0.335401 0.626017 x

x Se 15 0.733081 0.334465 0.874399 x

x Se 16 0.668131 0.662936 0.372785 x

x Se 17 0.867487 0.658329 0.127949 x

x Se 18 0.932819 0.334472 0.625669 x

x Se 19 0.932900 0.335003 0.873859 x

x Se 20 0.867631 0.659857 0.372557 x

x Nb 1 0.001790 0.006912 0.249984 x

x Nb 2 -0.001844 -0.006679 0.750015 x

x Nb 3 -0.000016 -0.000208 0.000039 x

x Nb 4 -0.000025 -0.000232 0.499950 x

x Nb 5 0.197611 -0.005884 0.249977 x

x Nb 6 0.201156 0.010626 0.749564 x

x Nb 7 0.199456 -0.000015 0.000110 x

x Nb 8 0.200044 0.002003 0.500147 x

x Nb 9 0.399700 -0.007365 0.250306 x

x Nb 10 0.399969 0.002238 0.749839 x

x Nb 11 0.399790 0.003070 -0.001249 x

x Nb 12 0.399045 0.000755 0.501090 x

x Nb 13 0.599975 -0.002404 0.250157 x

x Nb 14 0.600343 0.007696 0.749683 x

x Nb 15 0.600191 -0.003192 0.001290 x

x Nb 16 0.600972 -0.000736 0.498902 x

x Nb 17 0.798875 -0.010800 0.250447 x

x Nb 18 0.802421 0.005656 0.750027 x

x Nb 19 0.800579 0.000350 -0.000191 x

x Nb 20 0.799963 -0.001784 0.499912 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598575E+004 20071.83 <-- SCF

1 -3.62598649E+004 1.85950099E-004 20098.78 <-- SCF

2 -3.62598653E+004 9.62391764E-006 20121.03 <-- SCF

3 -3.62598631E+004 -5.38409966E-005 20147.20 <-- SCF

4 -3.62598607E+004 -6.05279514E-005 20171.94 <-- SCF

5 -3.62598607E+004 -6.17686032E-007 20192.12 <-- SCF

6 -3.62598607E+004 -7.24190749E-007 20209.53 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.86067342 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.03224 0.01117 -0.04095 \*

\* Se 2 -0.08046 0.00175 0.09882 \*

\* Se 3 -0.06123 -0.02850 -0.02718 \*

\* Se 4 0.04272 0.00644 0.02555 \*

\* Se 5 -0.01731 -0.02845 -0.05487 \*

\* Se 6 0.13210 0.02878 0.03903 \*

\* Se 7 0.01362 0.04748 0.10849 \*

\* Se 8 -0.01516 -0.01029 -0.01948 \*

\* Se 9 0.06406 0.03237 -0.06700 \*

\* Se 10 -0.02780 -0.04288 0.02229 \*

\* Se 11 -0.06407 -0.03059 0.06335 \*

\* Se 12 0.02795 0.04669 -0.01955 \*

\* Se 13 -0.01692 -0.05019 -0.09681 \*

\* Se 14 0.02002 0.00966 0.02011 \*

\* Se 15 0.02063 0.02612 0.05451 \*

\* Se 16 -0.13718 -0.02658 -0.04638 \*

\* Se 17 0.05832 0.03063 0.02213 \*

\* Se 18 -0.04356 -0.00469 -0.02778 \*

\* Se 19 -0.03356 -0.01258 0.04416 \*

\* Se 20 0.08028 -0.00388 -0.08842 \*

\* Nb 1 0.02489 -0.05660 0.01486 \*

\* Nb 2 -0.01859 0.04951 -0.01653 \*

\* Nb 3 -0.00008 0.00219 -0.00424 \*

\* Nb 4 0.00075 0.00188 0.00281 \*

\* Nb 5 0.01729 0.01116 -0.00247 \*

\* Nb 6 0.06645 0.03318 -0.01230 \*

\* Nb 7 0.02443 0.04518 -0.05831 \*

\* Nb 8 0.04483 0.04104 0.02050 \*

\* Nb 9 -0.04502 -0.06491 0.05465 \*

\* Nb 10 0.06799 0.12081 -0.04430 \*

\* Nb 11 0.04179 -0.02298 0.04030 \*

\* Nb 12 -0.03628 -0.04340 -0.05105 \*

\* Nb 13 -0.06162 -0.11877 0.04474 \*

\* Nb 14 0.04122 0.06047 -0.05495 \*

\* Nb 15 -0.04266 0.02388 -0.04429 \*

\* Nb 16 0.03530 0.04370 0.05270 \*

\* Nb 17 -0.07203 -0.02994 0.00985 \*

\* Nb 18 -0.01811 -0.00761 0.00122 \*

\* Nb 19 -0.02216 -0.04802 0.06221 \*

\* Nb 20 -0.04307 -0.04325 -0.02542 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.077260 0.041130 0.024874 \*

\* y 0.041130 -0.047967 0.124202 \*

\* z 0.024874 0.124202 -0.038343 \*

\* \*

\* Pressure: 0.0030 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000039 | -36259.859762 | <-- min BFGS

| trial step | 1.000000 | 0.000032 | -36259.860768 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 27 with line minimization (lambda= 5.369487)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8925435 -8.3281194 0.0023710 0.4197170 -0.0039062 0.0000034

0.0315086 3.3855388 -0.0009952 1.0324659 1.8462805 0.0004448

-0.0001436 -0.0032661 13.8917883 0.0000023 0.0001329 0.4522950

Lattice parameters(A) Cell Angles

a = 17.062984 alpha = 90.030318

b = 3.385686 beta = 89.985981

c = 13.891789 gamma = 118.681308

Current cell volume = 704.059269 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067102 0.665127 0.126012 x

x Se 2 0.132376 0.339778 0.627379 x

x Se 3 0.132517 0.341131 0.872213 x

x Se 4 0.067176 0.665552 0.374412 x

x Se 5 0.266864 0.665429 0.125560 x

x Se 6 0.332075 0.337432 0.627151 x

x Se 7 0.332357 0.339508 0.872350 x

x Se 8 0.266589 0.664593 0.373999 x

x Se 9 0.467491 0.655946 0.127969 x

x Se 10 0.532659 0.341561 0.626407 x

x Se 11 0.532506 0.344102 0.872031 x

x Se 12 0.467333 0.658477 0.373599 x

x Se 13 0.667661 0.660595 0.127610 x

x Se 14 0.733408 0.335331 0.626007 x

x Se 15 0.733127 0.334481 0.874442 x

x Se 16 0.667948 0.662678 0.372893 x

x Se 17 0.867462 0.658725 0.127816 x

x Se 18 0.932834 0.334508 0.625599 x

x Se 19 0.932909 0.334948 0.873974 x

x Se 20 0.867609 0.660091 0.372588 x

x Nb 1 0.001744 0.006492 0.250003 x

x Nb 2 -0.001792 -0.006279 0.749995 x

x Nb 3 -0.000015 -0.000195 0.000034 x

x Nb 4 -0.000023 -0.000218 0.499954 x

x Nb 5 0.197726 -0.005654 0.249979 x

x Nb 6 0.201138 0.010436 0.749569 x

x Nb 7 0.199495 0.000145 0.000050 x

x Nb 8 0.200067 0.002086 0.500161 x

x Nb 9 0.399679 -0.007437 0.250340 x

x Nb 10 0.400021 0.002642 0.749795 x

x Nb 11 0.399821 0.002941 -0.001173 x

x Nb 12 0.399065 0.000576 0.501018 x

x Nb 13 0.599930 -0.002786 0.250200 x

x Nb 14 0.600359 0.007734 0.749649 x

x Nb 15 0.600161 -0.003057 0.001208 x

x Nb 16 0.600950 -0.000559 0.498975 x

x Nb 17 0.798888 -0.010600 0.250440 x

x Nb 18 0.802304 0.005445 0.750024 x

x Nb 19 0.800539 0.000173 -0.000124 x

x Nb 20 0.799940 -0.001878 0.499891 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597993E+004 20312.50 <-- SCF

1 -3.62600742E+004 6.87213355E-003 20339.88 <-- SCF

2 -3.62600913E+004 4.27543357E-004 20367.88 <-- SCF

3 -3.62600802E+004 -2.77509286E-004 20394.47 <-- SCF

4 -3.62598530E+004 -5.67982930E-003 20420.47 <-- SCF

5 -3.62598675E+004 3.64204491E-004 20447.28 <-- SCF

6 -3.62598644E+004 -7.82884925E-005 20473.12 <-- SCF

7 -3.62598623E+004 -5.25862912E-005 20496.11 <-- SCF

8 -3.62598621E+004 -3.82342553E-006 20516.22 <-- SCF

9 -3.62598622E+004 1.57636321E-006 20534.12 <-- SCF

10 -3.62598623E+004 1.41006585E-006 20551.52 <-- SCF

11 -3.62598623E+004 1.04550753E-006 20568.55 <-- SCF

12 -3.62598623E+004 6.28482768E-007 20584.73 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.86232718 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.03810 -0.00662 -0.01089 \*

\* Se 2 -0.07712 0.02336 0.09955 \*

\* Se 3 -0.07178 -0.00052 -0.05374 \*

\* Se 4 0.05169 -0.00462 0.02171 \*

\* Se 5 -0.00343 -0.03561 -0.05064 \*

\* Se 6 0.06359 0.04781 0.06564 \*

\* Se 7 -0.02284 0.06495 0.02662 \*

\* Se 8 -0.00622 -0.02817 -0.02136 \*

\* Se 9 0.04828 0.00410 -0.01166 \*

\* Se 10 -0.00087 -0.02243 0.01609 \*

\* Se 11 -0.04715 -0.00202 0.00876 \*

\* Se 12 0.00184 0.02542 -0.01299 \*

\* Se 13 0.02138 -0.06490 -0.02001 \*

\* Se 14 0.00889 0.02782 0.02142 \*

\* Se 15 0.00532 0.03313 0.05108 \*

\* Se 16 -0.07096 -0.04665 -0.07118 \*

\* Se 17 0.06937 0.00120 0.05086 \*

\* Se 18 -0.05168 0.00629 -0.02321 \*

\* Se 19 -0.03859 0.00603 0.01255 \*

\* Se 20 0.07747 -0.02402 -0.09316 \*

\* Nb 1 0.03041 -0.02567 -0.00493 \*

\* Nb 2 -0.02882 0.02123 0.00375 \*

\* Nb 3 -0.00007 0.00033 -0.00239 \*

\* Nb 4 0.00075 0.00035 0.00142 \*

\* Nb 5 -0.01358 0.02650 -0.01464 \*

\* Nb 6 0.09232 0.01588 -0.00702 \*

\* Nb 7 0.01492 0.03620 -0.04126 \*

\* Nb 8 0.04702 0.03947 0.02414 \*

\* Nb 9 -0.03050 -0.03257 0.02979 \*

\* Nb 10 0.05181 0.08289 -0.00365 \*

\* Nb 11 0.03584 -0.00774 0.03333 \*

\* Nb 12 -0.04400 -0.03542 -0.04881 \*

\* Nb 13 -0.04895 -0.08108 0.00457 \*

\* Nb 14 0.02840 0.03005 -0.03019 \*

\* Nb 15 -0.03574 0.00742 -0.03562 \*

\* Nb 16 0.04391 0.03463 0.04990 \*

\* Nb 17 -0.09330 -0.01448 0.00555 \*

\* Nb 18 0.01405 -0.02493 0.01404 \*

\* Nb 19 -0.01371 -0.03726 0.04348 \*

\* Nb 20 -0.04606 -0.04038 -0.02689 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.043989 0.167033 0.029694 \*

\* y 0.167033 -0.047532 -0.045317 \*

\* z 0.029694 -0.045317 -0.054584 \*

\* \*

\* Pressure: 0.0194 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000039 | -36259.859762 | <-- min BFGS

| trial step | 1.000000 | 0.000032 | -36259.860768 | <-- min BFGS

| line step | 5.369487 | -4.797E-006 | -36259.862423 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 27 with enthalpy= -3.62598624E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 6.651201E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.280730E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.949592E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.670328E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 28 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000097 | -36259.862423 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 28 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8878183 -8.3306264 0.0042977 0.4198559 -0.0038949 0.0000291

0.0314142 3.3863575 -0.0022109 1.0328688 1.8458597 0.0010330

-0.0010295 -0.0072001 13.8949448 0.0000345 0.0002949 0.4521923

Lattice parameters(A) Cell Angles

a = 17.060085 alpha = 90.067133

b = 3.386504 beta = 89.974773

c = 13.894947 gamma = 118.698131

Current cell volume = 704.156309 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067144 0.665352 0.125921 x

x Se 2 0.132297 0.339978 0.627500 x

x Se 3 0.132452 0.341442 0.872088 x

x Se 4 0.067231 0.665840 0.374518 x

x Se 5 0.266885 0.665338 0.125381 x

x Se 6 0.332060 0.337720 0.627277 x

x Se 7 0.332337 0.339933 0.872236 x

x Se 8 0.266588 0.664450 0.374095 x

x Se 9 0.467479 0.655160 0.128061 x

x Se 10 0.532710 0.342175 0.626398 x

x Se 11 0.532518 0.344895 0.871937 x

x Se 12 0.467281 0.657871 0.373609 x

x Se 13 0.667681 0.660175 0.127724 x

x Se 14 0.733409 0.335469 0.625912 x

x Se 15 0.733105 0.334564 0.874621 x

x Se 16 0.667964 0.662400 0.372768 x

x Se 17 0.867525 0.658400 0.127943 x

x Se 18 0.932780 0.334226 0.625494 x

x Se 19 0.932868 0.334728 0.874065 x

x Se 20 0.867687 0.659877 0.372467 x

x Nb 1 0.001958 0.007252 0.249994 x

x Nb 2 -0.002009 -0.007024 0.750003 x

x Nb 3 -0.000017 -0.000211 0.000036 x

x Nb 4 -0.000025 -0.000236 0.499950 x

x Nb 5 0.197568 -0.006041 0.249962 x

x Nb 6 0.201225 0.011256 0.749537 x

x Nb 7 0.199453 0.000210 0.000028 x

x Nb 8 0.200085 0.002345 0.500194 x

x Nb 9 0.399648 -0.008084 0.250372 x

x Nb 10 0.400010 0.002928 0.749778 x

x Nb 11 0.399828 0.003180 -0.001280 x

x Nb 12 0.398982 0.000521 0.501108 x

x Nb 13 0.599938 -0.003079 0.250217 x

x Nb 14 0.600392 0.008404 0.749616 x

x Nb 15 0.600152 -0.003305 0.001318 x

x Nb 16 0.601034 -0.000502 0.498885 x

x Nb 17 0.798802 -0.011438 0.250471 x

x Nb 18 0.802464 0.005815 0.750041 x

x Nb 19 0.800586 0.000135 -0.000108 x

x Nb 20 0.799923 -0.002119 0.499862 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597885E+004 20687.94 <-- SCF

1 -3.62599701E+004 4.53978280E-003 20714.42 <-- SCF

2 -3.62599794E+004 2.31975924E-004 20742.80 <-- SCF

3 -3.62599239E+004 -1.38593936E-003 20769.77 <-- SCF

4 -3.62598665E+004 -1.43540544E-003 20795.92 <-- SCF

5 -3.62598667E+004 4.76987242E-006 20822.50 <-- SCF

6 -3.62598648E+004 -4.86929702E-005 20847.14 <-- SCF

7 -3.62598645E+004 -7.56971212E-006 20867.81 <-- SCF

8 -3.62598645E+004 5.92648790E-007 20886.14 <-- SCF

9 -3.62598645E+004 6.16670101E-007 20903.28 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.86451164 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02136 -0.00819 -0.00973 \*

\* Se 2 -0.05485 0.01756 0.07422 \*

\* Se 3 -0.05092 -0.01924 -0.04047 \*

\* Se 4 0.03968 0.00183 0.03339 \*

\* Se 5 -0.01008 -0.03332 -0.04686 \*

\* Se 6 0.08259 0.04789 0.05245 \*

\* Se 7 0.00151 0.05280 0.05579 \*

\* Se 8 -0.02213 -0.02225 -0.02258 \*

\* Se 9 0.04682 0.01740 -0.02008 \*

\* Se 10 -0.00780 -0.03261 0.00933 \*

\* Se 11 -0.04569 -0.01638 0.01789 \*

\* Se 12 0.00812 0.03607 -0.00599 \*

\* Se 13 -0.00318 -0.05505 -0.04781 \*

\* Se 14 0.02533 0.02145 0.02310 \*

\* Se 15 0.01236 0.03031 0.04699 \*

\* Se 16 -0.09053 -0.04621 -0.05974 \*

\* Se 17 0.04960 0.02114 0.03744 \*

\* Se 18 -0.03998 0.00010 -0.03532 \*

\* Se 19 -0.02204 0.00815 0.01061 \*

\* Se 20 0.05501 -0.01783 -0.06739 \*

\* Nb 1 0.03693 -0.03130 -0.00491 \*

\* Nb 2 -0.03400 0.02552 0.00362 \*

\* Nb 3 -0.00013 0.00097 -0.00288 \*

\* Nb 4 0.00105 0.00119 0.00220 \*

\* Nb 5 0.01228 0.01977 -0.01566 \*

\* Nb 6 0.07576 0.01210 -0.00355 \*

\* Nb 7 0.01785 0.03712 -0.04932 \*

\* Nb 8 0.04785 0.04137 0.03022 \*

\* Nb 9 -0.03207 -0.02756 0.02685 \*

\* Nb 10 0.05208 0.09450 -0.00031 \*

\* Nb 11 0.03815 -0.01095 0.03890 \*

\* Nb 12 -0.04215 -0.04371 -0.05147 \*

\* Nb 13 -0.04792 -0.09245 0.00147 \*

\* Nb 14 0.02912 0.02424 -0.02719 \*

\* Nb 15 -0.03788 0.01116 -0.04173 \*

\* Nb 16 0.04195 0.04353 0.05264 \*

\* Nb 17 -0.07812 -0.00987 0.00213 \*

\* Nb 18 -0.01220 -0.01732 0.01506 \*

\* Nb 19 -0.01675 -0.03896 0.05259 \*

\* Nb 20 -0.04696 -0.04297 -0.03389 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.010847 0.151594 0.020786 \*

\* y 0.151594 0.034639 -0.118911 \*

\* z 0.020786 -0.118911 -0.001826 \*

\* \*

\* Pressure: -0.0073 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000097 | -36259.862423 | <-- min BFGS

| trial step | 1.000000 | 0.000050 | -36259.864595 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 28 with line minimization (lambda= 2.044302)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8828837 -8.3332444 0.0063098 0.4200011 -0.0038829 0.0000559

0.0313156 3.3872126 -0.0034803 1.0332899 1.8454209 0.0016468

-0.0019547 -0.0113083 13.8982410 0.0000681 0.0004639 0.4520853

Lattice parameters(A) Cell Angles

a = 17.057058 alpha = 90.105559

b = 3.387359 beta = 89.963060

c = 13.898246 gamma = 118.715704

Current cell volume = 704.257338 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067187 0.665586 0.125826 x

x Se 2 0.132214 0.340187 0.627627 x

x Se 3 0.132383 0.341767 0.871957 x

x Se 4 0.067288 0.666140 0.374628 x

x Se 5 0.266908 0.665242 0.125193 x

x Se 6 0.332044 0.338020 0.627409 x

x Se 7 0.332317 0.340377 0.872116 x

x Se 8 0.266588 0.664302 0.374195 x

x Se 9 0.467466 0.654339 0.128157 x

x Se 10 0.532763 0.342816 0.626388 x

x Se 11 0.532531 0.345722 0.871840 x

x Se 12 0.467227 0.657238 0.373620 x

x Se 13 0.667703 0.659736 0.127844 x

x Se 14 0.733411 0.335613 0.625813 x

x Se 15 0.733083 0.334650 0.874809 x

x Se 16 0.667980 0.662110 0.372638 x

x Se 17 0.867591 0.658061 0.128074 x

x Se 18 0.932723 0.333933 0.625383 x

x Se 19 0.932825 0.334497 0.874160 x

x Se 20 0.867768 0.659654 0.372340 x

x Nb 1 0.002181 0.008045 0.249984 x

x Nb 2 -0.002235 -0.007801 0.750012 x

x Nb 3 -0.000018 -0.000228 0.000038 x

x Nb 4 -0.000028 -0.000255 0.499947 x

x Nb 5 0.197404 -0.006445 0.249944 x

x Nb 6 0.201316 0.012114 0.749504 x

x Nb 7 0.199408 0.000278 0.000005 x

x Nb 8 0.200104 0.002616 0.500228 x

x Nb 9 0.399617 -0.008760 0.250406 x

x Nb 10 0.399999 0.003227 0.749760 x

x Nb 11 0.399836 0.003429 -0.001392 x

x Nb 12 0.398895 0.000465 0.501201 x

x Nb 13 0.599946 -0.003385 0.250235 x

x Nb 14 0.600427 0.009103 0.749581 x

x Nb 15 0.600142 -0.003564 0.001432 x

x Nb 16 0.601123 -0.000444 0.498792 x

x Nb 17 0.798712 -0.012312 0.250505 x

x Nb 18 0.802631 0.006202 0.750058 x

x Nb 19 0.800634 0.000096 -0.000091 x

x Nb 20 0.799906 -0.002371 0.499832 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597812E+004 21006.22 <-- SCF

1 -3.62600288E+004 6.19139100E-003 21033.20 <-- SCF

2 -3.62600419E+004 3.26052170E-004 21061.67 <-- SCF

3 -3.62599975E+004 -1.10848391E-003 21088.81 <-- SCF

4 -3.62598635E+004 -3.35131619E-003 21115.11 <-- SCF

5 -3.62598694E+004 1.47130693E-004 21142.03 <-- SCF

6 -3.62598662E+004 -7.87746535E-005 21167.30 <-- SCF

7 -3.62598654E+004 -2.10218242E-005 21188.67 <-- SCF

8 -3.62598654E+004 -8.44663737E-007 21208.73 <-- SCF

9 -3.62598654E+004 6.64812336E-007 21226.75 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.86538196 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00679 -0.00707 -0.01276 \*

\* Se 2 -0.03076 0.01053 0.04656 \*

\* Se 3 -0.03345 -0.04022 -0.03109 \*

\* Se 4 0.02849 0.01051 0.04498 \*

\* Se 5 -0.01822 -0.03168 -0.03237 \*

\* Se 6 0.10142 0.05151 0.03342 \*

\* Se 7 0.02306 0.03108 0.09310 \*

\* Se 8 -0.03658 -0.01897 -0.02328 \*

\* Se 9 0.03904 0.04897 -0.03899 \*

\* Se 10 -0.01276 -0.03965 -0.00169 \*

\* Se 11 -0.03718 -0.04959 0.03788 \*

\* Se 12 0.01305 0.04370 0.00534 \*

\* Se 13 -0.02518 -0.03613 -0.08377 \*

\* Se 14 0.03976 0.01775 0.02421 \*

\* Se 15 0.02031 0.02844 0.03257 \*

\* Se 16 -0.11014 -0.04949 -0.04273 \*

\* Se 17 0.03350 0.04348 0.02789 \*

\* Se 18 -0.02875 -0.00817 -0.04716 \*

\* Se 19 -0.00719 0.00793 0.01260 \*

\* Se 20 0.03056 -0.00992 -0.04035 \*

\* Nb 1 0.04631 -0.03624 -0.00448 \*

\* Nb 2 -0.04323 0.02962 0.00316 \*

\* Nb 3 -0.00021 0.00126 -0.00318 \*

\* Nb 4 0.00123 0.00163 0.00271 \*

\* Nb 5 0.03448 0.01370 -0.01682 \*

\* Nb 6 0.05894 0.00873 -0.00122 \*

\* Nb 7 0.01888 0.03705 -0.05695 \*

\* Nb 8 0.04908 0.04128 0.03492 \*

\* Nb 9 -0.03286 -0.02439 0.02526 \*

\* Nb 10 0.05175 0.10587 0.00382 \*

\* Nb 11 0.04049 -0.01458 0.04521 \*

\* Nb 12 -0.04237 -0.05245 -0.05630 \*

\* Nb 13 -0.04689 -0.10331 -0.00232 \*

\* Nb 14 0.02907 0.02064 -0.02548 \*

\* Nb 15 -0.03991 0.01489 -0.04837 \*

\* Nb 16 0.04207 0.05234 0.05766 \*

\* Nb 17 -0.06145 -0.00591 -0.00013 \*

\* Nb 18 -0.03450 -0.01059 0.01636 \*

\* Nb 19 -0.01829 -0.03926 0.06079 \*

\* Nb 20 -0.04833 -0.04331 -0.03901 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.070354 0.130741 0.010500 \*

\* y 0.130741 0.118769 -0.193573 \*

\* z 0.010500 -0.193573 0.041859 \*

\* \*

\* Pressure: -0.0301 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000097 | -36259.862423 | <-- min BFGS

| trial step | 1.000000 | 0.000050 | -36259.864595 | <-- min BFGS

| line step | 2.044302 | -4.051E-006 | -36259.865430 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 28 with enthalpy= -3.62598654E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.519312E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.280877E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.803661E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.935731E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 29 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000035 | -36259.865430 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 29 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8818137 -8.3319666 0.0061669 0.4200393 -0.0038693 0.0000683

0.0311962 3.3865015 -0.0036377 1.0334424 1.8458436 0.0017458

-0.0023685 -0.0118198 13.8991372 0.0000841 0.0004848 0.4520562

Lattice parameters(A) Cell Angles

a = 17.055500 alpha = 90.110354

b = 3.386647 beta = 89.964000

c = 13.899142 gamma = 118.715623

Current cell volume = 704.090845 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067196 0.665677 0.125754 x

x Se 2 0.132190 0.340123 0.627616 x

x Se 3 0.132361 0.341686 0.871985 x

x Se 4 0.067304 0.666249 0.374701 x

x Se 5 0.266906 0.665193 0.125099 x

x Se 6 0.332073 0.338109 0.627389 x

x Se 7 0.332322 0.340433 0.872177 x

x Se 8 0.266585 0.664268 0.374263 x

x Se 9 0.467468 0.654357 0.128095 x

x Se 10 0.532776 0.342811 0.626339 x

x Se 11 0.532529 0.345707 0.871901 x

x Se 12 0.467214 0.657247 0.373671 x

x Se 13 0.667697 0.659676 0.127786 x

x Se 14 0.733415 0.335648 0.625745 x

x Se 15 0.733086 0.334698 0.874902 x

x Se 16 0.667950 0.662020 0.372657 x

x Se 17 0.867612 0.658142 0.128045 x

x Se 18 0.932707 0.333826 0.625310 x

x Se 19 0.932816 0.334405 0.874233 x

x Se 20 0.867792 0.659715 0.372353 x

x Nb 1 0.002206 0.008070 0.249984 x

x Nb 2 -0.002260 -0.007828 0.750012 x

x Nb 3 -0.000018 -0.000228 0.000037 x

x Nb 4 -0.000028 -0.000255 0.499947 x

x Nb 5 0.197395 -0.006452 0.249939 x

x Nb 6 0.201337 0.012243 0.749500 x

x Nb 7 0.199409 0.000338 -0.000013 x

x Nb 8 0.200115 0.002705 0.500237 x

x Nb 9 0.399608 -0.008882 0.250420 x

x Nb 10 0.400006 0.003396 0.749752 x

x Nb 11 0.399845 0.003450 -0.001387 x

x Nb 12 0.398879 0.000394 0.501192 x

x Nb 13 0.599939 -0.003549 0.250243 x

x Nb 14 0.600435 0.009220 0.749567 x

x Nb 15 0.600133 -0.003585 0.001427 x

x Nb 16 0.601139 -0.000373 0.498801 x

x Nb 17 0.798691 -0.012442 0.250507 x

x Nb 18 0.802640 0.006210 0.750063 x

x Nb 19 0.800634 0.000037 -0.000072 x

x Nb 20 0.799895 -0.002459 0.499821 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598608E+004 21329.77 <-- SCF

1 -3.62598835E+004 5.67892535E-004 21357.27 <-- SCF

2 -3.62598847E+004 3.15973428E-005 21381.67 <-- SCF

3 -3.62598810E+004 -9.36124164E-005 21408.30 <-- SCF

4 -3.62598661E+004 -3.71764875E-004 21434.44 <-- SCF

5 -3.62598666E+004 1.05342676E-005 21457.30 <-- SCF

6 -3.62598664E+004 -2.81891810E-006 21475.72 <-- SCF

7 -3.62598664E+004 -1.29465860E-007 21493.44 <-- SCF

8 -3.62598665E+004 6.84464898E-007 21509.86 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.86646034 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00990 -0.00831 -0.00727 \*

\* Se 2 -0.02397 0.01178 0.05063 \*

\* Se 3 -0.02925 -0.03617 -0.03874 \*

\* Se 4 0.03062 0.01444 0.04227 \*

\* Se 5 -0.00996 -0.03218 -0.02054 \*

\* Se 6 0.09381 0.05379 0.04122 \*

\* Se 7 0.02496 0.03415 0.07557 \*

\* Se 8 -0.03155 -0.02016 -0.02722 \*

\* Se 9 0.03703 0.04249 -0.01825 \*

\* Se 10 -0.00415 -0.03909 -0.00817 \*

\* Se 11 -0.03582 -0.04324 0.01752 \*

\* Se 12 0.00343 0.04293 0.01189 \*

\* Se 13 -0.02673 -0.03870 -0.06723 \*

\* Se 14 0.03485 0.01856 0.02852 \*

\* Se 15 0.01212 0.02884 0.02044 \*

\* Se 16 -0.10212 -0.05224 -0.05010 \*

\* Se 17 0.02981 0.03907 0.03597 \*

\* Se 18 -0.03091 -0.01227 -0.04494 \*

\* Se 19 -0.01016 0.00942 0.00677 \*

\* Se 20 0.02424 -0.01094 -0.04501 \*

\* Nb 1 0.05350 -0.03521 -0.00796 \*

\* Nb 2 -0.04987 0.02830 0.00675 \*

\* Nb 3 -0.00037 0.00167 -0.00333 \*

\* Nb 4 0.00128 0.00209 0.00293 \*

\* Nb 5 0.03205 0.01202 -0.01956 \*

\* Nb 6 0.06284 0.00561 -0.00062 \*

\* Nb 7 0.01924 0.03534 -0.05689 \*

\* Nb 8 0.05315 0.04084 0.03638 \*

\* Nb 9 -0.02843 -0.02014 0.02144 \*

\* Nb 10 0.05365 0.10311 0.01228 \*

\* Nb 11 0.04416 -0.01204 0.04468 \*

\* Nb 12 -0.04590 -0.05383 -0.05562 \*

\* Nb 13 -0.04876 -0.10082 -0.01073 \*

\* Nb 14 0.02472 0.01646 -0.02169 \*

\* Nb 15 -0.04395 0.01269 -0.04773 \*

\* Nb 16 0.04529 0.05427 0.05719 \*

\* Nb 17 -0.06595 -0.00261 -0.00051 \*

\* Nb 18 -0.03218 -0.00877 0.01927 \*

\* Nb 19 -0.01834 -0.03777 0.06109 \*

\* Nb 20 -0.05229 -0.04336 -0.04070 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.085234 0.113504 0.004908 \*

\* y 0.113504 0.070492 -0.202437 \*

\* z 0.004908 -0.202437 0.027090 \*

\* \*

\* Pressure: -0.0041 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000035 | -36259.865430 | <-- min BFGS

| trial step | 1.000000 | 0.000028 | -36259.866497 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 29 with line minimization (lambda= 5.117153)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8774084 -8.3267058 0.0055785 0.4201965 -0.0038130 0.0001193

0.0307045 3.3835738 -0.0042854 1.0340708 1.8475861 0.0021535

-0.0040722 -0.0139255 13.9028270 0.0001501 0.0005710 0.4519364

Lattice parameters(A) Cell Angles

a = 17.049086 alpha = 90.130104

b = 3.383716 beta = 89.967869

c = 13.902835 gamma = 118.715292

Current cell volume = 703.405310 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067236 0.666051 0.125456 x

x Se 2 0.132091 0.339859 0.627572 x

x Se 3 0.132271 0.341351 0.872099 x

x Se 4 0.067368 0.666695 0.375001 x

x Se 5 0.266898 0.664990 0.124713 x

x Se 6 0.332191 0.338475 0.627303 x

x Se 7 0.332342 0.340663 0.872428 x

x Se 8 0.266574 0.664128 0.374542 x

x Se 9 0.467478 0.654431 0.127839 x

x Se 10 0.532830 0.342793 0.626134 x

x Se 11 0.532521 0.345643 0.872152 x

x Se 12 0.467161 0.657285 0.373879 x

x Se 13 0.667673 0.659430 0.127549 x

x Se 14 0.733430 0.335793 0.625467 x

x Se 15 0.733096 0.334894 0.875289 x

x Se 16 0.667828 0.661651 0.372736 x

x Se 17 0.867699 0.658474 0.127924 x

x Se 18 0.932642 0.333388 0.625007 x

x Se 19 0.932775 0.334028 0.874533 x

x Se 20 0.867890 0.659968 0.372408 x

x Nb 1 0.002312 0.008171 0.249983 x

x Nb 2 -0.002363 -0.007940 0.750011 x

x Nb 3 -0.000019 -0.000228 0.000033 x

x Nb 4 -0.000028 -0.000254 0.499949 x

x Nb 5 0.197360 -0.006483 0.249918 x

x Nb 6 0.201420 0.012775 0.749486 x

x Nb 7 0.199415 0.000586 -0.000086 x

x Nb 8 0.200163 0.003069 0.500278 x

x Nb 9 0.399572 -0.009382 0.250478 x

x Nb 10 0.400037 0.004091 0.749720 x

x Nb 11 0.399883 0.003537 -0.001369 x

x Nb 12 0.398814 0.000103 0.501155 x

x Nb 13 0.599912 -0.004225 0.250276 x

x Nb 14 0.600469 0.009704 0.749508 x

x Nb 15 0.600095 -0.003673 0.001405 x

x Nb 16 0.601203 -0.000084 0.498840 x

x Nb 17 0.798605 -0.012977 0.250519 x

x Nb 18 0.802675 0.006247 0.750083 x

x Nb 19 0.800631 -0.000207 0.000003 x

x Nb 20 0.799849 -0.002821 0.499776 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597759E+004 21613.17 <-- SCF

1 -3.62601314E+004 8.88880531E-003 21640.14 <-- SCF

2 -3.62601492E+004 4.43828848E-004 21668.80 <-- SCF

3 -3.62600838E+004 -1.63531166E-003 21694.91 <-- SCF

4 -3.62598648E+004 -5.47423773E-003 21720.73 <-- SCF

5 -3.62598696E+004 1.19672925E-004 21746.80 <-- SCF

6 -3.62598680E+004 -3.94814970E-005 21770.97 <-- SCF

7 -3.62598678E+004 -5.27421801E-006 21793.38 <-- SCF

8 -3.62598679E+004 2.21941178E-006 21811.56 <-- SCF

9 -3.62598679E+004 5.27776031E-007 21829.08 <-- SCF

10 -3.62598679E+004 2.42225325E-007 21845.98 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.86791397 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01400 0.00330 0.00249 \*

\* Se 2 0.00058 0.01112 0.07414 \*

\* Se 3 -0.02017 -0.03093 -0.07797 \*

\* Se 4 0.03011 0.02571 0.01603 \*

\* Se 5 -0.00977 -0.02763 0.04490 \*

\* Se 6 0.04063 0.06061 0.07481 \*

\* Se 7 0.00608 0.03247 -0.01834 \*

\* Se 8 -0.02501 -0.02714 -0.04783 \*

\* Se 9 0.03307 0.02874 0.07236 \*

\* Se 10 0.02893 -0.04156 -0.02098 \*

\* Se 11 -0.03208 -0.02932 -0.07210 \*

\* Se 12 -0.02999 0.04453 0.02350 \*

\* Se 13 -0.00746 -0.03520 0.02134 \*

\* Se 14 0.02712 0.02449 0.04918 \*

\* Se 15 0.01153 0.02500 -0.04460 \*

\* Se 16 -0.04750 -0.06031 -0.08045 \*

\* Se 17 0.02207 0.03269 0.07654 \*

\* Se 18 -0.03057 -0.02433 -0.01979 \*

\* Se 19 -0.01405 -0.00144 -0.00379 \*

\* Se 20 0.00042 -0.00898 -0.07144 \*

\* Nb 1 0.06816 -0.02323 -0.01123 \*

\* Nb 2 -0.06552 0.01674 0.01057 \*

\* Nb 3 -0.00038 0.00185 -0.00282 \*

\* Nb 4 0.00150 0.00251 0.00305 \*

\* Nb 5 0.02829 0.00324 -0.01868 \*

\* Nb 6 0.05439 -0.00875 -0.00113 \*

\* Nb 7 0.00817 0.02441 -0.05711 \*

\* Nb 8 0.04985 0.03426 0.04534 \*

\* Nb 9 -0.03171 0.00287 0.00692 \*

\* Nb 10 0.05854 0.08352 0.03306 \*

\* Nb 11 0.04297 -0.00912 0.04245 \*

\* Nb 12 -0.04515 -0.05223 -0.04723 \*

\* Nb 13 -0.05462 -0.08158 -0.03106 \*

\* Nb 14 0.02804 -0.00602 -0.00711 \*

\* Nb 15 -0.04222 0.00986 -0.04490 \*

\* Nb 16 0.04485 0.05314 0.04913 \*

\* Nb 17 -0.05664 0.01154 0.00130 \*

\* Nb 18 -0.02845 -0.00032 0.01898 \*

\* Nb 19 -0.00821 -0.02722 0.06174 \*

\* Nb 20 -0.04979 -0.03728 -0.04926 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.185368 0.094653 -0.019577 \*

\* y 0.094653 -0.124102 -0.245495 \*

\* z -0.019577 -0.245495 -0.035024 \*

\* \*

\* Pressure: 0.1148 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000035 | -36259.865430 | <-- min BFGS

| trial step | 1.000000 | 0.000028 | -36259.866497 | <-- min BFGS

| line step | 5.117153 | -7.473E-006 | -36259.867938 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 29 with enthalpy= -3.62598679E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 6.267986E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.112000E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.721801E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.454951E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 30 ...

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Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000092 | -36259.867938 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 30 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8823427 -8.3277389 0.0033588 0.4200543 -0.0038177 0.0001242

0.0307576 3.3840902 -0.0034821 1.0336912 1.8472905 0.0018175

-0.0042117 -0.0113198 13.9007094 0.0001574 0.0004637 0.4520051

Lattice parameters(A) Cell Angles

a = 17.053896 alpha = 90.105767

b = 3.384232 beta = 89.981081

c = 13.900715 gamma = 118.709400

Current cell volume = 703.643957 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067252 0.666118 0.125446 x

x Se 2 0.132066 0.340031 0.627704 x

x Se 3 0.132252 0.341510 0.871982 x

x Se 4 0.067392 0.666797 0.375018 x

x Se 5 0.266895 0.664925 0.124686 x

x Se 6 0.332232 0.338798 0.627414 x

x Se 7 0.332360 0.340988 0.872369 x

x Se 8 0.266552 0.664035 0.374512 x

x Se 9 0.467492 0.654141 0.127921 x

x Se 10 0.532843 0.343045 0.626180 x

x Se 11 0.532507 0.345938 0.872069 x

x Se 12 0.467149 0.657042 0.373836 x

x Se 13 0.667655 0.659102 0.127612 x

x Se 14 0.733453 0.335884 0.625498 x

x Se 15 0.733100 0.334953 0.875316 x

x Se 16 0.667786 0.661330 0.372623 x

x Se 17 0.867717 0.658311 0.128040 x

x Se 18 0.932619 0.333290 0.624989 x

x Se 19 0.932759 0.333964 0.874543 x

x Se 20 0.867914 0.659790 0.372278 x

x Nb 1 0.002441 0.008561 0.249981 x

x Nb 2 -0.002493 -0.008328 0.750013 x

x Nb 3 -0.000020 -0.000234 0.000033 x

x Nb 4 -0.000028 -0.000260 0.499948 x

x Nb 5 0.197300 -0.006657 0.249905 x

x Nb 6 0.201469 0.013230 0.749468 x

x Nb 7 0.199399 0.000669 -0.000122 x

x Nb 8 0.200184 0.003271 0.500309 x

x Nb 9 0.399545 -0.009810 0.250504 x

x Nb 10 0.400051 0.004408 0.749705 x

x Nb 11 0.399898 0.003667 -0.001413 x

x Nb 12 0.398765 0.000000 0.501190 x

x Nb 13 0.599898 -0.004540 0.250292 x

x Nb 14 0.600497 0.010135 0.749481 x

x Nb 15 0.600078 -0.003808 0.001449 x

x Nb 16 0.601253 0.000020 0.498806 x

x Nb 17 0.798556 -0.013439 0.250537 x

x Nb 18 0.802736 0.006417 0.750095 x

x Nb 19 0.800649 -0.000279 0.000039 x

x Nb 20 0.799828 -0.003016 0.499745 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598443E+004 21949.67 <-- SCF

1 -3.62599035E+004 1.48004280E-003 21976.23 <-- SCF

2 -3.62599065E+004 7.36310173E-005 22004.16 <-- SCF

3 -3.62598880E+004 -4.61212234E-004 22030.59 <-- SCF

4 -3.62598706E+004 -4.36622167E-004 22055.94 <-- SCF

5 -3.62598706E+004 -1.17239118E-007 22080.72 <-- SCF

6 -3.62598701E+004 -1.01570420E-005 22100.70 <-- SCF

7 -3.62598701E+004 -6.49037262E-007 22119.12 <-- SCF

8 -3.62598701E+004 5.19084783E-007 22136.02 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.87013909 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01269 0.00354 -0.01229 \*

\* Se 2 0.00801 0.01135 0.04134 \*

\* Se 3 -0.01669 -0.03443 -0.05988 \*

\* Se 4 0.02957 0.02643 0.02464 \*

\* Se 5 -0.01105 -0.02763 0.03876 \*

\* Se 6 0.03128 0.06742 0.05732 \*

\* Se 7 0.00919 0.02081 -0.00169 \*

\* Se 8 -0.02271 -0.02274 -0.04072 \*

\* Se 9 0.02514 0.04213 0.04908 \*

\* Se 10 0.01893 -0.03950 -0.03141 \*

\* Se 11 -0.02442 -0.04412 -0.04789 \*

\* Se 12 -0.02092 0.04275 0.03457 \*

\* Se 13 -0.01042 -0.02447 0.00465 \*

\* Se 14 0.02486 0.02030 0.04243 \*

\* Se 15 0.01308 0.02524 -0.03858 \*

\* Se 16 -0.03717 -0.06726 -0.06384 \*

\* Se 17 0.01929 0.03698 0.05873 \*

\* Se 18 -0.03018 -0.02505 -0.02846 \*

\* Se 19 -0.01287 -0.00168 0.01082 \*

\* Se 20 -0.00709 -0.00871 -0.03986 \*

\* Nb 1 0.06864 -0.02384 -0.01428 \*

\* Nb 2 -0.06580 0.01707 0.01364 \*

\* Nb 3 -0.00040 0.00202 -0.00309 \*

\* Nb 4 0.00159 0.00278 0.00333 \*

\* Nb 5 0.02799 0.00232 -0.02301 \*

\* Nb 6 0.05941 -0.01264 0.00529 \*

\* Nb 7 0.00797 0.02757 -0.06148 \*

\* Nb 8 0.05332 0.03469 0.04822 \*

\* Nb 9 -0.03009 0.00784 0.00334 \*

\* Nb 10 0.05810 0.08689 0.03695 \*

\* Nb 11 0.04337 -0.01011 0.04378 \*

\* Nb 12 -0.04319 -0.05284 -0.04860 \*

\* Nb 13 -0.05391 -0.08493 -0.03476 \*

\* Nb 14 0.02621 -0.01104 -0.00349 \*

\* Nb 15 -0.04280 0.01104 -0.04625 \*

\* Nb 16 0.04284 0.05401 0.05048 \*

\* Nb 17 -0.06225 0.01567 -0.00491 \*

\* Nb 18 -0.02812 0.00077 0.02328 \*

\* Nb 19 -0.00793 -0.03056 0.06620 \*

\* Nb 20 -0.05345 -0.03802 -0.05235 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.117307 0.088972 -0.025536 \*

\* y 0.088972 -0.075502 -0.188517 \*

\* z -0.025536 -0.188517 -0.043396 \*

\* \*

\* Pressure: 0.0787 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000092 | -36259.867938 | <-- min BFGS

| trial step | 1.000000 | 0.000068 | -36259.870153 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 30 with line minimization (lambda= 3.894702)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8966261 -8.3307295 -0.0030666 0.4196432 -0.0038314 0.0001384

0.0309113 3.3855849 -0.0011569 1.0325939 1.8464365 0.0008449

-0.0046156 -0.0037770 13.8945795 0.0001786 0.0001529 0.4522042

Lattice parameters(A) Cell Angles

a = 17.067822 alpha = 90.035325

b = 3.385726 beta = 90.019304

c = 13.894581 gamma = 118.692374

Current cell volume = 704.334232 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067299 0.666310 0.125418 x

x Se 2 0.131993 0.340526 0.628086 x

x Se 3 0.132196 0.341970 0.871643 x

x Se 4 0.067459 0.667093 0.375067 x

x Se 5 0.266886 0.664736 0.124606 x

x Se 6 0.332350 0.339733 0.627736 x

x Se 7 0.332409 0.341931 0.872199 x

x Se 8 0.266490 0.663766 0.374424 x

x Se 9 0.467533 0.653301 0.128157 x

x Se 10 0.532878 0.343774 0.626311 x

x Se 11 0.532467 0.346793 0.871829 x

x Se 12 0.467113 0.656338 0.373710 x

x Se 13 0.667604 0.658151 0.127792 x

x Se 14 0.733520 0.336148 0.625588 x

x Se 15 0.733110 0.335124 0.875396 x

x Se 16 0.667664 0.660402 0.372296 x

x Se 17 0.867769 0.657838 0.128375 x

x Se 18 0.932552 0.333009 0.624938 x

x Se 19 0.932713 0.333780 0.874571 x

x Se 20 0.867985 0.659274 0.371903 x

x Nb 1 0.002817 0.009689 0.249974 x

x Nb 2 -0.002871 -0.009451 0.750017 x

x Nb 3 -0.000022 -0.000253 0.000032 x

x Nb 4 -0.000031 -0.000280 0.499946 x

x Nb 5 0.197127 -0.007159 0.249869 x

x Nb 6 0.201610 0.014550 0.749414 x

x Nb 7 0.199351 0.000911 -0.000229 x

x Nb 8 0.200246 0.003855 0.500400 x

x Nb 9 0.399466 -0.011049 0.250581 x

x Nb 10 0.400092 0.005325 0.749662 x

x Nb 11 0.399945 0.004043 -0.001539 x

x Nb 12 0.398623 -0.000297 0.501291 x

x Nb 13 0.599856 -0.005450 0.250336 x

x Nb 14 0.600576 0.011383 0.749403 x

x Nb 15 0.600030 -0.004196 0.001575 x

x Nb 16 0.601397 0.000321 0.498707 x

x Nb 17 0.798414 -0.014777 0.250589 x

x Nb 18 0.802913 0.006908 0.750131 x

x Nb 19 0.800702 -0.000488 0.000142 x

x Nb 20 0.799769 -0.003581 0.499655 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62596549E+004 22239.44 <-- SCF

1 -3.62601642E+004 1.27314812E-002 22266.19 <-- SCF

2 -3.62601897E+004 6.38358594E-004 22295.38 <-- SCF

3 -3.62600303E+004 -3.98436510E-003 22321.67 <-- SCF

4 -3.62598757E+004 -3.86407065E-003 22347.55 <-- SCF

5 -3.62598748E+004 -2.30659583E-005 22373.31 <-- SCF

6 -3.62598725E+004 -5.86143499E-005 22398.48 <-- SCF

7 -3.62598723E+004 -3.60893628E-006 22421.75 <-- SCF

8 -3.62598724E+004 2.26837845E-006 22440.88 <-- SCF

9 -3.62598724E+004 -1.33285777E-006 22458.94 <-- SCF

10 -3.62598724E+004 -5.99256669E-009 22476.41 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.87237255 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01467 0.00444 -0.03703 \*

\* Se 2 0.02437 0.01280 -0.02937 \*

\* Se 3 -0.01617 -0.05095 -0.02215 \*

\* Se 4 0.03237 0.02594 0.04743 \*

\* Se 5 -0.01251 -0.02588 0.03437 \*

\* Se 6 0.00807 0.08303 -0.02582 \*

\* Se 7 0.01628 -0.02828 0.06443 \*

\* Se 8 -0.02212 -0.01031 -0.02171 \*

\* Se 9 -0.00611 0.10195 -0.02688 \*

\* Se 10 -0.00164 -0.02930 -0.04952 \*

\* Se 11 0.00683 -0.10624 0.03008 \*

\* Se 12 -0.00290 0.03280 0.05489 \*

\* Se 13 -0.01734 0.02355 -0.06350 \*

\* Se 14 0.02382 0.00840 0.02422 \*

\* Se 15 0.01429 0.02414 -0.03342 \*

\* Se 16 -0.01052 -0.08599 0.01743 \*

\* Se 17 0.02136 0.05587 0.01969 \*

\* Se 18 -0.03314 -0.02464 -0.05193 \*

\* Se 19 -0.01520 -0.00264 0.03600 \*

\* Se 20 -0.02326 -0.00787 0.02723 \*

\* Nb 1 0.05902 -0.02817 -0.00776 \*

\* Nb 2 -0.05640 0.02064 0.00751 \*

\* Nb 3 -0.00029 0.00271 -0.00304 \*

\* Nb 4 0.00187 0.00350 0.00358 \*

\* Nb 5 0.04275 0.00175 -0.02510 \*

\* Nb 6 0.05958 -0.02635 0.01672 \*

\* Nb 7 0.01525 0.02724 -0.06132 \*

\* Nb 8 0.05345 0.03127 0.05099 \*

\* Nb 9 -0.03121 0.02684 -0.01002 \*

\* Nb 10 0.06764 0.08858 0.04784 \*

\* Nb 11 0.04663 -0.01693 0.06162 \*

\* Nb 12 -0.03733 -0.05178 -0.05981 \*

\* Nb 13 -0.06350 -0.08670 -0.04548 \*

\* Nb 14 0.02652 -0.03024 0.01042 \*

\* Nb 15 -0.04583 0.01818 -0.06400 \*

\* Nb 16 0.03655 0.05339 0.06182 \*

\* Nb 17 -0.06267 0.03008 -0.01577 \*

\* Nb 18 -0.04305 0.00188 0.02565 \*

\* Nb 19 -0.01605 -0.03133 0.06711 \*

\* Nb 20 -0.05406 -0.03540 -0.05539 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.076904 0.085348 -0.039505 \*

\* y 0.085348 0.042210 -0.023060 \*

\* z -0.039505 -0.023060 -0.031106 \*

\* \*

\* Pressure: -0.0293 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000092 | -36259.867938 | <-- min BFGS

| trial step | 1.000000 | 0.000068 | -36259.870153 | <-- min BFGS

| line step | 3.894702 | -8.242E-006 | -36259.872470 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 30 with enthalpy= -3.62598725E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.133180E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.212916E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.909884E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 8.534775E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 31 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000130 | -36259.872470 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 31 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8975541 -8.3366408 -0.0062339 0.4197234 -0.0036386 0.0001703

0.0293475 3.3852914 -0.0004439 1.0336138 1.8470645 0.0006180

-0.0056532 -0.0014860 13.8973071 0.0002213 0.0000574 0.4521154

Lattice parameters(A) Cell Angles

a = 17.071518 alpha = 90.013841

b = 3.385419 beta = 90.038270

c = 13.897308 gamma = 118.734590

Current cell volume = 704.276751 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067325 0.666457 0.125325 x

x Se 2 0.131933 0.340265 0.628174 x

x Se 3 0.132134 0.341476 0.871651 x

x Se 4 0.067502 0.667291 0.375151 x

x Se 5 0.266859 0.664539 0.124513 x

x Se 6 0.332510 0.340232 0.627744 x

x Se 7 0.332445 0.342098 0.872412 x

x Se 8 0.266462 0.663657 0.374430 x

x Se 9 0.467598 0.653935 0.128008 x

x Se 10 0.532863 0.343338 0.626276 x

x Se 11 0.532403 0.346166 0.871974 x

x Se 12 0.467128 0.656795 0.373750 x

x Se 13 0.667563 0.657957 0.127596 x

x Se 14 0.733553 0.336266 0.625582 x

x Se 15 0.733141 0.335317 0.875489 x

x Se 16 0.667496 0.659891 0.372276 x

x Se 17 0.867830 0.658341 0.128358 x

x Se 18 0.932508 0.332817 0.624849 x

x Se 19 0.932685 0.333626 0.874667 x

x Se 20 0.868045 0.659533 0.371828 x

x Nb 1 0.002828 0.009383 0.249981 x

x Nb 2 -0.002876 -0.009171 0.750008 x

x Nb 3 -0.000022 -0.000241 0.000026 x

x Nb 4 -0.000029 -0.000264 0.499951 x

x Nb 5 0.197182 -0.006972 0.249852 x

x Nb 6 0.201679 0.014744 0.749412 x

x Nb 7 0.199387 0.001195 -0.000323 x

x Nb 8 0.200304 0.004189 0.500444 x

x Nb 9 0.399423 -0.011315 0.250636 x

x Nb 10 0.400169 0.006117 0.749637 x

x Nb 11 0.399994 0.004020 -0.001444 x

x Nb 12 0.398586 -0.000681 0.501184 x

x Nb 13 0.599787 -0.006210 0.250363 x

x Nb 14 0.600614 0.011610 0.749348 x

x Nb 15 0.599980 -0.004168 0.001474 x

x Nb 16 0.601433 0.000702 0.498816 x

x Nb 17 0.798340 -0.014963 0.250589 x

x Nb 18 0.802857 0.006740 0.750146 x

x Nb 19 0.800667 -0.000787 0.000243 x

x Nb 20 0.799711 -0.003925 0.499603 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598265E+004 22579.84 <-- SCF

1 -3.62599977E+004 4.27833044E-003 22607.28 <-- SCF

2 -3.62600076E+004 2.47066272E-004 22635.58 <-- SCF

3 -3.62600019E+004 -1.41142500E-004 22662.44 <-- SCF

4 -3.62598689E+004 -3.32456925E-003 22688.25 <-- SCF

5 -3.62598783E+004 2.34948094E-004 22715.28 <-- SCF

6 -3.62598762E+004 -5.21508948E-005 22740.77 <-- SCF

7 -3.62598749E+004 -3.37532818E-005 22762.62 <-- SCF

8 -3.62598748E+004 -2.52922416E-006 22782.27 <-- SCF

9 -3.62598748E+004 1.10064867E-006 22800.50 <-- SCF

10 -3.62598749E+004 1.06094911E-006 22817.78 <-- SCF

11 -3.62598749E+004 7.01280032E-007 22834.27 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.87490120 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01402 0.00883 -0.03292 \*

\* Se 2 0.04723 0.02113 -0.03633 \*

\* Se 3 0.00175 -0.02925 -0.03008 \*

\* Se 4 0.02988 0.02339 0.03561 \*

\* Se 5 -0.00694 -0.01476 0.04254 \*

\* Se 6 -0.03417 0.09204 -0.01074 \*

\* Se 7 0.00210 -0.02760 -0.02558 \*

\* Se 8 -0.01761 -0.00207 -0.02390 \*

\* Se 9 -0.02839 0.06391 0.03352 \*

\* Se 10 0.01961 -0.02543 -0.05441 \*

\* Se 11 0.02858 -0.06921 -0.02885 \*

\* Se 12 -0.02521 0.02864 0.05988 \*

\* Se 13 -0.00341 0.02441 0.01915 \*

\* Se 14 0.01818 0.00037 0.02657 \*

\* Se 15 0.00799 0.01398 -0.04094 \*

\* Se 16 0.03537 -0.09621 0.00586 \*

\* Se 17 0.00381 0.03291 0.02964 \*

\* Se 18 -0.03023 -0.02231 -0.04000 \*

\* Se 19 -0.01437 -0.00752 0.03166 \*

\* Se 20 -0.04601 -0.01489 0.03188 \*

\* Nb 1 0.07161 -0.01975 -0.01615 \*

\* Nb 2 -0.07078 0.01361 0.01617 \*

\* Nb 3 -0.00023 0.00248 -0.00246 \*

\* Nb 4 0.00195 0.00335 0.00306 \*

\* Nb 5 0.02973 -0.00702 -0.03146 \*

\* Nb 6 0.06319 -0.02861 0.02343 \*

\* Nb 7 0.00433 0.01891 -0.05542 \*

\* Nb 8 0.05347 0.02496 0.05617 \*

\* Nb 9 -0.01793 0.03983 -0.02955 \*

\* Nb 10 0.05133 0.07239 0.07011 \*

\* Nb 11 0.04183 -0.01170 0.05329 \*

\* Nb 12 -0.03479 -0.04158 -0.04793 \*

\* Nb 13 -0.04901 -0.07087 -0.06794 \*

\* Nb 14 0.01385 -0.04222 0.02988 \*

\* Nb 15 -0.04062 0.01283 -0.05489 \*

\* Nb 16 0.03452 0.04344 0.04965 \*

\* Nb 17 -0.06470 0.03168 -0.02143 \*

\* Nb 18 -0.02936 0.00981 0.03217 \*

\* Nb 19 -0.00578 -0.02283 0.06051 \*

\* Nb 20 -0.05481 -0.02903 -0.05977 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.047993 0.037350 -0.065576 \*

\* y 0.037350 0.026107 0.022318 \*

\* z -0.065576 0.022318 0.003319 \*

\* \*

\* Pressure: -0.0258 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000130 | -36259.872470 | <-- min BFGS

| trial step | 1.000000 | 0.000055 | -36259.874959 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 31 with line minimization (lambda= 1.722958)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8982250 -8.3409144 -0.0085238 0.4197816 -0.0034992 0.0001934

0.0282169 3.3850791 0.0000715 1.0343517 1.8475193 0.0004539

-0.0064034 0.0001702 13.8992790 0.0002521 -0.0000117 0.4520513

Lattice parameters(A) Cell Angles

a = 17.074192 alpha = 89.998308

b = 3.385197 beta = 90.051978

c = 13.899281 gamma = 118.765112

Current cell volume = 704.234945 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067343 0.666563 0.125258 x

x Se 2 0.131890 0.340076 0.628237 x

x Se 3 0.132090 0.341118 0.871657 x

x Se 4 0.067533 0.667434 0.375211 x

x Se 5 0.266839 0.664397 0.124446 x

x Se 6 0.332627 0.340593 0.627749 x

x Se 7 0.332471 0.342219 0.872566 x

x Se 8 0.266441 0.663578 0.374435 x

x Se 9 0.467646 0.654394 0.127900 x

x Se 10 0.532853 0.343022 0.626251 x

x Se 11 0.532356 0.345712 0.872079 x

x Se 12 0.467139 0.657125 0.373778 x

x Se 13 0.667534 0.657817 0.127454 x

x Se 14 0.733578 0.336351 0.625578 x

x Se 15 0.733163 0.335457 0.875556 x

x Se 16 0.667375 0.659521 0.372262 x

x Se 17 0.867873 0.658705 0.128345 x

x Se 18 0.932476 0.332679 0.624786 x

x Se 19 0.932666 0.333516 0.874735 x

x Se 20 0.868089 0.659721 0.371775 x

x Nb 1 0.002836 0.009162 0.249986 x

x Nb 2 -0.002879 -0.008969 0.750002 x

x Nb 3 -0.000022 -0.000233 0.000022 x

x Nb 4 -0.000028 -0.000252 0.499954 x

x Nb 5 0.197222 -0.006836 0.249840 x

x Nb 6 0.201729 0.014884 0.749411 x

x Nb 7 0.199414 0.001401 -0.000390 x

x Nb 8 0.200346 0.004430 0.500475 x

x Nb 9 0.399391 -0.011507 0.250675 x

x Nb 10 0.400225 0.006690 0.749619 x

x Nb 11 0.400030 0.004004 -0.001376 x

x Nb 12 0.398559 -0.000959 0.501106 x

x Nb 13 0.599737 -0.006760 0.250382 x

x Nb 14 0.600642 0.011774 0.749309 x

x Nb 15 0.599945 -0.004148 0.001401 x

x Nb 16 0.601459 0.000979 0.498896 x

x Nb 17 0.798286 -0.015098 0.250588 x

x Nb 18 0.802817 0.006618 0.750158 x

x Nb 19 0.800641 -0.001003 0.000317 x

x Nb 20 0.799670 -0.004173 0.499566 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598492E+004 22937.58 <-- SCF

1 -3.62599682E+004 2.97407691E-003 22965.02 <-- SCF

2 -3.62599754E+004 1.80955924E-004 22992.59 <-- SCF

3 -3.62599835E+004 2.02332930E-004 23019.25 <-- SCF

4 -3.62598696E+004 -2.84829394E-003 23045.23 <-- SCF

5 -3.62598776E+004 1.99317446E-004 23071.95 <-- SCF

6 -3.62598764E+004 -2.87180378E-005 23096.73 <-- SCF

7 -3.62598754E+004 -2.54525789E-005 23118.34 <-- SCF

8 -3.62598753E+004 -2.20518844E-006 23137.25 <-- SCF

9 -3.62598754E+004 1.38760479E-006 23154.98 <-- SCF

10 -3.62598754E+004 1.33854314E-006 23172.61 <-- SCF

11 -3.62598755E+004 1.04175084E-006 23188.88 <-- SCF

12 -3.62598755E+004 7.17364618E-007 23205.05 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.87550542 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01378 0.01209 -0.02743 \*

\* Se 2 0.06327 0.02617 -0.04394 \*

\* Se 3 0.01459 -0.01583 -0.03401 \*

\* Se 4 0.02814 0.02126 0.02881 \*

\* Se 5 -0.00318 -0.00543 0.04746 \*

\* Se 6 -0.05895 0.09919 0.00113 \*

\* Se 7 -0.01222 -0.03077 -0.08702 \*

\* Se 8 -0.01475 0.00440 -0.02296 \*

\* Se 9 -0.04665 0.04056 0.07425 \*

\* Se 10 0.03533 -0.02347 -0.05894 \*

\* Se 11 0.04639 -0.04538 -0.06897 \*

\* Se 12 -0.04142 0.02603 0.06417 \*

\* Se 13 0.01040 0.02812 0.07641 \*

\* Se 14 0.01463 -0.00599 0.02574 \*

\* Se 15 0.00374 0.00540 -0.04527 \*

\* Se 16 0.06152 -0.10429 -0.00360 \*

\* Se 17 -0.00862 0.01868 0.03496 \*

\* Se 18 -0.02802 -0.02033 -0.03324 \*

\* Se 19 -0.01393 -0.01121 0.02600 \*

\* Se 20 -0.06179 -0.01894 0.03790 \*

\* Nb 1 0.08548 -0.01400 -0.01894 \*

\* Nb 2 -0.08572 0.00883 0.01916 \*

\* Nb 3 -0.00009 0.00230 -0.00197 \*

\* Nb 4 0.00211 0.00325 0.00272 \*

\* Nb 5 0.02125 -0.01409 -0.03428 \*

\* Nb 6 0.06685 -0.03028 0.02817 \*

\* Nb 7 0.00056 0.01449 -0.05124 \*

\* Nb 8 0.05217 0.02124 0.05791 \*

\* Nb 9 -0.01015 0.05012 -0.04341 \*

\* Nb 10 0.04259 0.06190 0.08437 \*

\* Nb 11 0.03940 -0.00923 0.04903 \*

\* Nb 12 -0.03294 -0.03495 -0.04086 \*

\* Nb 13 -0.04131 -0.06070 -0.08249 \*

\* Nb 14 0.00642 -0.05184 0.04376 \*

\* Nb 15 -0.03783 0.01024 -0.05020 \*

\* Nb 16 0.03297 0.03701 0.04235 \*

\* Nb 17 -0.06748 0.03280 -0.02544 \*

\* Nb 18 -0.02025 0.01625 0.03513 \*

\* Nb 19 -0.00235 -0.01831 0.05587 \*

\* Nb 20 -0.05395 -0.02532 -0.06113 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.029352 0.008507 -0.088060 \*

\* y 0.008507 0.024888 0.051492 \*

\* z -0.088060 0.051492 0.027965 \*

\* \*

\* Pressure: -0.0274 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000130 | -36259.872470 | <-- min BFGS

| trial step | 1.000000 | 0.000055 | -36259.874959 | <-- min BFGS

| line step | 1.722958 | 5.018E-006 | -36259.875559 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 31 with enthalpy= -3.62598756E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.722246E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.211366E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 5.214283E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 8.805970E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 32 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000036 | -36259.875559 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 32 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8971326 -8.3423481 -0.0083841 0.4198621 -0.0034097 0.0001998

0.0274852 3.3844135 -0.0000934 1.0349315 1.8481016 0.0005400

-0.0066174 -0.0003560 13.9013003 0.0002602 0.0000104 0.4519856

Lattice parameters(A) Cell Angles

a = 17.073939 alpha = 90.003271

b = 3.384525 beta = 90.051215

c = 13.901302 gamma = 118.783391

Current cell volume = 704.063796 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067369 0.666722 0.125137 x

x Se 2 0.131865 0.340351 0.628381 x

x Se 3 0.132072 0.341329 0.871538 x

x Se 4 0.067570 0.667650 0.375344 x

x Se 5 0.266825 0.664298 0.124312 x

x Se 6 0.332740 0.341252 0.627852 x

x Se 7 0.332529 0.342801 0.872567 x

x Se 8 0.266391 0.663438 0.374461 x

x Se 9 0.467669 0.654009 0.127944 x

x Se 10 0.532879 0.343369 0.626230 x

x Se 11 0.532334 0.346105 0.872032 x

x Se 12 0.467112 0.656794 0.373804 x

x Se 13 0.667474 0.657227 0.127460 x

x Se 14 0.733631 0.336489 0.625554 x

x Se 15 0.733179 0.335545 0.875691 x

x Se 16 0.667259 0.658865 0.372155 x

x Se 17 0.867888 0.658489 0.128461 x

x Se 18 0.932438 0.332472 0.624651 x

x Se 19 0.932640 0.333359 0.874858 x

x Se 20 0.868113 0.659436 0.371636 x

x Nb 1 0.003093 0.009929 0.249981 x

x Nb 2 -0.003137 -0.009738 0.750005 x

x Nb 3 -0.000024 -0.000242 0.000021 x

x Nb 4 -0.000029 -0.000261 0.499953 x

x Nb 5 0.197144 -0.007093 0.249811 x

x Nb 6 0.201815 0.015639 0.749381 x

x Nb 7 0.199388 0.001581 -0.000476 x

x Nb 8 0.200393 0.004833 0.500546 x

x Nb 9 0.399336 -0.012261 0.250722 x

x Nb 10 0.400261 0.007321 0.749594 x

x Nb 11 0.400072 0.004219 -0.001447 x

x Nb 12 0.398473 -0.001201 0.501165 x

x Nb 13 0.599702 -0.007383 0.250407 x

x Nb 14 0.600697 0.012529 0.749261 x

x Nb 15 0.599901 -0.004370 0.001472 x

x Nb 16 0.601546 0.001224 0.498839 x

x Nb 17 0.798200 -0.015863 0.250617 x

x Nb 18 0.802896 0.006872 0.750186 x

x Nb 19 0.800671 -0.001166 0.000401 x

x Nb 20 0.799624 -0.004567 0.499494 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598059E+004 23308.42 <-- SCF

1 -3.62599422E+004 3.40728014E-003 23333.72 <-- SCF

2 -3.62599517E+004 2.37650216E-004 23362.09 <-- SCF

3 -3.62599053E+004 -1.16070833E-003 23388.89 <-- SCF

4 -3.62598783E+004 -6.75670257E-004 23414.80 <-- SCF

5 -3.62598773E+004 -2.38612932E-005 23440.98 <-- SCF

6 -3.62598764E+004 -2.32079087E-005 23463.19 <-- SCF

7 -3.62598763E+004 -3.49367520E-006 23483.31 <-- SCF

8 -3.62598763E+004 6.11849845E-007 23501.45 <-- SCF

9 -3.62598763E+004 1.10629228E-007 23517.72 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.87629246 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01383 0.02187 -0.02882 \*

\* Se 2 0.06417 0.01667 -0.04978 \*

\* Se 3 0.00818 -0.02611 -0.03309 \*

\* Se 4 0.02877 0.02016 0.02410 \*

\* Se 5 -0.00746 0.00827 0.04540 \*

\* Se 6 -0.06212 0.09085 -0.01746 \*

\* Se 7 -0.01718 -0.05581 -0.09765 \*

\* Se 8 -0.01404 0.00881 -0.02128 \*

\* Se 9 -0.06402 0.06572 0.06467 \*

\* Se 10 0.03849 -0.02453 -0.06782 \*

\* Se 11 0.06373 -0.07237 -0.05788 \*

\* Se 12 -0.04551 0.02720 0.07323 \*

\* Se 13 0.01541 0.05380 0.08454 \*

\* Se 14 0.01414 -0.01036 0.02412 \*

\* Se 15 0.00815 -0.00707 -0.04239 \*

\* Se 16 0.06489 -0.09846 0.01523 \*

\* Se 17 -0.00139 0.02960 0.03351 \*

\* Se 18 -0.02841 -0.01933 -0.02934 \*

\* Se 19 -0.01403 -0.02119 0.02760 \*

\* Se 20 -0.06249 -0.00782 0.04361 \*

\* Nb 1 0.07593 -0.02061 -0.01795 \*

\* Nb 2 -0.07648 0.01543 0.01826 \*

\* Nb 3 0.00006 0.00256 -0.00187 \*

\* Nb 4 0.00239 0.00358 0.00282 \*

\* Nb 5 0.02175 -0.01653 -0.03543 \*

\* Nb 6 0.06807 -0.03398 0.03303 \*

\* Nb 7 0.00181 0.01426 -0.05382 \*

\* Nb 8 0.05149 0.02024 0.05928 \*

\* Nb 9 -0.00754 0.05953 -0.04872 \*

\* Nb 10 0.04438 0.06486 0.09025 \*

\* Nb 11 0.03816 -0.01088 0.05813 \*

\* Nb 12 -0.02985 -0.03395 -0.04724 \*

\* Nb 13 -0.04334 -0.06373 -0.08829 \*

\* Nb 14 0.00349 -0.06115 0.04929 \*

\* Nb 15 -0.03624 0.01195 -0.05929 \*

\* Nb 16 0.02997 0.03627 0.04864 \*

\* Nb 17 -0.06854 0.03671 -0.02989 \*

\* Nb 18 -0.02072 0.01874 0.03641 \*

\* Nb 19 -0.00407 -0.01835 0.05866 \*

\* Nb 20 -0.05384 -0.02484 -0.06274 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.007967 -0.018833 -0.088749 \*

\* y -0.018833 -0.024025 0.041605 \*

\* z -0.088749 0.041605 0.010292 \*

\* \*

\* Pressure: 0.0072 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000036 | -36259.875559 | <-- min BFGS

| trial step | 1.000000 | 0.000013 | -36259.876337 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 32 with line minimization (lambda= 1.586906)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8964914 -8.3431896 -0.0083021 0.4199094 -0.0033572 0.0002035

0.0270558 3.3840228 -0.0001903 1.0352720 1.8484436 0.0005905

-0.0067431 -0.0006649 13.9024866 0.0002649 0.0000233 0.4519470

Lattice parameters(A) Cell Angles

a = 17.073791 alpha = 90.006184

b = 3.384131 beta = 90.050767

c = 13.902488 gamma = 118.794122

Current cell volume = 703.963305 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067384 0.666815 0.125065 x

x Se 2 0.131850 0.340512 0.628465 x

x Se 3 0.132062 0.341452 0.871469 x

x Se 4 0.067592 0.667777 0.375421 x

x Se 5 0.266816 0.664240 0.124233 x

x Se 6 0.332807 0.341638 0.627912 x

x Se 7 0.332564 0.343142 0.872568 x

x Se 8 0.266362 0.663355 0.374477 x

x Se 9 0.467683 0.653783 0.127969 x

x Se 10 0.532894 0.343573 0.626218 x

x Se 11 0.532320 0.346336 0.872005 x

x Se 12 0.467097 0.656601 0.373819 x

x Se 13 0.667439 0.656880 0.127463 x

x Se 14 0.733662 0.336570 0.625540 x

x Se 15 0.733189 0.335596 0.875771 x

x Se 16 0.667191 0.658481 0.372092 x

x Se 17 0.867897 0.658363 0.128528 x

x Se 18 0.932417 0.332351 0.624572 x

x Se 19 0.932624 0.333268 0.874930 x

x Se 20 0.868127 0.659269 0.371554 x

x Nb 1 0.003243 0.010380 0.249979 x

x Nb 2 -0.003288 -0.010190 0.750006 x

x Nb 3 -0.000024 -0.000247 0.000020 x

x Nb 4 -0.000030 -0.000266 0.499953 x

x Nb 5 0.197099 -0.007244 0.249795 x

x Nb 6 0.201865 0.016081 0.749364 x

x Nb 7 0.199373 0.001686 -0.000526 x

x Nb 8 0.200421 0.005069 0.500587 x

x Nb 9 0.399303 -0.012704 0.250749 x

x Nb 10 0.400282 0.007691 0.749580 x

x Nb 11 0.400097 0.004346 -0.001489 x

x Nb 12 0.398422 -0.001344 0.501199 x

x Nb 13 0.599681 -0.007749 0.250422 x

x Nb 14 0.600730 0.012972 0.749233 x

x Nb 15 0.599876 -0.004500 0.001514 x

x Nb 16 0.601597 0.001368 0.498806 x

x Nb 17 0.798149 -0.016312 0.250633 x

x Nb 18 0.802943 0.007020 0.750202 x

x Nb 19 0.800688 -0.001262 0.000451 x

x Nb 20 0.799597 -0.004798 0.499452 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598517E+004 23621.19 <-- SCF

1 -3.62599161E+004 1.61045586E-003 23647.75 <-- SCF

2 -3.62599196E+004 8.69754459E-005 23675.53 <-- SCF

3 -3.62599072E+004 -3.11285888E-004 23702.19 <-- SCF

4 -3.62598756E+004 -7.88827901E-004 23728.08 <-- SCF

5 -3.62598774E+004 4.57408111E-005 23754.05 <-- SCF

6 -3.62598768E+004 -1.69086899E-005 23776.58 <-- SCF

7 -3.62598764E+004 -8.17409098E-006 23796.14 <-- SCF

8 -3.62598764E+004 -7.16785655E-007 23814.34 <-- SCF

9 -3.62598764E+004 5.03439330E-007 23832.25 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.87642611 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01517 0.02676 -0.02952 \*

\* Se 2 0.06527 0.01015 -0.05259 \*

\* Se 3 0.00524 -0.03278 -0.03082 \*

\* Se 4 0.02983 0.01883 0.02246 \*

\* Se 5 -0.00528 0.01781 0.04071 \*

\* Se 6 -0.05905 0.08232 -0.02870 \*

\* Se 7 -0.01572 -0.06886 -0.10124 \*

\* Se 8 -0.01157 0.01174 -0.02195 \*

\* Se 9 -0.07501 0.08178 0.05764 \*

\* Se 10 0.04118 -0.02511 -0.07091 \*

\* Se 11 0.07485 -0.08920 -0.05006 \*

\* Se 12 -0.04878 0.02774 0.07639 \*

\* Se 13 0.01385 0.06717 0.08650 \*

\* Se 14 0.01179 -0.01332 0.02492 \*

\* Se 15 0.00590 -0.01587 -0.03709 \*

\* Se 16 0.06150 -0.09150 0.02652 \*

\* Se 17 0.00201 0.03653 0.03100 \*

\* Se 18 -0.02914 -0.01806 -0.02819 \*

\* Se 19 -0.01534 -0.02621 0.02844 \*

\* Se 20 -0.06342 -0.00038 0.04627 \*

\* Nb 1 0.06887 -0.02546 -0.01822 \*

\* Nb 2 -0.06945 0.02018 0.01857 \*

\* Nb 3 -0.00003 0.00260 -0.00189 \*

\* Nb 4 0.00249 0.00376 0.00291 \*

\* Nb 5 0.02404 -0.01771 -0.03667 \*

\* Nb 6 0.07284 -0.03782 0.03640 \*

\* Nb 7 0.00408 0.01365 -0.05587 \*

\* Nb 8 0.05474 0.01873 0.06122 \*

\* Nb 9 -0.00210 0.06638 -0.05357 \*

\* Nb 10 0.04604 0.06633 0.09606 \*

\* Nb 11 0.04082 -0.01156 0.06257 \*

\* Nb 12 -0.02766 -0.03346 -0.05040 \*

\* Nb 13 -0.04505 -0.06521 -0.09408 \*

\* Nb 14 -0.00206 -0.06797 0.05432 \*

\* Nb 15 -0.03860 0.01294 -0.06406 \*

\* Nb 16 0.02766 0.03593 0.05182 \*

\* Nb 17 -0.07334 0.04057 -0.03304 \*

\* Nb 18 -0.02297 0.01995 0.03775 \*

\* Nb 19 -0.00649 -0.01799 0.06093 \*

\* Nb 20 -0.05709 -0.02336 -0.06453 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.032294 -0.035998 -0.092002 \*

\* y -0.035998 -0.053118 0.034758 \*

\* z -0.092002 0.034758 -0.003978 \*

\* \*

\* Pressure: 0.0298 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000036 | -36259.875559 | <-- min BFGS

| trial step | 1.000000 | 0.000013 | -36259.876337 | <-- min BFGS

| line step | 1.586906 | -1.374E-007 | -36259.876466 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 32 with enthalpy= -3.62598765E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.267049E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.267520E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.155408E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 9.200201E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 33 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000027 | -36259.876466 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 33 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8992575 -8.3462271 -0.0068242 0.4198619 -0.0033015 0.0001720

0.0266137 3.3844891 -0.0002345 1.0353891 1.8483233 0.0005313

-0.0056996 -0.0008027 13.9007295 0.0002236 0.0000296 0.4520041

Lattice parameters(A) Cell Angles

a = 17.077688 alpha = 90.007463

b = 3.384594 beta = 90.041774

c = 13.900731 gamma = 118.806026

Current cell volume = 704.050924 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067390 0.666821 0.125076 x

x Se 2 0.131854 0.340526 0.628524 x

x Se 3 0.132059 0.341340 0.871427 x

x Se 4 0.067602 0.667793 0.375406 x

x Se 5 0.266803 0.664196 0.124274 x

x Se 6 0.332857 0.341875 0.627944 x

x Se 7 0.332581 0.343202 0.872588 x

x Se 8 0.266343 0.663326 0.374412 x

x Se 9 0.467704 0.654003 0.127979 x

x Se 10 0.532883 0.343432 0.626239 x

x Se 11 0.532300 0.346115 0.871995 x

x Se 12 0.467107 0.656746 0.373800 x

x Se 13 0.667420 0.656810 0.127447 x

x Se 14 0.733682 0.336600 0.625605 x

x Se 15 0.733203 0.335640 0.875730 x

x Se 16 0.667138 0.658237 0.372056 x

x Se 17 0.867902 0.658482 0.128567 x

x Se 18 0.932407 0.332337 0.624585 x

x Se 19 0.932618 0.333261 0.874920 x

x Se 20 0.868123 0.659260 0.371499 x

x Nb 1 0.003266 0.010336 0.249979 x

x Nb 2 -0.003308 -0.010157 0.750006 x

x Nb 3 -0.000024 -0.000242 0.000017 x

x Nb 4 -0.000029 -0.000258 0.499955 x

x Nb 5 0.197124 -0.007193 0.249784 x

x Nb 6 0.201892 0.016140 0.749367 x

x Nb 7 0.199384 0.001780 -0.000568 x

x Nb 8 0.200447 0.005200 0.500614 x

x Nb 9 0.399287 -0.012769 0.250757 x

x Nb 10 0.400316 0.007988 0.749586 x

x Nb 11 0.400119 0.004350 -0.001454 x

x Nb 12 0.398408 -0.001491 0.501163 x

x Nb 13 0.599649 -0.008035 0.250416 x

x Nb 14 0.600744 0.013022 0.749225 x

x Nb 15 0.599854 -0.004501 0.001476 x

x Nb 16 0.601611 0.001516 0.498843 x

x Nb 17 0.798120 -0.016367 0.250629 x

x Nb 18 0.802917 0.006977 0.750213 x

x Nb 19 0.800676 -0.001362 0.000496 x

x Nb 20 0.799572 -0.004935 0.499422 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598695E+004 23935.66 <-- SCF

1 -3.62599104E+004 1.02052959E-003 23963.12 <-- SCF

2 -3.62599130E+004 6.54751617E-005 23988.41 <-- SCF

3 -3.62599204E+004 1.86663260E-004 24015.33 <-- SCF

4 -3.62598748E+004 -1.14023235E-003 24041.61 <-- SCF

5 -3.62598778E+004 7.32680135E-005 24066.67 <-- SCF

6 -3.62598775E+004 -7.84399942E-006 24088.19 <-- SCF

7 -3.62598771E+004 -9.50870930E-006 24107.81 <-- SCF

8 -3.62598770E+004 -9.82353870E-007 24125.84 <-- SCF

9 -3.62598770E+004 2.98051229E-007 24142.73 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.87704747 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01778 0.02606 -0.03127 \*

\* Se 2 0.06637 0.01210 -0.05828 \*

\* Se 3 0.00590 -0.02526 -0.02566 \*

\* Se 4 0.03268 0.01859 0.02513 \*

\* Se 5 0.00093 0.01658 0.04012 \*

\* Se 6 -0.05842 0.07859 -0.03488 \*

\* Se 7 -0.01758 -0.06625 -0.10601 \*

\* Se 8 -0.01061 0.01816 -0.01822 \*

\* Se 9 -0.08442 0.07063 0.05609 \*

\* Se 10 0.04553 -0.02248 -0.07117 \*

\* Se 11 0.08423 -0.07803 -0.04853 \*

\* Se 12 -0.05374 0.02513 0.07719 \*

\* Se 13 0.01585 0.06497 0.09034 \*

\* Se 14 0.01071 -0.01939 0.02131 \*

\* Se 15 -0.00071 -0.01486 -0.03650 \*

\* Se 16 0.06052 -0.08808 0.03383 \*

\* Se 17 0.00151 0.02874 0.02618 \*

\* Se 18 -0.03158 -0.01776 -0.03080 \*

\* Se 19 -0.01768 -0.02565 0.02989 \*

\* Se 20 -0.06408 -0.00222 0.05148 \*

\* Nb 1 0.07241 -0.02322 -0.01807 \*

\* Nb 2 -0.07353 0.01850 0.01836 \*

\* Nb 3 0.00013 0.00255 -0.00153 \*

\* Nb 4 0.00261 0.00369 0.00249 \*

\* Nb 5 0.01640 -0.01860 -0.03766 \*

\* Nb 6 0.07661 -0.03883 0.03690 \*

\* Nb 7 0.00376 0.01064 -0.04740 \*

\* Nb 8 0.05420 0.01731 0.05692 \*

\* Nb 9 0.00277 0.07022 -0.05607 \*

\* Nb 10 0.04012 0.06077 0.09853 \*

\* Nb 11 0.03954 -0.01071 0.06064 \*

\* Nb 12 -0.02625 -0.02979 -0.04977 \*

\* Nb 13 -0.03977 -0.05993 -0.09693 \*

\* Nb 14 -0.00657 -0.07146 0.05680 \*

\* Nb 15 -0.03775 0.01191 -0.06173 \*

\* Nb 16 0.02638 0.03231 0.05108 \*

\* Nb 17 -0.07648 0.04148 -0.03363 \*

\* Nb 18 -0.01490 0.02051 0.03877 \*

\* Nb 19 -0.00618 -0.01498 0.05217 \*

\* Nb 20 -0.05667 -0.02195 -0.06011 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.009899 -0.045599 -0.072681 \*

\* y -0.045599 -0.032059 0.031052 \*

\* z -0.072681 0.031052 -0.010206 \*

\* \*

\* Pressure: 0.0174 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000027 | -36259.876466 | <-- min BFGS

| trial step | 1.000000 | 0.000021 | -36259.877073 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 33 with line minimization (lambda= 4.621364)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9092746 -8.3572273 -0.0014723 0.4196902 -0.0031001 0.0000577

0.0250127 3.3861775 -0.0003948 1.0358130 1.8478880 0.0003163

-0.0019207 -0.0013020 13.8943662 0.0000739 0.0000522 0.4522110

Lattice parameters(A) Cell Angles

a = 17.091803 alpha = 90.012107

b = 3.386270 beta = 90.009219

c = 13.894366 gamma = 118.849102

Current cell volume = 704.367757 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067409 0.666840 0.125113 x

x Se 2 0.131869 0.340578 0.628735 x

x Se 3 0.132045 0.340936 0.871277 x

x Se 4 0.067637 0.667851 0.375349 x

x Se 5 0.266755 0.664035 0.124422 x

x Se 6 0.333041 0.342731 0.628058 x

x Se 7 0.332646 0.343419 0.872659 x

x Se 8 0.266277 0.663222 0.374179 x

x Se 9 0.467778 0.654796 0.128015 x

x Se 10 0.532844 0.342924 0.626317 x

x Se 11 0.532226 0.345315 0.871959 x

x Se 12 0.467143 0.657275 0.373732 x

x Se 13 0.667349 0.656557 0.127386 x

x Se 14 0.733754 0.336710 0.625842 x

x Se 15 0.733256 0.335800 0.875584 x

x Se 16 0.666947 0.657355 0.371927 x

x Se 17 0.867917 0.658912 0.128707 x

x Se 18 0.932370 0.332289 0.624633 x

x Se 19 0.932597 0.333236 0.874885 x

x Se 20 0.868109 0.659227 0.371299 x

x Nb 1 0.003346 0.010175 0.249979 x

x Nb 2 -0.003381 -0.010038 0.750003 x

x Nb 3 -0.000024 -0.000224 0.000009 x

x Nb 4 -0.000026 -0.000230 0.499962 x

x Nb 5 0.197215 -0.007008 0.249743 x

x Nb 6 0.201993 0.016353 0.749381 x

x Nb 7 0.199425 0.002117 -0.000718 x

x Nb 8 0.200540 0.005673 0.500710 x

x Nb 9 0.399227 -0.013004 0.250787 x

x Nb 10 0.400441 0.009064 0.749611 x

x Nb 11 0.400199 0.004364 -0.001327 x

x Nb 12 0.398355 -0.002025 0.501033 x

x Nb 13 0.599533 -0.009072 0.250395 x

x Nb 14 0.600795 0.013204 0.749195 x

x Nb 15 0.599776 -0.004504 0.001341 x

x Nb 16 0.601663 0.002054 0.498977 x

x Nb 17 0.798013 -0.016566 0.250614 x

x Nb 18 0.802826 0.006820 0.750252 x

x Nb 19 0.800635 -0.001728 0.000658 x

x Nb 20 0.799479 -0.005433 0.499315 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597845E+004 24245.97 <-- SCF

1 -3.62601196E+004 8.37865928E-003 24273.50 <-- SCF

2 -3.62601393E+004 4.90175477E-004 24301.95 <-- SCF

3 -3.62601121E+004 -6.79258463E-004 24329.20 <-- SCF

4 -3.62598693E+004 -6.06920686E-003 24355.48 <-- SCF

5 -3.62598843E+004 3.74910106E-004 24382.42 <-- SCF

6 -3.62598801E+004 -1.05800936E-004 24408.47 <-- SCF

7 -3.62598776E+004 -6.22902094E-005 24432.05 <-- SCF

8 -3.62598776E+004 7.28805746E-007 24452.59 <-- SCF

9 -3.62598777E+004 1.80725151E-006 24470.97 <-- SCF

10 -3.62598778E+004 1.92872125E-006 24488.59 <-- SCF

11 -3.62598778E+004 1.25566268E-006 24505.67 <-- SCF

12 -3.62598778E+004 7.18048763E-007 24522.30 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.87784357 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01925 0.02268 -0.04416 \*

\* Se 2 0.06552 0.01500 -0.09219 \*

\* Se 3 0.00565 0.00227 0.00046 \*

\* Se 4 0.03734 0.01620 0.04015 \*

\* Se 5 0.01773 0.01215 0.02933 \*

\* Se 6 -0.06771 0.05403 -0.06796 \*

\* Se 7 -0.03119 -0.05813 -0.12794 \*

\* Se 8 -0.00808 0.04167 0.00627 \*

\* Se 9 -0.11247 0.03174 0.04969 \*

\* Se 10 0.05524 -0.01421 -0.07553 \*

\* Se 11 0.11186 -0.03854 -0.04252 \*

\* Se 12 -0.06535 0.01608 0.08396 \*

\* Se 13 0.03023 0.05822 0.10996 \*

\* Se 14 0.00748 -0.04083 -0.00420 \*

\* Se 15 -0.01882 -0.01105 -0.02634 \*

\* Se 16 0.06912 -0.06350 0.07244 \*

\* Se 17 0.00164 -0.00002 0.00151 \*

\* Se 18 -0.03548 -0.01544 -0.04507 \*

\* Se 19 -0.01864 -0.02289 0.04160 \*

\* Se 20 -0.06281 -0.00535 0.08333 \*

\* Nb 1 0.07436 -0.01605 -0.01726 \*

\* Nb 2 -0.07669 0.01298 0.01737 \*

\* Nb 3 0.00054 0.00233 -0.00090 \*

\* Nb 4 0.00289 0.00339 0.00148 \*

\* Nb 5 -0.00796 -0.02284 -0.04240 \*

\* Nb 6 0.07895 -0.03793 0.04073 \*

\* Nb 7 -0.00286 0.00630 -0.03345 \*

\* Nb 8 0.04953 0.01370 0.04913 \*

\* Nb 9 0.01593 0.08339 -0.06383 \*

\* Nb 10 0.01760 0.04442 0.10472 \*

\* Nb 11 0.03205 -0.00827 0.05070 \*

\* Nb 12 -0.02480 -0.01595 -0.04134 \*

\* Nb 13 -0.01847 -0.04467 -0.10413 \*

\* Nb 14 -0.01862 -0.08360 0.06465 \*

\* Nb 15 -0.02958 0.00904 -0.05110 \*

\* Nb 16 0.02549 0.01851 0.04185 \*

\* Nb 17 -0.07758 0.04009 -0.03756 \*

\* Nb 18 0.01030 0.02378 0.04337 \*

\* Nb 19 0.00051 -0.01048 0.03679 \*

\* Nb 20 -0.05214 -0.01822 -0.05162 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.069659 -0.087491 -0.010169 \*

\* y -0.087491 0.041863 0.017119 \*

\* z -0.010169 0.017119 -0.027824 \*

\* \*

\* Pressure: -0.0279 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000027 | -36259.876466 | <-- min BFGS

| trial step | 1.000000 | 0.000021 | -36259.877073 | <-- min BFGS

| line step | 4.621364 | -3.388E-006 | -36259.877870 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 33 with enthalpy= -3.62598779E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 3.509663E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.439424E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.668698E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 8.749112E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 34 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000072 | -36259.877870 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 34 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9056006 -8.3534600 0.0026068 0.4197497 -0.0031800 -0.0000353

0.0256503 3.3857484 -0.0004121 1.0356240 1.8479286 0.0000903

0.0011598 -0.0013293 13.8966819 -0.0000480 0.0000554 0.4521357

Lattice parameters(A) Cell Angles

a = 17.086756 alpha = 90.012417

b = 3.385846 beta = 89.984408

c = 13.896682 gamma = 118.833265

Current cell volume = 704.296082 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067414 0.666929 0.125046 x

x Se 2 0.131893 0.340672 0.628655 x

x Se 3 0.132049 0.340953 0.871304 x

x Se 4 0.067648 0.667957 0.375419 x

x Se 5 0.266759 0.664063 0.124377 x

x Se 6 0.333005 0.342741 0.628009 x

x Se 7 0.332640 0.343312 0.872626 x

x Se 8 0.266276 0.663239 0.374241 x

x Se 9 0.467736 0.654706 0.128012 x

x Se 10 0.532875 0.343020 0.626234 x

x Se 11 0.532268 0.345395 0.871965 x

x Se 12 0.467110 0.657174 0.373817 x

x Se 13 0.667355 0.656663 0.127411 x

x Se 14 0.733754 0.336690 0.625780 x

x Se 15 0.733251 0.335773 0.875630 x

x Se 16 0.666985 0.657337 0.371977 x

x Se 17 0.867915 0.658904 0.128682 x

x Se 18 0.932360 0.332184 0.624561 x

x Se 19 0.932592 0.333149 0.874951 x

x Se 20 0.868086 0.659148 0.371373 x

x Nb 1 0.003388 0.010300 0.249968 x

x Nb 2 -0.003425 -0.010166 0.750014 x

x Nb 3 -0.000025 -0.000222 0.000009 x

x Nb 4 -0.000025 -0.000226 0.499963 x

x Nb 5 0.197208 -0.007056 0.249726 x

x Nb 6 0.202013 0.016385 0.749396 x

x Nb 7 0.199419 0.002113 -0.000734 x

x Nb 8 0.200553 0.005734 0.500735 x

x Nb 9 0.399230 -0.012922 0.250758 x

x Nb 10 0.400443 0.009127 0.749657 x

x Nb 11 0.400209 0.004400 -0.001318 x

x Nb 12 0.398343 -0.002065 0.501029 x

x Nb 13 0.599531 -0.009137 0.250349 x

x Nb 14 0.600792 0.013122 0.749224 x

x Nb 15 0.599766 -0.004538 0.001333 x

x Nb 16 0.601674 0.002098 0.498981 x

x Nb 17 0.797994 -0.016596 0.250601 x

x Nb 18 0.802833 0.006869 0.750271 x

x Nb 19 0.800641 -0.001729 0.000675 x

x Nb 20 0.799465 -0.005500 0.499289 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598706E+004 24625.27 <-- SCF

1 -3.62599003E+004 7.42560761E-004 24652.17 <-- SCF

2 -3.62599018E+004 3.94454234E-005 24677.78 <-- SCF

3 -3.62598943E+004 -1.87806477E-004 24704.06 <-- SCF

4 -3.62598794E+004 -3.72218957E-004 24729.72 <-- SCF

5 -3.62598800E+004 1.42533989E-005 24752.69 <-- SCF

6 -3.62598797E+004 -8.53858032E-006 24772.06 <-- SCF

7 -3.62598796E+004 -1.64507866E-006 24790.52 <-- SCF

8 -3.62598796E+004 4.80537584E-007 24808.16 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.87962976 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01898 0.02285 -0.03849 \*

\* Se 2 0.05878 0.01213 -0.07128 \*

\* Se 3 0.00420 0.00295 -0.00834 \*

\* Se 4 0.03376 0.01053 0.02878 \*

\* Se 5 0.01517 0.01206 0.02820 \*

\* Se 6 -0.05887 0.04949 -0.04419 \*

\* Se 7 -0.02690 -0.04754 -0.11305 \*

\* Se 8 -0.00702 0.03344 -0.00547 \*

\* Se 9 -0.09931 0.02963 0.04612 \*

\* Se 10 0.06251 -0.02047 -0.07851 \*

\* Se 11 0.09855 -0.03539 -0.04031 \*

\* Se 12 -0.07174 0.02201 0.08480 \*

\* Se 13 0.02656 0.04761 0.09739 \*

\* Se 14 0.00677 -0.03311 0.00794 \*

\* Se 15 -0.01599 -0.01100 -0.02490 \*

\* Se 16 0.05958 -0.05784 0.04850 \*

\* Se 17 0.00233 -0.00097 0.01016 \*

\* Se 18 -0.03167 -0.00968 -0.03418 \*

\* Se 19 -0.01847 -0.02305 0.03639 \*

\* Se 20 -0.05608 -0.00394 0.06377 \*

\* Nb 1 0.07298 -0.01346 -0.01481 \*

\* Nb 2 -0.07497 0.01042 0.01478 \*

\* Nb 3 0.00036 0.00242 -0.00090 \*

\* Nb 4 0.00309 0.00352 0.00145 \*

\* Nb 5 -0.00446 -0.01924 -0.04085 \*

\* Nb 6 0.07970 -0.03941 0.03923 \*

\* Nb 7 0.00118 0.00707 -0.03619 \*

\* Nb 8 0.05418 0.01598 0.04992 \*

\* Nb 9 0.01572 0.08462 -0.05814 \*

\* Nb 10 0.02230 0.04324 0.09560 \*

\* Nb 11 0.03526 -0.00992 0.05063 \*

\* Nb 12 -0.02678 -0.01780 -0.03967 \*

\* Nb 13 -0.02314 -0.04364 -0.09514 \*

\* Nb 14 -0.01874 -0.08506 0.05928 \*

\* Nb 15 -0.03289 0.01070 -0.05112 \*

\* Nb 16 0.02703 0.02039 0.04046 \*

\* Nb 17 -0.07847 0.04185 -0.03675 \*

\* Nb 18 0.00667 0.02030 0.04204 \*

\* Nb 19 -0.00343 -0.01120 0.03946 \*

\* Nb 20 -0.05672 -0.02051 -0.05260 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.048667 -0.055463 0.046676 \*

\* y -0.055463 0.023262 0.012950 \*

\* z 0.046676 0.012950 -0.007793 \*

\* \*

\* Pressure: -0.0214 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000072 | -36259.877870 | <-- min BFGS

| trial step | 1.000000 | 0.000057 | -36259.879686 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 34 with line minimization (lambda= 4.765688)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8917653 -8.3392738 0.0179674 0.4199745 -0.0034813 -0.0003857

0.0280514 3.3841323 -0.0004773 1.0349126 1.8480821 -0.0007594

0.0127602 -0.0014321 13.9054020 -0.0005071 0.0000679 0.4518526

Lattice parameters(A) Cell Angles

a = 17.067762 alpha = 90.013545

b = 3.384249 beta = 89.890927

c = 13.905408 gamma = 118.773563

Current cell volume = 704.024648 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067434 0.667265 0.124795 x

x Se 2 0.131982 0.341025 0.628356 x

x Se 3 0.132064 0.341021 0.871404 x

x Se 4 0.067690 0.668358 0.375681 x

x Se 5 0.266776 0.664169 0.124209 x

x Se 6 0.332869 0.342778 0.627822 x

x Se 7 0.332616 0.342910 0.872502 x

x Se 8 0.266275 0.663303 0.374477 x

x Se 9 0.467577 0.654367 0.128002 x

x Se 10 0.532991 0.343382 0.625923 x

x Se 11 0.532427 0.345697 0.871988 x

x Se 12 0.466983 0.656795 0.374137 x

x Se 13 0.667379 0.657061 0.127505 x

x Se 14 0.733753 0.336614 0.625550 x

x Se 15 0.733233 0.335672 0.875803 x

x Se 16 0.667127 0.657270 0.372167 x

x Se 17 0.867910 0.658871 0.128586 x

x Se 18 0.932319 0.331790 0.624292 x

x Se 19 0.932574 0.332823 0.875198 x

x Se 20 0.867999 0.658847 0.371655 x

x Nb 1 0.003546 0.010767 0.249927 x

x Nb 2 -0.003588 -0.010651 0.750057 x

x Nb 3 -0.000025 -0.000218 0.000009 x

x Nb 4 -0.000023 -0.000209 0.499965 x

x Nb 5 0.197183 -0.007235 0.249659 x

x Nb 6 0.202088 0.016505 0.749453 x

x Nb 7 0.199394 0.002099 -0.000794 x

x Nb 8 0.200605 0.005963 0.500831 x

x Nb 9 0.399242 -0.012612 0.250651 x

x Nb 10 0.400450 0.009365 0.749830 x

x Nb 11 0.400246 0.004535 -0.001285 x

x Nb 12 0.398300 -0.002216 0.501014 x

x Nb 13 0.599520 -0.009381 0.250178 x

x Nb 14 0.600778 0.012813 0.749333 x

x Nb 15 0.599731 -0.004664 0.001300 x

x Nb 16 0.601718 0.002263 0.498997 x

x Nb 17 0.797921 -0.016709 0.250551 x

x Nb 18 0.802861 0.007052 0.750339 x

x Nb 19 0.800663 -0.001732 0.000739 x

x Nb 20 0.799410 -0.005752 0.499192 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597574E+004 24911.61 <-- SCF

1 -3.62601007E+004 8.58308768E-003 24938.31 <-- SCF

2 -3.62601174E+004 4.17801138E-004 24966.84 <-- SCF

3 -3.62600247E+004 -2.31725306E-003 24992.75 <-- SCF

4 -3.62598833E+004 -3.53383522E-003 25018.34 <-- SCF

5 -3.62598835E+004 3.76097520E-006 25043.34 <-- SCF

6 -3.62598826E+004 -2.29275554E-005 25066.83 <-- SCF

7 -3.62598824E+004 -3.93730688E-006 25088.48 <-- SCF

8 -3.62598825E+004 1.49881468E-006 25106.42 <-- SCF

9 -3.62598825E+004 9.28170963E-007 25123.56 <-- SCF

10 -3.62598825E+004 6.15315733E-007 25139.81 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.88254103 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01218 0.01813 -0.00800 \*

\* Se 2 0.02601 0.00270 -0.01115 \*

\* Se 3 -0.00642 0.00713 -0.04393 \*

\* Se 4 0.01825 -0.01382 0.00055 \*

\* Se 5 -0.00045 0.01308 0.01965 \*

\* Se 6 -0.03836 0.03295 0.03711 \*

\* Se 7 -0.01312 -0.00835 -0.06349 \*

\* Se 8 -0.00808 0.00651 -0.04247 \*

\* Se 9 -0.05352 0.01915 0.04849 \*

\* Se 10 0.07894 -0.03515 -0.05333 \*

\* Se 11 0.05245 -0.02137 -0.04661 \*

\* Se 12 -0.08083 0.03195 0.04682 \*

\* Se 13 0.01488 0.00879 0.05937 \*

\* Se 14 0.00872 -0.00767 0.04531 \*

\* Se 15 0.00002 -0.01158 -0.01568 \*

\* Se 16 0.03683 -0.03682 -0.03297 \*

\* Se 17 0.00983 -0.00601 0.04615 \*

\* Se 18 -0.01570 0.01527 -0.00775 \*

\* Se 19 -0.01216 -0.01849 0.00756 \*

\* Se 20 -0.02424 0.00058 0.00802 \*

\* Nb 1 0.05403 -0.00087 0.00544 \*

\* Nb 2 -0.05515 -0.00118 -0.00592 \*

\* Nb 3 0.00000 0.00240 -0.00089 \*

\* Nb 4 0.00234 0.00335 0.00102 \*

\* Nb 5 -0.00644 -0.00294 -0.02127 \*

\* Nb 6 0.05085 -0.04709 0.01676 \*

\* Nb 7 0.00748 0.00674 -0.03528 \*

\* Nb 8 0.05045 0.01845 0.03389 \*

\* Nb 9 0.00179 0.08580 -0.01423 \*

\* Nb 10 0.03401 0.02741 0.03738 \*

\* Nb 11 0.03421 -0.01567 0.04007 \*

\* Nb 12 -0.03741 -0.01939 -0.02908 \*

\* Nb 13 -0.03362 -0.02830 -0.03705 \*

\* Nb 14 -0.00503 -0.08674 0.01639 \*

\* Nb 15 -0.03358 0.01633 -0.04054 \*

\* Nb 16 0.03735 0.02159 0.03081 \*

\* Nb 17 -0.05179 0.05062 -0.01651 \*

\* Nb 18 0.00750 0.00433 0.02274 \*

\* Nb 19 -0.00890 -0.01003 0.03868 \*

\* Nb 20 -0.05331 -0.02179 -0.03607 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.038234 0.053205 0.266858 \*

\* y 0.053205 -0.046559 0.001664 \*

\* z 0.266858 0.001664 0.037074 \*

\* \*

\* Pressure: 0.0159 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000072 | -36259.877870 | <-- min BFGS

| trial step | 1.000000 | 0.000057 | -36259.879686 | <-- min BFGS

| line step | 4.765688 | -4.602E-006 | -36259.882620 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 34 with enthalpy= -3.62598826E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.187603E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.015404E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.124288E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.668575E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 35 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000085 | -36259.882620 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 35 with trial guess (lambda= 1.000000)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.9000880 -8.3485587 0.0213499 0.4198763 -0.0032342 -0.0004526

0.0260688 3.3844930 -0.0006712 1.0357123 1.8484851 -0.0008439

0.0149699 -0.0020404 13.9034225 -0.0005948 0.0000942 0.4519171

Lattice parameters(A) Cell Angles

a = 17.079564 alpha = 90.019295

b = 3.384593 beta = 89.870450

c = 13.903431 gamma = 118.820709

Current cell volume = 704.163955 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067487 0.667544 0.124675 x

x Se 2 0.131950 0.341232 0.628502 x

x Se 3 0.131997 0.340853 0.871245 x

x Se 4 0.067777 0.668754 0.375808 x

x Se 5 0.266759 0.663964 0.124120 x

x Se 6 0.332963 0.343659 0.627935 x

x Se 7 0.332634 0.343229 0.872477 x

x Se 8 0.266225 0.663103 0.374451 x

x Se 9 0.467580 0.654397 0.128062 x

x Se 10 0.533038 0.343461 0.625863 x

x Se 11 0.532425 0.345657 0.871931 x

x Se 12 0.466931 0.656733 0.374208 x

x Se 13 0.667356 0.656713 0.127532 x

x Se 14 0.733809 0.336812 0.625580 x

x Se 15 0.733253 0.335871 0.875895 x

x Se 16 0.667027 0.656364 0.372043 x

x Se 17 0.867979 0.659062 0.128740 x

x Se 18 0.932233 0.331409 0.624156 x

x Se 19 0.932520 0.332544 0.875319 x

x Se 20 0.868032 0.658662 0.371514 x

x Nb 1 0.003790 0.011238 0.249909 x

x Nb 2 -0.003829 -0.011152 0.750073 x

x Nb 3 -0.000026 -0.000211 0.000003 x

x Nb 4 -0.000021 -0.000191 0.499969 x

x Nb 5 0.197142 -0.007362 0.249594 x

x Nb 6 0.202259 0.017259 0.749460 x

x Nb 7 0.199395 0.002431 -0.000949 x

x Nb 8 0.200713 0.006617 0.500958 x

x Nb 9 0.399179 -0.013096 0.250670 x

x Nb 10 0.400546 0.010529 0.749891 x

x Nb 11 0.400329 0.004745 -0.001230 x

x Nb 12 0.398183 -0.002766 0.500948 x

x Nb 13 0.599429 -0.010518 0.250121 x

x Nb 14 0.600835 0.013266 0.749313 x

x Nb 15 0.599649 -0.004869 0.001240 x

x Nb 16 0.601836 0.002821 0.499067 x

x Nb 17 0.797746 -0.017460 0.250545 x

x Nb 18 0.802904 0.007193 0.750404 x

x Nb 19 0.800664 -0.002076 0.000901 x

x Nb 20 0.799302 -0.006423 0.499057 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597804E+004 25243.45 <-- SCF

1 -3.62600163E+004 5.89812802E-003 25269.73 <-- SCF

2 -3.62600294E+004 3.26541661E-004 25298.12 <-- SCF

3 -3.62599675E+004 -1.54738332E-003 25324.80 <-- SCF

4 -3.62598845E+004 -2.07436410E-003 25350.66 <-- SCF

5 -3.62598884E+004 9.68101943E-005 25377.12 <-- SCF

6 -3.62598851E+004 -8.23537627E-005 25402.27 <-- SCF

7 -3.62598842E+004 -2.29299537E-005 25423.94 <-- SCF

8 -3.62598842E+004 1.24214359E-007 25443.34 <-- SCF

9 -3.62598842E+004 3.83096891E-007 25461.50 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.88421596 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00966 0.01624 -0.01024 \*

\* Se 2 0.03333 -0.01447 -0.01800 \*

\* Se 3 0.00053 0.00998 -0.02737 \*

\* Se 4 0.01774 -0.01860 -0.00352 \*

\* Se 5 0.00542 0.03654 0.00836 \*

\* Se 6 -0.02061 -0.01881 0.00230 \*

\* Se 7 0.00806 -0.02115 -0.04510 \*

\* Se 8 -0.00868 0.02258 -0.03890 \*

\* Se 9 -0.06583 0.02031 0.03262 \*

\* Se 10 0.08601 -0.03952 -0.05315 \*

\* Se 11 0.06407 -0.02210 -0.03118 \*

\* Se 12 -0.08580 0.03257 0.04297 \*

\* Se 13 -0.00575 0.02299 0.04024 \*

\* Se 14 0.00934 -0.02349 0.04221 \*

\* Se 15 -0.00671 -0.03435 -0.00361 \*

\* Se 16 0.01828 0.01730 0.00615 \*

\* Se 17 0.00257 -0.01006 0.03042 \*

\* Se 18 -0.01360 0.01973 -0.00385 \*

\* Se 19 -0.00933 -0.01701 0.00950 \*

\* Se 20 -0.03139 0.01667 0.01447 \*

\* Nb 1 0.05164 -0.00197 0.01087 \*

\* Nb 2 -0.05343 0.00124 -0.01152 \*

\* Nb 3 0.00029 0.00256 -0.00044 \*

\* Nb 4 0.00304 0.00348 0.00010 \*

\* Nb 5 -0.01171 -0.01386 -0.01885 \*

\* Nb 6 0.03716 -0.04584 0.01632 \*

\* Nb 7 0.00573 0.00187 -0.03209 \*

\* Nb 8 0.04926 0.01295 0.02990 \*

\* Nb 9 0.00873 0.09223 -0.01473 \*

\* Nb 10 0.02194 0.02053 0.02894 \*

\* Nb 11 0.02966 -0.01674 0.03267 \*

\* Nb 12 -0.03587 -0.01098 -0.01923 \*

\* Nb 13 -0.02342 -0.02231 -0.02943 \*

\* Nb 14 -0.01165 -0.09253 0.01733 \*

\* Nb 15 -0.02925 0.01724 -0.03264 \*

\* Nb 16 0.03521 0.01346 0.02091 \*

\* Nb 17 -0.03752 0.04955 -0.01668 \*

\* Nb 18 0.01290 0.01470 0.02052 \*

\* Nb 19 -0.00730 -0.00498 0.03500 \*

\* Nb 20 -0.05273 -0.01598 -0.03128 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.010310 -0.027781 0.297942 \*

\* y -0.027781 -0.017350 -0.015283 \*

\* z 0.297942 -0.015283 0.010157 \*

\* \*

\* Pressure: -0.0010 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000085 | -36259.882620 | <-- min BFGS

| trial step | 1.000000 | 0.000033 | -36259.884266 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 35 with line minimization (lambda= 1.654286)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9055335 -8.3546337 0.0235630 0.4198123 -0.0030726 -0.0004963

0.0247716 3.3847290 -0.0007981 1.0362356 1.8487493 -0.0008993

0.0164156 -0.0024384 13.9021273 -0.0006521 0.0001113 0.4519593

Lattice parameters(A) Cell Angles

a = 17.087287 alpha = 90.023063

b = 3.384820 beta = 89.857060

c = 13.902137 gamma = 118.851542

Current cell volume = 704.254807 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067521 0.667728 0.124596 x

x Se 2 0.131929 0.341368 0.628597 x

x Se 3 0.131953 0.340744 0.871141 x

x Se 4 0.067833 0.669013 0.375892 x

x Se 5 0.266748 0.663829 0.124062 x

x Se 6 0.333025 0.344235 0.628009 x

x Se 7 0.332646 0.343438 0.872460 x

x Se 8 0.266192 0.662972 0.374435 x

x Se 9 0.467582 0.654416 0.128100 x

x Se 10 0.533068 0.343512 0.625823 x

x Se 11 0.532423 0.345630 0.871894 x

x Se 12 0.466897 0.656693 0.374255 x

x Se 13 0.667341 0.656485 0.127550 x

x Se 14 0.733845 0.336942 0.625599 x

x Se 15 0.733266 0.336001 0.875956 x

x Se 16 0.666962 0.655771 0.371961 x

x Se 17 0.868025 0.659188 0.128840 x

x Se 18 0.932176 0.331160 0.624066 x

x Se 19 0.932485 0.332362 0.875398 x

x Se 20 0.868053 0.658541 0.371422 x

x Nb 1 0.003950 0.011546 0.249897 x

x Nb 2 -0.003987 -0.011480 0.750084 x

x Nb 3 -0.000027 -0.000207 -0.000001 x

x Nb 4 -0.000020 -0.000180 0.499972 x

x Nb 5 0.197115 -0.007445 0.249552 x

x Nb 6 0.202372 0.017753 0.749464 x

x Nb 7 0.199396 0.002649 -0.001050 x

x Nb 8 0.200783 0.007045 0.501040 x

x Nb 9 0.399138 -0.013413 0.250683 x

x Nb 10 0.400609 0.011290 0.749931 x

x Nb 11 0.400383 0.004882 -0.001194 x

x Nb 12 0.398106 -0.003125 0.500904 x

x Nb 13 0.599369 -0.011261 0.250083 x

x Nb 14 0.600873 0.013563 0.749300 x

x Nb 15 0.599595 -0.005003 0.001201 x

x Nb 16 0.601913 0.003186 0.499113 x

x Nb 17 0.797631 -0.017952 0.250540 x

x Nb 18 0.802932 0.007286 0.750447 x

x Nb 19 0.800665 -0.002301 0.001007 x

x Nb 20 0.799232 -0.006862 0.498969 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598396E+004 25564.62 <-- SCF

1 -3.62599560E+004 2.90844437E-003 25591.20 <-- SCF

2 -3.62599628E+004 1.71074910E-004 25619.52 <-- SCF

3 -3.62599401E+004 -5.69105220E-004 25646.59 <-- SCF

4 -3.62598832E+004 -1.42199248E-003 25672.58 <-- SCF

5 -3.62598869E+004 9.24960204E-005 25699.19 <-- SCF

6 -3.62598852E+004 -4.23176399E-005 25723.38 <-- SCF

7 -3.62598846E+004 -1.52379104E-005 25743.88 <-- SCF

8 -3.62598846E+004 -4.86947475E-007 25762.44 <-- SCF

9 -3.62598846E+004 3.90257283E-007 25780.62 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.88457407 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00710 0.01438 -0.00963 \*

\* Se 2 0.03441 -0.02815 -0.02280 \*

\* Se 3 0.00313 0.01001 -0.01765 \*

\* Se 4 0.01590 -0.02092 -0.00564 \*

\* Se 5 0.00877 0.05226 0.00292 \*

\* Se 6 -0.01465 -0.04994 -0.02055 \*

\* Se 7 0.01957 -0.02885 -0.03378 \*

\* Se 8 -0.01084 0.03351 -0.03692 \*

\* Se 9 -0.07421 0.02201 0.02372 \*

\* Se 10 0.09019 -0.04192 -0.05083 \*

\* Se 11 0.07222 -0.02344 -0.02268 \*

\* Se 12 -0.08809 0.03224 0.03887 \*

\* Se 13 -0.01697 0.03151 0.02850 \*

\* Se 14 0.01140 -0.03419 0.04032 \*

\* Se 15 -0.01067 -0.04969 0.00210 \*

\* Se 16 0.01266 0.05007 0.03178 \*

\* Se 17 -0.00058 -0.01097 0.02155 \*

\* Se 18 -0.01113 0.02171 -0.00182 \*

\* Se 19 -0.00676 -0.01535 0.00867 \*

\* Se 20 -0.03263 0.02950 0.01887 \*

\* Nb 1 0.05419 -0.00274 0.01481 \*

\* Nb 2 -0.05614 0.00292 -0.01556 \*

\* Nb 3 0.00029 0.00263 -0.00008 \*

\* Nb 4 0.00310 0.00353 -0.00037 \*

\* Nb 5 -0.01651 -0.02028 -0.01778 \*

\* Nb 6 0.02866 -0.04473 0.01715 \*

\* Nb 7 0.00531 -0.00160 -0.02889 \*

\* Nb 8 0.04820 0.00904 0.02604 \*

\* Nb 9 0.01239 0.09755 -0.01493 \*

\* Nb 10 0.01430 0.01524 0.02341 \*

\* Nb 11 0.02798 -0.01904 0.02858 \*

\* Nb 12 -0.03594 -0.00586 -0.01369 \*

\* Nb 13 -0.01646 -0.01757 -0.02437 \*

\* Nb 14 -0.01518 -0.09730 0.01786 \*

\* Nb 15 -0.02776 0.01958 -0.02838 \*

\* Nb 16 0.03501 0.00852 0.01517 \*

\* Nb 17 -0.02892 0.04867 -0.01788 \*

\* Nb 18 0.01775 0.02091 0.01952 \*

\* Nb 19 -0.00714 -0.00141 0.03149 \*

\* Nb 20 -0.05196 -0.01187 -0.02711 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.034840 -0.077722 0.323479 \*

\* y -0.077722 -0.003985 -0.023745 \*

\* z 0.323479 -0.023745 -0.007756 \*

\* \*

\* Pressure: -0.0077 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000085 | -36259.882620 | <-- min BFGS

| trial step | 1.000000 | 0.000033 | -36259.884266 | <-- min BFGS

| line step | 1.654286 | 1.268E-006 | -36259.884624 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 35 with enthalpy= -3.62598846E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 5.009279E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.116970E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.089736E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.234786E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 36 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000042 | -36259.884624 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 36 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9057597 -8.3541142 0.0214818 0.4198171 -0.0030527 -0.0004488

0.0246078 3.3842482 -0.0007889 1.0363301 1.8490615 -0.0007845

0.0148467 -0.0024222 13.9041411 -0.0005898 0.0001096 0.4518937

Lattice parameters(A) Cell Angles

a = 17.087228 alpha = 90.022893

b = 3.384338 beta = 89.869719

c = 13.904149 gamma = 118.852368

Current cell volume = 704.248823 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067523 0.667742 0.124604 x

x Se 2 0.131959 0.341395 0.628572 x

x Se 3 0.131960 0.340644 0.871131 x

x Se 4 0.067840 0.669026 0.375881 x

x Se 5 0.266744 0.663851 0.124115 x

x Se 6 0.333017 0.344285 0.627994 x

x Se 7 0.332645 0.343299 0.872435 x

x Se 8 0.266184 0.662992 0.374392 x

x Se 9 0.467562 0.654593 0.128120 x

x Se 10 0.533080 0.343393 0.625798 x

x Se 11 0.532444 0.345443 0.871876 x

x Se 12 0.466883 0.656806 0.374281 x

x Se 13 0.667342 0.656619 0.127570 x

x Se 14 0.733853 0.336922 0.625643 x

x Se 15 0.733271 0.335982 0.875905 x

x Se 16 0.666970 0.655708 0.371976 x

x Se 17 0.868021 0.659301 0.128850 x

x Se 18 0.932170 0.331150 0.624073 x

x Se 19 0.932483 0.332347 0.875389 x

x Se 20 0.868024 0.658531 0.371445 x

x Nb 1 0.003950 0.011469 0.249892 x

x Nb 2 -0.003987 -0.011414 0.750088 x

x Nb 3 -0.000026 -0.000199 -0.000002 x

x Nb 4 -0.000019 -0.000167 0.499974 x

x Nb 5 0.197146 -0.007387 0.249535 x

x Nb 6 0.202393 0.017644 0.749485 x

x Nb 7 0.199406 0.002684 -0.001079 x

x Nb 8 0.200808 0.007126 0.501068 x

x Nb 9 0.399139 -0.013199 0.250660 x

x Nb 10 0.400633 0.011438 0.749975 x

x Nb 11 0.400402 0.004865 -0.001142 x

x Nb 12 0.398101 -0.003234 0.500860 x

x Nb 13 0.599346 -0.011405 0.250040 x

x Nb 14 0.600869 0.013337 0.749325 x

x Nb 15 0.599577 -0.004980 0.001148 x

x Nb 16 0.601917 0.003299 0.499159 x

x Nb 17 0.797609 -0.017835 0.250521 x

x Nb 18 0.802901 0.007236 0.750464 x

x Nb 19 0.800653 -0.002350 0.001041 x

x Nb 20 0.799206 -0.006956 0.498940 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598771E+004 25884.09 <-- SCF

1 -3.62599131E+004 8.99508104E-004 25911.56 <-- SCF

2 -3.62599152E+004 5.20490535E-005 25937.36 <-- SCF

3 -3.62599138E+004 -3.56938216E-005 25964.47 <-- SCF

4 -3.62598846E+004 -7.27903946E-004 25990.77 <-- SCF

5 -3.62598864E+004 4.51575096E-005 26016.27 <-- SCF

6 -3.62598859E+004 -1.35463294E-005 26037.94 <-- SCF

7 -3.62598856E+004 -6.42856838E-006 26057.22 <-- SCF

8 -3.62598856E+004 -3.45030589E-007 26074.55 <-- SCF

9 -3.62598857E+004 1.10926072E-006 26093.61 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.88567459 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00982 0.01458 -0.01172 \*

\* Se 2 0.02649 -0.02600 -0.01888 \*

\* Se 3 -0.00084 0.01726 -0.01472 \*

\* Se 4 0.01654 -0.02045 -0.00542 \*

\* Se 5 0.01218 0.04665 0.00001 \*

\* Se 6 -0.01075 -0.05329 -0.01427 \*

\* Se 7 0.02165 -0.01745 -0.01933 \*

\* Se 8 -0.00981 0.03645 -0.03875 \*

\* Se 9 -0.07034 0.01180 0.01807 \*

\* Se 10 0.08963 -0.03919 -0.04518 \*

\* Se 11 0.06834 -0.01241 -0.01793 \*

\* Se 12 -0.08574 0.02785 0.03237 \*

\* Se 13 -0.01863 0.02049 0.01630 \*

\* Se 14 0.00995 -0.03663 0.04197 \*

\* Se 15 -0.01433 -0.04458 0.00512 \*

\* Se 16 0.00863 0.05447 0.02579 \*

\* Se 17 0.00258 -0.01865 0.01881 \*

\* Se 18 -0.01169 0.02158 -0.00213 \*

\* Se 19 -0.00943 -0.01559 0.01069 \*

\* Se 20 -0.02491 0.02630 0.01536 \*

\* Nb 1 0.05706 0.00008 0.01726 \*

\* Nb 2 -0.05927 0.00082 -0.01810 \*

\* Nb 3 0.00025 0.00252 0.00015 \*

\* Nb 4 0.00297 0.00338 -0.00067 \*

\* Nb 5 -0.02748 -0.01861 -0.01251 \*

\* Nb 6 0.02834 -0.04217 0.01174 \*

\* Nb 7 0.00448 -0.00286 -0.02241 \*

\* Nb 8 0.04782 0.00964 0.01902 \*

\* Nb 9 0.00981 0.09469 -0.00634 \*

\* Nb 10 0.01038 0.01120 0.01188 \*

\* Nb 11 0.02623 -0.01999 0.02449 \*

\* Nb 12 -0.04021 -0.00310 -0.00894 \*

\* Nb 13 -0.01246 -0.01378 -0.01322 \*

\* Nb 14 -0.01253 -0.09425 0.00932 \*

\* Nb 15 -0.02627 0.02046 -0.02414 \*

\* Nb 16 0.03907 0.00560 0.01036 \*

\* Nb 17 -0.02866 0.04605 -0.01292 \*

\* Nb 18 0.02890 0.01909 0.01414 \*

\* Nb 19 -0.00625 0.00022 0.02469 \*

\* Nb 20 -0.05153 -0.01216 -0.01995 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.041641 -0.080672 0.296408 \*

\* y -0.080672 -0.028974 -0.025123 \*

\* z 0.296408 -0.025123 0.014967 \*

\* \*

\* Pressure: -0.0092 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000042 | -36259.884624 | <-- min BFGS

| trial step | 1.000000 | 0.000034 | -36259.885724 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 36 with line minimization (lambda= 5.385004)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9067516 -8.3518363 0.0123558 0.4198380 -0.0029655 -0.0002409

0.0238895 3.3821396 -0.0007490 1.0367453 1.8504315 -0.0002810

0.0079669 -0.0023511 13.9129717 -0.0003170 0.0001023 0.4516065

Lattice parameters(A) Cell Angles

a = 17.086971 alpha = 90.022139

b = 3.382224 beta = 89.925213

c = 13.912974 gamma = 118.855995

Current cell volume = 704.221946 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067531 0.667807 0.124640 x

x Se 2 0.132090 0.341512 0.628459 x

x Se 3 0.131990 0.340206 0.871087 x

x Se 4 0.067871 0.669080 0.375833 x

x Se 5 0.266724 0.663946 0.124347 x

x Se 6 0.332979 0.344507 0.627926 x

x Se 7 0.332637 0.342690 0.872326 x

x Se 8 0.266152 0.663080 0.374208 x

x Se 9 0.467473 0.655369 0.128208 x

x Se 10 0.533134 0.342873 0.625689 x

x Se 11 0.532532 0.344621 0.871802 x

x Se 12 0.466820 0.657301 0.374395 x

x Se 13 0.667347 0.657205 0.127658 x

x Se 14 0.733887 0.336831 0.625835 x

x Se 15 0.733292 0.335900 0.875681 x

x Se 16 0.667006 0.655433 0.372040 x

x Se 17 0.868003 0.659797 0.128895 x

x Se 18 0.932141 0.331110 0.624105 x

x Se 19 0.932474 0.332280 0.875350 x

x Se 20 0.867898 0.658487 0.371548 x

x Nb 1 0.003949 0.011128 0.249874 x

x Nb 2 -0.003984 -0.011128 0.750106 x

x Nb 3 -0.000025 -0.000164 -0.000009 x

x Nb 4 -0.000012 -0.000109 0.499983 x

x Nb 5 0.197284 -0.007132 0.249461 x

x Nb 6 0.202485 0.017166 0.749575 x

x Nb 7 0.199452 0.002836 -0.001209 x

x Nb 8 0.200918 0.007479 0.501187 x

x Nb 9 0.399145 -0.012261 0.250557 x

x Nb 10 0.400738 0.012088 0.750168 x

x Nb 11 0.400486 0.004789 -0.000916 x

x Nb 12 0.398079 -0.003711 0.500665 x

x Nb 13 0.599247 -0.012036 0.249850 x

x Nb 14 0.600853 0.012346 0.749430 x

x Nb 15 0.599497 -0.004881 0.000916 x

x Nb 16 0.601939 0.003793 0.499358 x

x Nb 17 0.797514 -0.017322 0.250435 x

x Nb 18 0.802764 0.007019 0.750541 x

x Nb 19 0.800602 -0.002566 0.001187 x

x Nb 20 0.799091 -0.007369 0.498808 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597247E+004 26197.02 <-- SCF

1 -3.62604149E+004 1.72549193E-002 26224.12 <-- SCF

2 -3.62604538E+004 9.74494068E-004 26252.30 <-- SCF

3 -3.62603776E+004 -1.90462619E-003 26278.91 <-- SCF

4 -3.62598757E+004 -1.25496574E-002 26305.14 <-- SCF

5 -3.62599002E+004 6.14147831E-004 26331.83 <-- SCF

6 -3.62598901E+004 -2.54346955E-004 26357.97 <-- SCF

7 -3.62598865E+004 -8.96650984E-005 26381.64 <-- SCF

8 -3.62598867E+004 4.73295631E-006 26402.58 <-- SCF

9 -3.62598869E+004 5.18991573E-006 26421.67 <-- SCF

10 -3.62598870E+004 4.21721011E-006 26439.19 <-- SCF

11 -3.62598872E+004 2.93370788E-006 26456.50 <-- SCF

12 -3.62598873E+004 2.48243243E-006 26473.86 <-- SCF

13 -3.62598873E+004 2.23240139E-006 26490.12 <-- SCF

14 -3.62598874E+004 1.87987321E-006 26506.72 <-- SCF

15 -3.62598875E+004 1.57790598E-006 26522.84 <-- SCF

16 -3.62598875E+004 1.30425889E-006 26539.00 <-- SCF

17 -3.62598876E+004 1.09256314E-006 26554.92 <-- SCF

18 -3.62598876E+004 9.29280165E-007 26570.80 <-- SCF

19 -3.62598876E+004 8.50322043E-007 26586.80 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.88764594 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01721 0.01698 -0.02596 \*

\* Se 2 -0.00489 -0.01750 -0.00086 \*

\* Se 3 -0.01847 0.04592 -0.00036 \*

\* Se 4 0.01757 -0.01842 -0.00856 \*

\* Se 5 0.02817 0.02549 -0.02081 \*

\* Se 6 0.00851 -0.06632 0.01708 \*

\* Se 7 0.03701 0.03019 0.04175 \*

\* Se 8 -0.00618 0.04832 -0.04489 \*

\* Se 9 -0.05077 -0.01985 -0.01490 \*

\* Se 10 0.07389 -0.02018 -0.02231 \*

\* Se 11 0.04948 0.02092 0.01212 \*

\* Se 12 -0.06256 0.00317 0.00953 \*

\* Se 13 -0.03184 -0.02569 -0.03520 \*

\* Se 14 0.00329 -0.04531 0.04515 \*

\* Se 15 -0.03153 -0.02547 0.02537 \*

\* Se 16 -0.01157 0.07138 -0.00419 \*

\* Se 17 0.01657 -0.04954 0.00483 \*

\* Se 18 -0.01200 0.02112 0.00097 \*

\* Se 19 -0.01646 -0.01804 0.02414 \*

\* Se 20 0.00535 0.01325 -0.00085 \*

\* Nb 1 0.04905 0.00828 0.02471 \*

\* Nb 2 -0.05284 -0.00393 -0.02645 \*

\* Nb 3 0.00047 0.00112 0.00142 \*

\* Nb 4 0.00309 0.00178 -0.00285 \*

\* Nb 5 -0.05889 -0.01697 0.00714 \*

\* Nb 6 0.02269 -0.03232 -0.00862 \*

\* Nb 7 0.00293 -0.00430 -0.00527 \*

\* Nb 8 0.04483 0.00919 -0.00589 \*

\* Nb 9 0.00259 0.08892 0.01939 \*

\* Nb 10 -0.00903 -0.00658 -0.02633 \*

\* Nb 11 0.01641 -0.02200 -0.00122 \*

\* Nb 12 -0.05535 0.00678 0.01274 \*

\* Nb 13 0.00569 0.00316 0.02373 \*

\* Nb 14 -0.00459 -0.08775 -0.01599 \*

\* Nb 15 -0.01727 0.02166 0.00238 \*

\* Nb 16 0.05386 -0.00553 -0.01200 \*

\* Nb 17 -0.02211 0.03578 0.00539 \*

\* Nb 18 0.06088 0.01592 -0.00567 \*

\* Nb 19 -0.00408 0.00478 0.00463 \*

\* Nb 20 -0.04909 -0.00839 0.00669 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.072932 -0.094076 0.157999 \*

\* y -0.094076 -0.130290 -0.021154 \*

\* z 0.157999 -0.021154 0.114291 \*

\* \*

\* Pressure: -0.0190 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000042 | -36259.884624 | <-- min BFGS

| trial step | 1.000000 | 0.000034 | -36259.885724 | <-- min BFGS

| line step | 5.385004 | 1.265E-006 | -36259.887704 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 36 with enthalpy= -3.62598877E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.700708E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 9.104684E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.777039E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.579987E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 37 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000109 | -36259.887704 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 37 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9017758 -8.3525829 0.0032155 0.4199014 -0.0031019 -0.0000295

0.0250006 3.3842914 -0.0007666 1.0363354 1.8489178 0.0002540

0.0009578 -0.0024472 13.9062639 -0.0000400 0.0001026 0.4518241

Lattice parameters(A) Cell Angles

a = 17.082991 alpha = 90.023032

b = 3.384384 beta = 89.980843

c = 13.906264 gamma = 118.847784

Current cell volume = 704.223887 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067572 0.668136 0.124405 x

x Se 2 0.132101 0.341841 0.628495 x

x Se 3 0.131967 0.340323 0.871015 x

x Se 4 0.067936 0.669428 0.376060 x

x Se 5 0.266713 0.663934 0.124151 x

x Se 6 0.333071 0.345193 0.627945 x

x Se 7 0.332700 0.343105 0.872330 x

x Se 8 0.266094 0.663008 0.374287 x

x Se 9 0.467427 0.655050 0.128211 x

x Se 10 0.533225 0.343217 0.625525 x

x Se 11 0.532577 0.344930 0.871800 x

x Se 12 0.466725 0.656959 0.374562 x

x Se 13 0.667282 0.656780 0.127652 x

x Se 14 0.733948 0.336899 0.625761 x

x Se 15 0.733304 0.335905 0.875882 x

x Se 16 0.666912 0.654732 0.372022 x

x Se 17 0.868028 0.659691 0.128964 x

x Se 18 0.932078 0.330780 0.623868 x

x Se 19 0.932433 0.331953 0.875586 x

x Se 20 0.867887 0.658173 0.371511 x

x Nb 1 0.004261 0.011941 0.249865 x

x Nb 2 -0.004297 -0.011957 0.750113 x

x Nb 3 -0.000027 -0.000163 -0.000012 x

x Nb 4 -0.000011 -0.000097 0.499984 x

x Nb 5 0.197212 -0.007440 0.249399 x

x Nb 6 0.202620 0.017902 0.749577 x

x Nb 7 0.199433 0.003071 -0.001348 x

x Nb 8 0.201014 0.008072 0.501309 x

x Nb 9 0.399092 -0.012731 0.250567 x

x Nb 10 0.400802 0.013003 0.750214 x

x Nb 11 0.400561 0.005020 -0.000927 x

x Nb 12 0.397961 -0.004133 0.500676 x

x Nb 13 0.599183 -0.012943 0.249806 x

x Nb 14 0.600903 0.012802 0.749421 x

x Nb 15 0.599422 -0.005112 0.000926 x

x Nb 16 0.602057 0.004226 0.499350 x

x Nb 17 0.797377 -0.018056 0.250434 x

x Nb 18 0.802839 0.007333 0.750604 x

x Nb 19 0.800622 -0.002802 0.001330 x

x Nb 20 0.798993 -0.007974 0.498682 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597750E+004 26690.09 <-- SCF

1 -3.62600207E+004 6.14256711E-003 26716.33 <-- SCF

2 -3.62600350E+004 3.58619424E-004 26745.75 <-- SCF

3 -3.62599568E+004 -1.95442069E-003 26772.47 <-- SCF

4 -3.62598924E+004 -1.61197745E-003 26798.36 <-- SCF

5 -3.62598924E+004 1.00622700E-006 26824.66 <-- SCF

6 -3.62598901E+004 -5.65084700E-005 26849.11 <-- SCF

7 -3.62598898E+004 -9.42857500E-006 26870.48 <-- SCF

8 -3.62598899E+004 2.52674250E-006 26889.86 <-- SCF

9 -3.62598899E+004 -6.59822707E-008 26907.39 <-- SCF

10 -3.62598899E+004 2.36871736E-007 26923.53 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.88987583 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00545 -0.00867 -0.01501 \*

\* Se 2 -0.00654 -0.02861 0.00935 \*

\* Se 3 -0.02290 0.04245 -0.00806 \*

\* Se 4 0.00791 -0.03744 -0.02180 \*

\* Se 5 0.02212 0.03940 -0.02826 \*

\* Se 6 0.00091 -0.07974 0.02125 \*

\* Se 7 0.04020 0.03178 0.03626 \*

\* Se 8 -0.01542 0.04071 -0.05160 \*

\* Se 9 -0.05521 -0.01658 -0.00926 \*

\* Se 10 0.06918 -0.00602 -0.00946 \*

\* Se 11 0.05274 0.01834 0.00524 \*

\* Se 12 -0.05748 -0.01216 0.00597 \*

\* Se 13 -0.03441 -0.02724 -0.02879 \*

\* Se 14 0.01303 -0.03741 0.05128 \*

\* Se 15 -0.02545 -0.03815 0.03262 \*

\* Se 16 -0.00260 0.08559 -0.00873 \*

\* Se 17 0.02042 -0.04650 0.01261 \*

\* Se 18 -0.00215 0.03931 0.01336 \*

\* Se 19 -0.00484 0.00683 0.01277 \*

\* Se 20 0.00681 0.02337 -0.01142 \*

\* Nb 1 0.03206 0.01481 0.02389 \*

\* Nb 2 -0.03494 -0.01037 -0.02630 \*

\* Nb 3 0.00052 0.00174 0.00110 \*

\* Nb 4 0.00310 0.00239 -0.00333 \*

\* Nb 5 -0.05284 -0.00642 0.01674 \*

\* Nb 6 0.00304 -0.04139 -0.01452 \*

\* Nb 7 0.00370 -0.00801 -0.00209 \*

\* Nb 8 0.04318 0.00766 -0.01382 \*

\* Nb 9 0.00904 0.10266 0.02207 \*

\* Nb 10 -0.00563 -0.02512 -0.03664 \*

\* Nb 11 0.01578 -0.02249 -0.00036 \*

\* Nb 12 -0.05258 0.00869 0.01578 \*

\* Nb 13 0.00269 0.02122 0.03339 \*

\* Nb 14 -0.01069 -0.10171 -0.01923 \*

\* Nb 15 -0.01715 0.02249 0.00092 \*

\* Nb 16 0.05086 -0.00685 -0.01542 \*

\* Nb 17 -0.00371 0.04541 0.01047 \*

\* Nb 18 0.05412 0.00588 -0.01591 \*

\* Nb 19 -0.00473 0.00783 0.00095 \*

\* Nb 20 -0.04759 -0.00768 0.01396 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.027116 -0.034635 0.046311 \*

\* y -0.034635 -0.044450 -0.017412 \*

\* z 0.046311 -0.017412 0.016663 \*

\* \*

\* Pressure: 0.0002 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000109 | -36259.887704 | <-- min BFGS

| trial step | 1.000000 | 0.000036 | -36259.889943 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 37 with line minimization (lambda= 1.483752)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8993688 -8.3529440 -0.0012061 0.4199322 -0.0031678 0.0000729

0.0255381 3.3853323 -0.0007751 1.0361377 1.8481863 0.0005128

-0.0024329 -0.0024937 13.9030189 0.0000942 0.0001028 0.4519296

Lattice parameters(A) Cell Angles

a = 17.081067 alpha = 90.023470

b = 3.385429 beta = 90.007766

c = 13.903019 gamma = 118.843819

Current cell volume = 704.224452 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067592 0.668295 0.124291 x

x Se 2 0.132107 0.341999 0.628513 x

x Se 3 0.131956 0.340380 0.870981 x

x Se 4 0.067967 0.669597 0.376169 x

x Se 5 0.266707 0.663929 0.124057 x

x Se 6 0.333115 0.345525 0.627954 x

x Se 7 0.332731 0.343306 0.872332 x

x Se 8 0.266066 0.662973 0.374325 x

x Se 9 0.467405 0.654896 0.128213 x

x Se 10 0.533269 0.343383 0.625447 x

x Se 11 0.532599 0.345079 0.871799 x

x Se 12 0.466679 0.656793 0.374642 x

x Se 13 0.667250 0.656575 0.127649 x

x Se 14 0.733978 0.336932 0.625725 x

x Se 15 0.733310 0.335908 0.875979 x

x Se 16 0.666866 0.654393 0.372012 x

x Se 17 0.868041 0.659640 0.128998 x

x Se 18 0.932048 0.330620 0.623754 x

x Se 19 0.932413 0.331795 0.875699 x

x Se 20 0.867882 0.658021 0.371494 x

x Nb 1 0.004412 0.012334 0.249860 x

x Nb 2 -0.004449 -0.012358 0.750117 x

x Nb 3 -0.000027 -0.000162 -0.000013 x

x Nb 4 -0.000010 -0.000091 0.499985 x

x Nb 5 0.197177 -0.007590 0.249369 x

x Nb 6 0.202686 0.018259 0.749578 x

x Nb 7 0.199424 0.003184 -0.001415 x

x Nb 8 0.201061 0.008359 0.501368 x

x Nb 9 0.399066 -0.012958 0.250572 x

x Nb 10 0.400833 0.013445 0.750236 x

x Nb 11 0.400597 0.005132 -0.000933 x

x Nb 12 0.397904 -0.004338 0.500682 x

x Nb 13 0.599153 -0.013382 0.249784 x

x Nb 14 0.600927 0.013023 0.749417 x

x Nb 15 0.599386 -0.005223 0.000930 x

x Nb 16 0.602114 0.004435 0.499346 x

x Nb 17 0.797310 -0.018412 0.250433 x

x Nb 18 0.802875 0.007485 0.750634 x

x Nb 19 0.800632 -0.002917 0.001399 x

x Nb 20 0.798946 -0.008266 0.498621 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598624E+004 27026.38 <-- SCF

1 -3.62599533E+004 2.27324678E-003 27053.59 <-- SCF

2 -3.62599586E+004 1.30274372E-004 27081.08 <-- SCF

3 -3.62599496E+004 -2.24733962E-004 27108.09 <-- SCF

4 -3.62598874E+004 -1.55494070E-003 27134.06 <-- SCF

5 -3.62598921E+004 1.18261543E-004 27160.72 <-- SCF

6 -3.62598909E+004 -2.96074705E-005 27184.39 <-- SCF

7 -3.62598902E+004 -1.69270614E-005 27204.92 <-- SCF

8 -3.62598902E+004 -4.30798600E-007 27223.58 <-- SCF

9 -3.62598903E+004 7.18155646E-007 27241.38 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.89025233 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00058 -0.02231 -0.01565 \*

\* Se 2 -0.00600 -0.03285 0.01695 \*

\* Se 3 -0.02475 0.04152 -0.01251 \*

\* Se 4 0.00574 -0.04593 -0.02669 \*

\* Se 5 0.02289 0.04633 -0.03510 \*

\* Se 6 0.00217 -0.08350 0.02490 \*

\* Se 7 0.04589 0.03404 0.03509 \*

\* Se 8 -0.01887 0.03721 -0.05626 \*

\* Se 9 -0.05748 -0.01513 -0.00837 \*

\* Se 10 0.06652 0.00094 -0.01224 \*

\* Se 11 0.05467 0.01723 0.00387 \*

\* Se 12 -0.05521 -0.01906 0.01335 \*

\* Se 13 -0.03989 -0.02954 -0.02739 \*

\* Se 14 0.01656 -0.03382 0.05556 \*

\* Se 15 -0.02648 -0.04403 0.03864 \*

\* Se 16 -0.00325 0.08968 -0.01256 \*

\* Se 17 0.02207 -0.04576 0.01718 \*

\* Se 18 -0.00010 0.04697 0.01874 \*

\* Se 19 0.00021 0.02009 0.01321 \*

\* Se 20 0.00631 0.02715 -0.01940 \*

\* Nb 1 0.02835 0.01886 0.02236 \*

\* Nb 2 -0.03069 -0.01446 -0.02517 \*

\* Nb 3 0.00044 0.00201 0.00091 \*

\* Nb 4 0.00330 0.00268 -0.00359 \*

\* Nb 5 -0.04790 -0.00133 0.01954 \*

\* Nb 6 -0.00152 -0.04689 -0.01590 \*

\* Nb 7 0.00645 -0.00869 -0.00345 \*

\* Nb 8 0.04711 0.00709 -0.01726 \*

\* Nb 9 0.01509 0.11026 0.02231 \*

\* Nb 10 -0.00524 -0.03447 -0.03996 \*

\* Nb 11 0.02016 -0.02272 -0.00151 \*

\* Nb 12 -0.05086 0.00898 0.01715 \*

\* Nb 13 0.00239 0.03028 0.03621 \*

\* Nb 14 -0.01654 -0.10942 -0.01962 \*

\* Nb 15 -0.02167 0.02278 0.00188 \*

\* Nb 16 0.04892 -0.00700 -0.01703 \*

\* Nb 17 0.00036 0.05116 0.01133 \*

\* Nb 18 0.04895 0.00109 -0.01883 \*

\* Nb 19 -0.00729 0.00806 0.00216 \*

\* Nb 20 -0.05141 -0.00750 0.01717 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.008889 -0.009615 -0.012742 \*

\* y -0.009615 -0.001730 -0.016018 \*

\* z -0.012742 -0.016018 -0.029338 \*

\* \*

\* Pressure: 0.0074 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000109 | -36259.887704 | <-- min BFGS

| trial step | 1.000000 | 0.000036 | -36259.889943 | <-- min BFGS

| line step | 1.483752 | 8.020E-006 | -36259.890325 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 37 with enthalpy= -3.62598903E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 6.551729E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.135012E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.955346E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.933806E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 38 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000013 | -36259.890325 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 38 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8955976 -8.3513154 -0.0044440 0.4200071 -0.0032245 0.0001357

0.0259911 3.3854406 -0.0005689 1.0360874 1.8479889 0.0005799

-0.0045063 -0.0018372 13.9049804 0.0001766 0.0000746 0.4518659

Lattice parameters(A) Cell Angles

a = 17.076982 alpha = 90.017340

b = 3.385540 beta = 90.027405

c = 13.904981 gamma = 118.837585

Current cell volume = 704.220704 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067585 0.668267 0.124271 x

x Se 2 0.132133 0.342130 0.628518 x

x Se 3 0.131983 0.340573 0.870966 x

x Se 4 0.067956 0.669536 0.376185 x

x Se 5 0.266705 0.664015 0.124050 x

x Se 6 0.333132 0.345554 0.627960 x

x Se 7 0.332764 0.343465 0.872317 x

x Se 8 0.266049 0.663007 0.374313 x

x Se 9 0.467394 0.654699 0.128238 x

x Se 10 0.533281 0.343540 0.625439 x

x Se 11 0.532610 0.345279 0.871773 x

x Se 12 0.466669 0.656629 0.374648 x

x Se 13 0.667219 0.656425 0.127663 x

x Se 14 0.733995 0.336897 0.625737 x

x Se 15 0.733311 0.335820 0.875986 x

x Se 16 0.666850 0.654369 0.372011 x

x Se 17 0.868012 0.659440 0.129014 x

x Se 18 0.932060 0.330684 0.623737 x

x Se 19 0.932420 0.331825 0.875719 x

x Se 20 0.867855 0.657885 0.371487 x

x Nb 1 0.004478 0.012621 0.249864 x

x Nb 2 -0.004516 -0.012638 0.750112 x

x Nb 3 -0.000027 -0.000165 -0.000012 x

x Nb 4 -0.000010 -0.000094 0.499983 x

x Nb 5 0.197160 -0.007689 0.249369 x

x Nb 6 0.202677 0.018310 0.749569 x

x Nb 7 0.199412 0.003158 -0.001420 x

x Nb 8 0.201064 0.008385 0.501376 x

x Nb 9 0.399061 -0.013021 0.250575 x

x Nb 10 0.400828 0.013389 0.750224 x

x Nb 11 0.400601 0.005167 -0.000974 x

x Nb 12 0.397893 -0.004318 0.500728 x

x Nb 13 0.599157 -0.013333 0.249796 x

x Nb 14 0.600932 0.013094 0.749415 x

x Nb 15 0.599381 -0.005261 0.000972 x

x Nb 16 0.602125 0.004417 0.499300 x

x Nb 17 0.797319 -0.018464 0.250441 x

x Nb 18 0.802894 0.007580 0.750634 x

x Nb 19 0.800644 -0.002885 0.001402 x

x Nb 20 0.798943 -0.008290 0.498615 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598846E+004 27344.58 <-- SCF

1 -3.62598967E+004 3.03942207E-004 27370.52 <-- SCF

2 -3.62598975E+004 1.83421317E-005 27394.42 <-- SCF

3 -3.62598937E+004 -9.53458741E-005 27420.53 <-- SCF

4 -3.62598908E+004 -7.24250805E-005 27445.98 <-- SCF

5 -3.62598907E+004 -8.45227541E-007 27468.89 <-- SCF

6 -3.62598906E+004 -1.85435508E-006 27486.33 <-- SCF

7 -3.62598906E+004 -3.76231008E-007 27503.77 <-- SCF

8 -3.62598906E+004 2.55186481E-007 27519.66 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.89064262 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00120 -0.02560 -0.01326 \*

\* Se 2 -0.01720 -0.03494 0.01754 \*

\* Se 3 -0.03701 0.03332 -0.01558 \*

\* Se 4 0.00381 -0.04628 -0.02407 \*

\* Se 5 0.01755 0.03968 -0.03685 \*

\* Se 6 -0.00472 -0.08225 0.02541 \*

\* Se 7 0.03796 0.03132 0.03259 \*

\* Se 8 -0.02330 0.03237 -0.05781 \*

\* Se 9 -0.05832 -0.00836 -0.01060 \*

\* Se 10 0.06762 -0.00248 -0.01719 \*

\* Se 11 0.05533 0.01068 0.00610 \*

\* Se 12 -0.05675 -0.01507 0.01851 \*

\* Se 13 -0.03201 -0.02739 -0.02464 \*

\* Se 14 0.02095 -0.02828 0.05683 \*

\* Se 15 -0.02066 -0.03704 0.03993 \*

\* Se 16 0.00380 0.08787 -0.01458 \*

\* Se 17 0.03451 -0.03717 0.02008 \*

\* Se 18 0.00154 0.04719 0.01622 \*

\* Se 19 0.00168 0.02326 0.01115 \*

\* Se 20 0.01747 0.02961 -0.01977 \*

\* Nb 1 0.02323 0.01683 0.02333 \*

\* Nb 2 -0.02528 -0.01302 -0.02603 \*

\* Nb 3 0.00037 0.00207 0.00100 \*

\* Nb 4 0.00316 0.00275 -0.00349 \*

\* Nb 5 -0.05217 0.00499 0.02123 \*

\* Nb 6 0.00027 -0.04794 -0.01875 \*

\* Nb 7 0.00564 -0.00829 -0.00214 \*

\* Nb 8 0.04690 0.00856 -0.01857 \*

\* Nb 9 0.01440 0.10998 0.02588 \*

\* Nb 10 -0.00275 -0.03178 -0.04043 \*

\* Nb 11 0.01984 -0.02181 0.00277 \*

\* Nb 12 -0.05507 0.00717 0.01443 \*

\* Nb 13 0.00073 0.02783 0.03721 \*

\* Nb 14 -0.01589 -0.10955 -0.02326 \*

\* Nb 15 -0.02140 0.02193 -0.00249 \*

\* Nb 16 0.05324 -0.00526 -0.01417 \*

\* Nb 17 -0.00159 0.05220 0.01454 \*

\* Nb 18 0.05281 -0.00498 -0.02058 \*

\* Nb 19 -0.00629 0.00725 0.00131 \*

\* Nb 20 -0.05117 -0.00939 0.01819 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.005180 0.000840 -0.048388 \*

\* y 0.000840 0.004183 0.000537 \*

\* z -0.048388 0.000537 -0.016435 \*

\* \*

\* Pressure: 0.0058 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000013 | -36259.890325 | <-- min BFGS

| trial step | 1.000000 | 6.752E-006 | -36259.890732 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 38 with line minimization (lambda= 2.127364)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8913462 -8.3494793 -0.0080943 0.4200917 -0.0032884 0.0002065

0.0265017 3.3855628 -0.0003364 1.0360307 1.8477663 0.0006556

-0.0068438 -0.0010969 13.9071918 0.0002696 0.0000428 0.4517941

Lattice parameters(A) Cell Angles

a = 17.072377 alpha = 90.010432

b = 3.385667 beta = 90.049548

c = 13.907193 gamma = 118.830560

Current cell volume = 704.216355 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067577 0.668234 0.124249 x

x Se 2 0.132163 0.342277 0.628523 x

x Se 3 0.132014 0.340791 0.870949 x

x Se 4 0.067943 0.669467 0.376203 x

x Se 5 0.266704 0.664112 0.124042 x

x Se 6 0.333151 0.345588 0.627966 x

x Se 7 0.332801 0.343644 0.872300 x

x Se 8 0.266029 0.663045 0.374300 x

x Se 9 0.467382 0.654476 0.128267 x

x Se 10 0.533293 0.343717 0.625431 x

x Se 11 0.532621 0.345504 0.871744 x

x Se 12 0.466658 0.656445 0.374655 x

x Se 13 0.667183 0.656255 0.127679 x

x Se 14 0.734013 0.336857 0.625749 x

x Se 15 0.733312 0.335721 0.875995 x

x Se 16 0.666832 0.654342 0.372009 x

x Se 17 0.867981 0.659215 0.129033 x

x Se 18 0.932074 0.330757 0.623718 x

x Se 19 0.932429 0.331858 0.875740 x

x Se 20 0.867825 0.657732 0.371480 x

x Nb 1 0.004553 0.012944 0.249869 x

x Nb 2 -0.004593 -0.012954 0.750107 x

x Nb 3 -0.000028 -0.000169 -0.000011 x

x Nb 4 -0.000010 -0.000098 0.499981 x

x Nb 5 0.197140 -0.007801 0.249370 x

x Nb 6 0.202667 0.018367 0.749559 x

x Nb 7 0.199399 0.003129 -0.001426 x

x Nb 8 0.201067 0.008414 0.501384 x

x Nb 9 0.399056 -0.013092 0.250578 x

x Nb 10 0.400821 0.013325 0.750210 x

x Nb 11 0.400606 0.005207 -0.001020 x

x Nb 12 0.397881 -0.004296 0.500779 x

x Nb 13 0.599161 -0.013279 0.249809 x

x Nb 14 0.600938 0.013173 0.749412 x

x Nb 15 0.599376 -0.005304 0.001020 x

x Nb 16 0.602138 0.004396 0.499248 x

x Nb 17 0.797330 -0.018523 0.250451 x

x Nb 18 0.802914 0.007688 0.750634 x

x Nb 19 0.800658 -0.002849 0.001405 x

x Nb 20 0.798940 -0.008316 0.498608 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598833E+004 27622.89 <-- SCF

1 -3.62598962E+004 3.21834498E-004 27646.81 <-- SCF

2 -3.62598968E+004 1.49773276E-005 27670.58 <-- SCF

3 -3.62598919E+004 -1.21064133E-004 27696.16 <-- SCF

4 -3.62598911E+004 -2.11205121E-005 27721.02 <-- SCF

5 -3.62598908E+004 -7.77132312E-006 27742.47 <-- SCF

6 -3.62598908E+004 -1.07748490E-007 27758.39 <-- SCF

7 -3.62598908E+004 1.27188972E-006 27776.58 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.89082144 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00032 -0.02901 -0.01655 \*

\* Se 2 -0.02512 -0.03812 0.01531 \*

\* Se 3 -0.04941 0.02272 -0.01154 \*

\* Se 4 0.00550 -0.04681 -0.02047 \*

\* Se 5 0.01701 0.03282 -0.04161 \*

\* Se 6 -0.00847 -0.08107 0.02573 \*

\* Se 7 0.03423 0.02725 0.03446 \*

\* Se 8 -0.02250 0.02670 -0.05842 \*

\* Se 9 -0.05811 0.00218 -0.01688 \*

\* Se 10 0.06763 -0.00719 -0.01922 \*

\* Se 11 0.05542 0.00028 0.01257 \*

\* Se 12 -0.05727 -0.00970 0.02087 \*

\* Se 13 -0.02877 -0.02397 -0.02649 \*

\* Se 14 0.01993 -0.02184 0.05699 \*

\* Se 15 -0.01993 -0.02978 0.04430 \*

\* Se 16 0.00760 0.08611 -0.01666 \*

\* Se 17 0.04711 -0.02609 0.01568 \*

\* Se 18 -0.00014 0.04755 0.01321 \*

\* Se 19 0.00015 0.02655 0.01454 \*

\* Se 20 0.02528 0.03325 -0.01688 \*

\* Nb 1 0.01875 0.01553 0.02072 \*

\* Nb 2 -0.02057 -0.01207 -0.02334 \*

\* Nb 3 0.00029 0.00191 0.00110 \*

\* Nb 4 0.00314 0.00263 -0.00366 \*

\* Nb 5 -0.05152 0.00981 0.02084 \*

\* Nb 6 0.00619 -0.04776 -0.01910 \*

\* Nb 7 0.00653 -0.00714 -0.00198 \*

\* Nb 8 0.04968 0.01034 -0.01911 \*

\* Nb 9 0.01725 0.10881 0.02585 \*

\* Nb 10 0.00174 -0.03062 -0.03919 \*

\* Nb 11 0.02380 -0.02005 0.00473 \*

\* Nb 12 -0.05579 0.00563 0.01099 \*

\* Nb 13 -0.00360 0.02665 0.03608 \*

\* Nb 14 -0.01852 -0.10854 -0.02302 \*

\* Nb 15 -0.02535 0.02017 -0.00442 \*

\* Nb 16 0.05401 -0.00395 -0.01070 \*

\* Nb 17 -0.00779 0.05189 0.01516 \*

\* Nb 18 0.05220 -0.00979 -0.02010 \*

\* Nb 19 -0.00706 0.00600 0.00122 \*

\* Nb 20 -0.05384 -0.01129 0.01900 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.023035 0.009141 -0.082540 \*

\* y 0.009141 0.005584 0.015462 \*

\* z -0.082540 0.015462 -0.000220 \*

\* \*

\* Pressure: 0.0059 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000013 | -36259.890325 | <-- min BFGS

| trial step | 1.000000 | 6.752E-006 | -36259.890732 | <-- min BFGS

| line step | 2.127364 | 3.250E-007 | -36259.890925 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 38 with enthalpy= -3.62598909E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.499087E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.131582E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.313446E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 8.254028E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 39 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000012 | -36259.890925 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 39 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8904049 -8.3485816 -0.0076215 0.4201006 -0.0033201 0.0001993

0.0267575 3.3856354 -0.0004016 1.0359192 1.8476493 0.0006655

-0.0066096 -0.0013038 13.9079759 0.0002601 0.0000515 0.4517686

Lattice parameters(A) Cell Angles

a = 17.071117 alpha = 90.012382

b = 3.385741 beta = 90.046704

c = 13.907978 gamma = 118.825158

Current cell volume = 704.256160 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067581 0.668260 0.124216 x

x Se 2 0.132164 0.342300 0.628520 x

x Se 3 0.132007 0.340836 0.870940 x

x Se 4 0.067950 0.669484 0.376228 x

x Se 5 0.266708 0.664154 0.124008 x

x Se 6 0.333149 0.345582 0.627970 x

x Se 7 0.332811 0.343711 0.872294 x

x Se 8 0.266022 0.663054 0.374306 x

x Se 9 0.467361 0.654365 0.128271 x

x Se 10 0.533318 0.343816 0.625403 x

x Se 11 0.532642 0.345613 0.871739 x

x Se 12 0.466634 0.656338 0.374684 x

x Se 13 0.667174 0.656193 0.127685 x

x Se 14 0.734020 0.336848 0.625744 x

x Se 15 0.733308 0.335679 0.876030 x

x Se 16 0.666834 0.654350 0.372008 x

x Se 17 0.867987 0.659168 0.129043 x

x Se 18 0.932068 0.330745 0.623691 x

x Se 19 0.932424 0.331832 0.875772 x

x Se 20 0.867824 0.657708 0.371482 x

x Nb 1 0.004595 0.013086 0.249871 x

x Nb 2 -0.004636 -0.013095 0.750105 x

x Nb 3 -0.000028 -0.000168 -0.000011 x

x Nb 4 -0.000010 -0.000094 0.499980 x

x Nb 5 0.197119 -0.007869 0.249366 x

x Nb 6 0.202681 0.018421 0.749556 x

x Nb 7 0.199395 0.003139 -0.001438 x

x Nb 8 0.201083 0.008495 0.501393 x

x Nb 9 0.399055 -0.013053 0.250579 x

x Nb 10 0.400824 0.013372 0.750212 x

x Nb 11 0.400616 0.005233 -0.001027 x

x Nb 12 0.397860 -0.004343 0.500789 x

x Nb 13 0.599158 -0.013330 0.249807 x

x Nb 14 0.600939 0.013135 0.749411 x

x Nb 15 0.599366 -0.005331 0.001027 x

x Nb 16 0.602159 0.004445 0.499239 x

x Nb 17 0.797316 -0.018575 0.250453 x

x Nb 18 0.802936 0.007755 0.750638 x

x Nb 19 0.800662 -0.002858 0.001417 x

x Nb 20 0.798922 -0.008400 0.498599 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598883E+004 27879.52 <-- SCF

1 -3.62599187E+004 7.58214751E-004 27907.73 <-- SCF

2 -3.62599212E+004 6.38195032E-005 27931.08 <-- SCF

3 -3.62599252E+004 9.94007491E-005 27957.14 <-- SCF

4 -3.62598891E+004 -9.03229552E-004 27983.05 <-- SCF

5 -3.62598918E+004 6.76585853E-005 28007.39 <-- SCF

6 -3.62598915E+004 -6.60973548E-006 28028.05 <-- SCF

7 -3.62598912E+004 -7.74153089E-006 28046.92 <-- SCF

8 -3.62598911E+004 -1.16762460E-006 28064.84 <-- SCF

9 -3.62598911E+004 3.26627058E-007 28082.31 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.89114891 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00194 -0.03412 -0.01553 \*

\* Se 2 -0.02476 -0.03653 0.01660 \*

\* Se 3 -0.04688 0.02174 -0.01626 \*

\* Se 4 0.00428 -0.04797 -0.01651 \*

\* Se 5 0.01566 0.03301 -0.04337 \*

\* Se 6 -0.00452 -0.07955 0.02540 \*

\* Se 7 0.03677 0.02887 0.03363 \*

\* Se 8 -0.02305 0.02533 -0.06037 \*

\* Se 9 -0.05606 0.00349 -0.01322 \*

\* Se 10 0.06534 -0.00531 -0.02488 \*

\* Se 11 0.05337 -0.00087 0.00885 \*

\* Se 12 -0.05555 -0.01088 0.02779 \*

\* Se 13 -0.03139 -0.02580 -0.02577 \*

\* Se 14 0.02054 -0.02046 0.05894 \*

\* Se 15 -0.01859 -0.02961 0.04549 \*

\* Se 16 0.00375 0.08428 -0.01746 \*

\* Se 17 0.04453 -0.02491 0.02007 \*

\* Se 18 0.00105 0.04855 0.00957 \*

\* Se 19 0.00239 0.03156 0.01349 \*

\* Se 20 0.02481 0.03173 -0.01801 \*

\* Nb 1 0.01047 0.01315 0.02148 \*

\* Nb 2 -0.01208 -0.01012 -0.02419 \*

\* Nb 3 0.00023 0.00209 0.00072 \*

\* Nb 4 0.00320 0.00286 -0.00324 \*

\* Nb 5 -0.04674 0.01530 0.02242 \*

\* Nb 6 0.00365 -0.05234 -0.01950 \*

\* Nb 7 0.00973 -0.00746 -0.00269 \*

\* Nb 8 0.05046 0.00968 -0.02146 \*

\* Nb 9 0.01919 0.10914 0.02984 \*

\* Nb 10 0.00736 -0.03139 -0.04028 \*

\* Nb 11 0.02676 -0.02041 0.00964 \*

\* Nb 12 -0.05374 0.00238 0.00671 \*

\* Nb 13 -0.00844 0.02773 0.03761 \*

\* Nb 14 -0.02062 -0.10940 -0.02726 \*

\* Nb 15 -0.02839 0.02057 -0.00939 \*

\* Nb 16 0.05193 -0.00088 -0.00624 \*

\* Nb 17 -0.00538 0.05638 0.01587 \*

\* Nb 18 0.04723 -0.01497 -0.02189 \*

\* Nb 19 -0.01015 0.00602 0.00230 \*

\* Nb 20 -0.05442 -0.01090 0.02112 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.011429 0.010089 -0.080016 \*

\* y 0.010089 0.013674 0.016894 \*

\* z -0.080016 0.016894 0.000026 \*

\* \*

\* Pressure: -0.0008 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000012 | -36259.890925 | <-- min BFGS

| trial step | 1.000000 | 0.000012 | -36259.891258 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 39 with line minimization (lambda= 23.066800)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8696336 -8.3287720 0.0028133 0.4202994 -0.0040206 0.0000418

0.0324026 3.3872375 -0.0018406 1.0334612 1.8450729 0.0008844

-0.0014407 -0.0058675 13.9252801 0.0000517 0.0002447 0.4512072

Lattice parameters(A) Cell Angles

a = 17.043311 alpha = 90.055330

b = 3.387393 beta = 89.983916

c = 13.925281 gamma = 118.705961

Current cell volume = 705.132201 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067678 0.668835 0.123500 x

x Se 2 0.132197 0.342811 0.628449 x

x Se 3 0.131860 0.341832 0.870743 x

x Se 4 0.068120 0.669849 0.376771 x

x Se 5 0.266796 0.665084 0.123267 x

x Se 6 0.333104 0.345448 0.628050 x

x Se 7 0.333034 0.345187 0.872158 x

x Se 8 0.265853 0.663260 0.374442 x

x Se 9 0.466895 0.651922 0.128362 x

x Se 10 0.533870 0.346006 0.624792 x

x Se 11 0.533097 0.348021 0.871643 x

x Se 12 0.466106 0.653961 0.375307 x

x Se 13 0.666972 0.654832 0.127818 x

x Se 14 0.734183 0.336656 0.625616 x

x Se 15 0.733206 0.334748 0.876799 x

x Se 16 0.666881 0.654523 0.371991 x

x Se 17 0.868136 0.658122 0.129267 x

x Se 18 0.931924 0.330483 0.623091 x

x Se 19 0.932333 0.331246 0.876472 x

x Se 20 0.867794 0.657174 0.371522 x

x Nb 1 0.005533 0.016210 0.249917 x

x Nb 2 -0.005593 -0.016191 0.750044 x

x Nb 3 -0.000030 -0.000149 -0.000006 x

x Nb 4 0.000003 -0.000016 0.499961 x

x Nb 5 0.196653 -0.009361 0.249294 x

x Nb 6 0.202996 0.019602 0.749500 x

x Nb 7 0.199309 0.003350 -0.001707 x

x Nb 8 0.201441 0.010281 0.501603 x

x Nb 9 0.399034 -0.012192 0.250617 x

x Nb 10 0.400877 0.014390 0.750240 x

x Nb 11 0.400833 0.005815 -0.001164 x

x Nb 12 0.397392 -0.005368 0.501011 x

x Nb 13 0.599088 -0.014449 0.249766 x

x Nb 14 0.600953 0.012289 0.749389 x

x Nb 15 0.599142 -0.005929 0.001168 x

x Nb 16 0.602624 0.005514 0.499024 x

x Nb 17 0.796998 -0.019713 0.250497 x

x Nb 18 0.803415 0.009243 0.750717 x

x Nb 19 0.800750 -0.003075 0.001683 x

x Nb 20 0.798544 -0.010252 0.498387 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62589162E+004 28185.39 <-- SCF

1 -3.62610168E+004 5.25146607E-002 28210.67 <-- SCF

2 -3.62611599E+004 3.57680037E-003 28240.34 <-- SCF

3 -3.62603526E+004 -2.01809740E-002 28266.69 <-- SCF

4 -3.62599243E+004 -1.07078551E-002 28292.53 <-- SCF

5 -3.62598941E+004 -7.55260831E-004 28317.83 <-- SCF

6 -3.62598908E+004 -8.33534480E-005 28345.23 <-- SCF

7 -3.62598908E+004 6.14480313E-007 28368.95 <-- SCF

8 -3.62598910E+004 4.87793258E-006 28389.88 <-- SCF

9 -3.62598910E+004 8.29393690E-007 28408.91 <-- SCF

10 -3.62598912E+004 3.78254052E-006 28426.08 <-- SCF

11 -3.62598913E+004 3.25266689E-006 28442.59 <-- SCF

12 -3.62598914E+004 2.91292105E-006 28458.77 <-- SCF

13 -3.62598915E+004 2.34170023E-006 28474.75 <-- SCF

14 -3.62598916E+004 2.03221066E-006 28490.73 <-- SCF

15 -3.62598917E+004 1.78363221E-006 28507.09 <-- SCF

16 -3.62598917E+004 1.70260093E-006 28522.97 <-- SCF

17 -3.62598918E+004 1.33233047E-006 28538.92 <-- SCF

18 -3.62598918E+004 1.19395650E-006 28554.81 <-- SCF

19 -3.62598919E+004 1.08449463E-006 28570.81 <-- SCF

20 -3.62598919E+004 9.79936240E-007 28586.75 <-- SCF

21 -3.62598919E+004 8.67250247E-007 28602.84 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.89193954 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02850 -0.10868 0.01729 \*

\* Se 2 -0.05425 -0.03297 0.06920 \*

\* Se 3 -0.04382 -0.06556 -0.03671 \*

\* Se 4 -0.00241 -0.05734 -0.07298 \*

\* Se 5 -0.03697 -0.00643 0.04822 \*

\* Se 6 0.05308 -0.04547 0.05201 \*

\* Se 7 0.04269 0.01361 0.05937 \*

\* Se 8 -0.05004 -0.01536 -0.11740 \*

\* Se 9 0.02239 0.06850 -0.00841 \*

\* Se 10 -0.03010 -0.03030 -0.05993 \*

\* Se 11 -0.02542 -0.06661 0.00683 \*

\* Se 12 0.03763 0.03258 0.05961 \*

\* Se 13 -0.04375 -0.01627 -0.05227 \*

\* Se 14 0.04761 0.01946 0.11704 \*

\* Se 15 0.03958 0.01484 -0.06240 \*

\* Se 16 -0.05289 0.04351 -0.06749 \*

\* Se 17 0.04196 0.06700 0.03339 \*

\* Se 18 0.00280 0.06026 0.09295 \*

\* Se 19 0.02882 0.10620 -0.01659 \*

\* Se 20 0.05347 0.03079 -0.06434 \*

\* Nb 1 -0.05011 0.00582 0.01162 \*

\* Nb 2 0.05146 -0.00662 -0.01531 \*

\* Nb 3 -0.00084 0.00068 0.00019 \*

\* Nb 4 0.00363 0.00193 -0.00349 \*

\* Nb 5 -0.00533 0.06546 0.00090 \*

\* Nb 6 -0.05104 -0.06573 -0.00527 \*

\* Nb 7 0.01582 0.00188 -0.01482 \*

\* Nb 8 0.04871 -0.00168 -0.03024 \*

\* Nb 9 -0.00288 0.07231 0.04438 \*

\* Nb 10 0.06090 -0.06391 -0.06149 \*

\* Nb 11 0.04189 -0.02241 0.01534 \*

\* Nb 12 -0.06739 -0.02051 0.00438 \*

\* Nb 13 -0.05843 0.06205 0.06356 \*

\* Nb 14 0.00399 -0.07853 -0.04166 \*

\* Nb 15 -0.04408 0.02229 -0.01391 \*

\* Nb 16 0.06586 0.01709 -0.00200 \*

\* Nb 17 0.04742 0.06623 0.00620 \*

\* Nb 18 0.00521 -0.06402 -0.00213 \*

\* Nb 19 -0.01498 -0.00407 0.01578 \*

\* Nb 20 -0.05168 -0.00003 0.03061 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.101437 0.109697 0.042269 \*

\* y 0.109697 0.202814 -0.086401 \*

\* z 0.042269 -0.086401 0.274820 \*

\* \*

\* Pressure: -0.1930 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000012 | -36259.890925 | <-- min BFGS

| trial step | 1.000000 | 0.000012 | -36259.891258 | <-- min BFGS

| line step | 23.066800 | -0.000014 | -36259.892076 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 39 with quad minimization (lambda= 10.895546)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8810903 -8.3396983 -0.0029421 0.4201895 -0.0036342 0.0001287

0.0292890 3.3863538 -0.0010469 1.0348162 1.8464926 0.0007637

-0.0042917 -0.0033503 13.9157357 0.0001667 0.0001381 0.4515167

Lattice parameters(A) Cell Angles

a = 17.058647 alpha = 90.031659

b = 3.386481 beta = 90.018553

c = 13.915737 gamma = 118.771702

Current cell volume = 704.649562 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067625 0.668518 0.123895 x

x Se 2 0.132179 0.342529 0.628488 x

x Se 3 0.131941 0.341283 0.870852 x

x Se 4 0.068027 0.669647 0.376471 x

x Se 5 0.266747 0.664571 0.123676 x

x Se 6 0.333129 0.345522 0.628006 x

x Se 7 0.332911 0.344373 0.872233 x

x Se 8 0.265946 0.663147 0.374367 x

x Se 9 0.467152 0.653269 0.128312 x

x Se 10 0.533566 0.344798 0.625129 x

x Se 11 0.532846 0.346693 0.871696 x

x Se 12 0.466397 0.655272 0.374963 x

x Se 13 0.667083 0.655583 0.127745 x

x Se 14 0.734093 0.336762 0.625686 x

x Se 15 0.733262 0.335262 0.876375 x

x Se 16 0.666855 0.654428 0.372000 x

x Se 17 0.868054 0.658699 0.129143 x

x Se 18 0.932003 0.330627 0.623422 x

x Se 19 0.932383 0.331569 0.876086 x

x Se 20 0.867810 0.657468 0.371500 x

x Nb 1 0.005016 0.014487 0.249892 x

x Nb 2 -0.005065 -0.014483 0.750078 x

x Nb 3 -0.000029 -0.000159 -0.000009 x

x Nb 4 -0.000004 -0.000059 0.499972 x

x Nb 5 0.196910 -0.008538 0.249334 x

x Nb 6 0.202823 0.018950 0.749531 x

x Nb 7 0.199356 0.003233 -0.001559 x

x Nb 8 0.201244 0.009296 0.501488 x

x Nb 9 0.399046 -0.012667 0.250596 x

x Nb 10 0.400848 0.013828 0.750224 x

x Nb 11 0.400713 0.005494 -0.001088 x

x Nb 12 0.397650 -0.004802 0.500889 x

x Nb 13 0.599127 -0.013831 0.249789 x

x Nb 14 0.600945 0.012755 0.749401 x

x Nb 15 0.599265 -0.005599 0.001090 x

x Nb 16 0.602367 0.004924 0.499142 x

x Nb 17 0.797173 -0.019085 0.250473 x

x Nb 18 0.803151 0.008422 0.750673 x

x Nb 19 0.800701 -0.002956 0.001536 x

x Nb 20 0.798753 -0.009231 0.498504 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62595972E+004 28706.06 <-- SCF

1 -3.62602464E+004 1.62306886E-002 28731.48 <-- SCF

2 -3.62602871E+004 1.01598357E-003 28760.73 <-- SCF

3 -3.62600417E+004 -6.13471063E-003 28786.95 <-- SCF

4 -3.62599037E+004 -3.44960578E-003 28812.78 <-- SCF

5 -3.62598951E+004 -2.14211659E-004 28837.89 <-- SCF

6 -3.62598935E+004 -4.09737214E-005 28862.89 <-- SCF

7 -3.62598935E+004 -8.91664288E-007 28885.83 <-- SCF

8 -3.62598935E+004 2.61060100E-007 28904.31 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.89347673 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02053 -0.07733 -0.01574 \*

\* Se 2 -0.03748 -0.02947 0.04766 \*

\* Se 3 -0.04866 -0.00793 -0.03748 \*

\* Se 4 -0.00616 -0.05793 -0.02178 \*

\* Se 5 -0.00458 0.02342 -0.03709 \*

\* Se 6 0.02293 -0.06016 0.04800 \*

\* Se 7 0.04245 0.02924 0.03847 \*

\* Se 8 -0.03944 0.00231 -0.09468 \*

\* Se 9 -0.01926 0.03348 -0.00226 \*

\* Se 10 0.03567 -0.00353 -0.05621 \*

\* Se 11 0.01676 -0.03053 -0.00100 \*

\* Se 12 -0.02914 -0.00381 0.06358 \*

\* Se 13 -0.03965 -0.02860 -0.03097 \*

\* Se 14 0.03717 0.00216 0.09367 \*

\* Se 15 0.00182 -0.01591 0.02899 \*

\* Se 16 -0.02339 0.06170 -0.05048 \*

\* Se 17 0.04710 0.00682 0.03864 \*

\* Se 18 0.00991 0.05707 0.02513 \*

\* Se 19 0.02123 0.07404 0.01395 \*

\* Se 20 0.03769 0.02582 -0.04654 \*

\* Nb 1 0.00004 0.01320 0.01584 \*

\* Nb 2 -0.00055 -0.01211 -0.01909 \*

\* Nb 3 -0.00001 0.00138 0.00047 \*

\* Nb 4 0.00405 0.00235 -0.00326 \*

\* Nb 5 -0.04186 0.04486 0.01199 \*

\* Nb 6 -0.01565 -0.06858 -0.01533 \*

\* Nb 7 0.00565 -0.00491 -0.00666 \*

\* Nb 8 0.05774 0.00414 -0.02450 \*

\* Nb 9 0.01842 0.10119 0.03378 \*

\* Nb 10 0.03184 -0.04671 -0.04644 \*

\* Nb 11 0.04308 -0.02091 0.01438 \*

\* Nb 12 -0.07150 -0.00873 0.00563 \*

\* Nb 13 -0.03138 0.04419 0.04588 \*

\* Nb 14 -0.01892 -0.10404 -0.03131 \*

\* Nb 15 -0.04508 0.02095 -0.01359 \*

\* Nb 16 0.06984 0.00811 -0.00457 \*

\* Nb 17 0.01397 0.07085 0.01368 \*

\* Nb 18 0.04239 -0.04404 -0.01201 \*

\* Nb 19 -0.00507 0.00334 0.00688 \*

\* Nb 20 -0.06143 -0.00542 0.02439 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.074650 0.009135 -0.033501 \*

\* y 0.009135 0.102401 -0.035473 \*

\* z -0.033501 -0.035473 0.056630 \*

\* \*

\* Pressure: -0.0779 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000012 | -36259.890925 | <-- min BFGS

| trial step | 1.000000 | 0.000012 | -36259.891258 | <-- min BFGS

| line step | 23.066800 | -0.000014 | -36259.892076 | <-- min BFGS

| quad step | 10.895546 | 7.194E-006 | -36259.893561 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 39 with enthalpy= -3.62598936E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 6.591742E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.102792E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.194336E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.024007E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 40 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000459 | -36259.893561 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 40 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8317188 -8.3013767 0.0092579 0.4209396 -0.0048099 -0.0000874

0.0387000 3.3868924 -0.0021751 1.0317355 1.8433590 0.0006981

0.0028196 -0.0068628 13.9542403 -0.0001185 0.0002905 0.4502708

Lattice parameters(A) Cell Angles

a = 16.996847 alpha = 90.064837

b = 3.387114 beta = 89.944927

c = 13.954242 gamma = 118.581283

Current cell volume = 705.452150 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067813 0.669439 0.122679 x

x Se 2 0.132320 0.343472 0.628690 x

x Se 3 0.131674 0.342486 0.870219 x

x Se 4 0.068374 0.670139 0.377299 x

x Se 5 0.266834 0.666320 0.122651 x

x Se 6 0.333358 0.346325 0.628346 x

x Se 7 0.333488 0.347476 0.872087 x

x Se 8 0.265495 0.663533 0.374080 x

x Se 9 0.466357 0.650162 0.128570 x

x Se 10 0.534565 0.347952 0.624118 x

x Se 11 0.533621 0.349723 0.871424 x

x Se 12 0.465443 0.651765 0.376009 x

x Se 13 0.666539 0.652657 0.127906 x

x Se 14 0.734539 0.336418 0.625994 x

x Se 15 0.733156 0.333519 0.877457 x

x Se 16 0.666617 0.653661 0.371762 x

x Se 17 0.868326 0.657440 0.129813 x

x Se 18 0.931706 0.330356 0.622469 x

x Se 19 0.932201 0.330612 0.877272 x

x Se 20 0.867676 0.656512 0.371254 x

x Nb 1 0.006859 0.019965 0.250005 x

x Nb 2 -0.006935 -0.019977 0.749932 x

x Nb 3 -0.000032 -0.000080 -0.000012 x

x Nb 4 0.000028 0.000157 0.499945 x

x Nb 5 0.196227 -0.010963 0.249145 x

x Nb 6 0.203532 0.020956 0.749455 x

x Nb 7 0.199278 0.004123 -0.002313 x

x Nb 8 0.202098 0.013426 0.502024 x

x Nb 9 0.398931 -0.010769 0.250709 x

x Nb 10 0.401162 0.017263 0.750301 x

x Nb 11 0.401273 0.006487 -0.001095 x

x Nb 12 0.396685 -0.007654 0.501080 x

x Nb 13 0.598795 -0.017408 0.249691 x

x Nb 14 0.601031 0.010789 0.749320 x

x Nb 15 0.598697 -0.006604 0.001094 x

x Nb 16 0.603322 0.007867 0.498970 x

x Nb 17 0.796449 -0.020969 0.250522 x

x Nb 18 0.803859 0.010895 0.750877 x

x Nb 19 0.800780 -0.003919 0.002305 x

x Nb 20 0.797858 -0.013545 0.497946 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62562051E+004 29007.84 <-- SCF

1 -3.62635277E+004 1.83064421E-001 29032.75 <-- SCF

2 -3.62640971E+004 1.42344264E-002 29061.77 <-- SCF

3 -3.62612388E+004 -7.14574800E-002 29088.86 <-- SCF

4 -3.62600394E+004 -2.99852240E-002 29114.81 <-- SCF

5 -3.62599300E+004 -2.73469051E-003 29141.03 <-- SCF

6 -3.62598807E+004 -1.23146381E-003 29167.44 <-- SCF

7 -3.62598757E+004 -1.25110757E-004 29194.45 <-- SCF

8 -3.62598773E+004 3.89825218E-005 29220.12 <-- SCF

9 -3.62598763E+004 -2.39763358E-005 29242.70 <-- SCF

10 -3.62598765E+004 4.62302731E-006 29262.50 <-- SCF

11 -3.62598768E+004 6.07650455E-006 29280.42 <-- SCF

12 -3.62598770E+004 5.02682564E-006 29297.70 <-- SCF

13 -3.62598771E+004 3.81238533E-006 29314.44 <-- SCF

14 -3.62598772E+004 2.95131976E-006 29330.47 <-- SCF

15 -3.62598773E+004 2.27956126E-006 29346.44 <-- SCF

16 -3.62598774E+004 1.93600507E-006 29362.47 <-- SCF

17 -3.62598775E+004 1.63413405E-006 29378.44 <-- SCF

18 -3.62598775E+004 1.28174632E-006 29394.41 <-- SCF

19 -3.62598776E+004 1.06464764E-006 29410.31 <-- SCF

20 -3.62598776E+004 8.93007673E-007 29426.28 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.87760515 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02099 -0.16245 0.15211 \*

\* Se 2 -0.09596 -0.01976 0.06468 \*

\* Se 3 -0.02495 -0.11497 0.02297 \*

\* Se 4 0.01253 -0.07716 -0.11933 \*

\* Se 5 -0.11361 -0.09895 0.07268 \*

\* Se 6 0.06511 -0.00981 0.01520 \*

\* Se 7 0.01955 0.02020 0.07898 \*

\* Se 8 -0.02551 -0.08044 -0.10756 \*

\* Se 9 0.06175 0.04912 -0.01572 \*

\* Se 10 -0.19216 -0.01485 -0.02580 \*

\* Se 11 -0.06470 -0.04914 0.01961 \*

\* Se 12 0.19536 0.02429 0.03253 \*

\* Se 13 -0.02997 -0.02659 -0.07510 \*

\* Se 14 0.02114 0.07669 0.10402 \*

\* Se 15 0.12330 0.10028 -0.07545 \*

\* Se 16 -0.06609 0.00488 -0.05218 \*

\* Se 17 0.02075 0.12032 -0.03125 \*

\* Se 18 -0.01083 0.11226 0.11263 \*

\* Se 19 0.02137 0.15935 -0.15132 \*

\* Se 20 0.09350 0.01966 -0.05151 \*

\* Nb 1 -0.14984 0.01567 -0.00236 \*

\* Nb 2 0.15326 -0.01807 -0.00142 \*

\* Nb 3 -0.00151 -0.00166 0.00137 \*

\* Nb 4 0.00441 0.00035 -0.00507 \*

\* Nb 5 0.01692 0.12864 -0.03581 \*

\* Nb 6 -0.10262 -0.08392 0.02620 \*

\* Nb 7 0.02607 0.01276 0.00098 \*

\* Nb 8 0.03842 -0.03319 -0.05922 \*

\* Nb 9 -0.01719 0.03997 0.04888 \*

\* Nb 10 0.09857 -0.14363 -0.08518 \*

\* Nb 11 0.04062 -0.02316 0.00351 \*

\* Nb 12 -0.07560 -0.01071 0.01742 \*

\* Nb 13 -0.09364 0.14404 0.09460 \*

\* Nb 14 0.02341 -0.05187 -0.04493 \*

\* Nb 15 -0.04315 0.02273 0.00197 \*

\* Nb 16 0.07495 0.00068 -0.01236 \*

\* Nb 17 0.09879 0.07804 -0.01680 \*

\* Nb 18 -0.01730 -0.12644 0.03345 \*

\* Nb 19 -0.02383 -0.01478 0.00097 \*

\* Nb 20 -0.04032 0.03161 0.06361 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.011651 0.315191 0.116660 \*

\* y 0.315191 0.244890 -0.101559 \*

\* z 0.116660 -0.101559 0.489666 \*

\* \*

\* Pressure: -0.2410 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000459 | -36259.893561 | <-- min BFGS

| trial step | 1.000000 | -0.001602 | -36259.877662 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 40 with line minimization (lambda= 0.222632)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8700986 -8.3311667 -0.0002260 0.4203557 -0.0038956 0.0000806

0.0313842 3.3864737 -0.0012980 1.0341299 1.8457934 0.0007489

-0.0027085 -0.0041323 13.9243081 0.0001032 0.0001720 0.4512387

Lattice parameters(A) Cell Angles

a = 17.044887 alpha = 90.039067

b = 3.386619 beta = 90.002172

c = 13.924309 gamma = 118.729322

Current cell volume = 704.829775 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067666 0.668723 0.123624 x

x Se 2 0.132210 0.342739 0.628533 x

x Se 3 0.131882 0.341551 0.870711 x

x Se 4 0.068104 0.669757 0.376656 x

x Se 5 0.266767 0.664960 0.123448 x

x Se 6 0.333180 0.345701 0.628081 x

x Se 7 0.333039 0.345064 0.872201 x

x Se 8 0.265846 0.663232 0.374303 x

x Se 9 0.466975 0.652578 0.128369 x

x Se 10 0.533788 0.345501 0.624904 x

x Se 11 0.533019 0.347367 0.871635 x

x Se 12 0.466185 0.654491 0.375196 x

x Se 13 0.666962 0.654931 0.127781 x

x Se 14 0.734192 0.336686 0.625755 x

x Se 15 0.733238 0.334874 0.876616 x

x Se 16 0.666802 0.654257 0.371947 x

x Se 17 0.868115 0.658418 0.129292 x

x Se 18 0.931937 0.330567 0.623210 x

x Se 19 0.932343 0.331356 0.876350 x

x Se 20 0.867781 0.657255 0.371445 x

x Nb 1 0.005426 0.015706 0.249917 x

x Nb 2 -0.005481 -0.015706 0.750045 x

x Nb 3 -0.000030 -0.000142 -0.000009 x

x Nb 4 0.000003 -0.000011 0.499966 x

x Nb 5 0.196758 -0.009078 0.249292 x

x Nb 6 0.202981 0.019397 0.749514 x

x Nb 7 0.199339 0.003431 -0.001727 x

x Nb 8 0.201434 0.010216 0.501607 x

x Nb 9 0.399020 -0.012244 0.250621 x

x Nb 10 0.400918 0.014593 0.750241 x

x Nb 11 0.400838 0.005715 -0.001090 x

x Nb 12 0.397435 -0.005437 0.500931 x

x Nb 13 0.599053 -0.014628 0.249767 x

x Nb 14 0.600964 0.012317 0.749383 x

x Nb 15 0.599139 -0.005823 0.001091 x

x Nb 16 0.602580 0.005579 0.499104 x

x Nb 17 0.797012 -0.019505 0.250484 x

x Nb 18 0.803309 0.008973 0.750719 x

x Nb 19 0.800719 -0.003170 0.001707 x

x Nb 20 0.798554 -0.010191 0.498380 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62576757E+004 29529.72 <-- SCF

1 -3.62622445E+004 1.14220595E-001 29555.11 <-- SCF

2 -3.62626004E+004 8.89779415E-003 29584.52 <-- SCF

3 -3.62609509E+004 -4.12384323E-002 29611.19 <-- SCF

4 -3.62599684E+004 -2.45624187E-002 29637.39 <-- SCF

5 -3.62599343E+004 -8.51845530E-004 29664.14 <-- SCF

6 -3.62598960E+004 -9.58896490E-004 29690.89 <-- SCF

7 -3.62598937E+004 -5.60973826E-005 29717.58 <-- SCF

8 -3.62598950E+004 3.23847653E-005 29742.20 <-- SCF

9 -3.62598941E+004 -2.24621969E-005 29763.69 <-- SCF

10 -3.62598941E+004 -1.20731766E-006 29783.52 <-- SCF

11 -3.62598941E+004 1.42709212E-006 29801.83 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.89411518 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02617 -0.10578 -0.00566 \*

\* Se 2 -0.04957 -0.02396 0.05497 \*

\* Se 3 -0.04344 -0.03134 -0.02273 \*

\* Se 4 -0.00702 -0.06155 -0.04116 \*

\* Se 5 -0.02095 -0.00538 0.00684 \*

\* Se 6 0.04192 -0.04672 0.04740 \*

\* Se 7 0.04239 0.02894 0.03755 \*

\* Se 8 -0.04267 -0.01940 -0.10698 \*

\* Se 9 0.00937 0.04540 -0.00896 \*

\* Se 10 -0.00580 -0.00838 -0.06764 \*

\* Se 11 -0.01228 -0.04290 0.00723 \*

\* Se 12 0.01324 0.00872 0.06989 \*

\* Se 13 -0.04250 -0.03044 -0.03180 \*

\* Se 14 0.03892 0.02537 0.10426 \*

\* Se 15 0.02070 0.01417 -0.02217 \*

\* Se 16 -0.04136 0.04557 -0.05774 \*

\* Se 17 0.04183 0.03197 0.02192 \*

\* Se 18 0.00874 0.06181 0.05890 \*

\* Se 19 0.02662 0.10267 0.00485 \*

\* Se 20 0.04932 0.02076 -0.05151 \*

\* Nb 1 -0.02649 0.02184 0.01106 \*

\* Nb 2 0.02735 -0.02125 -0.01419 \*

\* Nb 3 -0.00027 0.00074 0.00037 \*

\* Nb 4 0.00385 0.00225 -0.00378 \*

\* Nb 5 -0.02905 0.06436 0.00079 \*

\* Nb 6 -0.03793 -0.07819 -0.00289 \*

\* Nb 7 0.01019 0.00085 -0.00464 \*

\* Nb 8 0.04558 -0.00748 -0.03812 \*

\* Nb 9 0.01373 0.09617 0.03556 \*

\* Nb 10 0.05203 -0.06645 -0.05810 \*

\* Nb 11 0.04757 -0.02295 0.01144 \*

\* Nb 12 -0.06448 -0.00407 0.00766 \*

\* Nb 13 -0.04993 0.06463 0.05960 \*

\* Nb 14 -0.01271 -0.10110 -0.03298 \*

\* Nb 15 -0.04934 0.02234 -0.00967 \*

\* Nb 16 0.06312 0.00137 -0.00558 \*

\* Nb 17 0.03490 0.07837 0.00370 \*

\* Nb 18 0.02888 -0.06349 -0.00146 \*

\* Nb 19 -0.00937 -0.00286 0.00494 \*

\* Nb 20 -0.04888 0.00537 0.03881 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.088473 0.015602 -0.001974 \*

\* y 0.015602 0.119834 -0.051360 \*

\* z -0.001974 -0.051360 0.089876 \*

\* \*

\* Pressure: -0.0994 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000459 | -36259.893561 | <-- min BFGS

| trial step | 1.000000 | -0.001602 | -36259.877662 | <-- min BFGS

| line step | 0.222632 | 0.000118 | -36259.894226 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 40 with enthalpy= -3.62598942E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.662261E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.168004E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.281619E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.198341E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 41 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000242 | -36259.894226 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 41 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8535551 -8.3186150 0.0071286 0.4205848 -0.0043283 -0.0000660

0.0348592 3.3873103 -0.0016942 1.0328794 1.8442895 0.0005545

0.0021320 -0.0053835 13.9336337 -0.0000896 0.0002265 0.4509367

Lattice parameters(A) Cell Angles

a = 17.024321 alpha = 90.050702

b = 3.387490 beta = 89.957542

c = 13.933635 gamma = 118.661050

Current cell volume = 705.091596 A\*\*3

-------------------------------

Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067650 0.668278 0.123669 x

x Se 2 0.132313 0.342278 0.628528 x

x Se 3 0.131839 0.341530 0.870615 x

x Se 4 0.068104 0.668938 0.376398 x

x Se 5 0.266815 0.665940 0.123611 x

x Se 6 0.333130 0.344441 0.628146 x

x Se 7 0.333201 0.345333 0.872207 x

x Se 8 0.265750 0.663744 0.373795 x

x Se 9 0.466708 0.652613 0.128440 x

x Se 10 0.534034 0.345608 0.624818 x

x Se 11 0.533275 0.347305 0.871555 x

x Se 12 0.465970 0.654197 0.375284 x

x Se 13 0.666819 0.654762 0.127788 x

x Se 14 0.734279 0.336211 0.626263 x

x Se 15 0.733179 0.333922 0.876471 x

x Se 16 0.666851 0.655552 0.371934 x

x Se 17 0.868159 0.658403 0.129410 x

x Se 18 0.931958 0.331453 0.623426 x

x Se 19 0.932361 0.331770 0.876294 x

x Se 20 0.867682 0.657697 0.371431 x

x Nb 1 0.005460 0.015834 0.250012 x

x Nb 2 -0.005522 -0.015828 0.749939 x

x Nb 3 -0.000027 -0.000084 -0.000008 x

x Nb 4 0.000019 0.000098 0.499955 x

x Nb 5 0.196715 -0.009276 0.249337 x

x Nb 6 0.202993 0.018074 0.749511 x

x Nb 7 0.199394 0.003365 -0.001803 x

x Nb 8 0.201654 0.010811 0.501589 x

x Nb 9 0.399097 -0.009634 0.250633 x

x Nb 10 0.400975 0.014255 0.750197 x

x Nb 11 0.400958 0.005466 -0.000934 x

x Nb 12 0.397274 -0.005979 0.500885 x

x Nb 13 0.598989 -0.014366 0.249798 x

x Nb 14 0.600876 0.009670 0.749387 x

x Nb 15 0.599017 -0.005569 0.000934 x

x Nb 16 0.602734 0.006143 0.499154 x

x Nb 17 0.796995 -0.018105 0.250472 x

x Nb 18 0.803354 0.009201 0.750679 x

x Nb 19 0.800656 -0.003171 0.001791 x

x Nb 20 0.798314 -0.010878 0.498391 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62596154E+004 29905.12 <-- SCF

1 -3.62602943E+004 1.69733305E-002 29932.19 <-- SCF

2 -3.62603272E+004 8.23110098E-004 29961.16 <-- SCF

3 -3.62601947E+004 -3.31240393E-003 29988.03 <-- SCF

4 -3.62598968E+004 -7.44734485E-003 30014.11 <-- SCF

5 -3.62599078E+004 2.73434352E-004 30040.80 <-- SCF

6 -3.62598983E+004 -2.35554751E-004 30066.69 <-- SCF

7 -3.62598966E+004 -4.45810882E-005 30090.25 <-- SCF

8 -3.62598966E+004 1.94822609E-008 30111.67 <-- SCF

9 -3.62598966E+004 9.95745497E-007 30129.88 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.89659316 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.03034 -0.09899 -0.01984 \*

\* Se 2 -0.05811 0.02819 0.03742 \*

\* Se 3 -0.02898 -0.04201 0.00434 \*

\* Se 4 -0.01637 -0.03650 0.01727 \*

\* Se 5 -0.04444 -0.07406 -0.04167 \*

\* Se 6 0.07739 0.02824 0.02901 \*

\* Se 7 0.02870 0.03905 0.02412 \*

\* Se 8 -0.01306 -0.07039 -0.03776 \*

\* Se 9 0.07163 0.01987 -0.01337 \*

\* Se 10 -0.05915 -0.00593 -0.07453 \*

\* Se 11 -0.07434 -0.01853 0.01719 \*

\* Se 12 0.06248 0.01901 0.07652 \*

\* Se 13 -0.03545 -0.04386 -0.02182 \*

\* Se 14 0.01071 0.06931 0.03521 \*

\* Se 15 0.04534 0.07930 0.02349 \*

\* Se 16 -0.07358 -0.03492 -0.06068 \*

\* Se 17 0.02655 0.04789 -0.01029 \*

\* Se 18 0.02004 0.03802 -0.00672 \*

\* Se 19 0.02834 0.09860 0.02166 \*

\* Se 20 0.05609 -0.02746 -0.02768 \*

\* Nb 1 -0.05051 0.01442 -0.00899 \*

\* Nb 2 0.05291 -0.01504 0.00643 \*

\* Nb 3 -0.00176 -0.00088 0.00119 \*

\* Nb 4 0.00301 0.00109 -0.00357 \*

\* Nb 5 -0.02794 0.09619 -0.03342 \*

\* Nb 6 -0.03980 -0.06244 0.01931 \*

\* Nb 7 0.01297 0.01680 0.00918 \*

\* Nb 8 0.03271 -0.01131 -0.05120 \*

\* Nb 9 0.00408 0.03612 0.03938 \*

\* Nb 10 0.06251 -0.08599 -0.04616 \*

\* Nb 11 0.03696 -0.01295 -0.00880 \*

\* Nb 12 -0.06970 -0.01660 0.02140 \*

\* Nb 13 -0.05917 0.08746 0.05388 \*

\* Nb 14 0.00018 -0.04416 -0.03582 \*

\* Nb 15 -0.03896 0.01316 0.01388 \*

\* Nb 16 0.06859 0.01030 -0.01709 \*

\* Nb 17 0.03661 0.05892 -0.01137 \*

\* Nb 18 0.02819 -0.09357 0.03245 \*

\* Nb 19 -0.01075 -0.01719 -0.00733 \*

\* Nb 20 -0.03358 0.01084 0.05478 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.048875 0.167271 0.094205 \*

\* y 0.167271 0.200177 -0.078109 \*

\* z 0.094205 -0.078109 0.237359 \*

\* \*

\* Pressure: -0.1621 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000242 | -36259.894226 | <-- min BFGS

| trial step | 1.000000 | -0.000066 | -36259.896687 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 41 with enthalpy= -3.62598967E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 6.152251E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.185486E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 8.353721E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.373591E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 42 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000161 | -36259.896687 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 42 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8672807 -8.3304973 0.0036580 0.4204383 -0.0038906 -0.0000234

0.0313340 3.3861164 -0.0010450 1.0343591 1.8460013 0.0003841

0.0007435 -0.0033138 13.9243665 -0.0000328 0.0001396 0.4512367

Lattice parameters(A) Cell Angles

a = 17.042102 alpha = 90.031288

b = 3.386261 beta = 89.978367

c = 13.924367 gamma = 118.732786

Current cell volume = 704.619823 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067650 0.668127 0.123764 x

x Se 2 0.132225 0.341769 0.628607 x

x Se 3 0.131774 0.341022 0.870648 x

x Se 4 0.068108 0.668834 0.376296 x

x Se 5 0.266808 0.665751 0.123646 x

x Se 6 0.333192 0.344352 0.628173 x

x Se 7 0.333174 0.345262 0.872383 x

x Se 8 0.265769 0.663651 0.373722 x

x Se 9 0.466792 0.653279 0.128325 x

x Se 10 0.533975 0.345045 0.624902 x

x Se 11 0.533192 0.346652 0.871664 x

x Se 12 0.466033 0.654773 0.375199 x

x Se 13 0.666844 0.654820 0.127632 x

x Se 14 0.734262 0.336315 0.626334 x

x Se 15 0.733188 0.334113 0.876433 x

x Se 16 0.666783 0.655644 0.371896 x

x Se 17 0.868220 0.658908 0.129371 x

x Se 18 0.931953 0.331555 0.623529 x

x Se 19 0.932359 0.331912 0.876201 x

x Se 20 0.867770 0.658191 0.371364 x

x Nb 1 0.005262 0.015058 0.250028 x

x Nb 2 -0.005318 -0.015061 0.749922 x

x Nb 3 -0.000026 -0.000075 -0.000011 x

x Nb 4 0.000021 0.000107 0.499957 x

x Nb 5 0.196777 -0.008930 0.249365 x

x Nb 6 0.202977 0.017762 0.749504 x

x Nb 7 0.199438 0.003459 -0.001785 x

x Nb 8 0.201652 0.010746 0.501533 x

x Nb 9 0.399102 -0.009437 0.250687 x

x Nb 10 0.400999 0.014288 0.750134 x

x Nb 11 0.400954 0.005306 -0.000845 x

x Nb 12 0.397296 -0.006069 0.500786 x

x Nb 13 0.598970 -0.014381 0.249862 x

x Nb 14 0.600870 0.009449 0.749333 x

x Nb 15 0.599021 -0.005407 0.000842 x

x Nb 16 0.602710 0.006222 0.499254 x

x Nb 17 0.797007 -0.017788 0.250476 x

x Nb 18 0.803290 0.008868 0.750650 x

x Nb 19 0.800612 -0.003276 0.001776 x

x Nb 20 0.798317 -0.010817 0.498443 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598277E+004 30233.34 <-- SCF

1 -3.62599912E+004 4.08611413E-003 30260.00 <-- SCF

2 -3.62599997E+004 2.13186382E-004 30289.39 <-- SCF

3 -3.62599709E+004 -7.20794751E-004 30316.58 <-- SCF

4 -3.62598982E+004 -1.81609873E-003 30342.53 <-- SCF

5 -3.62599017E+004 8.60299756E-005 30369.27 <-- SCF

6 -3.62598999E+004 -4.53107459E-005 30393.94 <-- SCF

7 -3.62598993E+004 -1.42824453E-005 30414.95 <-- SCF

8 -3.62598993E+004 -8.01777643E-007 30434.48 <-- SCF

9 -3.62598993E+004 1.01967926E-006 30451.92 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.89930875 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02773 -0.07906 -0.02347 \*

\* Se 2 -0.03279 0.03379 0.01191 \*

\* Se 3 0.00153 -0.02918 -0.00148 \*

\* Se 4 -0.01463 -0.02519 0.02565 \*

\* Se 5 -0.03466 -0.04487 -0.04200 \*

\* Se 6 0.05243 0.02876 0.01336 \*

\* Se 7 0.02358 0.03998 -0.03892 \*

\* Se 8 -0.00459 -0.04674 -0.02335 \*

\* Se 9 0.06760 0.01551 0.02397 \*

\* Se 10 -0.04318 -0.00265 -0.08359 \*

\* Se 11 -0.06963 -0.01532 -0.01814 \*

\* Se 12 0.04607 0.01525 0.08685 \*

\* Se 13 -0.02998 -0.04224 0.03413 \*

\* Se 14 0.00197 0.04583 0.02232 \*

\* Se 15 0.03493 0.05011 0.02739 \*

\* Se 16 -0.04881 -0.03657 -0.04102 \*

\* Se 17 -0.00254 0.03481 -0.00306 \*

\* Se 18 0.01970 0.02610 -0.02360 \*

\* Se 19 0.02529 0.07824 0.02392 \*

\* Se 20 0.03111 -0.03176 -0.00475 \*

\* Nb 1 -0.01791 0.00537 -0.01132 \*

\* Nb 2 0.01857 -0.00558 0.00955 \*

\* Nb 3 -0.00136 -0.00103 0.00177 \*

\* Nb 4 0.00369 0.00094 -0.00319 \*

\* Nb 5 -0.04295 0.07261 -0.03810 \*

\* Nb 6 -0.02789 -0.04898 0.02499 \*

\* Nb 7 -0.00007 0.01014 0.00881 \*

\* Nb 8 0.03404 -0.01666 -0.04361 \*

\* Nb 9 0.00782 0.03266 0.01627 \*

\* Nb 10 0.04946 -0.07478 -0.01682 \*

\* Nb 11 0.04137 -0.01110 -0.00897 \*

\* Nb 12 -0.07608 -0.01472 0.02752 \*

\* Nb 13 -0.04777 0.07623 0.02487 \*

\* Nb 14 -0.00343 -0.04005 -0.01276 \*

\* Nb 15 -0.04294 0.01157 0.01464 \*

\* Nb 16 0.07609 0.00898 -0.02314 \*

\* Nb 17 0.02602 0.04494 -0.01566 \*

\* Nb 18 0.04388 -0.07056 0.03779 \*

\* Nb 19 0.00101 -0.01052 -0.00682 \*

\* Nb 20 -0.03720 0.01576 0.04805 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.030422 0.024874 0.062102 \*

\* y 0.024874 0.062012 -0.036557 \*

\* z 0.062102 -0.036557 0.057007 \*

\* \*

\* Pressure: -0.0498 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000161 | -36259.896687 | <-- min BFGS

| trial step | 1.000000 | 0.000035 | -36259.899379 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 42 with enthalpy= -3.62598994E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 6.730655E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 9.948396E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.191850E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 6.210173E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 43 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000048 | -36259.899379 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 43 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8684771 -8.3343550 -0.0025346 0.4204908 -0.0037348 0.0000845

0.0300702 3.3855194 -0.0004404 1.0351499 1.8467058 0.0003927

-0.0028116 -0.0013850 13.9232364 0.0001093 0.0000577 0.4512734

Lattice parameters(A) Cell Angles

a = 17.045031 alpha = 90.013255

b = 3.385653 beta = 90.015826

c = 13.923237 gamma = 118.763422

Current cell volume = 704.350495 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067668 0.668106 0.123652 x

x Se 2 0.132200 0.341679 0.628696 x

x Se 3 0.131722 0.340957 0.870581 x

x Se 4 0.068145 0.668803 0.376362 x

x Se 5 0.266805 0.665842 0.123528 x

x Se 6 0.333296 0.344546 0.628238 x

x Se 7 0.333255 0.345755 0.872476 x

x Se 8 0.265710 0.663620 0.373637 x

x Se 9 0.466760 0.653241 0.128297 x

x Se 10 0.534055 0.345138 0.624818 x

x Se 11 0.533221 0.346691 0.871687 x

x Se 12 0.465963 0.654652 0.375287 x

x Se 13 0.666765 0.654338 0.127552 x

x Se 14 0.734322 0.336356 0.626420 x

x Se 15 0.733190 0.334024 0.876553 x

x Se 16 0.666674 0.655455 0.371836 x

x Se 17 0.868270 0.658964 0.129440 x

x Se 18 0.931921 0.331615 0.623450 x

x Se 19 0.932341 0.331923 0.876311 x

x Se 20 0.867795 0.658267 0.371278 x

x Nb 1 0.005419 0.015457 0.250051 x

x Nb 2 -0.005476 -0.015465 0.749893 x

x Nb 3 -0.000027 -0.000063 -0.000013 x

x Nb 4 0.000025 0.000137 0.499954 x

x Nb 5 0.196724 -0.009047 0.249350 x

x Nb 6 0.203052 0.017891 0.749486 x

x Nb 7 0.199449 0.003641 -0.001877 x

x Nb 8 0.201760 0.011250 0.501572 x

x Nb 9 0.399079 -0.009228 0.250743 x

x Nb 10 0.401060 0.014762 0.750092 x

x Nb 11 0.401028 0.005369 -0.000820 x

x Nb 12 0.397179 -0.006502 0.500777 x

x Nb 13 0.598911 -0.014861 0.249901 x

x Nb 14 0.600888 0.009217 0.749282 x

x Nb 15 0.598945 -0.005472 0.000816 x

x Nb 16 0.602825 0.006660 0.499265 x

x Nb 17 0.796928 -0.017903 0.250489 x

x Nb 18 0.803345 0.008997 0.750665 x

x Nb 19 0.800602 -0.003469 0.001872 x

x Nb 20 0.798205 -0.011342 0.498401 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598540E+004 30555.02 <-- SCF

1 -3.62599714E+004 2.93574557E-003 30581.52 <-- SCF

2 -3.62599781E+004 1.68118261E-004 30609.64 <-- SCF

3 -3.62599627E+004 -3.85771274E-004 30636.45 <-- SCF

4 -3.62598982E+004 -1.61248577E-003 30662.09 <-- SCF

5 -3.62599026E+004 1.11175910E-004 30688.59 <-- SCF

6 -3.62599009E+004 -4.45232109E-005 30713.45 <-- SCF

7 -3.62599003E+004 -1.52496623E-005 30733.89 <-- SCF

8 -3.62599001E+004 -2.57099611E-006 30752.50 <-- SCF

9 -3.62599002E+004 8.28331046E-007 30770.86 <-- SCF

10 -3.62599002E+004 8.56619327E-007 30787.78 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.90021608 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02987 -0.07135 -0.02006 \*

\* Se 2 -0.02658 0.03031 -0.00390 \*

\* Se 3 0.01172 -0.04253 0.00512 \*

\* Se 4 -0.00883 -0.01470 0.02906 \*

\* Se 5 -0.03193 -0.04357 -0.02002 \*

\* Se 6 0.02653 0.02801 -0.00791 \*

\* Se 7 0.01954 0.02959 -0.06917 \*

\* Se 8 -0.00035 -0.03676 -0.00959 \*

\* Se 9 0.07207 0.02357 0.04079 \*

\* Se 10 -0.05904 -0.01107 -0.08798 \*

\* Se 11 -0.07421 -0.02426 -0.03361 \*

\* Se 12 0.06100 0.02518 0.09103 \*

\* Se 13 -0.02658 -0.03121 0.05977 \*

\* Se 14 -0.00123 0.03375 0.01150 \*

\* Se 15 0.03339 0.04835 0.00201 \*

\* Se 16 -0.02369 -0.03665 -0.02113 \*

\* Se 17 -0.01206 0.04898 -0.01047 \*

\* Se 18 0.01203 0.01501 -0.02274 \*

\* Se 19 0.02743 0.07168 0.02146 \*

\* Se 20 0.02509 -0.02644 0.01058 \*

\* Nb 1 -0.02872 -0.00712 -0.02051 \*

\* Nb 2 0.02928 0.00685 0.01867 \*

\* Nb 3 -0.00147 -0.00129 0.00181 \*

\* Nb 4 0.00369 0.00069 -0.00350 \*

\* Nb 5 -0.03977 0.06766 -0.04707 \*

\* Nb 6 -0.03007 -0.03867 0.03351 \*

\* Nb 7 -0.00170 0.00974 0.01000 \*

\* Nb 8 0.03083 -0.02120 -0.04265 \*

\* Nb 9 0.00744 0.01757 0.00564 \*

\* Nb 10 0.05005 -0.07586 -0.00278 \*

\* Nb 11 0.03738 -0.00893 -0.00993 \*

\* Nb 12 -0.07255 -0.01458 0.03084 \*

\* Nb 13 -0.04879 0.07789 0.01136 \*

\* Nb 14 -0.00223 -0.02519 -0.00252 \*

\* Nb 15 -0.03880 0.00959 0.01606 \*

\* Nb 16 0.07262 0.00841 -0.02640 \*

\* Nb 17 0.02883 0.03362 -0.02248 \*

\* Nb 18 0.04089 -0.06539 0.04620 \*

\* Nb 19 0.00233 -0.01005 -0.00821 \*

\* Nb 20 -0.03366 0.02037 0.04721 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.033655 -0.007124 -0.003461 \*

\* y -0.007124 -0.003906 0.008163 \*

\* z -0.003461 0.008163 0.002302 \*

\* \*

\* Pressure: 0.0118 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000048 | -36259.899379 | <-- min BFGS

| trial step | 1.000000 | 8.980E-006 | -36259.900277 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 43 with enthalpy= -3.62599003E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.242908E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.124371E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.389134E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.365487E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 44 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000015 | -36259.900277 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 44 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8722055 -8.3379673 -0.0033104 0.4204417 -0.0036328 0.0000990

0.0292532 3.3855839 -0.0003824 1.0354578 1.8469178 0.0004042

-0.0032894 -0.0012025 13.9209171 0.0001284 0.0000499 0.4513486

Lattice parameters(A) Cell Angles

a = 17.050050 alpha = 90.011537

b = 3.385710 beta = 90.020513

c = 13.920918 gamma = 118.781720

Current cell volume = 704.328897 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067669 0.668031 0.123612 x

x Se 2 0.132211 0.341636 0.628688 x

x Se 3 0.131709 0.340861 0.870571 x

x Se 4 0.068158 0.668743 0.376377 x

x Se 5 0.266802 0.665898 0.123512 x

x Se 6 0.333317 0.344567 0.628234 x

x Se 7 0.333285 0.345847 0.872499 x

x Se 8 0.265685 0.663626 0.373578 x

x Se 9 0.466733 0.653354 0.128292 x

x Se 10 0.534091 0.345084 0.624749 x

x Se 11 0.533247 0.346571 0.871692 x

x Se 12 0.465930 0.654692 0.375359 x

x Se 13 0.666736 0.654249 0.127530 x

x Se 14 0.734346 0.336353 0.626480 x

x Se 15 0.733192 0.333973 0.876570 x

x Se 16 0.666652 0.655428 0.371838 x

x Se 17 0.868284 0.659064 0.129451 x

x Se 18 0.931912 0.331689 0.623428 x

x Se 19 0.932339 0.331992 0.876350 x

x Se 20 0.867786 0.658314 0.371286 x

x Nb 1 0.005460 0.015530 0.250057 x

x Nb 2 -0.005516 -0.015545 0.749885 x

x Nb 3 -0.000027 -0.000053 -0.000014 x

x Nb 4 0.000028 0.000159 0.499953 x

x Nb 5 0.196719 -0.009030 0.249335 x

x Nb 6 0.203081 0.017756 0.749496 x

x Nb 7 0.199460 0.003706 -0.001919 x

x Nb 8 0.201818 0.011459 0.501588 x

x Nb 9 0.399081 -0.008880 0.250747 x

x Nb 10 0.401096 0.014909 0.750102 x

x Nb 11 0.401069 0.005369 -0.000779 x

x Nb 12 0.397127 -0.006736 0.500753 x

x Nb 13 0.598875 -0.015010 0.249892 x

x Nb 14 0.600885 0.008853 0.749280 x

x Nb 15 0.598904 -0.005469 0.000775 x

x Nb 16 0.602876 0.006894 0.499292 x

x Nb 17 0.796897 -0.017759 0.250480 x

x Nb 18 0.803350 0.008990 0.750681 x

x Nb 19 0.800589 -0.003548 0.001917 x

x Nb 20 0.798144 -0.011571 0.498382 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598881E+004 30891.41 <-- SCF

1 -3.62599391E+004 1.27539342E-003 30918.48 <-- SCF

2 -3.62599421E+004 7.54321876E-005 30944.33 <-- SCF

3 -3.62599488E+004 1.67721111E-004 30971.16 <-- SCF

4 -3.62598982E+004 -1.26494018E-003 30997.17 <-- SCF

5 -3.62599017E+004 8.73607726E-005 31022.81 <-- SCF

6 -3.62599010E+004 -1.67371054E-005 31045.05 <-- SCF

7 -3.62599006E+004 -1.01574986E-005 31064.50 <-- SCF

8 -3.62599006E+004 -1.63239299E-006 31082.73 <-- SCF

9 -3.62599006E+004 3.52177833E-007 31100.25 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.90058800 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02831 -0.06342 -0.01727 \*

\* Se 2 -0.02659 0.02862 -0.00300 \*

\* Se 3 0.01456 -0.04398 0.00350 \*

\* Se 4 -0.00543 -0.00831 0.02959 \*

\* Se 5 -0.02725 -0.04212 -0.01860 \*

\* Se 6 0.02333 0.02572 -0.00463 \*

\* Se 7 0.02083 0.02712 -0.07402 \*

\* Se 8 0.00337 -0.03047 -0.00612 \*

\* Se 9 0.07802 0.02518 0.04382 \*

\* Se 10 -0.06821 -0.01390 -0.08462 \*

\* Se 11 -0.08022 -0.02581 -0.03693 \*

\* Se 12 0.07034 0.02860 0.08805 \*

\* Se 13 -0.02799 -0.02886 0.06442 \*

\* Se 14 -0.00430 0.02681 0.00977 \*

\* Se 15 0.02912 0.04638 0.00043 \*

\* Se 16 -0.02095 -0.03419 -0.02405 \*

\* Se 17 -0.01521 0.05041 -0.00934 \*

\* Se 18 0.00785 0.00874 -0.02243 \*

\* Se 19 0.02581 0.06434 0.01907 \*

\* Se 20 0.02506 -0.02482 0.00963 \*

\* Nb 1 -0.03113 -0.01513 -0.02095 \*

\* Nb 2 0.03159 0.01502 0.01887 \*

\* Nb 3 -0.00156 -0.00135 0.00178 \*

\* Nb 4 0.00374 0.00066 -0.00374 \*

\* Nb 5 -0.04458 0.06433 -0.04803 \*

\* Nb 6 -0.02919 -0.02947 0.03280 \*

\* Nb 7 -0.00035 0.00938 0.01299 \*

\* Nb 8 0.03195 -0.02233 -0.04594 \*

\* Nb 9 0.00630 0.00493 0.00707 \*

\* Nb 10 0.04819 -0.07387 -0.00512 \*

\* Nb 11 0.03584 -0.00963 -0.01343 \*

\* Nb 12 -0.07651 -0.01463 0.03405 \*

\* Nb 13 -0.04694 0.07598 0.01336 \*

\* Nb 14 -0.00083 -0.01252 -0.00425 \*

\* Nb 15 -0.03732 0.01028 0.01955 \*

\* Nb 16 0.07674 0.00813 -0.02988 \*

\* Nb 17 0.02813 0.02414 -0.02192 \*

\* Nb 18 0.04572 -0.06202 0.04678 \*

\* Nb 19 0.00123 -0.00958 -0.01159 \*

\* Nb 20 -0.03484 0.02164 0.05034 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.028228 -0.027768 -0.010163 \*

\* y -0.027768 -0.013511 0.013841 \*

\* z -0.010163 0.013841 -0.013974 \*

\* \*

\* Pressure: 0.0186 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000015 | -36259.900277 | <-- min BFGS

| trial step | 1.000000 | 9.964E-006 | -36259.900652 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 44 with line minimization (lambda= 2.879515)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8792131 -8.3447566 -0.0047685 0.4203495 -0.0034412 0.0001263

0.0277174 3.3857051 -0.0002732 1.0360366 1.8473166 0.0004258

-0.0041875 -0.0008593 13.9165579 0.0001644 0.0000351 0.4514899

Lattice parameters(A) Cell Angles

a = 17.059483 alpha = 90.008303

b = 3.385819 beta = 90.029322

c = 13.916559 gamma = 118.816104

Current cell volume = 704.288007 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067672 0.667891 0.123536 x

x Se 2 0.132230 0.341557 0.628671 x

x Se 3 0.131685 0.340680 0.870552 x

x Se 4 0.068182 0.668630 0.376407 x

x Se 5 0.266797 0.666004 0.123482 x

x Se 6 0.333356 0.344607 0.628227 x

x Se 7 0.333341 0.346020 0.872542 x

x Se 8 0.265639 0.663636 0.373467 x

x Se 9 0.466681 0.653566 0.128283 x

x Se 10 0.534159 0.344981 0.624618 x

x Se 11 0.533296 0.346345 0.871703 x

x Se 12 0.465868 0.654768 0.375494 x

x Se 13 0.666681 0.654082 0.127489 x

x Se 14 0.734392 0.336349 0.626594 x

x Se 15 0.733195 0.333878 0.876601 x

x Se 16 0.666609 0.655378 0.371844 x

x Se 17 0.868310 0.659254 0.129471 x

x Se 18 0.931895 0.331829 0.623385 x

x Se 19 0.932336 0.332123 0.876423 x

x Se 20 0.867767 0.658403 0.371302 x

x Nb 1 0.005535 0.015668 0.250068 x

x Nb 2 -0.005592 -0.015695 0.749870 x

x Nb 3 -0.000027 -0.000035 -0.000016 x

x Nb 4 0.000035 0.000201 0.499952 x

x Nb 5 0.196710 -0.008998 0.249305 x

x Nb 6 0.203136 0.017503 0.749514 x

x Nb 7 0.199482 0.003827 -0.001996 x

x Nb 8 0.201927 0.011851 0.501619 x

x Nb 9 0.399082 -0.008226 0.250756 x

x Nb 10 0.401164 0.015183 0.750120 x

x Nb 11 0.401146 0.005369 -0.000702 x

x Nb 12 0.397030 -0.007174 0.500707 x

x Nb 13 0.598809 -0.015289 0.249875 x

x Nb 14 0.600878 0.008169 0.749277 x

x Nb 15 0.598827 -0.005464 0.000697 x

x Nb 16 0.602971 0.007335 0.499342 x

x Nb 17 0.796839 -0.017489 0.250461 x

x Nb 18 0.803361 0.008976 0.750712 x

x Nb 19 0.800566 -0.003695 0.002001 x

x Nb 20 0.798029 -0.012000 0.498347 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598586E+004 31203.69 <-- SCF

1 -3.62599664E+004 2.69565792E-003 31230.23 <-- SCF

2 -3.62599721E+004 1.42457634E-004 31258.28 <-- SCF

3 -3.62599545E+004 -4.38560608E-004 31285.00 <-- SCF

4 -3.62599001E+004 -1.36191299E-003 31311.02 <-- SCF

5 -3.62599030E+004 7.42859633E-005 31337.31 <-- SCF

6 -3.62599013E+004 -4.32079500E-005 31361.70 <-- SCF

7 -3.62599008E+004 -1.21432575E-005 31381.95 <-- SCF

8 -3.62599008E+004 -7.19148993E-007 31400.47 <-- SCF

9 -3.62599008E+004 9.09517162E-007 31417.91 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.90083261 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02679 -0.04848 -0.00914 \*

\* Se 2 -0.02740 0.02650 0.00059 \*

\* Se 3 0.01929 -0.04594 0.00043 \*

\* Se 4 -0.00016 0.00297 0.02935 \*

\* Se 5 -0.02250 -0.03973 -0.01531 \*

\* Se 6 0.01616 0.02219 0.00198 \*

\* Se 7 0.02105 0.02221 -0.08501 \*

\* Se 8 0.00705 -0.01882 -0.00404 \*

\* Se 9 0.08968 0.02925 0.04826 \*

\* Se 10 -0.08818 -0.01436 -0.07523 \*

\* Se 11 -0.09183 -0.02983 -0.04195 \*

\* Se 12 0.08992 0.03008 0.08020 \*

\* Se 13 -0.02863 -0.02437 0.07472 \*

\* Se 14 -0.00675 0.01455 0.01067 \*

\* Se 15 0.02516 0.04291 -0.00296 \*

\* Se 16 -0.01480 -0.03032 -0.02986 \*

\* Se 17 -0.02055 0.05234 -0.00731 \*

\* Se 18 0.00109 -0.00220 -0.02080 \*

\* Se 19 0.02435 0.05037 0.01161 \*

\* Se 20 0.02560 -0.02285 0.00592 \*

\* Nb 1 -0.03730 -0.02827 -0.02275 \*

\* Nb 2 0.03787 0.02845 0.02018 \*

\* Nb 3 -0.00176 -0.00167 0.00174 \*

\* Nb 4 0.00365 0.00028 -0.00424 \*

\* Nb 5 -0.05369 0.05837 -0.05124 \*

\* Nb 6 -0.03167 -0.01273 0.03214 \*

\* Nb 7 -0.00093 0.00892 0.01745 \*

\* Nb 8 0.02813 -0.02578 -0.05109 \*

\* Nb 9 0.00382 -0.01665 0.00824 \*

\* Nb 10 0.04510 -0.07096 -0.00743 \*

\* Nb 11 0.03190 -0.01006 -0.02013 \*

\* Nb 12 -0.08015 -0.01332 0.03971 \*

\* Nb 13 -0.04402 0.07334 0.01507 \*

\* Nb 14 0.00229 0.00918 -0.00605 \*

\* Nb 15 -0.03342 0.01072 0.02622 \*

\* Nb 16 0.08079 0.00618 -0.03608 \*

\* Nb 17 0.03123 0.00675 -0.02138 \*

\* Nb 18 0.05507 -0.05591 0.04915 \*

\* Nb 19 0.00200 -0.00875 -0.01712 \*

\* Nb 20 -0.03067 0.02545 0.05548 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.015433 -0.077997 -0.026511 \*

\* y -0.077997 -0.036320 0.021583 \*

\* z -0.026511 0.021583 -0.069397 \*

\* \*

\* Pressure: 0.0404 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000015 | -36259.900277 | <-- min BFGS

| trial step | 1.000000 | 9.964E-006 | -36259.900652 | <-- min BFGS

| line step | 2.879515 | -2.692E-006 | -36259.900903 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 44 with enthalpy= -3.62599009E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.567024E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.241887E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.484853E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 7.799694E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 45 ...

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Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000020 | -36259.900903 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 45 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8787797 -8.3427438 -0.0030648 0.4203291 -0.0035002 0.0000971

0.0281942 3.3857111 -0.0004494 1.0357346 1.8471699 0.0004288

-0.0032286 -0.0014206 13.9178117 0.0001260 0.0000589 0.4514493

Lattice parameters(A) Cell Angles

a = 17.058120 alpha = 90.013564

b = 3.385829 beta = 90.019027

c = 13.917812 gamma = 118.802855

Current cell volume = 704.386893 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067665 0.667832 0.123539 x

x Se 2 0.132225 0.341602 0.628682 x

x Se 3 0.131693 0.340732 0.870546 x

x Se 4 0.068176 0.668613 0.376410 x

x Se 5 0.266794 0.665967 0.123475 x

x Se 6 0.333358 0.344625 0.628237 x

x Se 7 0.333346 0.346088 0.872514 x

x Se 8 0.265640 0.663615 0.373472 x

x Se 9 0.466697 0.653515 0.128304 x

x Se 10 0.534144 0.345019 0.624617 x

x Se 11 0.533280 0.346397 0.871683 x

x Se 12 0.465884 0.654743 0.375495 x

x Se 13 0.666676 0.654012 0.127516 x

x Se 14 0.734390 0.336367 0.626588 x

x Se 15 0.733199 0.333919 0.876604 x

x Se 16 0.666609 0.655359 0.371829 x

x Se 17 0.868301 0.659202 0.129477 x

x Se 18 0.931901 0.331846 0.623385 x

x Se 19 0.932343 0.332183 0.876421 x

x Se 20 0.867772 0.658356 0.371292 x

x Nb 1 0.005539 0.015713 0.250063 x

x Nb 2 -0.005596 -0.015735 0.749874 x

x Nb 3 -0.000027 -0.000040 -0.000015 x

x Nb 4 0.000034 0.000197 0.499950 x

x Nb 5 0.196692 -0.009009 0.249300 x

x Nb 6 0.203121 0.017522 0.749514 x

x Nb 7 0.199475 0.003810 -0.001983 x

x Nb 8 0.201920 0.011810 0.501603 x

x Nb 9 0.399083 -0.008313 0.250760 x

x Nb 10 0.401161 0.015087 0.750108 x

x Nb 11 0.401143 0.005391 -0.000729 x

x Nb 12 0.397023 -0.007157 0.500736 x

x Nb 13 0.598812 -0.015193 0.249888 x

x Nb 14 0.600879 0.008259 0.749273 x

x Nb 15 0.598829 -0.005488 0.000726 x

x Nb 16 0.602979 0.007313 0.499313 x

x Nb 17 0.796853 -0.017515 0.250463 x

x Nb 18 0.803380 0.008986 0.750717 x

x Nb 19 0.800574 -0.003672 0.001986 x

x Nb 20 0.798036 -0.011955 0.498366 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598989E+004 31521.53 <-- SCF

1 -3.62599054E+004 1.62077869E-004 31548.86 <-- SCF

2 -3.62599057E+004 8.24262684E-006 31569.34 <-- SCF

3 -3.62599045E+004 -3.13521574E-005 31595.78 <-- SCF

4 -3.62599014E+004 -7.63643818E-005 31621.39 <-- SCF

5 -3.62599016E+004 3.78113279E-006 31641.97 <-- SCF

6 -3.62599015E+004 -1.98064337E-006 31659.66 <-- SCF

7 -3.62599014E+004 -8.67554500E-007 31676.42 <-- SCF

8 -3.62599015E+004 6.97794500E-007 31694.69 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.90147364 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02797 -0.04797 -0.00858 \*

\* Se 2 -0.02953 0.02174 -0.00034 \*

\* Se 3 0.01478 -0.04788 0.00102 \*

\* Se 4 -0.00193 0.00215 0.02928 \*

\* Se 5 -0.02559 -0.03919 -0.01450 \*

\* Se 6 0.01017 0.02071 -0.00303 \*

\* Se 7 0.01437 0.01590 -0.07559 \*

\* Se 8 0.00391 -0.01873 -0.00313 \*

\* Se 9 0.08556 0.03202 0.04325 \*

\* Se 10 -0.08513 -0.01769 -0.07980 \*

\* Se 11 -0.08740 -0.03270 -0.03702 \*

\* Se 12 0.08706 0.03256 0.08440 \*

\* Se 13 -0.02192 -0.01807 0.06567 \*

\* Se 14 -0.00333 0.01457 0.00947 \*

\* Se 15 0.02839 0.04234 -0.00304 \*

\* Se 16 -0.00895 -0.02825 -0.02257 \*

\* Se 17 -0.01591 0.05404 -0.00784 \*

\* Se 18 0.00273 -0.00127 -0.02082 \*

\* Se 19 0.02549 0.04989 0.01059 \*

\* Se 20 0.02780 -0.01798 0.00677 \*

\* Nb 1 -0.03876 -0.02751 -0.02160 \*

\* Nb 2 0.03913 0.02771 0.01898 \*

\* Nb 3 -0.00185 -0.00198 0.00177 \*

\* Nb 4 0.00356 0.00006 -0.00445 \*

\* Nb 5 -0.06054 0.05966 -0.05160 \*

\* Nb 6 -0.03551 -0.01063 0.03084 \*

\* Nb 7 -0.00603 0.00801 0.01728 \*

\* Nb 8 0.02690 -0.02651 -0.04980 \*

\* Nb 9 0.00599 -0.01873 0.01060 \*

\* Nb 10 0.04361 -0.07108 -0.01030 \*

\* Nb 11 0.02852 -0.00791 -0.02421 \*

\* Nb 12 -0.08482 -0.01121 0.04352 \*

\* Nb 13 -0.04258 0.07346 0.01778 \*

\* Nb 14 0.00036 0.01153 -0.00869 \*

\* Nb 15 -0.03026 0.00857 0.03031 \*

\* Nb 16 0.08578 0.00414 -0.04024 \*

\* Nb 17 0.03484 0.00474 -0.02025 \*

\* Nb 18 0.06187 -0.05720 0.04925 \*

\* Nb 19 0.00720 -0.00760 -0.01744 \*

\* Nb 20 -0.03001 0.02630 0.05408 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.004766 -0.051291 -0.009238 \*

\* y -0.051291 -0.013667 0.009053 \*

\* z -0.009238 0.009053 -0.030083 \*

\* \*

\* Pressure: 0.0130 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000020 | -36259.900903 | <-- min BFGS

| trial step | 1.000000 | 0.000018 | -36259.901509 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 45 with line minimization (lambda= 7.341681)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8760310 -8.3299798 0.0077394 0.4202003 -0.0038744 -0.0000874

0.0312173 3.3857497 -0.0015668 1.0338211 1.8462419 0.0004485

0.0028522 -0.0049798 13.9257627 -0.0001172 0.0002099 0.4511916

Lattice parameters(A) Cell Angles

a = 17.049484 alpha = 90.046893

b = 3.385894 beta = 89.953742

c = 13.925764 gamma = 118.718817

Current cell volume = 705.013262 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067621 0.667456 0.123553 x

x Se 2 0.132190 0.341883 0.628753 x

x Se 3 0.131742 0.341064 0.870505 x

x Se 4 0.068135 0.668504 0.376428 x

x Se 5 0.266769 0.665727 0.123432 x

x Se 6 0.333367 0.344740 0.628300 x

x Se 7 0.333375 0.346517 0.872332 x

x Se 8 0.265651 0.663480 0.373508 x

x Se 9 0.466799 0.653193 0.128434 x

x Se 10 0.534044 0.345256 0.624614 x

x Se 11 0.533176 0.346728 0.871558 x

x Se 12 0.465986 0.654585 0.375502 x

x Se 13 0.666641 0.653570 0.127686 x

x Se 14 0.734377 0.336480 0.626554 x

x Se 15 0.733224 0.334174 0.876620 x

x Se 16 0.666607 0.655240 0.371733 x

x Se 17 0.868247 0.658870 0.129511 x

x Se 18 0.931943 0.331952 0.623385 x

x Se 19 0.932385 0.332562 0.876410 x

x Se 20 0.867803 0.658058 0.371229 x

x Nb 1 0.005563 0.016000 0.250037 x

x Nb 2 -0.005623 -0.015992 0.749899 x

x Nb 3 -0.000029 -0.000073 -0.000008 x

x Nb 4 0.000033 0.000171 0.499941 x

x Nb 5 0.196574 -0.009082 0.249268 x

x Nb 6 0.203031 0.017637 0.749516 x

x Nb 7 0.199432 0.003702 -0.001895 x

x Nb 8 0.201876 0.011549 0.501501 x

x Nb 9 0.399089 -0.008863 0.250789 x

x Nb 10 0.401140 0.014477 0.750035 x

x Nb 11 0.401127 0.005532 -0.000900 x

x Nb 12 0.396975 -0.007048 0.500921 x

x Nb 13 0.598829 -0.014586 0.249971 x

x Nb 14 0.600886 0.008830 0.749245 x

x Nb 15 0.598842 -0.005642 0.000909 x

x Nb 16 0.603028 0.007173 0.499131 x

x Nb 17 0.796946 -0.017677 0.250475 x

x Nb 18 0.803498 0.009048 0.750747 x

x Nb 19 0.800620 -0.003525 0.001890 x

x Nb 20 0.798080 -0.011669 0.498481 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598030E+004 31797.86 <-- SCF

1 -3.62601625E+004 8.98669189E-003 31825.38 <-- SCF

2 -3.62601835E+004 5.25463176E-004 31853.73 <-- SCF

3 -3.62601773E+004 -1.55209623E-004 31880.94 <-- SCF

4 -3.62598895E+004 -7.19509995E-003 31907.22 <-- SCF

5 -3.62599093E+004 4.94102292E-004 31934.16 <-- SCF

6 -3.62599051E+004 -1.03343279E-004 31960.56 <-- SCF

7 -3.62599028E+004 -5.90416617E-005 31983.53 <-- SCF

8 -3.62599024E+004 -8.69708372E-006 32004.44 <-- SCF

9 -3.62599024E+004 -3.41015127E-007 32023.38 <-- SCF

10 -3.62599025E+004 1.87801537E-006 32041.44 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.90249751 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.03038 -0.04846 -0.01738 \*

\* Se 2 -0.03869 0.00701 -0.01766 \*

\* Se 3 -0.01088 -0.04984 0.02158 \*

\* Se 4 -0.00646 -0.00679 0.03316 \*

\* Se 5 -0.01791 -0.03968 -0.00320 \*

\* Se 6 -0.01350 0.01762 -0.02565 \*

\* Se 7 -0.00566 -0.01408 -0.01372 \*

\* Se 8 0.00207 -0.02660 -0.00802 \*

\* Se 9 0.05194 0.04031 0.00891 \*

\* Se 10 -0.06138 -0.02050 -0.09642 \*

\* Se 11 -0.05297 -0.04125 -0.00361 \*

\* Se 12 0.06328 0.03174 0.09942 \*

\* Se 13 -0.00115 0.01144 0.00698 \*

\* Se 14 -0.00074 0.02294 0.01255 \*

\* Se 15 0.02081 0.04227 -0.00885 \*

\* Se 16 0.01431 -0.02259 0.01332 \*

\* Se 17 0.00994 0.05412 -0.02678 \*

\* Se 18 0.00740 0.00792 -0.02532 \*

\* Se 19 0.02822 0.05020 0.01859 \*

\* Se 20 0.03777 -0.00336 0.02283 \*

\* Nb 1 -0.05035 -0.02495 -0.01622 \*

\* Nb 2 0.05143 0.02331 0.01390 \*

\* Nb 3 -0.00142 -0.00082 -0.00016 \*

\* Nb 4 0.00328 0.00080 -0.00219 \*

\* Nb 5 -0.03732 0.05963 -0.04927 \*

\* Nb 6 -0.02178 -0.02661 0.02629 \*

\* Nb 7 0.00325 0.00820 0.00079 \*

\* Nb 8 0.03456 -0.02050 -0.02992 \*

\* Nb 9 0.00368 0.00246 0.00939 \*

\* Nb 10 0.06000 -0.05375 -0.00596 \*

\* Nb 11 0.03128 -0.00984 0.00215 \*

\* Nb 12 -0.08070 -0.01628 0.00837 \*

\* Nb 13 -0.05838 0.05561 0.00959 \*

\* Nb 14 -0.00106 -0.00805 -0.00772 \*

\* Nb 15 -0.03259 0.01041 0.00115 \*

\* Nb 16 0.08220 0.01121 -0.00677 \*

\* Nb 17 0.02162 0.02289 -0.02117 \*

\* Nb 18 0.03805 -0.05678 0.04644 \*

\* Nb 19 -0.00320 -0.00870 -0.00083 \*

\* Nb 20 -0.03858 0.01935 0.03144 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.139697 0.036192 0.105851 \*

\* y 0.036192 0.087138 -0.063309 \*

\* z 0.105851 -0.063309 0.160478 \*

\* \*

\* Pressure: -0.1291 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000020 | -36259.900903 | <-- min BFGS

| trial step | 1.000000 | 0.000018 | -36259.901509 | <-- min BFGS

| line step | 7.341681 | -4.052E-006 | -36259.902589 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 45 with enthalpy= -3.62599026E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 4.214135E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.220450E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.535459E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.604777E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 46 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000107 | -36259.902589 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 46 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8797127 -8.3323489 0.0064357 0.4201280 -0.0038166 -0.0000592

0.0307592 3.3859283 -0.0015384 1.0338827 1.8462838 0.0005077

0.0019178 -0.0049019 13.9218316 -0.0000800 0.0002058 0.4513190

Lattice parameters(A) Cell Angles

a = 17.053854 alpha = 90.046133

b = 3.386068 beta = 89.961635

c = 13.921833 gamma = 118.727497

Current cell volume = 704.972689 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067595 0.667013 0.123470 x

x Se 2 0.132167 0.341709 0.628679 x

x Se 3 0.131713 0.340728 0.870545 x

x Se 4 0.068147 0.668317 0.376477 x

x Se 5 0.266755 0.665644 0.123355 x

x Se 6 0.333370 0.344614 0.628257 x

x Se 7 0.333418 0.346671 0.872305 x

x Se 8 0.265633 0.663416 0.373435 x

x Se 9 0.466798 0.653619 0.128435 x

x Se 10 0.534058 0.344970 0.624381 x

x Se 11 0.533172 0.346282 0.871566 x

x Se 12 0.465982 0.654893 0.375741 x

x Se 13 0.666595 0.653407 0.127703 x

x Se 14 0.734391 0.336538 0.626632 x

x Se 15 0.733238 0.334289 0.876677 x

x Se 16 0.666604 0.655337 0.371747 x

x Se 17 0.868276 0.659230 0.129469 x

x Se 18 0.931939 0.332169 0.623333 x

x Se 19 0.932409 0.332993 0.876492 x

x Se 20 0.867826 0.658246 0.371308 x

x Nb 1 0.005532 0.015827 0.250028 x

x Nb 2 -0.005592 -0.015823 0.749902 x

x Nb 3 -0.000030 -0.000064 -0.000006 x

x Nb 4 0.000043 0.000220 0.499934 x

x Nb 5 0.196519 -0.008889 0.249202 x

x Nb 6 0.203031 0.017043 0.749570 x

x Nb 7 0.199453 0.003773 -0.001914 x

x Nb 8 0.201987 0.011773 0.501444 x

x Nb 9 0.399117 -0.007985 0.250801 x

x Nb 10 0.401220 0.014297 0.750036 x

x Nb 11 0.401210 0.005521 -0.000841 x

x Nb 12 0.396835 -0.007572 0.500915 x

x Nb 13 0.598750 -0.014408 0.249978 x

x Nb 14 0.600859 0.007914 0.749241 x

x Nb 15 0.598758 -0.005628 0.000857 x

x Nb 16 0.603167 0.007675 0.499144 x

x Nb 17 0.796943 -0.017086 0.250433 x

x Nb 18 0.803556 0.008881 0.750813 x

x Nb 19 0.800597 -0.003621 0.001914 x

x Nb 20 0.797961 -0.011935 0.498541 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598516E+004 32144.48 <-- SCF

1 -3.62599606E+004 2.72606739E-003 32170.70 <-- SCF

2 -3.62599665E+004 1.46740814E-004 32199.28 <-- SCF

3 -3.62599371E+004 -7.35295725E-004 32225.97 <-- SCF

4 -3.62599060E+004 -7.77797070E-004 32251.97 <-- SCF

5 -3.62599056E+004 -9.19224603E-006 32277.41 <-- SCF

6 -3.62599052E+004 -9.88816737E-006 32298.41 <-- SCF

7 -3.62599051E+004 -3.09178591E-006 32318.95 <-- SCF

8 -3.62599051E+004 2.37199964E-007 32336.19 <-- SCF

9 -3.62599051E+004 2.42495239E-007 32352.19 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.90509687 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02706 -0.02608 -0.00625 \*

\* Se 2 -0.02083 0.00694 -0.00170 \*

\* Se 3 0.00446 -0.03323 0.00762 \*

\* Se 4 -0.00289 -0.00149 0.02293 \*

\* Se 5 -0.00855 -0.02887 0.01379 \*

\* Se 6 -0.01462 0.01980 0.00247 \*

\* Se 7 -0.00651 -0.02680 -0.00093 \*

\* Se 8 0.00315 -0.01612 -0.01990 \*

\* Se 9 0.04936 0.03322 0.01499 \*

\* Se 10 -0.07723 -0.01231 -0.08610 \*

\* Se 11 -0.04941 -0.03396 -0.01182 \*

\* Se 12 0.07761 0.02288 0.08718 \*

\* Se 13 0.00015 0.02366 -0.00322 \*

\* Se 14 -0.00057 0.01266 0.02557 \*

\* Se 15 0.01180 0.02934 -0.02068 \*

\* Se 16 0.01499 -0.02221 -0.00291 \*

\* Se 17 -0.00648 0.03555 -0.01260 \*

\* Se 18 0.00265 0.00311 -0.01555 \*

\* Se 19 0.02592 0.02860 0.00737 \*

\* Se 20 0.02028 -0.00461 0.00587 \*

\* Nb 1 -0.04724 -0.03292 -0.01584 \*

\* Nb 2 0.04800 0.03143 0.01328 \*

\* Nb 3 -0.00168 -0.00122 -0.00091 \*

\* Nb 4 0.00267 0.00059 -0.00215 \*

\* Nb 5 -0.03900 0.04644 -0.04494 \*

\* Nb 6 -0.02657 -0.01063 0.01346 \*

\* Nb 7 0.00171 0.00372 -0.00184 \*

\* Nb 8 0.02879 -0.02479 -0.02841 \*

\* Nb 9 0.00999 -0.01703 0.01538 \*

\* Nb 10 0.05593 -0.04188 -0.01714 \*

\* Nb 11 0.02773 -0.00471 -0.00745 \*

\* Nb 12 -0.08110 -0.01061 0.01181 \*

\* Nb 13 -0.05554 0.04366 0.01754 \*

\* Nb 14 -0.00823 0.01296 -0.01489 \*

\* Nb 15 -0.02951 0.00496 0.00951 \*

\* Nb 16 0.08369 0.00544 -0.01197 \*

\* Nb 17 0.02841 0.00739 -0.01173 \*

\* Nb 18 0.04041 -0.04371 0.04097 \*

\* Nb 19 -0.00142 -0.00344 -0.00016 \*

\* Nb 20 -0.03327 0.02425 0.02935 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.150186 -0.014632 0.087968 \*

\* y -0.014632 0.076570 -0.068833 \*

\* z 0.087968 -0.068833 0.086726 \*

\* \*

\* Pressure: -0.1045 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000107 | -36259.902589 | <-- min BFGS

| trial step | 1.000000 | 0.000075 | -36259.905188 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 46 with line minimization (lambda= 3.385137)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8884940 -8.3379995 0.0033261 0.4199558 -0.0036790 0.0000081

0.0296663 3.3863544 -0.0014707 1.0340298 1.8463840 0.0006490

-0.0003110 -0.0047161 13.9124552 0.0000089 0.0001961 0.4516231

Lattice parameters(A) Cell Angles

a = 17.064276 alpha = 90.044316

b = 3.386485 beta = 89.980459

c = 13.912456 gamma = 118.748196

Current cell volume = 704.875475 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067533 0.665957 0.123273 x

x Se 2 0.132111 0.341295 0.628502 x

x Se 3 0.131644 0.339927 0.870640 x

x Se 4 0.068176 0.667872 0.376593 x

x Se 5 0.266721 0.665446 0.123174 x

x Se 6 0.333378 0.344314 0.628154 x

x Se 7 0.333518 0.347040 0.872242 x

x Se 8 0.265591 0.663261 0.373259 x

x Se 9 0.466795 0.654636 0.128436 x

x Se 10 0.534090 0.344291 0.623826 x

x Se 11 0.533162 0.345219 0.871584 x

x Se 12 0.465973 0.655626 0.376312 x

x Se 13 0.666487 0.653018 0.127746 x

x Se 14 0.734426 0.336675 0.626820 x

x Se 15 0.733270 0.334564 0.876813 x

x Se 16 0.666598 0.655568 0.371782 x

x Se 17 0.868346 0.660089 0.129368 x

x Se 18 0.931931 0.332689 0.623208 x

x Se 19 0.932465 0.334020 0.876686 x

x Se 20 0.867882 0.658693 0.371496 x

x Nb 1 0.005457 0.015414 0.250007 x

x Nb 2 -0.005517 -0.015419 0.749908 x

x Nb 3 -0.000033 -0.000043 -0.000002 x

x Nb 4 0.000064 0.000338 0.499918 x

x Nb 5 0.196385 -0.008429 0.249044 x

x Nb 6 0.203030 0.015624 0.749697 x

x Nb 7 0.199504 0.003945 -0.001957 x

x Nb 8 0.202251 0.012307 0.501306 x

x Nb 9 0.399185 -0.005889 0.250830 x

x Nb 10 0.401411 0.013868 0.750040 x

x Nb 11 0.401408 0.005495 -0.000699 x

x Nb 12 0.396501 -0.008822 0.500902 x

x Nb 13 0.598561 -0.013984 0.249995 x

x Nb 14 0.600794 0.005728 0.749233 x

x Nb 15 0.598556 -0.005595 0.000732 x

x Nb 16 0.603496 0.008873 0.499175 x

x Nb 17 0.796935 -0.015675 0.250332 x

x Nb 18 0.803694 0.008484 0.750970 x

x Nb 19 0.800542 -0.003848 0.001971 x

x Nb 20 0.797677 -0.012569 0.498685 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62596027E+004 32454.84 <-- SCF

1 -3.62602643E+004 1.65389730E-002 32480.98 <-- SCF

2 -3.62602990E+004 8.68441187E-004 32510.25 <-- SCF

3 -3.62601335E+004 -4.13934513E-003 32537.11 <-- SCF

4 -3.62599122E+004 -5.53190359E-003 32563.06 <-- SCF

5 -3.62599140E+004 4.64167995E-005 32589.77 <-- SCF

6 -3.62599085E+004 -1.39214713E-004 32616.02 <-- SCF

7 -3.62599076E+004 -2.21892590E-005 32639.33 <-- SCF

8 -3.62599076E+004 1.14515209E-006 32660.45 <-- SCF

9 -3.62599076E+004 -2.13550502E-007 32678.42 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.90762575 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.01122 0.03026 0.02128 \*

\* Se 2 0.01844 0.00091 0.03456 \*

\* Se 3 0.03587 0.00367 -0.03219 \*

\* Se 4 0.00354 0.01053 -0.00600 \*

\* Se 5 0.00977 0.00055 0.04988 \*

\* Se 6 -0.01695 0.02622 0.07196 \*

\* Se 7 -0.00945 -0.06165 0.02800 \*

\* Se 8 -0.00104 0.01067 -0.05612 \*

\* Se 9 0.04448 0.03246 0.02143 \*

\* Se 10 -0.12515 0.01385 -0.03898 \*

\* Se 11 -0.04228 -0.03410 -0.02168 \*

\* Se 12 0.11296 -0.00454 0.03580 \*

\* Se 13 0.00500 0.05793 -0.02556 \*

\* Se 14 0.00904 -0.01298 0.06434 \*

\* Se 15 -0.00562 -0.00478 -0.04745 \*

\* Se 16 0.01793 -0.02077 -0.04269 \*

\* Se 17 -0.04024 -0.00611 0.02825 \*

\* Se 18 -0.00698 -0.00804 0.00730 \*

\* Se 19 0.01181 -0.02777 -0.02293 \*

\* Se 20 -0.01770 -0.00144 -0.03159 \*

\* Nb 1 -0.03857 -0.05419 -0.01509 \*

\* Nb 2 0.04176 0.05115 0.01286 \*

\* Nb 3 -0.00246 -0.00050 -0.00336 \*

\* Nb 4 0.00128 0.00124 0.00005 \*

\* Nb 5 -0.03934 0.01060 -0.03343 \*

\* Nb 6 -0.03938 0.02933 -0.01407 \*

\* Nb 7 -0.00274 -0.00820 -0.01152 \*

\* Nb 8 0.01815 -0.03426 -0.01881 \*

\* Nb 9 0.01211 -0.06494 0.02818 \*

\* Nb 10 0.04289 -0.01127 -0.03887 \*

\* Nb 11 0.01223 0.00466 -0.02539 \*

\* Nb 12 -0.08431 -0.00092 0.01333 \*

\* Nb 13 -0.04240 0.01262 0.03170 \*

\* Nb 14 -0.01219 0.06408 -0.02934 \*

\* Nb 15 -0.01408 -0.00503 0.02462 \*

\* Nb 16 0.09010 -0.00258 -0.01716 \*

\* Nb 17 0.04253 -0.03009 0.00754 \*

\* Nb 18 0.04096 -0.00632 0.02757 \*

\* Nb 19 0.00400 0.00785 0.00701 \*

\* Nb 20 -0.02274 0.03191 0.01657 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.168407 -0.103730 0.040940 \*

\* y -0.103730 0.057798 -0.074770 \*

\* z 0.040940 -0.074770 -0.046684 \*

\* \*

\* Pressure: -0.0598 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000107 | -36259.902589 | <-- min BFGS

| trial step | 1.000000 | 0.000075 | -36259.905188 | <-- min BFGS

| line step | 3.385137 | -2.010E-006 | -36259.907737 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 46 with enthalpy= -3.62599077E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.287020E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.318117E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.184156E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.684071E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 47 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000106 | -36259.907737 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 47 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8770490 -8.3286854 0.0001013 0.4201498 -0.0039137 0.0000407

0.0315384 3.3857943 -0.0007486 1.0335229 1.8461222 0.0004194

-0.0013718 -0.0023940 13.9170643 0.0000525 0.0000993 0.4514735

Lattice parameters(A) Cell Angles

a = 17.049739 alpha = 90.022576

b = 3.385941 beta = 89.999773

c = 13.917065 gamma = 118.707917

Current cell volume = 704.666866 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067471 0.665320 0.123330 x

x Se 2 0.132083 0.341273 0.628522 x

x Se 3 0.131682 0.339791 0.870652 x

x Se 4 0.068132 0.667558 0.376544 x

x Se 5 0.266684 0.665207 0.123224 x

x Se 6 0.333409 0.344261 0.628171 x

x Se 7 0.333563 0.347260 0.872132 x

x Se 8 0.265597 0.663172 0.373157 x

x Se 9 0.466915 0.655112 0.128516 x

x Se 10 0.533965 0.343911 0.623745 x

x Se 11 0.533039 0.344739 0.871513 x

x Se 12 0.466105 0.656085 0.376396 x

x Se 13 0.666434 0.652773 0.127844 x

x Se 14 0.734417 0.336747 0.626926 x

x Se 15 0.733308 0.334836 0.876731 x

x Se 16 0.666571 0.655597 0.371723 x

x Se 17 0.868305 0.660244 0.129347 x

x Se 18 0.931979 0.333015 0.623270 x

x Se 19 0.932524 0.334650 0.876632 x

x Se 20 0.867908 0.658716 0.371489 x

x Nb 1 0.005327 0.015034 0.249987 x

x Nb 2 -0.005387 -0.015027 0.749924 x

x Nb 3 -0.000035 -0.000057 0.000002 x

x Nb 4 0.000070 0.000354 0.499909 x

x Nb 5 0.196337 -0.008161 0.248984 x

x Nb 6 0.202921 0.015019 0.749741 x

x Nb 7 0.199509 0.003899 -0.001891 x

x Nb 8 0.202269 0.012095 0.501172 x

x Nb 9 0.399211 -0.005619 0.250860 x

x Nb 10 0.401460 0.013226 0.749976 x

x Nb 11 0.401437 0.005472 -0.000742 x

x Nb 12 0.396419 -0.009048 0.500988 x

x Nb 13 0.598513 -0.013336 0.250070 x

x Nb 14 0.600776 0.005438 0.749209 x

x Nb 15 0.598523 -0.005577 0.000788 x

x Nb 16 0.603578 0.009058 0.499095 x

x Nb 17 0.797043 -0.015101 0.250304 x

x Nb 18 0.803744 0.008233 0.751027 x

x Nb 19 0.800538 -0.003798 0.001904 x

x Nb 20 0.797653 -0.012370 0.498828 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598466E+004 32781.80 <-- SCF

1 -3.62599734E+004 3.16839628E-003 32807.36 <-- SCF

2 -3.62599805E+004 1.77869536E-004 32835.97 <-- SCF

3 -3.62599480E+004 -8.13329103E-004 32862.20 <-- SCF

4 -3.62599109E+004 -9.27067399E-004 32887.86 <-- SCF

5 -3.62599109E+004 3.48737003E-007 32913.33 <-- SCF

6 -3.62599101E+004 -1.86998287E-005 32935.45 <-- SCF

7 -3.62599099E+004 -4.93528486E-006 32955.47 <-- SCF

8 -3.62599100E+004 5.58818677E-007 32973.34 <-- SCF

9 -3.62599100E+004 6.32886009E-007 32989.97 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.90998929 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00127 0.04984 0.00714 \*

\* Se 2 0.03065 -0.00488 0.02387 \*

\* Se 3 0.02972 0.02854 -0.02306 \*

\* Se 4 -0.00143 0.00847 0.00029 \*

\* Se 5 0.02716 0.00693 0.04059 \*

\* Se 6 -0.03810 0.03051 0.07051 \*

\* Se 7 -0.02296 -0.07970 0.06443 \*

\* Se 8 -0.01100 0.01301 -0.07183 \*

\* Se 9 0.00372 0.02293 -0.00337 \*

\* Se 10 -0.10223 0.00835 -0.04973 \*

\* Se 11 0.00095 -0.02464 0.00128 \*

\* Se 12 0.08699 0.00014 0.04602 \*

\* Se 13 0.01978 0.07637 -0.05905 \*

\* Se 14 0.02058 -0.01436 0.07849 \*

\* Se 15 -0.02480 -0.01264 -0.03202 \*

\* Se 16 0.03995 -0.02105 -0.02339 \*

\* Se 17 -0.03460 -0.03336 0.02185 \*

\* Se 18 -0.00249 -0.01001 -0.00342 \*

\* Se 19 0.00108 -0.04657 -0.01124 \*

\* Se 20 -0.02926 0.00374 -0.02217 \*

\* Nb 1 -0.03288 -0.05289 -0.01470 \*

\* Nb 2 0.03473 0.04982 0.01241 \*

\* Nb 3 -0.00194 -0.00029 -0.00392 \*

\* Nb 4 0.00120 0.00096 0.00093 \*

\* Nb 5 -0.03519 0.00053 -0.02781 \*

\* Nb 6 -0.02967 0.02741 -0.02552 \*

\* Nb 7 -0.00265 -0.01199 -0.01785 \*

\* Nb 8 0.02367 -0.03196 -0.00963 \*

\* Nb 9 0.02382 -0.05907 0.02673 \*

\* Nb 10 0.03929 0.00557 -0.03608 \*

\* Nb 11 0.01371 0.00830 -0.01505 \*

\* Nb 12 -0.09585 0.00300 -0.00438 \*

\* Nb 13 -0.03975 -0.00502 0.02477 \*

\* Nb 14 -0.02650 0.06055 -0.02911 \*

\* Nb 15 -0.01557 -0.00936 0.01241 \*

\* Nb 16 0.10311 -0.00554 -0.00169 \*

\* Nb 17 0.03517 -0.02712 0.01428 \*

\* Nb 18 0.03724 0.00334 0.02120 \*

\* Nb 19 0.00299 0.01200 0.01194 \*

\* Nb 20 -0.02992 0.03015 0.00589 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.079831 -0.054850 0.019682 \*

\* y -0.054850 0.043798 -0.025159 \*

\* z 0.019682 -0.025159 -0.026478 \*

\* \*

\* Pressure: -0.0324 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000106 | -36259.907737 | <-- min BFGS

| trial step | 1.000000 | 0.000053 | -36259.910042 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 47 with line minimization (lambda= 1.996600)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8656429 -8.3194029 -0.0031125 0.4203436 -0.0041478 0.0000733

0.0334041 3.3852361 -0.0000290 1.0330175 1.8458619 0.0001908

-0.0024290 -0.0000798 13.9216577 0.0000961 0.0000029 0.4513245

Lattice parameters(A) Cell Angles

a = 17.035252 alpha = 90.000918

b = 3.385401 beta = 90.019032

c = 13.921658 gamma = 118.667753

Current cell volume = 704.458309 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067409 0.664685 0.123387 x

x Se 2 0.132054 0.341251 0.628541 x

x Se 3 0.131720 0.339655 0.870664 x

x Se 4 0.068089 0.667245 0.376496 x

x Se 5 0.266648 0.664969 0.123275 x

x Se 6 0.333439 0.344209 0.628189 x

x Se 7 0.333607 0.347480 0.872023 x

x Se 8 0.265603 0.663083 0.373055 x

x Se 9 0.467033 0.655587 0.128596 x

x Se 10 0.533840 0.343533 0.623664 x

x Se 11 0.532917 0.344260 0.871442 x

x Se 12 0.466237 0.656542 0.376480 x

x Se 13 0.666381 0.652529 0.127943 x

x Se 14 0.734409 0.336819 0.627033 x

x Se 15 0.733346 0.335107 0.876649 x

x Se 16 0.666545 0.655625 0.371663 x

x Se 17 0.868264 0.660398 0.129327 x

x Se 18 0.932027 0.333340 0.623332 x

x Se 19 0.932583 0.335279 0.876577 x

x Se 20 0.867933 0.658737 0.371482 x

x Nb 1 0.005197 0.014656 0.249967 x

x Nb 2 -0.005256 -0.014637 0.749940 x

x Nb 3 -0.000036 -0.000071 0.000007 x

x Nb 4 0.000075 0.000369 0.499899 x

x Nb 5 0.196288 -0.007893 0.248925 x

x Nb 6 0.202813 0.014415 0.749786 x

x Nb 7 0.199513 0.003853 -0.001825 x

x Nb 8 0.202288 0.011884 0.501039 x

x Nb 9 0.399237 -0.005349 0.250889 x

x Nb 10 0.401508 0.012585 0.749912 x

x Nb 11 0.401467 0.005449 -0.000785 x

x Nb 12 0.396337 -0.009272 0.501075 x

x Nb 13 0.598465 -0.012691 0.250146 x

x Nb 14 0.600759 0.005149 0.749186 x

x Nb 15 0.598490 -0.005560 0.000843 x

x Nb 16 0.603660 0.009242 0.499014 x

x Nb 17 0.797150 -0.014529 0.250276 x

x Nb 18 0.803794 0.007982 0.751083 x

x Nb 19 0.800535 -0.003748 0.001838 x

x Nb 20 0.797629 -0.012171 0.498971 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598472E+004 33092.94 <-- SCF

1 -3.62599857E+004 3.46120495E-003 33118.81 <-- SCF

2 -3.62599929E+004 1.80703568E-004 33147.33 <-- SCF

3 -3.62599565E+004 -9.10038402E-004 33173.47 <-- SCF

4 -3.62599113E+004 -1.12992928E-003 33199.06 <-- SCF

5 -3.62599119E+004 1.54674304E-005 33224.05 <-- SCF

6 -3.62599111E+004 -2.19275670E-005 33245.20 <-- SCF

7 -3.62599108E+004 -5.95302909E-006 33265.97 <-- SCF

8 -3.62599109E+004 1.51296671E-006 33284.05 <-- SCF

9 -3.62599109E+004 2.10201396E-007 33301.05 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.91088312 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01424 0.06733 -0.00390 \*

\* Se 2 0.04545 -0.00827 0.01321 \*

\* Se 3 0.02531 0.05377 -0.01291 \*

\* Se 4 -0.00582 0.00672 0.00564 \*

\* Se 5 0.04541 0.01156 0.03091 \*

\* Se 6 -0.06220 0.03705 0.06808 \*

\* Se 7 -0.03763 -0.09555 0.10068 \*

\* Se 8 -0.02263 0.01302 -0.08414 \*

\* Se 9 -0.04335 0.00934 -0.03304 \*

\* Se 10 -0.07160 0.00305 -0.05426 \*

\* Se 11 0.04904 -0.01144 0.02783 \*

\* Se 12 0.05460 0.00346 0.05414 \*

\* Se 13 0.03631 0.09242 -0.09319 \*

\* Se 14 0.03330 -0.01364 0.08842 \*

\* Se 15 -0.04342 -0.01918 -0.01489 \*

\* Se 16 0.06516 -0.02332 -0.00331 \*

\* Se 17 -0.03107 -0.06120 0.01384 \*

\* Se 18 0.00085 -0.01225 -0.01298 \*

\* Se 19 -0.01061 -0.06338 -0.00206 \*

\* Se 20 -0.04312 0.00636 -0.01331 \*

\* Nb 1 -0.02783 -0.05059 -0.01438 \*

\* Nb 2 0.02848 0.04761 0.01239 \*

\* Nb 3 -0.00180 -0.00022 -0.00505 \*

\* Nb 4 0.00076 0.00083 0.00186 \*

\* Nb 5 -0.02658 -0.00905 -0.01961 \*

\* Nb 6 -0.01911 0.02669 -0.03911 \*

\* Nb 7 -0.00170 -0.01502 -0.02605 \*

\* Nb 8 0.02286 -0.02929 0.00112 \*

\* Nb 9 0.03477 -0.05251 0.02576 \*

\* Nb 10 0.03530 0.02433 -0.03399 \*

\* Nb 11 0.01210 0.01386 -0.00721 \*

\* Nb 12 -0.09494 0.00816 -0.02073 \*

\* Nb 13 -0.03739 -0.02386 0.01847 \*

\* Nb 14 -0.04023 0.05664 -0.02968 \*

\* Nb 15 -0.01396 -0.01523 0.00274 \*

\* Nb 16 0.10335 -0.00972 0.01216 \*

\* Nb 17 0.02669 -0.02505 0.02265 \*

\* Nb 18 0.02994 0.01199 0.01228 \*

\* Nb 19 0.00134 0.01617 0.01810 \*

\* Nb 20 -0.03026 0.02842 -0.00646 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.007320 -0.019755 -0.004591 \*

\* y -0.019755 0.019714 0.020515 \*

\* z -0.004591 0.020515 -0.029783 \*

\* \*

\* Pressure: 0.0058 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000106 | -36259.907737 | <-- min BFGS

| trial step | 1.000000 | 0.000053 | -36259.910042 | <-- min BFGS

| line step | 1.996600 | -1.600E-006 | -36259.910926 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 47 with enthalpy= -3.62599109E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.971107E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.438164E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 5.762488E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.978253E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

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Starting BFGS iteration 48 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000032 | -36259.910926 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 48 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8638777 -8.3164698 -0.0020991 0.4203670 -0.0041966 0.0000577

0.0337907 3.3847239 -0.0001654 1.0328670 1.8460248 0.0002111

-0.0019163 -0.0005203 13.9243788 0.0000756 0.0000213 0.4512363

Lattice parameters(A) Cell Angles

a = 17.032279 alpha = 90.005019

b = 3.384893 beta = 90.012897

c = 13.924379 gamma = 118.655413

Current cell volume = 704.450191 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067412 0.664553 0.123318 x

x Se 2 0.132068 0.341208 0.628615 x

x Se 3 0.131697 0.339414 0.870587 x

x Se 4 0.068119 0.667163 0.376514 x

x Se 5 0.266627 0.665007 0.123276 x

x Se 6 0.333537 0.344482 0.628244 x

x Se 7 0.333693 0.347756 0.872055 x

x Se 8 0.265539 0.663070 0.372876 x

x Se 9 0.467018 0.655996 0.128614 x

x Se 10 0.533874 0.343296 0.623550 x

x Se 11 0.532930 0.343838 0.871424 x

x Se 12 0.466208 0.656773 0.376601 x

x Se 13 0.666294 0.652245 0.127915 x

x Se 14 0.734474 0.336838 0.627216 x

x Se 15 0.733367 0.335082 0.876645 x

x Se 16 0.666444 0.655340 0.371604 x

x Se 17 0.868287 0.660650 0.129400 x

x Se 18 0.932003 0.333449 0.623300 x

x Se 19 0.932579 0.335402 0.876645 x

x Se 20 0.867921 0.658790 0.371412 x

x Nb 1 0.005290 0.014701 0.249974 x

x Nb 2 -0.005348 -0.014703 0.749926 x

x Nb 3 -0.000037 -0.000054 0.000004 x

x Nb 4 0.000082 0.000417 0.499898 x

x Nb 5 0.196275 -0.007849 0.248873 x

x Nb 6 0.202875 0.014257 0.749806 x

x Nb 7 0.199540 0.004059 -0.001935 x

x Nb 8 0.202422 0.012367 0.501073 x

x Nb 9 0.399226 -0.004899 0.250920 x

x Nb 10 0.401614 0.013102 0.749909 x

x Nb 11 0.401567 0.005476 -0.000702 x

x Nb 12 0.396201 -0.009879 0.501025 x

x Nb 13 0.598363 -0.013201 0.250150 x

x Nb 14 0.600765 0.004656 0.749161 x

x Nb 15 0.598390 -0.005582 0.000759 x

x Nb 16 0.603795 0.009846 0.499069 x

x Nb 17 0.797084 -0.014355 0.250256 x

x Nb 18 0.803809 0.007967 0.751135 x

x Nb 19 0.800507 -0.003981 0.001955 x

x Nb 20 0.797489 -0.012697 0.498932 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598610E+004 33404.20 <-- SCF

1 -3.62599979E+004 3.42278621E-003 33431.19 <-- SCF

2 -3.62600055E+004 1.89916541E-004 33459.09 <-- SCF

3 -3.62599925E+004 -3.24663605E-004 33486.20 <-- SCF

4 -3.62599102E+004 -2.05820622E-003 33512.19 <-- SCF

5 -3.62599147E+004 1.14529468E-004 33538.77 <-- SCF

6 -3.62599123E+004 -6.11020525E-005 33564.38 <-- SCF

7 -3.62599116E+004 -1.77523788E-005 33585.09 <-- SCF

8 -3.62599115E+004 -1.28767423E-006 33604.00 <-- SCF

9 -3.62599116E+004 3.27670367E-007 33621.94 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.91155177 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02052 0.06998 -0.00624 \*

\* Se 2 0.04626 -0.00121 -0.00234 \*

\* Se 3 0.03158 0.07020 0.00446 \*

\* Se 4 0.00478 0.00484 0.00771 \*

\* Se 5 0.05643 0.00657 0.02497 \*

\* Se 6 -0.08352 0.03377 0.04483 \*

\* Se 7 -0.04076 -0.09168 0.09519 \*

\* Se 8 -0.03001 0.01167 -0.09380 \*

\* Se 9 -0.04542 0.00097 -0.03410 \*

\* Se 10 -0.08422 0.02149 -0.05489 \*

\* Se 11 0.05189 -0.00413 0.02945 \*

\* Se 12 0.06757 -0.01549 0.06217 \*

\* Se 13 0.03959 0.08952 -0.08980 \*

\* Se 14 0.03997 -0.01015 0.09546 \*

\* Se 15 -0.05471 -0.01481 -0.00878 \*

\* Se 16 0.08883 -0.02081 0.01999 \*

\* Se 17 -0.03816 -0.07804 -0.00273 \*

\* Se 18 -0.01001 -0.01145 -0.01520 \*

\* Se 19 -0.01709 -0.06618 -0.00089 \*

\* Se 20 -0.04439 -0.00093 0.00127 \*

\* Nb 1 -0.03824 -0.04934 -0.01886 \*

\* Nb 2 0.03888 0.04710 0.01641 \*

\* Nb 3 -0.00220 -0.00021 -0.00490 \*

\* Nb 4 0.00078 0.00085 0.00154 \*

\* Nb 5 -0.03356 -0.00676 -0.02469 \*

\* Nb 6 -0.02017 0.02821 -0.03738 \*

\* Nb 7 -0.00260 -0.01640 -0.01614 \*

\* Nb 8 0.02094 -0.03349 -0.00604 \*

\* Nb 9 0.04176 -0.05423 0.02201 \*

\* Nb 10 0.03280 0.01195 -0.03296 \*

\* Nb 11 0.01017 0.01595 -0.01477 \*

\* Nb 12 -0.09828 0.01663 -0.01368 \*

\* Nb 13 -0.03602 -0.01137 0.01698 \*

\* Nb 14 -0.04642 0.05885 -0.02599 \*

\* Nb 15 -0.01224 -0.01726 0.01076 \*

\* Nb 16 0.10683 -0.01812 0.00488 \*

\* Nb 17 0.02828 -0.02684 0.02099 \*

\* Nb 18 0.03674 0.00984 0.01709 \*

\* Nb 19 0.00229 0.01784 0.00720 \*

\* Nb 20 -0.02888 0.03267 0.00080 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.002735 -0.005476 0.003540 \*

\* y -0.005476 -0.004723 0.008442 \*

\* z 0.003540 0.008442 -0.017110 \*

\* \*

\* Pressure: 0.0082 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000032 | -36259.910926 | <-- min BFGS

| trial step | 1.000000 | 0.000016 | -36259.911611 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 48 with line minimization (lambda= 2.061310)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8620043 -8.3133568 -0.0010236 0.4203919 -0.0042485 0.0000411

0.0342010 3.3841802 -0.0003101 1.0327073 1.8461977 0.0002327

-0.0013721 -0.0009879 13.9272667 0.0000539 0.0000408 0.4511428

Lattice parameters(A) Cell Angles

a = 17.029124 alpha = 90.009370

b = 3.384353 beta = 90.006386

c = 13.927267 gamma = 118.642313

Current cell volume = 704.441502 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067414 0.664413 0.123244 x

x Se 2 0.132083 0.341163 0.628694 x

x Se 3 0.131672 0.339159 0.870505 x

x Se 4 0.068151 0.667076 0.376534 x

x Se 5 0.266606 0.665046 0.123277 x

x Se 6 0.333640 0.344771 0.628303 x

x Se 7 0.333783 0.348049 0.872089 x

x Se 8 0.265471 0.663056 0.372687 x

x Se 9 0.467002 0.656430 0.128634 x

x Se 10 0.533910 0.343044 0.623429 x

x Se 11 0.532943 0.343390 0.871406 x

x Se 12 0.466178 0.657018 0.376730 x

x Se 13 0.666201 0.651944 0.127886 x

x Se 14 0.734544 0.336857 0.627411 x

x Se 15 0.733389 0.335055 0.876641 x

x Se 16 0.666338 0.655037 0.371540 x

x Se 17 0.868312 0.660917 0.129479 x

x Se 18 0.931977 0.333565 0.623267 x

x Se 19 0.932575 0.335532 0.876717 x

x Se 20 0.867907 0.658846 0.371338 x

x Nb 1 0.005390 0.014750 0.249982 x

x Nb 2 -0.005446 -0.014773 0.749913 x

x Nb 3 -0.000038 -0.000036 -0.000000 x

x Nb 4 0.000090 0.000468 0.499896 x

x Nb 5 0.196261 -0.007801 0.248817 x

x Nb 6 0.202941 0.014089 0.749827 x

x Nb 7 0.199569 0.004277 -0.002051 x

x Nb 8 0.202563 0.012880 0.501109 x

x Nb 9 0.399214 -0.004421 0.250953 x

x Nb 10 0.401725 0.013650 0.749906 x

x Nb 11 0.401672 0.005504 -0.000615 x

x Nb 12 0.396057 -0.010523 0.500972 x

x Nb 13 0.598254 -0.013743 0.250155 x

x Nb 14 0.600772 0.004132 0.749134 x

x Nb 15 0.598283 -0.005606 0.000671 x

x Nb 16 0.603938 0.010487 0.499127 x

x Nb 17 0.797014 -0.014171 0.250235 x

x Nb 18 0.803825 0.007951 0.751190 x

x Nb 19 0.800477 -0.004228 0.002079 x

x Nb 20 0.797340 -0.013254 0.498891 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598542E+004 33725.08 <-- SCF

1 -3.62600385E+004 4.60643849E-003 33752.17 <-- SCF

2 -3.62600485E+004 2.51868466E-004 33780.11 <-- SCF

3 -3.62600435E+004 -1.27015342E-004 33807.23 <-- SCF

4 -3.62599067E+004 -3.41765684E-003 33833.66 <-- SCF

5 -3.62599162E+004 2.35162184E-004 33860.48 <-- SCF

6 -3.62599130E+004 -7.79127260E-005 33886.55 <-- SCF

7 -3.62599119E+004 -2.94418690E-005 33908.17 <-- SCF

8 -3.62599117E+004 -5.10734663E-006 33927.84 <-- SCF

9 -3.62599117E+004 5.25936126E-007 33946.44 <-- SCF

10 -3.62599117E+004 1.39772867E-006 33963.88 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.91172889 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02489 0.07286 -0.01090 \*

\* Se 2 0.04290 0.00577 -0.01802 \*

\* Se 3 0.03747 0.08690 0.02214 \*

\* Se 4 0.01031 0.00216 0.01257 \*

\* Se 5 0.06804 0.00172 0.01556 \*

\* Se 6 -0.10414 0.03055 0.02297 \*

\* Se 7 -0.04789 -0.08920 0.08721 \*

\* Se 8 -0.03597 0.00692 -0.09661 \*

\* Se 9 -0.04506 -0.00696 -0.03651 \*

\* Se 10 -0.09724 0.03851 -0.06043 \*

\* Se 11 0.05261 0.00275 0.03223 \*

\* Se 12 0.08265 -0.03401 0.07389 \*

\* Se 13 0.04725 0.08821 -0.08312 \*

\* Se 14 0.04414 -0.00231 0.09580 \*

\* Se 15 -0.06635 -0.01045 0.00094 \*

\* Se 16 0.10872 -0.01875 0.04054 \*

\* Se 17 -0.04479 -0.09502 -0.01905 \*

\* Se 18 -0.01591 -0.00997 -0.02013 \*

\* Se 19 -0.02169 -0.06917 0.00251 \*

\* Se 20 -0.04163 -0.00806 0.01581 \*

\* Nb 1 -0.04777 -0.04580 -0.02155 \*

\* Nb 2 0.04798 0.04457 0.01922 \*

\* Nb 3 -0.00225 -0.00048 -0.00449 \*

\* Nb 4 0.00059 0.00040 0.00132 \*

\* Nb 5 -0.04352 -0.00603 -0.03043 \*

\* Nb 6 -0.01798 0.03120 -0.03521 \*

\* Nb 7 -0.00648 -0.01711 -0.00779 \*

\* Nb 8 0.01602 -0.03772 -0.00937 \*

\* Nb 9 0.04379 -0.05648 0.01638 \*

\* Nb 10 0.02294 0.00086 -0.02860 \*

\* Nb 11 0.00567 0.01459 -0.02071 \*

\* Nb 12 -0.10295 0.02331 -0.00934 \*

\* Nb 13 -0.02680 0.00001 0.01247 \*

\* Nb 14 -0.04794 0.06200 -0.02075 \*

\* Nb 15 -0.00772 -0.01601 0.01713 \*

\* Nb 16 0.11211 -0.02480 0.00026 \*

\* Nb 17 0.02707 -0.03026 0.01891 \*

\* Nb 18 0.04701 0.00908 0.02268 \*

\* Nb 19 0.00599 0.01895 -0.00207 \*

\* Nb 20 -0.02409 0.03731 0.00454 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.003159 0.014309 0.012230 \*

\* y 0.014309 -0.025130 0.000183 \*

\* z 0.012230 0.000183 -0.000706 \*

\* \*

\* Pressure: 0.0097 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000032 | -36259.910926 | <-- min BFGS

| trial step | 1.000000 | 0.000016 | -36259.911611 | <-- min BFGS

| line step | 2.061310 | -8.238E-007 | -36259.911819 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 48 with enthalpy= -3.62599118E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.233366E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.336243E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 5.718458E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.513007E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 49 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000025 | -36259.911819 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 49 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8584202 -8.3110127 -0.0015973 0.4204451 -0.0043358 0.0000556

0.0349015 3.3844229 -0.0003328 1.0324729 1.8458540 0.0002788

-0.0018518 -0.0010683 13.9282231 0.0000729 0.0000436 0.4511118

Lattice parameters(A) Cell Angles

a = 17.024852 alpha = 90.010107

b = 3.384603 beta = 90.009879

c = 13.928223 gamma = 118.629499

Current cell volume = 704.451130 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067393 0.664134 0.123191 x

x Se 2 0.132109 0.341080 0.628631 x

x Se 3 0.131677 0.339080 0.870530 x

x Se 4 0.068148 0.666840 0.376542 x

x Se 5 0.266608 0.665177 0.123263 x

x Se 6 0.333630 0.344534 0.628277 x

x Se 7 0.333836 0.348115 0.872089 x

x Se 8 0.265440 0.663107 0.372570 x

x Se 9 0.466962 0.656648 0.128637 x

x Se 10 0.533931 0.342889 0.623261 x

x Se 11 0.532980 0.343158 0.871406 x

x Se 12 0.466164 0.657161 0.376902 x

x Se 13 0.666148 0.651885 0.127881 x

x Se 14 0.734573 0.336810 0.627532 x

x Se 15 0.733386 0.334942 0.876649 x

x Se 16 0.666349 0.655271 0.371569 x

x Se 17 0.868307 0.660998 0.129455 x

x Se 18 0.931987 0.333822 0.623250 x

x Se 19 0.932596 0.335805 0.876767 x

x Se 20 0.867882 0.658935 0.371401 x

x Nb 1 0.005380 0.014680 0.249984 x

x Nb 2 -0.005438 -0.014704 0.749904 x

x Nb 3 -0.000038 -0.000026 0.000001 x

x Nb 4 0.000097 0.000509 0.499891 x

x Nb 5 0.196224 -0.007743 0.248778 x

x Nb 6 0.202924 0.013556 0.749852 x

x Nb 7 0.199584 0.004277 -0.002071 x

x Nb 8 0.202652 0.013038 0.501072 x

x Nb 9 0.399246 -0.003624 0.250961 x

x Nb 10 0.401780 0.013458 0.749895 x

x Nb 11 0.401735 0.005477 -0.000578 x

x Nb 12 0.395946 -0.010894 0.500978 x

x Nb 13 0.598198 -0.013565 0.250167 x

x Nb 14 0.600739 0.003312 0.749132 x

x Nb 15 0.598218 -0.005579 0.000638 x

x Nb 16 0.604047 0.010850 0.499124 x

x Nb 17 0.797029 -0.013629 0.250212 x

x Nb 18 0.803864 0.007914 0.751228 x

x Nb 19 0.800460 -0.004248 0.002101 x

x Nb 20 0.797243 -0.013450 0.498928 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598790E+004 34067.20 <-- SCF

1 -3.62599585E+004 1.98655021E-003 34093.61 <-- SCF

2 -3.62599626E+004 1.04078979E-004 34121.48 <-- SCF

3 -3.62599529E+004 -2.44697875E-004 34148.20 <-- SCF

4 -3.62599117E+004 -1.02885308E-003 34173.91 <-- SCF

5 -3.62599139E+004 5.48724254E-005 34200.08 <-- SCF

6 -3.62599127E+004 -3.04855609E-005 34223.92 <-- SCF

7 -3.62599124E+004 -7.49038663E-006 34243.80 <-- SCF

8 -3.62599124E+004 -1.96600024E-007 34261.97 <-- SCF

9 -3.62599124E+004 5.35472385E-007 34279.22 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.91238688 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02973 0.07890 -0.01420 \*

\* Se 2 0.04491 0.01069 -0.00964 \*

\* Se 3 0.03803 0.09129 0.01372 \*

\* Se 4 0.01245 0.00367 0.01062 \*

\* Se 5 0.06744 -0.00801 0.01777 \*

\* Se 6 -0.09734 0.04804 0.04220 \*

\* Se 7 -0.05261 -0.09145 0.08600 \*

\* Se 8 -0.04054 -0.00040 -0.10273 \*

\* Se 9 -0.03348 -0.00918 -0.03705 \*

\* Se 10 -0.10955 0.04693 -0.06779 \*

\* Se 11 0.04208 0.00393 0.03252 \*

\* Se 12 0.09810 -0.04170 0.08291 \*

\* Se 13 0.05147 0.09036 -0.08035 \*

\* Se 14 0.04826 0.00650 0.10042 \*

\* Se 15 -0.06574 -0.00229 -0.00005 \*

\* Se 16 0.10222 -0.03341 0.02204 \*

\* Se 17 -0.04593 -0.09939 -0.01113 \*

\* Se 18 -0.01935 -0.01431 -0.01942 \*

\* Se 19 -0.02707 -0.07530 0.00476 \*

\* Se 20 -0.04359 -0.01289 0.00825 \*

\* Nb 1 -0.05105 -0.04861 -0.02403 \*

\* Nb 2 0.05112 0.04749 0.02173 \*

\* Nb 3 -0.00253 -0.00073 -0.00455 \*

\* Nb 4 0.00040 0.00011 0.00153 \*

\* Nb 5 -0.04260 -0.00503 -0.03084 \*

\* Nb 6 -0.01834 0.03845 -0.03834 \*

\* Nb 7 -0.00616 -0.01586 -0.00733 \*

\* Nb 8 0.01684 -0.03910 -0.01269 \*

\* Nb 9 0.04353 -0.06865 0.02192 \*

\* Nb 10 0.02421 0.00265 -0.03247 \*

\* Nb 11 0.00609 0.01503 -0.02374 \*

\* Nb 12 -0.10873 0.02416 -0.01053 \*

\* Nb 13 -0.02783 -0.00134 0.01659 \*

\* Nb 14 -0.04818 0.07454 -0.02660 \*

\* Nb 15 -0.00849 -0.01650 0.01988 \*

\* Nb 16 0.11817 -0.02615 0.00135 \*

\* Nb 17 0.02737 -0.03790 0.02165 \*

\* Nb 18 0.04626 0.00784 0.02283 \*

\* Nb 19 0.00536 0.01844 -0.00307 \*

\* Nb 20 -0.02491 0.03918 0.00786 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.016511 0.026206 0.005432 \*

\* y 0.026206 -0.009709 -0.004232 \*

\* z 0.005432 -0.004232 -0.004259 \*

\* \*

\* Pressure: 0.0102 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000025 | -36259.911819 | <-- min BFGS

| trial step | 1.000000 | 0.000019 | -36259.912487 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 49 with line minimization (lambda= 3.980525)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8477374 -8.3040260 -0.0033073 0.4206042 -0.0045959 0.0000986

0.0369894 3.3851463 -0.0004007 1.0317748 1.8448303 0.0004162

-0.0032814 -0.0013080 13.9310736 0.0001295 0.0000520 0.4510195

Lattice parameters(A) Cell Angles

a = 17.012118 alpha = 90.012309

b = 3.385348 beta = 90.020292

c = 13.931074 gamma = 118.591316

Current cell volume = 704.479365 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067329 0.663301 0.123032 x

x Se 2 0.132185 0.340832 0.628442 x

x Se 3 0.131690 0.338845 0.870605 x

x Se 4 0.068138 0.666135 0.376566 x

x Se 5 0.266614 0.665567 0.123220 x

x Se 6 0.333601 0.343829 0.628199 x

x Se 7 0.333994 0.348311 0.872092 x

x Se 8 0.265349 0.663258 0.372219 x

x Se 9 0.466842 0.657295 0.128647 x

x Se 10 0.533993 0.342429 0.622761 x

x Se 11 0.533090 0.342467 0.871405 x

x Se 12 0.466122 0.657586 0.377416 x

x Se 13 0.665991 0.651710 0.127867 x

x Se 14 0.734659 0.336670 0.627892 x

x Se 15 0.733375 0.334607 0.876674 x

x Se 16 0.666383 0.655968 0.371653 x

x Se 17 0.868293 0.661240 0.129385 x

x Se 18 0.932018 0.334587 0.623201 x

x Se 19 0.932658 0.336619 0.876916 x

x Se 20 0.867808 0.659198 0.371589 x

x Nb 1 0.005352 0.014473 0.249993 x

x Nb 2 -0.005413 -0.014500 0.749880 x

x Nb 3 -0.000040 0.000002 0.000003 x

x Nb 4 0.000119 0.000631 0.499874 x

x Nb 5 0.196112 -0.007570 0.248661 x

x Nb 6 0.202876 0.011969 0.749925 x

x Nb 7 0.199629 0.004276 -0.002132 x

x Nb 8 0.202918 0.013509 0.500961 x

x Nb 9 0.399341 -0.001248 0.250984 x

x Nb 10 0.401943 0.012888 0.749860 x

x Nb 11 0.401923 0.005399 -0.000470 x

x Nb 12 0.395617 -0.012000 0.500996 x

x Nb 13 0.598032 -0.013034 0.250203 x

x Nb 14 0.600642 0.000867 0.749127 x

x Nb 15 0.598026 -0.005501 0.000542 x

x Nb 16 0.604375 0.011932 0.499115 x

x Nb 17 0.797074 -0.012012 0.250145 x

x Nb 18 0.803982 0.007805 0.751342 x

x Nb 19 0.800409 -0.004305 0.002168 x

x Nb 20 0.796952 -0.014034 0.499040 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62596202E+004 34382.44 <-- SCF

1 -3.62602025E+004 1.45561836E-002 34408.28 <-- SCF

2 -3.62602347E+004 8.05033672E-004 34437.34 <-- SCF

3 -3.62600805E+004 -3.85371013E-003 34463.98 <-- SCF

4 -3.62599189E+004 -4.04161810E-003 34490.17 <-- SCF

5 -3.62599196E+004 1.81488599E-005 34516.62 <-- SCF

6 -3.62599132E+004 -1.60147022E-004 34542.23 <-- SCF

7 -3.62599124E+004 -1.94362669E-005 34565.08 <-- SCF

8 -3.62599125E+004 2.58647110E-006 34585.23 <-- SCF

9 -3.62599125E+004 1.97870865E-007 34603.06 <-- SCF

10 -3.62599125E+004 4.72600860E-007 34619.39 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.91253302 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.03681 0.09120 -0.02453 \*

\* Se 2 0.04644 0.02058 0.01714 \*

\* Se 3 0.03938 0.10399 -0.01192 \*

\* Se 4 0.01694 0.01189 0.00061 \*

\* Se 5 0.06437 -0.03288 0.02264 \*

\* Se 6 -0.07933 0.10238 0.10927 \*

\* Se 7 -0.06799 -0.10021 0.07678 \*

\* Se 8 -0.04904 -0.03168 -0.10450 \*

\* Se 9 0.00719 -0.02387 -0.04105 \*

\* Se 10 -0.16023 0.07015 -0.05148 \*

\* Se 11 0.00411 0.01641 0.03693 \*

\* Se 12 0.15356 -0.06138 0.04525 \*

\* Se 13 0.06587 0.09947 -0.06495 \*

\* Se 14 0.05813 0.04079 0.09669 \*

\* Se 15 -0.06203 0.01908 -0.00065 \*

\* Se 16 0.08387 -0.08244 -0.04365 \*

\* Se 17 -0.04876 -0.11135 0.01428 \*

\* Se 18 -0.02749 -0.03209 -0.01237 \*

\* Se 19 -0.03601 -0.08781 0.01502 \*

\* Se 20 -0.04503 -0.02220 -0.01459 \*

\* Nb 1 -0.06824 -0.05780 -0.02892 \*

\* Nb 2 0.06928 0.05599 0.02888 \*

\* Nb 3 -0.00356 -0.00110 -0.00459 \*

\* Nb 4 -0.00068 -0.00040 0.00383 \*

\* Nb 5 -0.04503 -0.00704 -0.03233 \*

\* Nb 6 -0.02344 0.06624 -0.04764 \*

\* Nb 7 -0.00991 -0.01280 -0.00555 \*

\* Nb 8 0.00623 -0.04149 -0.01377 \*

\* Nb 9 0.04257 -0.11050 0.03349 \*

\* Nb 10 0.01462 0.01396 -0.03764 \*

\* Nb 11 -0.00591 0.01932 -0.03612 \*

\* Nb 12 -0.12597 0.02625 -0.01002 \*

\* Nb 13 -0.01730 -0.01127 0.02413 \*

\* Nb 14 -0.04767 0.11739 -0.03769 \*

\* Nb 15 0.00297 -0.02101 0.03339 \*

\* Nb 16 0.13626 -0.02832 0.00234 \*

\* Nb 17 0.03175 -0.06599 0.03147 \*

\* Nb 18 0.04819 0.01061 0.02533 \*

\* Nb 19 0.00918 0.01622 -0.00423 \*

\* Nb 20 -0.01407 0.04170 0.01075 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.060226 0.086007 -0.014743 \*

\* y 0.086007 0.040768 -0.009120 \*

\* z -0.014743 -0.009120 0.014442 \*

\* \*

\* Pressure: 0.0017 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000025 | -36259.911819 | <-- min BFGS

| trial step | 1.000000 | 0.000019 | -36259.912487 | <-- min BFGS

| line step | 3.980525 | -0.000021 | -36259.912609 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: reverting to earlier configuration

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8584202 -8.3110127 -0.0015973 0.4204451 -0.0043358 0.0000556

0.0349015 3.3844229 -0.0003328 1.0324729 1.8458540 0.0002788

-0.0018518 -0.0010683 13.9282231 0.0000729 0.0000436 0.4511118

Lattice parameters(A) Cell Angles

a = 17.024852 alpha = 90.010107

b = 3.384603 beta = 90.009879

c = 13.928223 gamma = 118.629499

Current cell volume = 704.451130 A\*\*3

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Cell Contents

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x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067393 0.664134 0.123191 x

x Se 2 0.132109 0.341080 0.628631 x

x Se 3 0.131677 0.339080 0.870530 x

x Se 4 0.068148 0.666840 0.376542 x

x Se 5 0.266608 0.665177 0.123263 x

x Se 6 0.333630 0.344534 0.628277 x

x Se 7 0.333836 0.348115 0.872089 x

x Se 8 0.265440 0.663107 0.372570 x

x Se 9 0.466962 0.656648 0.128637 x

x Se 10 0.533931 0.342889 0.623261 x

x Se 11 0.532980 0.343158 0.871406 x

x Se 12 0.466164 0.657161 0.376902 x

x Se 13 0.666148 0.651885 0.127881 x

x Se 14 0.734573 0.336810 0.627532 x

x Se 15 0.733386 0.334942 0.876649 x

x Se 16 0.666349 0.655271 0.371569 x

x Se 17 0.868307 0.660998 0.129455 x

x Se 18 0.931987 0.333822 0.623250 x

x Se 19 0.932596 0.335805 0.876767 x

x Se 20 0.867882 0.658935 0.371401 x

x Nb 1 0.005380 0.014680 0.249984 x

x Nb 2 -0.005438 -0.014704 0.749904 x

x Nb 3 -0.000038 -0.000026 0.000001 x

x Nb 4 0.000097 0.000509 0.499891 x

x Nb 5 0.196224 -0.007743 0.248778 x

x Nb 6 0.202924 0.013556 0.749852 x

x Nb 7 0.199584 0.004277 -0.002071 x

x Nb 8 0.202652 0.013038 0.501072 x

x Nb 9 0.399246 -0.003624 0.250961 x

x Nb 10 0.401780 0.013458 0.749895 x

x Nb 11 0.401735 0.005477 -0.000578 x

x Nb 12 0.395946 -0.010894 0.500978 x

x Nb 13 0.598198 -0.013565 0.250167 x

x Nb 14 0.600739 0.003312 0.749132 x

x Nb 15 0.598218 -0.005579 0.000638 x

x Nb 16 0.604047 0.010850 0.499124 x

x Nb 17 0.797029 -0.013629 0.250212 x

x Nb 18 0.803864 0.007914 0.751228 x

x Nb 19 0.800460 -0.004248 0.002101 x

x Nb 20 0.797243 -0.013450 0.498928 x

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BFGS: finished iteration 49 with enthalpy= -3.62599125E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.669525E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.371085E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.556897E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.620573E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 50 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000135 | -36259.912487 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 50 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8438938 -8.2990559 -0.0039489 0.4206421 -0.0047256 0.0001021

0.0380275 3.3849251 -0.0002082 1.0313176 1.8446396 0.0003421

-0.0033887 -0.0006899 13.9355495 0.0001346 0.0000262 0.4508746

Lattice parameters(A) Cell Angles

a = 17.006338 alpha = 90.006517

b = 3.385139 beta = 90.024081

c = 13.935550 gamma = 118.565413

Current cell volume = 704.596127 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067276 0.662486 0.122788 x

x Se 2 0.132210 0.340853 0.628384 x

x Se 3 0.131694 0.338637 0.870588 x

x Se 4 0.068160 0.665682 0.376718 x

x Se 5 0.266591 0.665570 0.123074 x

x Se 6 0.333667 0.343923 0.628219 x

x Se 7 0.334168 0.348871 0.872054 x

x Se 8 0.265229 0.663113 0.371898 x

x Se 9 0.466824 0.657954 0.128711 x

x Se 10 0.533979 0.341980 0.622198 x

x Se 11 0.533100 0.341768 0.871354 x

x Se 12 0.466152 0.658080 0.378003 x

x Se 13 0.665809 0.651127 0.127891 x

x Se 14 0.734778 0.336818 0.628228 x

x Se 15 0.733397 0.334655 0.876788 x

x Se 16 0.666321 0.655853 0.371616 x

x Se 17 0.868284 0.661467 0.129397 x

x Se 18 0.932014 0.335094 0.623032 x

x Se 19 0.932708 0.337420 0.877152 x

x Se 20 0.867783 0.659198 0.371657 x

x Nb 1 0.005459 0.014553 0.249964 x

x Nb 2 -0.005522 -0.014591 0.749891 x

x Nb 3 -0.000045 0.000013 0.000003 x

x Nb 4 0.000140 0.000744 0.499857 x

x Nb 5 0.195930 -0.007421 0.248473 x

x Nb 6 0.202878 0.010982 0.749999 x

x Nb 7 0.199655 0.004462 -0.002247 x

x Nb 8 0.203217 0.014199 0.500869 x

x Nb 9 0.399394 0.000270 0.251053 x

x Nb 10 0.402170 0.012816 0.749808 x

x Nb 11 0.402154 0.005541 -0.000421 x

x Nb 12 0.395184 -0.013440 0.501058 x

x Nb 13 0.597805 -0.012973 0.250263 x

x Nb 14 0.600590 -0.000729 0.749075 x

x Nb 15 0.597789 -0.005648 0.000508 x

x Nb 16 0.604809 0.013332 0.499066 x

x Nb 17 0.797069 -0.011022 0.250084 x

x Nb 18 0.804173 0.007728 0.751524 x

x Nb 19 0.800381 -0.004530 0.002287 x

x Nb 20 0.796628 -0.014831 0.499135 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62588235E+004 34726.69 <-- SCF

1 -3.62610743E+004 5.62705321E-002 34753.03 <-- SCF

2 -3.62612031E+004 3.21939505E-003 34782.62 <-- SCF

3 -3.62605776E+004 -1.56366168E-002 34809.55 <-- SCF

4 -3.62599342E+004 -1.60869662E-002 34835.41 <-- SCF

5 -3.62599373E+004 7.95289677E-005 34862.09 <-- SCF

6 -3.62599152E+004 -5.54260583E-004 34888.47 <-- SCF

7 -3.62599118E+004 -8.34815541E-005 34913.66 <-- SCF

8 -3.62599123E+004 1.07906095E-005 34937.08 <-- SCF

9 -3.62599121E+004 -3.55918771E-006 34957.31 <-- SCF

10 -3.62599121E+004 2.30130215E-007 34975.31 <-- SCF

11 -3.62599122E+004 9.84232753E-007 34992.72 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.91216264 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.03744 0.09504 -0.03589 \*

\* Se 2 0.04793 0.00859 0.02727 \*

\* Se 3 0.03723 0.11410 -0.01543 \*

\* Se 4 0.03039 0.02411 -0.01850 \*

\* Se 5 0.07452 -0.02460 0.03559 \*

\* Se 6 -0.09438 0.09293 0.12845 \*

\* Se 7 -0.08083 -0.12118 0.07696 \*

\* Se 8 -0.04488 -0.04895 -0.09317 \*

\* Se 9 0.00525 -0.04291 -0.05590 \*

\* Se 10 -0.19008 0.07343 0.01095 \*

\* Se 11 0.00879 0.03378 0.04995 \*

\* Se 12 0.18504 -0.07207 -0.02491 \*

\* Se 13 0.08089 0.12305 -0.05888 \*

\* Se 14 0.05345 0.05901 0.07251 \*

\* Se 15 -0.07594 0.00925 -0.01433 \*

\* Se 16 0.09794 -0.06951 -0.05533 \*

\* Se 17 -0.04784 -0.12251 0.02140 \*

\* Se 18 -0.03784 -0.04808 -0.00585 \*

\* Se 19 -0.03730 -0.09160 0.02941 \*

\* Se 20 -0.04612 -0.01079 -0.02281 \*

\* Nb 1 -0.08829 -0.06755 -0.02787 \*

\* Nb 2 0.08904 0.06629 0.03037 \*

\* Nb 3 -0.00417 -0.00094 -0.00425 \*

\* Nb 4 -0.00155 -0.00066 0.00641 \*

\* Nb 5 -0.04526 -0.02529 -0.02874 \*

\* Nb 6 -0.02653 0.09068 -0.05955 \*

\* Nb 7 -0.01127 -0.01996 -0.00437 \*

\* Nb 8 0.00318 -0.04763 -0.01177 \*

\* Nb 9 0.04816 -0.13698 0.04147 \*

\* Nb 10 0.00547 0.02999 -0.03987 \*

\* Nb 11 -0.01426 0.02533 -0.03781 \*

\* Nb 12 -0.14633 0.03888 -0.02192 \*

\* Nb 13 -0.00879 -0.02677 0.02737 \*

\* Nb 14 -0.05448 0.14703 -0.04431 \*

\* Nb 15 0.01082 -0.02715 0.03626 \*

\* Nb 16 0.15821 -0.03954 0.01562 \*

\* Nb 17 0.03570 -0.08935 0.04236 \*

\* Nb 18 0.04823 0.02883 0.02361 \*

\* Nb 19 0.00979 0.02500 -0.00493 \*

\* Nb 20 -0.01134 0.04871 0.01044 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.062510 0.109530 -0.011564 \*

\* y 0.109530 0.069794 0.004941 \*

\* z -0.011564 0.004941 0.065740 \*

\* \*

\* Pressure: -0.0243 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000135 | -36259.912487 | <-- min BFGS

| trial step | 1.000000 | -0.000213 | -36259.912257 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 50 with line minimization (lambda= 0.386843)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8528008 -8.3063873 -0.0025070 0.4205212 -0.0044866 0.0000735

0.0361108 3.3846172 -0.0002846 1.0320258 1.8453839 0.0003034

-0.0024463 -0.0009219 13.9310573 0.0000968 0.0000369 0.4510200

Lattice parameters(A) Cell Angles

a = 17.017690 alpha = 90.008717

b = 3.384810 beta = 90.015371

c = 13.931058 gamma = 118.604709

Current cell volume = 704.507399 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067348 0.663496 0.123035 x

x Se 2 0.132148 0.340992 0.628535 x

x Se 3 0.131683 0.338909 0.870552 x

x Se 4 0.068152 0.666392 0.376610 x

x Se 5 0.266601 0.665329 0.123190 x

x Se 6 0.333645 0.344298 0.628254 x

x Se 7 0.333964 0.348407 0.872076 x

x Se 8 0.265358 0.663109 0.372310 x

x Se 9 0.466909 0.657153 0.128666 x

x Se 10 0.533950 0.342537 0.622850 x

x Se 11 0.533026 0.342620 0.871386 x

x Se 12 0.466160 0.657516 0.377328 x

x Se 13 0.666017 0.651592 0.127885 x

x Se 14 0.734652 0.336813 0.627801 x

x Se 15 0.733390 0.334831 0.876703 x

x Se 16 0.666338 0.655496 0.371587 x

x Se 17 0.868299 0.661180 0.129433 x

x Se 18 0.931998 0.334314 0.623166 x

x Se 19 0.932639 0.336430 0.876916 x

x Se 20 0.867844 0.659036 0.371500 x

x Nb 1 0.005410 0.014631 0.249976 x

x Nb 2 -0.005470 -0.014661 0.749899 x

x Nb 3 -0.000041 -0.000011 0.000002 x

x Nb 4 0.000114 0.000600 0.499878 x

x Nb 5 0.196110 -0.007618 0.248660 x

x Nb 6 0.202906 0.012560 0.749909 x

x Nb 7 0.199611 0.004349 -0.002139 x

x Nb 8 0.202871 0.013487 0.500993 x

x Nb 9 0.399303 -0.002118 0.250996 x

x Nb 10 0.401931 0.013210 0.749861 x

x Nb 11 0.401897 0.005502 -0.000518 x

x Nb 12 0.395651 -0.011879 0.501009 x

x Nb 13 0.598046 -0.013336 0.250204 x

x Nb 14 0.600681 0.001748 0.749110 x

x Nb 15 0.598052 -0.005606 0.000588 x

x Nb 16 0.604342 0.011810 0.499101 x

x Nb 17 0.797045 -0.012620 0.250163 x

x Nb 18 0.803984 0.007842 0.751343 x

x Nb 19 0.800430 -0.004357 0.002173 x

x Nb 20 0.797005 -0.013985 0.499008 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62595060E+004 35096.42 <-- SCF

1 -3.62602809E+004 1.93732965E-002 35121.88 <-- SCF

2 -3.62603406E+004 1.49323271E-003 35151.00 <-- SCF

3 -3.62601105E+004 -5.75303267E-003 35177.48 <-- SCF

4 -3.62599246E+004 -4.64736494E-003 35203.36 <-- SCF

5 -3.62599185E+004 -1.53184545E-004 35229.55 <-- SCF

6 -3.62599139E+004 -1.14090350E-004 35255.53 <-- SCF

7 -3.62599135E+004 -1.13945199E-005 35278.83 <-- SCF

8 -3.62599135E+004 1.39201406E-006 35298.72 <-- SCF

9 -3.62599135E+004 -1.94798572E-006 35316.81 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.91345998 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.03429 0.08517 -0.02494 \*

\* Se 2 0.04532 0.00834 0.00580 \*

\* Se 3 0.04055 0.10045 0.00084 \*

\* Se 4 0.01320 0.00639 0.00303 \*

\* Se 5 0.07119 -0.01558 0.02654 \*

\* Se 6 -0.09530 0.06446 0.08015 \*

\* Se 7 -0.06384 -0.10224 0.08106 \*

\* Se 8 -0.04724 -0.01680 -0.11970 \*

\* Se 9 -0.02058 -0.01554 -0.03919 \*

\* Se 10 -0.14065 0.06218 -0.07031 \*

\* Se 11 0.03054 0.00854 0.03502 \*

\* Se 12 0.13535 -0.05549 0.06640 \*

\* Se 13 0.06323 0.10208 -0.07042 \*

\* Se 14 0.05543 0.02575 0.11406 \*

\* Se 15 -0.07036 0.00336 -0.00643 \*

\* Se 16 0.09977 -0.04646 -0.01221 \*

\* Se 17 -0.04957 -0.10845 0.00303 \*

\* Se 18 -0.02155 -0.02313 -0.01656 \*

\* Se 19 -0.03296 -0.08262 0.01527 \*

\* Se 20 -0.04409 -0.01056 -0.00476 \*

\* Nb 1 -0.06067 -0.05800 -0.02438 \*

\* Nb 2 0.06147 0.05607 0.02398 \*

\* Nb 3 -0.00340 -0.00014 -0.00431 \*

\* Nb 4 0.00113 0.00052 0.00337 \*

\* Nb 5 -0.04738 -0.01161 -0.03078 \*

\* Nb 6 -0.02397 0.05570 -0.04544 \*

\* Nb 7 -0.01059 -0.01595 -0.00629 \*

\* Nb 8 0.02009 -0.04322 -0.01140 \*

\* Nb 9 0.04646 -0.09631 0.02568 \*

\* Nb 10 0.02134 0.01448 -0.03429 \*

\* Nb 11 0.01067 0.01392 -0.02682 \*

\* Nb 12 -0.13950 0.03070 -0.01292 \*

\* Nb 13 -0.02439 -0.01217 0.01984 \*

\* Nb 14 -0.05213 0.10312 -0.02976 \*

\* Nb 15 -0.01421 -0.01575 0.02404 \*

\* Nb 16 0.14976 -0.03174 0.00533 \*

\* Nb 17 0.03198 -0.05481 0.02911 \*

\* Nb 18 0.05024 0.01544 0.02401 \*

\* Nb 19 0.01012 0.01773 -0.00294 \*

\* Nb 20 -0.02976 0.04217 0.00727 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.027039 0.042009 -0.000109 \*

\* y 0.042009 0.026628 -0.001581 \*

\* z -0.000109 -0.001581 0.003055 \*

\* \*

\* Pressure: -0.0009 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000135 | -36259.912487 | <-- min BFGS

| trial step | 1.000000 | -0.000213 | -36259.912257 | <-- min BFGS

| line step | 0.386843 | 0.000092 | -36259.913525 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 50 with enthalpy= -3.62599135E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.596939E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.690934E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.061346E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.200909E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 51 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000190 | -36259.913525 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 51 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8359585 -8.2890696 -0.0054443 0.4207303 -0.0049763 0.0001440

0.0400293 3.3843352 -0.0003476 1.0304721 1.8443612 0.0005071

-0.0047854 -0.0011599 13.9420587 0.0001900 0.0000440 0.4506642

Lattice parameters(A) Cell Angles

a = 16.994539 alpha = 90.010883

b = 3.384572 beta = 90.033198

c = 13.942060 gamma = 118.515082

Current cell volume = 704.654711 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067194 0.661247 0.122461 x

x Se 2 0.132248 0.340822 0.628297 x

x Se 3 0.131701 0.338438 0.870559 x

x Se 4 0.068186 0.664907 0.376893 x

x Se 5 0.266580 0.665679 0.122889 x

x Se 6 0.333711 0.343790 0.628278 x

x Se 7 0.334410 0.349581 0.871983 x

x Se 8 0.265053 0.662922 0.371357 x

x Se 9 0.466774 0.658843 0.128823 x

x Se 10 0.533946 0.341320 0.621361 x

x Se 11 0.533138 0.340817 0.871261 x

x Se 12 0.466210 0.658794 0.378869 x

x Se 13 0.665556 0.650396 0.127944 x

x Se 14 0.734952 0.337022 0.628788 x

x Se 15 0.733406 0.334621 0.876930 x

x Se 16 0.666284 0.655972 0.371553 x

x Se 17 0.868269 0.661678 0.129421 x

x Se 18 0.932015 0.335942 0.622828 x

x Se 19 0.932785 0.338638 0.877464 x

x Se 20 0.867746 0.659252 0.371759 x

x Nb 1 0.005570 0.014547 0.249924 x

x Nb 2 -0.005637 -0.014594 0.749903 x

x Nb 3 -0.000052 0.000028 0.000004 x

x Nb 4 0.000173 0.000919 0.499831 x

x Nb 5 0.195630 -0.007249 0.248197 x

x Nb 6 0.202855 0.009363 0.750099 x

x Nb 7 0.199692 0.004657 -0.002392 x

x Nb 8 0.203666 0.015142 0.500702 x

x Nb 9 0.399498 0.002743 0.251161 x

x Nb 10 0.402497 0.012490 0.749709 x

x Nb 11 0.402493 0.005736 -0.000359 x

x Nb 12 0.394510 -0.015579 0.501160 x

x Nb 13 0.597475 -0.012676 0.250369 x

x Nb 14 0.600487 -0.003314 0.748994 x

x Nb 15 0.597439 -0.005855 0.000469 x

x Nb 16 0.605486 0.015415 0.498978 x

x Nb 17 0.797087 -0.009393 0.250000 x

x Nb 18 0.804486 0.007666 0.751791 x

x Nb 19 0.800341 -0.004785 0.002436 x

x Nb 20 0.796140 -0.015943 0.499307 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62578408E+004 35420.20 <-- SCF

1 -3.62618559E+004 1.00377716E-001 35447.02 <-- SCF

2 -3.62621204E+004 6.61384790E-003 35476.92 <-- SCF

3 -3.62608705E+004 -3.12472488E-002 35503.92 <-- SCF

4 -3.62599689E+004 -2.25411633E-002 35530.03 <-- SCF

5 -3.62599369E+004 -7.99671625E-004 35556.59 <-- SCF

6 -3.62599099E+004 -6.75512358E-004 35583.11 <-- SCF

7 -3.62599074E+004 -6.11587499E-005 35609.22 <-- SCF

8 -3.62599078E+004 1.06276560E-005 35634.05 <-- SCF

9 -3.62599073E+004 -1.34411723E-005 35655.44 <-- SCF

10 -3.62599073E+004 -4.96755349E-007 35674.23 <-- SCF

11 -3.62599073E+004 1.31285965E-006 35691.52 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.90734473 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.03462 0.11074 -0.03935 \*

\* Se 2 0.05079 -0.00714 0.03856 \*

\* Se 3 0.03546 0.11774 -0.01639 \*

\* Se 4 0.04641 0.05609 -0.03488 \*

\* Se 5 0.07590 -0.01816 0.03884 \*

\* Se 6 -0.10841 0.09396 0.14884 \*

\* Se 7 -0.08976 -0.14009 0.07506 \*

\* Se 8 -0.03048 -0.07690 -0.00131 \*

\* Se 9 0.01116 -0.06808 -0.08882 \*

\* Se 10 -0.22804 0.09652 0.14868 \*

\* Se 11 0.00509 0.05775 0.07920 \*

\* Se 12 0.24443 -0.12982 -0.14885 \*

\* Se 13 0.08929 0.14536 -0.05086 \*

\* Se 14 0.04445 0.08351 -0.02606 \*

\* Se 15 -0.08483 0.00208 -0.02324 \*

\* Se 16 0.10630 -0.06612 -0.07357 \*

\* Se 17 -0.04886 -0.12587 0.02495 \*

\* Se 18 -0.04612 -0.07511 -0.00917 \*

\* Se 19 -0.03484 -0.10140 0.03638 \*

\* Se 20 -0.04956 0.00562 -0.03306 \*

\* Nb 1 -0.11735 -0.08366 -0.02996 \*

\* Nb 2 0.11577 0.08422 0.03469 \*

\* Nb 3 -0.00564 -0.00073 -0.00441 \*

\* Nb 4 -0.00341 -0.00082 0.00923 \*

\* Nb 5 -0.03536 -0.04484 -0.02718 \*

\* Nb 6 -0.03366 0.12858 -0.07605 \*

\* Nb 7 -0.00732 -0.02426 -0.00700 \*

\* Nb 8 -0.00586 -0.05330 -0.00908 \*

\* Nb 9 0.06153 -0.18079 0.05140 \*

\* Nb 10 -0.00323 0.05152 -0.04186 \*

\* Nb 11 -0.02533 0.03471 -0.04634 \*

\* Nb 12 -0.17544 0.05486 -0.03769 \*

\* Nb 13 -0.00201 -0.04589 0.03054 \*

\* Nb 14 -0.07136 0.19603 -0.05447 \*

\* Nb 15 0.01967 -0.03601 0.04481 \*

\* Nb 16 0.18683 -0.05316 0.03210 \*

\* Nb 17 0.04216 -0.12565 0.05725 \*

\* Nb 18 0.03740 0.04879 0.02307 \*

\* Nb 19 0.00318 0.03299 -0.00325 \*

\* Nb 20 -0.00359 0.05673 0.00927 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.099969 0.160496 -0.035943 \*

\* y 0.160496 0.080754 -0.016809 \*

\* z -0.035943 -0.016809 0.100920 \*

\* \*

\* Pressure: -0.0272 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000190 | -36259.913525 | <-- min BFGS

| trial step | 1.000000 | -0.000682 | -36259.907424 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 51 with line minimization (lambda= 0.217641)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8491352 -8.3026183 -0.0031463 0.4205666 -0.0045931 0.0000889

0.0369636 3.3845558 -0.0002983 1.0316876 1.8451610 0.0003478

-0.0029554 -0.0009737 13.9334516 0.0001171 0.0000385 0.4509425

Lattice parameters(A) Cell Angles

a = 17.012651 alpha = 90.009187

b = 3.384758 beta = 90.019250

c = 13.933452 gamma = 118.585209

Current cell volume = 704.539669 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067314 0.663007 0.122910 x

x Se 2 0.132170 0.340955 0.628483 x

x Se 3 0.131687 0.338806 0.870554 x

x Se 4 0.068160 0.666069 0.376672 x

x Se 5 0.266597 0.665405 0.123124 x

x Se 6 0.333659 0.344187 0.628260 x

x Se 7 0.334061 0.348663 0.872056 x

x Se 8 0.265292 0.663068 0.372102 x

x Se 9 0.466879 0.657521 0.128700 x

x Se 10 0.533949 0.342273 0.622526 x

x Se 11 0.533051 0.342228 0.871359 x

x Se 12 0.466171 0.657795 0.377664 x

x Se 13 0.665917 0.651332 0.127898 x

x Se 14 0.734717 0.336859 0.628016 x

x Se 15 0.733393 0.334785 0.876752 x

x Se 16 0.666326 0.655600 0.371579 x

x Se 17 0.868292 0.661288 0.129430 x

x Se 18 0.932001 0.334668 0.623092 x

x Se 19 0.932671 0.336910 0.877035 x

x Se 20 0.867823 0.659083 0.371557 x

x Nb 1 0.005445 0.014613 0.249965 x

x Nb 2 -0.005507 -0.014646 0.749900 x

x Nb 3 -0.000043 -0.000003 0.000002 x

x Nb 4 0.000127 0.000669 0.499868 x

x Nb 5 0.196006 -0.007538 0.248559 x

x Nb 6 0.202895 0.011865 0.749950 x

x Nb 7 0.199629 0.004416 -0.002194 x

x Nb 8 0.203044 0.013847 0.500930 x

x Nb 9 0.399346 -0.001060 0.251032 x

x Nb 10 0.402054 0.013053 0.749828 x

x Nb 11 0.402027 0.005553 -0.000483 x

x Nb 12 0.395403 -0.012684 0.501042 x

x Nb 13 0.597922 -0.013192 0.250240 x

x Nb 14 0.600639 0.000646 0.749085 x

x Nb 15 0.597919 -0.005660 0.000562 x

x Nb 16 0.604591 0.012594 0.499074 x

x Nb 17 0.797054 -0.011918 0.250127 x

x Nb 18 0.804093 0.007804 0.751440 x

x Nb 19 0.800410 -0.004450 0.002230 x

x Nb 20 0.796817 -0.014411 0.499073 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62586491E+004 35794.80 <-- SCF

1 -3.62610947E+004 6.11409953E-002 35820.64 <-- SCF

2 -3.62612776E+004 4.57099219E-003 35850.38 <-- SCF

3 -3.62605411E+004 -1.84119860E-002 35877.09 <-- SCF

4 -3.62599470E+004 -1.48516428E-002 35903.11 <-- SCF

5 -3.62599300E+004 -4.25050686E-004 35929.55 <-- SCF

6 -3.62599153E+004 -3.67565441E-004 35955.91 <-- SCF

7 -3.62599136E+004 -4.29174074E-005 35980.84 <-- SCF

8 -3.62599140E+004 9.50990852E-006 36003.94 <-- SCF

9 -3.62599137E+004 -7.55528909E-006 36024.19 <-- SCF

10 -3.62599137E+004 2.65846481E-007 36042.25 <-- SCF

11 -3.62599137E+004 8.02667665E-007 36059.20 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.91373632 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.03471 0.08783 -0.03468 \*

\* Se 2 0.04697 0.00479 0.01337 \*

\* Se 3 0.04028 0.10442 -0.00036 \*

\* Se 4 0.02112 0.01436 -0.00687 \*

\* Se 5 0.07489 -0.01840 0.03151 \*

\* Se 6 -0.09565 0.07277 0.09200 \*

\* Se 7 -0.07342 -0.10973 0.08332 \*

\* Se 8 -0.04589 -0.03383 -0.11478 \*

\* Se 9 -0.01433 -0.02685 -0.04715 \*

\* Se 10 -0.16321 0.06815 -0.03980 \*

\* Se 11 0.02487 0.02018 0.04237 \*

\* Se 12 0.15699 -0.06204 0.02909 \*

\* Se 13 0.07483 0.11111 -0.06961 \*

\* Se 14 0.05402 0.04426 0.10418 \*

\* Se 15 -0.07467 0.00612 -0.01181 \*

\* Se 16 0.09837 -0.05418 -0.02149 \*

\* Se 17 -0.04881 -0.11093 0.00489 \*

\* Se 18 -0.02987 -0.03497 -0.01263 \*

\* Se 19 -0.03425 -0.08610 0.02660 \*

\* Se 20 -0.04596 -0.00681 -0.01124 \*

\* Nb 1 -0.06908 -0.06984 -0.02740 \*

\* Nb 2 0.07423 0.06383 0.02882 \*

\* Nb 3 -0.00475 0.00372 -0.00555 \*

\* Nb 4 -0.00137 0.00291 0.00733 \*

\* Nb 5 -0.04189 -0.01202 -0.02974 \*

\* Nb 6 -0.02516 0.07105 -0.05209 \*

\* Nb 7 -0.00641 -0.01630 -0.00387 \*

\* Nb 8 0.01612 -0.04653 -0.01098 \*

\* Nb 9 0.04908 -0.11350 0.03257 \*

\* Nb 10 0.01753 0.02429 -0.03682 \*

\* Nb 11 -0.00008 0.00953 -0.03130 \*

\* Nb 12 -0.13571 0.03474 -0.01950 \*

\* Nb 13 -0.01776 -0.02193 0.02296 \*

\* Nb 14 -0.05504 0.11992 -0.03578 \*

\* Nb 15 -0.00514 -0.01191 0.02825 \*

\* Nb 16 0.14721 -0.03129 0.01415 \*

\* Nb 17 0.02910 -0.06723 0.03474 \*

\* Nb 18 0.04206 0.02082 0.02357 \*

\* Nb 19 0.00736 0.01163 -0.00295 \*

\* Nb 20 -0.02132 0.03796 0.00668 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.032604 0.059590 -0.002679 \*

\* y 0.059590 0.037949 -0.002403 \*

\* z -0.002679 -0.002403 0.013753 \*

\* \*

\* Pressure: -0.0064 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000190 | -36259.913525 | <-- min BFGS

| trial step | 1.000000 | -0.000682 | -36259.907424 | <-- min BFGS

| line step | 0.217641 | 0.000039 | -36259.913828 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 51 with enthalpy= -3.62599138E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.551677E-006 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.812911E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.752381E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 5.958952E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 52 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000092 | -36259.913828 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 52 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8485267 -8.3029624 -0.0048519 0.4205802 -0.0045994 0.0001292

0.0370159 3.3847796 -0.0003168 1.0316956 1.8450230 0.0004559

-0.0042908 -0.0010440 13.9340959 0.0001699 0.0000403 0.4509217

Lattice parameters(A) Cell Angles

a = 17.012288 alpha = 90.009847

b = 3.384982 beta = 90.029645

c = 13.934097 gamma = 118.586376

Current cell volume = 704.596024 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067297 0.662923 0.122850 x

x Se 2 0.132177 0.341002 0.628356 x

x Se 3 0.131718 0.339082 0.870647 x

x Se 4 0.068147 0.665978 0.376737 x

x Se 5 0.266637 0.665428 0.123051 x

x Se 6 0.333535 0.343862 0.628229 x

x Se 7 0.334022 0.348343 0.872059 x

x Se 8 0.265295 0.662979 0.372099 x

x Se 9 0.466865 0.657397 0.128676 x

x Se 10 0.533864 0.342213 0.622321 x

x Se 11 0.533066 0.342345 0.871386 x

x Se 12 0.466251 0.657878 0.377873 x

x Se 13 0.665954 0.651645 0.127887 x

x Se 14 0.734716 0.336961 0.628021 x

x Se 15 0.733353 0.334762 0.876822 x

x Se 16 0.666457 0.655956 0.371644 x

x Se 17 0.868255 0.660989 0.129340 x

x Se 18 0.932015 0.334733 0.623027 x

x Se 19 0.932688 0.337006 0.877089 x

x Se 20 0.867815 0.659035 0.371684 x

x Nb 1 0.005357 0.014371 0.249930 x

x Nb 2 -0.005420 -0.014393 0.749931 x

x Nb 3 -0.000046 -0.000017 0.000003 x

x Nb 4 0.000130 0.000679 0.499863 x

x Nb 5 0.195912 -0.007550 0.248505 x

x Nb 6 0.202823 0.011556 0.749947 x

x Nb 7 0.199613 0.004250 -0.002138 x

x Nb 8 0.203059 0.013615 0.500840 x

x Nb 9 0.399406 -0.000801 0.251044 x

x Nb 10 0.402065 0.012506 0.749791 x

x Nb 11 0.402037 0.005615 -0.000546 x

x Nb 12 0.395286 -0.012838 0.501105 x

x Nb 13 0.597907 -0.012658 0.250270 x

x Nb 14 0.600582 0.000398 0.749074 x

x Nb 15 0.597905 -0.005734 0.000631 x

x Nb 16 0.604714 0.012741 0.499007 x

x Nb 17 0.797132 -0.011612 0.250127 x

x Nb 18 0.804190 0.007832 0.751487 x

x Nb 19 0.800426 -0.004278 0.002164 x

x Nb 20 0.796794 -0.014201 0.499167 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598766E+004 36162.47 <-- SCF

1 -3.62600350E+004 3.96013677E-003 36189.75 <-- SCF

2 -3.62600443E+004 2.31822151E-004 36217.00 <-- SCF

3 -3.62600389E+004 -1.34023542E-004 36243.88 <-- SCF

4 -3.62599096E+004 -3.23186673E-003 36270.22 <-- SCF

5 -3.62599190E+004 2.34966060E-004 36296.91 <-- SCF

6 -3.62599171E+004 -4.91495459E-005 36322.09 <-- SCF

7 -3.62599158E+004 -3.28423566E-005 36343.81 <-- SCF

8 -3.62599157E+004 -2.05664357E-006 36363.45 <-- SCF

9 -3.62599157E+004 1.88376911E-006 36381.19 <-- SCF

10 -3.62599158E+004 1.48129653E-006 36398.27 <-- SCF

11 -3.62599159E+004 1.30385982E-006 36415.16 <-- SCF

12 -3.62599159E+004 9.69510423E-007 36431.44 <-- SCF

13 -3.62599159E+004 7.85128325E-007 36447.48 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.91592686 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02606 0.08588 -0.02756 \*

\* Se 2 0.04670 -0.00562 0.03408 \*

\* Se 3 0.03095 0.08301 -0.02670 \*

\* Se 4 0.01473 0.01805 -0.02425 \*

\* Se 5 0.05787 -0.01078 0.04797 \*

\* Se 6 -0.07624 0.07436 0.12406 \*

\* Se 7 -0.06696 -0.10913 0.07709 \*

\* Se 8 -0.05129 -0.02726 -0.12995 \*

\* Se 9 -0.01157 -0.01963 -0.03291 \*

\* Se 10 -0.16378 0.05561 -0.01363 \*

\* Se 11 0.02201 0.01343 0.02857 \*

\* Se 12 0.16235 -0.05527 0.00309 \*

\* Se 13 0.06845 0.11059 -0.05988 \*

\* Se 14 0.05891 0.03729 0.11909 \*

\* Se 15 -0.05931 -0.00132 -0.03023 \*

\* Se 16 0.07450 -0.05774 -0.06487 \*

\* Se 17 -0.03836 -0.08899 0.03085 \*

\* Se 18 -0.02116 -0.03670 0.00047 \*

\* Se 19 -0.02608 -0.08442 0.02060 \*

\* Se 20 -0.04539 0.00418 -0.03110 \*

\* Nb 1 -0.06534 -0.07159 -0.02328 \*

\* Nb 2 0.06940 0.06643 0.02490 \*

\* Nb 3 -0.00496 0.00310 -0.00510 \*

\* Nb 4 -0.00149 0.00178 0.00765 \*

\* Nb 5 -0.02840 -0.02097 -0.02164 \*

\* Nb 6 -0.03107 0.07971 -0.05461 \*

\* Nb 7 -0.00356 -0.01379 -0.01142 \*

\* Nb 8 0.01440 -0.04058 -0.00787 \*

\* Nb 9 0.05114 -0.12098 0.04115 \*

\* Nb 10 0.01463 0.04146 -0.03306 \*

\* Nb 11 0.00036 0.00748 -0.02818 \*

\* Nb 12 -0.13910 0.02685 -0.02934 \*

\* Nb 13 -0.01433 -0.03839 0.02310 \*

\* Nb 14 -0.05721 0.12836 -0.04391 \*

\* Nb 15 -0.00470 -0.00933 0.02512 \*

\* Nb 16 0.14994 -0.02319 0.02564 \*

\* Nb 17 0.03474 -0.07581 0.03902 \*

\* Nb 18 0.02870 0.02832 0.01707 \*

\* Nb 19 0.00400 0.01088 0.00506 \*

\* Nb 20 -0.01952 0.03473 0.00490 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.031964 0.048369 -0.025118 \*

\* y 0.048369 0.072561 -0.000130 \*

\* z -0.025118 -0.000130 0.048577 \*

\* \*

\* Pressure: -0.0297 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000092 | -36259.913828 | <-- min BFGS

| trial step | 1.000000 | 0.000062 | -36259.916018 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 52 with line minimization (lambda= 3.062003)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8472718 -8.3036720 -0.0083688 0.4206083 -0.0046125 0.0002122

0.0371237 3.3852410 -0.0003548 1.0317121 1.8447386 0.0006789

-0.0070445 -0.0011890 13.9354243 0.0002789 0.0000442 0.4508788

Lattice parameters(A) Cell Angles

a = 17.011541 alpha = 90.011210

b = 3.385445 beta = 90.051079

c = 13.935426 gamma = 118.588782

Current cell volume = 704.712174 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067263 0.662751 0.122724 x

x Se 2 0.132192 0.341099 0.628094 x

x Se 3 0.131783 0.339650 0.870838 x

x Se 4 0.068120 0.665791 0.376873 x

x Se 5 0.266722 0.665474 0.122899 x

x Se 6 0.333279 0.343192 0.628165 x

x Se 7 0.333941 0.347685 0.872065 x

x Se 8 0.265302 0.662793 0.372091 x

x Se 9 0.466837 0.657144 0.128627 x

x Se 10 0.533690 0.342089 0.621898 x

x Se 11 0.533098 0.342585 0.871441 x

x Se 12 0.466417 0.658052 0.378305 x

x Se 13 0.666031 0.652291 0.127864 x

x Se 14 0.734713 0.337172 0.628032 x

x Se 15 0.733268 0.334713 0.876967 x

x Se 16 0.666727 0.656690 0.371778 x

x Se 17 0.868180 0.660373 0.129153 x

x Se 18 0.932042 0.334866 0.622891 x

x Se 19 0.932724 0.337203 0.877201 x

x Se 20 0.867799 0.658936 0.371947 x

x Nb 1 0.005176 0.013873 0.249859 x

x Nb 2 -0.005243 -0.013870 0.749996 x

x Nb 3 -0.000051 -0.000045 0.000005 x

x Nb 4 0.000137 0.000699 0.499852 x

x Nb 5 0.195719 -0.007574 0.248394 x

x Nb 6 0.202675 0.010920 0.749940 x

x Nb 7 0.199581 0.003910 -0.002021 x

x Nb 8 0.203089 0.013136 0.500656 x

x Nb 9 0.399531 -0.000268 0.251068 x

x Nb 10 0.402087 0.011379 0.749716 x

x Nb 11 0.402058 0.005742 -0.000676 x

x Nb 12 0.395046 -0.013156 0.501236 x

x Nb 13 0.597876 -0.011555 0.250331 x

x Nb 14 0.600464 -0.000115 0.749051 x

x Nb 15 0.597878 -0.005886 0.000773 x

x Nb 16 0.604967 0.013043 0.498868 x

x Nb 17 0.797293 -0.010981 0.250127 x

x Nb 18 0.804390 0.007891 0.751585 x

x Nb 19 0.800457 -0.003922 0.002026 x

x Nb 20 0.796746 -0.013769 0.499361 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597523E+004 36551.00 <-- SCF

1 -3.62603320E+004 1.44936385E-002 36578.41 <-- SCF

2 -3.62603638E+004 7.93941781E-004 36606.11 <-- SCF

3 -3.62602639E+004 -2.49689222E-003 36632.94 <-- SCF

4 -3.62599042E+004 -8.99191569E-003 36658.98 <-- SCF

5 -3.62599301E+004 6.47359371E-004 36685.80 <-- SCF

6 -3.62599219E+004 -2.06037293E-004 36711.95 <-- SCF

7 -3.62599177E+004 -1.03598756E-004 36735.72 <-- SCF

8 -3.62599174E+004 -8.89709797E-006 36757.31 <-- SCF

9 -3.62599176E+004 5.06877314E-006 36775.72 <-- SCF

10 -3.62599177E+004 3.38905060E-006 36793.53 <-- SCF

11 -3.62599178E+004 2.45438452E-006 36810.94 <-- SCF

12 -3.62599179E+004 1.67327599E-006 36827.16 <-- SCF

13 -3.62599179E+004 1.42425996E-006 36843.47 <-- SCF

14 -3.62599180E+004 1.31032710E-006 36859.64 <-- SCF

15 -3.62599180E+004 1.16855700E-006 36875.75 <-- SCF

16 -3.62599181E+004 1.00258493E-006 36891.78 <-- SCF

17 -3.62599181E+004 8.97938679E-007 36907.86 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.91811019 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01038 0.07926 -0.01848 \*

\* Se 2 0.04195 -0.02914 0.07094 \*

\* Se 3 0.01645 0.03972 -0.06932 \*

\* Se 4 0.00255 0.02474 -0.05372 \*

\* Se 5 0.02195 0.00733 0.07690 \*

\* Se 6 -0.02140 0.06735 0.17931 \*

\* Se 7 -0.04650 -0.10761 0.06217 \*

\* Se 8 -0.05962 -0.01449 -0.16838 \*

\* Se 9 -0.00585 -0.00483 -0.00538 \*

\* Se 10 -0.17554 0.04984 0.02826 \*

\* Se 11 0.01473 -0.00032 0.00230 \*

\* Se 12 0.18766 -0.07233 -0.03396 \*

\* Se 13 0.04713 0.10881 -0.03713 \*

\* Se 14 0.06675 0.02405 0.15787 \*

\* Se 15 -0.02621 -0.01827 -0.06363 \*

\* Se 16 0.00642 -0.05498 -0.15001 \*

\* Se 17 -0.02153 -0.04434 0.07186 \*

\* Se 18 -0.00443 -0.03776 0.02282 \*

\* Se 19 -0.01100 -0.07779 0.01422 \*

\* Se 20 -0.03916 0.02868 -0.06685 \*

\* Nb 1 -0.05768 -0.07587 -0.01788 \*

\* Nb 2 0.06001 0.07311 0.02040 \*

\* Nb 3 -0.00468 0.00249 -0.00430 \*

\* Nb 4 -0.00112 0.00082 0.00844 \*

\* Nb 5 -0.00088 -0.03906 -0.00773 \*

\* Nb 6 -0.04276 0.09555 -0.06020 \*

\* Nb 7 -0.00023 -0.00896 -0.02479 \*

\* Nb 8 0.01952 -0.03182 0.00107 \*

\* Nb 9 0.05760 -0.13560 0.05714 \*

\* Nb 10 0.01027 0.07318 -0.02526 \*

\* Nb 11 0.00312 0.00622 -0.02386 \*

\* Nb 12 -0.15442 0.01802 -0.04744 \*

\* Nb 13 -0.00847 -0.06798 0.02292 \*

\* Nb 14 -0.06390 0.14577 -0.05865 \*

\* Nb 15 -0.00699 -0.00643 0.02028 \*

\* Nb 16 0.16312 -0.01336 0.04762 \*

\* Nb 17 0.04528 -0.09059 0.04874 \*

\* Nb 18 0.00145 0.04447 0.00605 \*

\* Nb 19 -0.00006 0.01071 0.01942 \*

\* Nb 20 -0.02392 0.03137 -0.00171 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.042790 0.019476 -0.082307 \*

\* y 0.019476 0.139521 -0.008202 \*

\* z -0.082307 -0.008202 0.082573 \*

\* \*

\* Pressure: -0.0598 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000092 | -36259.913828 | <-- min BFGS

| trial step | 1.000000 | 0.000062 | -36259.916018 | <-- min BFGS

| line step | 3.062003 | 8.597E-006 | -36259.918200 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 52 with enthalpy= -3.62599182E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.093245E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.039620E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 9.730908E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.395209E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 53 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000253 | -36259.918200 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 53 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8502804 -8.3042608 -0.0073574 0.4205356 -0.0045898 0.0001860

0.0369469 3.3851951 -0.0003077 1.0316208 1.8448185 0.0005948

-0.0061750 -0.0010389 13.9332118 0.0002448 0.0000383 0.4509504

Lattice parameters(A) Cell Angles

a = 17.014454 alpha = 90.009756

b = 3.385397 beta = 90.044854

c = 13.933213 gamma = 118.588552

Current cell volume = 704.712591 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067238 0.662638 0.122726 x

x Se 2 0.132264 0.341253 0.628063 x

x Se 3 0.131875 0.340198 0.870862 x

x Se 4 0.068097 0.665449 0.376839 x

x Se 5 0.266798 0.665606 0.123006 x

x Se 6 0.333128 0.342954 0.628288 x

x Se 7 0.333910 0.346966 0.872160 x

x Se 8 0.265230 0.662579 0.371694 x

x Se 9 0.466844 0.657464 0.128640 x

x Se 10 0.533418 0.341470 0.621604 x

x Se 11 0.533099 0.342253 0.871429 x

x Se 12 0.466675 0.658701 0.378619 x

x Se 13 0.666054 0.652980 0.127772 x

x Se 14 0.734797 0.337443 0.628433 x

x Se 15 0.733194 0.334560 0.876867 x

x Se 16 0.666887 0.657014 0.371763 x

x Se 17 0.868073 0.659761 0.129129 x

x Se 18 0.932063 0.335140 0.622907 x

x Se 19 0.932751 0.337344 0.877182 x

x Se 20 0.867729 0.658783 0.371985 x

x Nb 1 0.004991 0.012979 0.249792 x

x Nb 2 -0.005056 -0.012981 0.750052 x

x Nb 3 -0.000058 -0.000060 -0.000002 x

x Nb 4 0.000146 0.000747 0.499847 x

x Nb 5 0.195588 -0.007527 0.248256 x

x Nb 6 0.202552 0.010286 0.749905 x

x Nb 7 0.199585 0.003730 -0.002011 x

x Nb 8 0.203196 0.012889 0.500513 x

x Nb 9 0.399646 0.000199 0.251143 x

x Nb 10 0.402210 0.010941 0.749602 x

x Nb 11 0.402137 0.005854 -0.000726 x

x Nb 12 0.394717 -0.013926 0.501268 x

x Nb 13 0.597748 -0.011122 0.250422 x

x Nb 14 0.600347 -0.000594 0.748975 x

x Nb 15 0.597792 -0.006022 0.000827 x

x Nb 16 0.605311 0.013812 0.498824 x

x Nb 17 0.797427 -0.010322 0.250141 x

x Nb 18 0.804528 0.007913 0.751703 x

x Nb 19 0.800453 -0.003748 0.001997 x

x Nb 20 0.796617 -0.013603 0.499501 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597854E+004 37010.97 <-- SCF

1 -3.62600373E+004 6.29881161E-003 37035.34 <-- SCF

2 -3.62600552E+004 4.46641267E-004 37063.83 <-- SCF

3 -3.62599654E+004 -2.24398033E-003 37090.08 <-- SCF

4 -3.62599299E+004 -8.87857193E-004 37115.88 <-- SCF

5 -3.62599261E+004 -9.54852876E-005 37141.72 <-- SCF

6 -3.62599246E+004 -3.86752021E-005 37165.59 <-- SCF

7 -3.62599245E+004 -8.34338307E-007 37186.44 <-- SCF

8 -3.62599246E+004 1.16843264E-006 37204.81 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.92456928 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00084 0.07612 -0.02621 \*

\* Se 2 0.02830 -0.03483 0.06465 \*

\* Se 3 -0.01159 0.00289 -0.06074 \*

\* Se 4 0.00384 0.03361 -0.05738 \*

\* Se 5 0.00120 0.01797 0.07418 \*

\* Se 6 0.01184 0.02993 0.12902 \*

\* Se 7 -0.02801 -0.08542 0.01864 \*

\* Se 8 -0.06619 -0.02494 -0.10224 \*

\* Se 9 -0.00605 -0.01605 -0.00904 \*

\* Se 10 -0.17344 0.08050 0.01923 \*

\* Se 11 0.01252 0.01291 0.00707 \*

\* Se 12 0.18177 -0.11523 -0.02828 \*

\* Se 13 0.02913 0.08656 0.00855 \*

\* Se 14 0.06644 0.03273 0.07699 \*

\* Se 15 -0.00532 -0.02559 -0.05352 \*

\* Se 16 -0.02620 -0.02758 -0.14291 \*

\* Se 17 0.01108 -0.00433 0.06292 \*

\* Se 18 -0.00125 -0.04441 0.02812 \*

\* Se 19 -0.00072 -0.07513 0.02345 \*

\* Se 20 -0.02453 0.03552 -0.05882 \*

\* Nb 1 -0.05827 -0.07232 -0.01716 \*

\* Nb 2 0.05859 0.07202 0.02097 \*

\* Nb 3 -0.00426 0.00195 -0.00208 \*

\* Nb 4 -0.00089 -0.00061 0.00927 \*

\* Nb 5 0.00097 -0.05112 -0.00806 \*

\* Nb 6 -0.04081 0.10678 -0.04901 \*

\* Nb 7 -0.00063 -0.01010 -0.02232 \*

\* Nb 8 0.02136 -0.02922 0.00090 \*

\* Nb 9 0.07646 -0.13615 0.06514 \*

\* Nb 10 -0.00477 0.07977 0.00045 \*

\* Nb 11 0.00114 0.00940 -0.02745 \*

\* Nb 12 -0.16798 0.02286 -0.05977 \*

\* Nb 13 0.00934 -0.07307 0.00948 \*

\* Nb 14 -0.08103 0.14855 -0.06418 \*

\* Nb 15 -0.00457 -0.00882 0.02456 \*

\* Nb 16 0.17514 -0.01670 0.06780 \*

\* Nb 17 0.04106 -0.10127 0.04713 \*

\* Nb 18 -0.00039 0.05489 0.00976 \*

\* Nb 19 -0.00005 0.01504 0.01730 \*

\* Nb 20 -0.02237 0.03290 0.00362 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.043310 0.001313 -0.063429 \*

\* y 0.001313 0.153662 -0.012034 \*

\* z -0.063429 -0.012034 0.051361 \*

\* \*

\* Pressure: -0.0539 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000253 | -36259.918200 | <-- min BFGS

| trial step | 1.000000 | 0.000193 | -36259.924644 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 53 with line minimization (lambda= 4.226538)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8599875 -8.3061605 -0.0040942 0.4203011 -0.0045167 0.0001015

0.0363766 3.3850468 -0.0001557 1.0313266 1.8450762 0.0003230

-0.0033697 -0.0005547 13.9260732 0.0001351 0.0000193 0.4511814

Lattice parameters(A) Cell Angles

a = 17.023852 alpha = 90.005067

b = 3.385242 beta = 90.024767

c = 13.926074 gamma = 118.587816

Current cell volume = 704.713602 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067156 0.662274 0.122732 x

x Se 2 0.132495 0.341748 0.627964 x

x Se 3 0.132173 0.341964 0.870940 x

x Se 4 0.068022 0.664345 0.376732 x

x Se 5 0.267046 0.666031 0.123352 x

x Se 6 0.332643 0.342187 0.628684 x

x Se 7 0.333811 0.344645 0.872468 x

x Se 8 0.264995 0.661887 0.370412 x

x Se 9 0.466866 0.658498 0.128683 x

x Se 10 0.532543 0.339476 0.620657 x

x Se 11 0.533101 0.341180 0.871387 x

x Se 12 0.467508 0.660798 0.379632 x

x Se 13 0.666130 0.655202 0.127474 x

x Se 14 0.735071 0.338316 0.629728 x

x Se 15 0.732954 0.334064 0.876544 x

x Se 16 0.667402 0.658059 0.371716 x

x Se 17 0.867728 0.657784 0.129051 x

x Se 18 0.932130 0.336025 0.622960 x

x Se 19 0.932839 0.337800 0.877120 x

x Se 20 0.867502 0.658288 0.372108 x

x Nb 1 0.004393 0.010093 0.249574 x

x Nb 2 -0.004452 -0.010112 0.750236 x

x Nb 3 -0.000079 -0.000105 -0.000024 x

x Nb 4 0.000177 0.000902 0.499832 x

x Nb 5 0.195167 -0.007376 0.247812 x

x Nb 6 0.202158 0.008243 0.749791 x

x Nb 7 0.199596 0.003152 -0.001979 x

x Nb 8 0.203542 0.012095 0.500053 x

x Nb 9 0.400019 0.001706 0.251387 x

x Nb 10 0.402606 0.009529 0.749233 x

x Nb 11 0.402391 0.006215 -0.000887 x

x Nb 12 0.393657 -0.016411 0.501374 x

x Nb 13 0.597337 -0.009725 0.250714 x

x Nb 14 0.599969 -0.002139 0.748730 x

x Nb 15 0.597513 -0.006463 0.001001 x

x Nb 16 0.606423 0.016293 0.498682 x

x Nb 17 0.797859 -0.008194 0.250186 x

x Nb 18 0.804973 0.007986 0.752086 x

x Nb 19 0.800438 -0.003189 0.001904 x

x Nb 20 0.796199 -0.013070 0.499953 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62584744E+004 37308.23 <-- SCF

1 -3.62614914E+004 7.54239324E-002 37334.80 <-- SCF

2 -3.62616655E+004 4.35273126E-003 37364.33 <-- SCF

3 -3.62606831E+004 -2.45604295E-002 37391.38 <-- SCF

4 -3.62599638E+004 -1.79817194E-002 37417.67 <-- SCF

5 -3.62599662E+004 5.96406123E-005 37444.50 <-- SCF

6 -3.62599361E+004 -7.53318853E-004 37470.53 <-- SCF

7 -3.62599307E+004 -1.33933036E-004 37496.45 <-- SCF

8 -3.62599317E+004 2.46498826E-005 37520.48 <-- SCF

9 -3.62599315E+004 -4.86810847E-006 37541.56 <-- SCF

10 -3.62599316E+004 1.80634772E-006 37559.83 <-- SCF

11 -3.62599316E+004 1.86887833E-006 37577.91 <-- SCF

12 -3.62599317E+004 2.02462181E-006 37595.47 <-- SCF

13 -3.62599318E+004 1.69498052E-006 37612.53 <-- SCF

14 -3.62599318E+004 1.30926878E-006 37628.89 <-- SCF

15 -3.62599319E+004 9.78970734E-007 37645.59 <-- SCF

16 -3.62599319E+004 7.90692586E-007 37661.94 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.93191741 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.03289 0.06060 -0.04787 \*

\* Se 2 -0.01453 -0.05882 0.02170 \*

\* Se 3 -0.07515 -0.11475 -0.01985 \*

\* Se 4 0.00321 0.05501 -0.06124 \*

\* Se 5 -0.01699 0.05220 0.02159 \*

\* Se 6 0.07588 -0.08715 -0.01136 \*

\* Se 7 0.07454 0.03101 -0.14673 \*

\* Se 8 -0.13072 -0.03074 0.04858 \*

\* Se 9 -0.00922 -0.05096 -0.00935 \*

\* Se 10 -0.08152 0.09120 0.00441 \*

\* Se 11 0.00888 0.04844 0.01214 \*

\* Se 12 0.10857 -0.08883 -0.04061 \*

\* Se 13 -0.07130 -0.02645 0.16866 \*

\* Se 14 0.12072 0.03470 -0.05208 \*

\* Se 15 0.01464 -0.05337 0.01438 \*

\* Se 16 -0.08851 0.06304 -0.11104 \*

\* Se 17 0.07553 0.11786 0.01861 \*

\* Se 18 0.01151 -0.05946 0.02434 \*

\* Se 19 0.02499 -0.06625 0.04707 \*

\* Se 20 0.02010 0.05745 -0.02387 \*

\* Nb 1 -0.05145 -0.05671 -0.00575 \*

\* Nb 2 0.04835 0.05636 0.01009 \*

\* Nb 3 -0.00554 0.00040 0.00125 \*

\* Nb 4 -0.00095 -0.00668 0.01049 \*

\* Nb 5 0.03820 -0.10738 0.00039 \*

\* Nb 6 -0.03697 0.15473 -0.02175 \*

\* Nb 7 -0.00088 0.00027 -0.00467 \*

\* Nb 8 0.03732 -0.01049 0.00888 \*

\* Nb 9 0.12753 -0.14921 0.08206 \*

\* Nb 10 -0.05868 0.13127 0.10318 \*

\* Nb 11 -0.00447 0.01367 -0.02196 \*

\* Nb 12 -0.23055 0.03281 -0.10997 \*

\* Nb 13 0.06779 -0.12315 -0.05737 \*

\* Nb 14 -0.12630 0.16150 -0.07704 \*

\* Nb 15 0.00213 -0.01548 0.01773 \*

\* Nb 16 0.22462 -0.02361 0.13667 \*

\* Nb 17 0.02218 -0.15192 0.04531 \*

\* Nb 18 -0.03954 0.10053 0.01237 \*

\* Nb 19 -0.00190 0.00268 0.00890 \*

\* Nb 20 -0.02864 0.01567 0.00370 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.075493 -0.054742 -0.031360 \*

\* y -0.054742 0.202944 -0.015932 \*

\* z -0.031360 -0.015932 -0.057464 \*

\* \*

\* Pressure: -0.0233 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000253 | -36259.918200 | <-- min BFGS

| trial step | 1.000000 | 0.000193 | -36259.924644 | <-- min BFGS

| line step | 4.226538 | 5.498E-007 | -36259.932022 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 53 with enthalpy= -3.62599320E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 3.455252E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.639873E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.464014E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.029438E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 54 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000263 | -36259.932022 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 54 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8627516 -8.2901682 -0.0015412 0.4201138 -0.0047210 0.0000284

0.0379988 3.3814657 0.0000925 1.0299718 1.8465506 0.0000317

-0.0009398 0.0002854 13.9319263 0.0000396 -0.0000128 0.4509919

Lattice parameters(A) Cell Angles

a = 17.018469 alpha = 89.997302

b = 3.381679 beta = 90.009136

c = 13.931926 gamma = 118.508143

Current cell volume = 704.577933 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067236 0.663270 0.122619 x

x Se 2 0.132463 0.342104 0.628172 x

x Se 3 0.132146 0.342348 0.870798 x

x Se 4 0.068100 0.665088 0.376886 x

x Se 5 0.267083 0.665848 0.123249 x

x Se 6 0.332668 0.343050 0.628879 x

x Se 7 0.333745 0.344398 0.872548 x

x Se 8 0.264944 0.661552 0.370467 x

x Se 9 0.466882 0.658039 0.128658 x

x Se 10 0.532440 0.339690 0.620694 x

x Se 11 0.533098 0.341655 0.871404 x

x Se 12 0.467587 0.660617 0.379604 x

x Se 13 0.666189 0.655408 0.127412 x

x Se 14 0.735137 0.338681 0.629673 x

x Se 15 0.732923 0.334187 0.876677 x

x Se 16 0.667376 0.657238 0.371582 x

x Se 17 0.867748 0.657359 0.129187 x

x Se 18 0.932040 0.335223 0.622795 x

x Se 19 0.932762 0.336836 0.877228 x

x Se 20 0.867535 0.657929 0.371905 x

x Nb 1 0.004559 0.010150 0.249525 x

x Nb 2 -0.004615 -0.010193 0.750286 x

x Nb 3 -0.000083 -0.000127 -0.000035 x

x Nb 4 0.000170 0.000865 0.499844 x

x Nb 5 0.195099 -0.007781 0.247755 x

x Nb 6 0.202262 0.009740 0.749710 x

x Nb 7 0.199564 0.003339 -0.002087 x

x Nb 8 0.203542 0.012299 0.500162 x

x Nb 9 0.399989 -0.000070 0.251456 x

x Nb 10 0.402635 0.010813 0.749222 x

x Nb 11 0.402390 0.006540 -0.000957 x

x Nb 12 0.393534 -0.016651 0.501329 x

x Nb 13 0.597310 -0.010971 0.250712 x

x Nb 14 0.599993 -0.000343 0.748649 x

x Nb 15 0.597513 -0.006803 0.001058 x

x Nb 16 0.606556 0.016564 0.498718 x

x Nb 17 0.797761 -0.009685 0.250247 x

x Nb 18 0.805044 0.008401 0.752133 x

x Nb 19 0.800474 -0.003348 0.002002 x

x Nb 20 0.796201 -0.013260 0.499835 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597591E+004 37765.12 <-- SCF

1 -3.62600662E+004 7.67680562E-003 37790.66 <-- SCF

2 -3.62600887E+004 5.63898505E-004 37820.06 <-- SCF

3 -3.62599989E+004 -2.24558303E-003 37846.81 <-- SCF

4 -3.62599412E+004 -1.44406284E-003 37872.91 <-- SCF

5 -3.62599389E+004 -5.58124994E-005 37899.14 <-- SCF

6 -3.62599371E+004 -4.45150163E-005 37923.12 <-- SCF

7 -3.62599369E+004 -5.65444205E-006 37944.73 <-- SCF

8 -3.62599370E+004 1.61330500E-006 37963.31 <-- SCF

9 -3.62599370E+004 -5.29496523E-008 37980.50 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.93698206 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.04862 0.00854 -0.02250 \*

\* Se 2 -0.02150 -0.05789 -0.01288 \*

\* Se 3 -0.09048 -0.12655 0.00559 \*

\* Se 4 -0.00650 0.01891 -0.06232 \*

\* Se 5 -0.02549 0.05716 0.05215 \*

\* Se 6 0.06993 -0.08999 -0.06677 \*

\* Se 7 0.09227 0.06609 -0.18222 \*

\* Se 8 -0.11225 -0.02546 0.03853 \*

\* Se 9 -0.01306 -0.06271 0.01535 \*

\* Se 10 -0.05674 0.09198 -0.02490 \*

\* Se 11 0.00739 0.06247 -0.01022 \*

\* Se 12 0.09021 -0.09798 -0.02382 \*

\* Se 13 -0.08683 -0.06024 0.19718 \*

\* Se 14 0.09751 0.02785 -0.04055 \*

\* Se 15 0.02247 -0.05429 -0.02662 \*

\* Se 16 -0.09326 0.08723 -0.06712 \*

\* Se 17 0.09475 0.12941 -0.00486 \*

\* Se 18 0.02525 -0.02061 0.03057 \*

\* Se 19 0.04206 -0.02433 0.02577 \*

\* Se 20 0.02601 0.05434 0.01039 \*

\* Nb 1 -0.06185 -0.02016 0.00011 \*

\* Nb 2 0.05827 0.02030 0.00396 \*

\* Nb 3 -0.00431 0.00064 0.00313 \*

\* Nb 4 0.00108 -0.00697 0.00851 \*

\* Nb 5 0.04675 -0.09752 -0.00033 \*

\* Nb 6 -0.04584 0.11400 -0.00140 \*

\* Nb 7 -0.00245 -0.00340 0.00147 \*

\* Nb 8 0.04143 -0.00984 0.01232 \*

\* Nb 9 0.12186 -0.09578 0.07156 \*

\* Nb 10 -0.05489 0.09197 0.12567 \*

\* Nb 11 -0.00279 0.00668 -0.01640 \*

\* Nb 12 -0.22722 0.03728 -0.10640 \*

\* Nb 13 0.06517 -0.08584 -0.07285 \*

\* Nb 14 -0.11655 0.10649 -0.06451 \*

\* Nb 15 0.00217 -0.00927 0.01352 \*

\* Nb 16 0.21897 -0.02814 0.13762 \*

\* Nb 17 0.02759 -0.11186 0.03126 \*

\* Nb 18 -0.04868 0.08865 0.01598 \*

\* Nb 19 -0.00046 0.00460 0.00474 \*

\* Nb 20 -0.03137 0.01428 0.00131 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.010274 0.055465 0.008226 \*

\* y 0.055465 0.057456 -0.002015 \*

\* z 0.008226 -0.002015 -0.033122 \*

\* \*

\* Pressure: -0.0047 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000263 | -36259.932022 | <-- min BFGS

| trial step | 1.000000 | 0.000098 | -36259.937128 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 54 with line minimization (lambda= 1.595000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8643963 -8.2806528 -0.0000222 0.4200026 -0.0048427 -0.0000150

0.0389641 3.3793349 0.0002403 1.0291657 1.8474300 -0.0001415

0.0005059 0.0007852 13.9354090 -0.0000171 -0.0000319 0.4508791

Lattice parameters(A) Cell Angles

a = 17.015272 alpha = 89.992675

b = 3.379560 beta = 89.999829

c = 13.935409 gamma = 118.460693

Current cell volume = 704.496536 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067283 0.663863 0.122551 x

x Se 2 0.132444 0.342316 0.628296 x

x Se 3 0.132130 0.342577 0.870713 x

x Se 4 0.068146 0.665530 0.376977 x

x Se 5 0.267106 0.665739 0.123188 x

x Se 6 0.332682 0.343563 0.628994 x

x Se 7 0.333706 0.344251 0.872595 x

x Se 8 0.264914 0.661353 0.370500 x

x Se 9 0.466891 0.657766 0.128644 x

x Se 10 0.532379 0.339817 0.620716 x

x Se 11 0.533096 0.341937 0.871413 x

x Se 12 0.467634 0.660509 0.379588 x

x Se 13 0.666224 0.655531 0.127375 x

x Se 14 0.735176 0.338899 0.629640 x

x Se 15 0.732905 0.334260 0.876756 x

x Se 16 0.667361 0.656749 0.371503 x

x Se 17 0.867760 0.657105 0.129267 x

x Se 18 0.931986 0.334745 0.622697 x

x Se 19 0.932716 0.336262 0.877293 x

x Se 20 0.867554 0.657716 0.371785 x

x Nb 1 0.004658 0.010183 0.249496 x

x Nb 2 -0.004712 -0.010241 0.750316 x

x Nb 3 -0.000085 -0.000140 -0.000042 x

x Nb 4 0.000166 0.000843 0.499851 x

x Nb 5 0.195058 -0.008022 0.247721 x

x Nb 6 0.202323 0.010632 0.749661 x

x Nb 7 0.199545 0.003451 -0.002151 x

x Nb 8 0.203542 0.012420 0.500226 x

x Nb 9 0.399972 -0.001126 0.251496 x

x Nb 10 0.402653 0.011577 0.749215 x

x Nb 11 0.402389 0.006733 -0.000998 x

x Nb 12 0.393461 -0.016793 0.501302 x

x Nb 13 0.597294 -0.011713 0.250711 x

x Nb 14 0.600007 0.000726 0.748602 x

x Nb 15 0.597512 -0.007005 0.001092 x

x Nb 16 0.606636 0.016725 0.498740 x

x Nb 17 0.797704 -0.010571 0.250283 x

x Nb 18 0.805086 0.008648 0.752161 x

x Nb 19 0.800496 -0.003442 0.002060 x

x Nb 20 0.796203 -0.013373 0.499764 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598736E+004 38083.91 <-- SCF

1 -3.62600258E+004 3.80508369E-003 38110.91 <-- SCF

2 -3.62600333E+004 1.86988566E-004 38138.72 <-- SCF

3 -3.62600054E+004 -6.97914184E-004 38165.69 <-- SCF

4 -3.62599367E+004 -1.71529763E-003 38191.88 <-- SCF

5 -3.62599403E+004 8.76719848E-005 38218.56 <-- SCF

6 -3.62599386E+004 -4.22032772E-005 38242.80 <-- SCF

7 -3.62599380E+004 -1.35303469E-005 38263.08 <-- SCF

8 -3.62599379E+004 -1.92542149E-006 38282.81 <-- SCF

9 -3.62599380E+004 9.32251700E-007 38300.47 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.93798226 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.05802 -0.02888 -0.00722 \*

\* Se 2 -0.03311 -0.05795 -0.02897 \*

\* Se 3 -0.10147 -0.13226 0.02136 \*

\* Se 4 -0.01556 -0.00371 -0.06506 \*

\* Se 5 -0.03104 0.05843 0.06538 \*

\* Se 6 0.06190 -0.08181 -0.09309 \*

\* Se 7 0.09791 0.08584 -0.19757 \*

\* Se 8 -0.10285 -0.02308 0.03261 \*

\* Se 9 -0.01499 -0.07068 0.02680 \*

\* Se 10 -0.04355 0.09250 -0.04223 \*

\* Se 11 0.00664 0.07125 -0.02026 \*

\* Se 12 0.08106 -0.10378 -0.01396 \*

\* Se 13 -0.09168 -0.07983 0.20952 \*

\* Se 14 0.08618 0.02446 -0.03337 \*

\* Se 15 0.02911 -0.05376 -0.04667 \*

\* Se 16 -0.09372 0.08935 -0.04873 \*

\* Se 17 0.10837 0.13497 -0.01894 \*

\* Se 18 0.03398 0.00719 0.03758 \*

\* Se 19 0.05271 0.00783 0.01136 \*

\* Se 20 0.03705 0.05322 0.02545 \*

\* Nb 1 -0.06637 0.00364 0.00143 \*

\* Nb 2 0.06341 -0.00327 0.00231 \*

\* Nb 3 -0.00365 0.00056 0.00395 \*

\* Nb 4 0.00208 -0.00714 0.00779 \*

\* Nb 5 0.04757 -0.09057 -0.00368 \*

\* Nb 6 -0.04804 0.09135 0.01117 \*

\* Nb 7 -0.00328 -0.00440 0.00437 \*

\* Nb 8 0.04344 -0.00916 0.01507 \*

\* Nb 9 0.11658 -0.06515 0.06510 \*

\* Nb 10 -0.05251 0.06957 0.13998 \*

\* Nb 11 -0.00218 0.00188 -0.01391 \*

\* Nb 12 -0.23074 0.03886 -0.10546 \*

\* Nb 13 0.06371 -0.06454 -0.08271 \*

\* Nb 14 -0.10927 0.07509 -0.05707 \*

\* Nb 15 0.00253 -0.00496 0.01194 \*

\* Nb 16 0.22152 -0.02930 0.13897 \*

\* Nb 17 0.02835 -0.08956 0.02252 \*

\* Nb 18 -0.04970 0.08064 0.02098 \*

\* Nb 19 0.00088 0.00436 0.00356 \*

\* Nb 20 -0.03321 0.01278 -0.00034 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.025970 0.122479 0.034236 \*

\* y 0.122479 -0.030623 0.007366 \*

\* z 0.034236 0.007366 -0.025500 \*

\* \*

\* Pressure: 0.0101 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000263 | -36259.932022 | <-- min BFGS

| trial step | 1.000000 | 0.000098 | -36259.937128 | <-- min BFGS

| line step | 1.595000 | 7.256E-006 | -36259.938127 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 54 with enthalpy= -3.62599381E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.526431E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.631407E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 9.562801E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.224792E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 55 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000089 | -36259.938127 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 55 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8680544 -8.2844636 -0.0017298 0.4199916 -0.0046746 0.0000260

0.0376045 3.3785706 0.0002068 1.0298454 1.8482546 -0.0000249

-0.0008556 0.0006649 13.9392775 0.0000368 -0.0000280 0.4507540

Lattice parameters(A) Cell Angles

a = 17.020323 alpha = 89.993800

b = 3.378780 beta = 90.010226

c = 13.939278 gamma = 118.488812

Current cell volume = 704.551083 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067288 0.663801 0.122484 x

x Se 2 0.132437 0.342550 0.628410 x

x Se 3 0.132119 0.342476 0.870587 x

x Se 4 0.068189 0.665659 0.377045 x

x Se 5 0.267088 0.665531 0.123191 x

x Se 6 0.332747 0.344240 0.629103 x

x Se 7 0.333744 0.344483 0.872506 x

x Se 8 0.264843 0.661066 0.370351 x

x Se 9 0.466940 0.657981 0.128750 x

x Se 10 0.532299 0.339632 0.620575 x

x Se 11 0.533048 0.341707 0.871314 x

x Se 12 0.467710 0.660752 0.379736 x

x Se 13 0.666178 0.655261 0.127461 x

x Se 14 0.735251 0.339184 0.629795 x

x Se 15 0.732926 0.334472 0.876749 x

x Se 16 0.667292 0.656049 0.371374 x

x Se 17 0.867770 0.657223 0.129385 x

x Se 18 0.931947 0.334624 0.622620 x

x Se 19 0.932709 0.336322 0.877358 x

x Se 20 0.867562 0.657503 0.371680 x

x Nb 1 0.004777 0.010279 0.249455 x

x Nb 2 -0.004829 -0.010360 0.750353 x

x Nb 3 -0.000089 -0.000145 -0.000046 x

x Nb 4 0.000171 0.000868 0.499851 x

x Nb 5 0.194991 -0.008044 0.247609 x

x Nb 6 0.202389 0.010932 0.749680 x

x Nb 7 0.199545 0.003659 -0.002254 x

x Nb 8 0.203660 0.012814 0.500259 x

x Nb 9 0.399966 -0.001373 0.251541 x

x Nb 10 0.402772 0.012216 0.749245 x

x Nb 11 0.402485 0.006935 -0.000990 x

x Nb 12 0.393245 -0.017522 0.501279 x

x Nb 13 0.597180 -0.012322 0.250691 x

x Nb 14 0.600011 0.000946 0.748560 x

x Nb 15 0.597415 -0.007211 0.001086 x

x Nb 16 0.606855 0.017449 0.498770 x

x Nb 17 0.797636 -0.010881 0.250271 x

x Nb 18 0.805157 0.008699 0.752271 x

x Nb 19 0.800497 -0.003659 0.002165 x

x Nb 20 0.796079 -0.013797 0.499730 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598749E+004 38404.41 <-- SCF

1 -3.62600235E+004 3.71545844E-003 38430.55 <-- SCF

2 -3.62600317E+004 2.05427841E-004 38458.88 <-- SCF

3 -3.62599890E+004 -1.06697273E-003 38485.59 <-- SCF

4 -3.62599418E+004 -1.18015761E-003 38511.03 <-- SCF

5 -3.62599419E+004 1.01212552E-006 38537.22 <-- SCF

6 -3.62599402E+004 -4.08115411E-005 38560.80 <-- SCF

7 -3.62599400E+004 -4.68346821E-006 38580.84 <-- SCF

8 -3.62599401E+004 5.11319288E-007 38599.98 <-- SCF

9 -3.62599401E+004 -1.50544251E-008 38617.02 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.94005512 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.05851 -0.02737 -0.01443 \*

\* Se 2 -0.03402 -0.07766 -0.04609 \*

\* Se 3 -0.10700 -0.12801 0.04950 \*

\* Se 4 -0.01137 -0.00512 -0.06641 \*

\* Se 5 -0.01873 0.07675 0.05756 \*

\* Se 6 0.05563 -0.09666 -0.11749 \*

\* Se 7 0.09548 0.07632 -0.16410 \*

\* Se 8 -0.09400 -0.00489 0.04677 \*

\* Se 9 -0.03668 -0.08060 0.00184 \*

\* Se 10 -0.03654 0.08324 -0.02888 \*

\* Se 11 0.02922 0.08136 0.00308 \*

\* Se 12 0.06676 -0.09452 -0.03241 \*

\* Se 13 -0.08399 -0.06865 0.17893 \*

\* Se 14 0.06665 0.00576 -0.06116 \*

\* Se 15 0.01770 -0.07247 -0.03599 \*

\* Se 16 -0.09888 0.10915 -0.02204 \*

\* Se 17 0.11597 0.12821 -0.04172 \*

\* Se 18 0.03166 0.00918 0.03943 \*

\* Se 19 0.05575 0.00584 0.01953 \*

\* Se 20 0.03911 0.06996 0.04177 \*

\* Nb 1 -0.07101 -0.00063 0.00643 \*

\* Nb 2 0.06870 0.00163 -0.00119 \*

\* Nb 3 -0.00249 0.00019 0.00442 \*

\* Nb 4 0.00312 -0.00725 0.00791 \*

\* Nb 5 0.04625 -0.10446 0.00374 \*

\* Nb 6 -0.04744 0.09752 0.00424 \*

\* Nb 7 -0.00029 -0.00703 0.00567 \*

\* Nb 8 0.04533 -0.01098 0.01257 \*

\* Nb 9 0.11958 -0.06396 0.06979 \*

\* Nb 10 -0.06561 0.07407 0.13148 \*

\* Nb 11 -0.00757 0.00198 -0.01418 \*

\* Nb 12 -0.23874 0.04886 -0.10787 \*

\* Nb 13 0.07692 -0.07036 -0.07531 \*

\* Nb 14 -0.11101 0.07480 -0.05984 \*

\* Nb 15 0.01007 -0.00595 0.01392 \*

\* Nb 16 0.23106 -0.03936 0.14120 \*

\* Nb 17 0.03041 -0.09478 0.02814 \*

\* Nb 18 -0.04629 0.09337 0.01527 \*

\* Nb 19 -0.00143 0.00772 0.00244 \*

\* Nb 20 -0.03380 0.01481 0.00347 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.015863 0.067166 0.006930 \*

\* y 0.067166 -0.030921 0.003419 \*

\* z 0.006930 0.003419 0.005020 \*

\* \*

\* Pressure: 0.0033 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000089 | -36259.938127 | <-- min BFGS

| trial step | 1.000000 | 0.000049 | -36259.940173 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 55 with line minimization (lambda= 2.256503)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8726509 -8.2892520 -0.0038754 0.4199781 -0.0044634 0.0000775

0.0358961 3.3776103 0.0001648 1.0307004 1.8492919 0.0001216

-0.0025664 0.0005137 13.9441383 0.0001045 -0.0000231 0.4505969

Lattice parameters(A) Cell Angles

a = 17.026669 alpha = 89.995206

b = 3.377801 beta = 90.023280

c = 13.944139 gamma = 118.524153

Current cell volume = 704.619172 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067293 0.663723 0.122401 x

x Se 2 0.132429 0.342845 0.628552 x

x Se 3 0.132105 0.342350 0.870429 x

x Se 4 0.068241 0.665822 0.377130 x

x Se 5 0.267066 0.665270 0.123194 x

x Se 6 0.332829 0.345090 0.629239 x

x Se 7 0.333792 0.344775 0.872394 x

x Se 8 0.264754 0.660706 0.370164 x

x Se 9 0.467001 0.658251 0.128883 x

x Se 10 0.532199 0.339400 0.620398 x

x Se 11 0.532988 0.341418 0.871190 x

x Se 12 0.467807 0.661057 0.379922 x

x Se 13 0.666121 0.654921 0.127569 x

x Se 14 0.735346 0.339542 0.629991 x

x Se 15 0.732953 0.334737 0.876739 x

x Se 16 0.667206 0.655170 0.371211 x

x Se 17 0.867782 0.657372 0.129534 x

x Se 18 0.931898 0.334472 0.622523 x

x Se 19 0.932701 0.336397 0.877439 x

x Se 20 0.867571 0.657235 0.371549 x

x Nb 1 0.004928 0.010399 0.249403 x

x Nb 2 -0.004977 -0.010509 0.750399 x

x Nb 3 -0.000093 -0.000151 -0.000051 x

x Nb 4 0.000178 0.000900 0.499853 x

x Nb 5 0.194907 -0.008072 0.247467 x

x Nb 6 0.202471 0.011310 0.749704 x

x Nb 7 0.199544 0.003920 -0.002383 x

x Nb 8 0.203809 0.013308 0.500301 x

x Nb 9 0.399960 -0.001682 0.251597 x

x Nb 10 0.402921 0.013019 0.749282 x

x Nb 11 0.402605 0.007189 -0.000980 x

x Nb 12 0.392974 -0.018438 0.501250 x

x Nb 13 0.597036 -0.013088 0.250666 x

x Nb 14 0.600017 0.001222 0.748507 x

x Nb 15 0.597292 -0.007469 0.001077 x

x Nb 16 0.607131 0.018358 0.498808 x

x Nb 17 0.797551 -0.011269 0.250256 x

x Nb 18 0.805245 0.008762 0.752408 x

x Nb 19 0.800500 -0.003931 0.002298 x

x Nb 20 0.795925 -0.014330 0.499687 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598368E+004 38720.42 <-- SCF

1 -3.62601116E+004 6.87015237E-003 38747.38 <-- SCF

2 -3.62601270E+004 3.84256499E-004 38775.55 <-- SCF

3 -3.62600676E+004 -1.48609507E-003 38802.47 <-- SCF

4 -3.62599408E+004 -3.16914721E-003 38828.30 <-- SCF

5 -3.62599461E+004 1.33440417E-004 38854.97 <-- SCF

6 -3.62599418E+004 -1.07304105E-004 38881.08 <-- SCF

7 -3.62599409E+004 -2.34367672E-005 38903.47 <-- SCF

8 -3.62599409E+004 5.58033218E-008 38923.67 <-- SCF

9 -3.62599409E+004 4.97035008E-007 38941.45 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.94091491 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.05975 -0.02601 -0.02927 \*

\* Se 2 -0.03642 -0.10379 -0.06836 \*

\* Se 3 -0.11019 -0.12440 0.08679 \*

\* Se 4 -0.00984 -0.00659 -0.06543 \*

\* Se 5 -0.00363 0.09942 0.04224 \*

\* Se 6 0.03633 -0.12143 -0.14952 \*

\* Se 7 0.08560 0.06062 -0.11305 \*

\* Se 8 -0.07093 0.02072 0.08189 \*

\* Se 9 -0.06131 -0.08934 -0.03356 \*

\* Se 10 -0.01750 0.06877 -0.00671 \*

\* Se 11 0.05488 0.09085 0.03630 \*

\* Se 12 0.04022 -0.08068 -0.05919 \*

\* Se 13 -0.06832 -0.05052 0.12990 \*

\* Se 14 0.03409 -0.02044 -0.10918 \*

\* Se 15 0.00325 -0.09504 -0.01837 \*

\* Se 16 -0.09042 0.13396 0.01195 \*

\* Se 17 0.12184 0.12213 -0.07315 \*

\* Se 18 0.03166 0.01143 0.04161 \*

\* Se 19 0.05954 0.00432 0.03466 \*

\* Se 20 0.04219 0.09279 0.06239 \*

\* Nb 1 -0.08099 -0.00473 0.01332 \*

\* Nb 2 0.07989 0.00672 -0.00724 \*

\* Nb 3 -0.00142 0.00035 0.00524 \*

\* Nb 4 0.00441 -0.00713 0.00801 \*

\* Nb 5 0.04353 -0.12348 0.01151 \*

\* Nb 6 -0.05201 0.10254 -0.00040 \*

\* Nb 7 0.00087 -0.01219 0.00997 \*

\* Nb 8 0.04345 -0.01260 0.01012 \*

\* Nb 9 0.12468 -0.05904 0.07120 \*

\* Nb 10 -0.08161 0.08120 0.12436 \*

\* Nb 11 -0.01349 0.00004 -0.01345 \*

\* Nb 12 -0.24815 0.05919 -0.10969 \*

\* Nb 13 0.09249 -0.07897 -0.06929 \*

\* Nb 14 -0.11494 0.07139 -0.05939 \*

\* Nb 15 0.01755 -0.00455 0.01460 \*

\* Nb 16 0.24221 -0.04832 0.14303 \*

\* Nb 17 0.03745 -0.09846 0.03128 \*

\* Nb 18 -0.04226 0.11155 0.00947 \*

\* Nb 19 -0.00159 0.01340 -0.00124 \*

\* Nb 20 -0.03136 0.01632 0.00666 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.000062 0.004160 -0.026777 \*

\* y 0.004160 -0.037256 0.001209 \*

\* z -0.026777 0.001209 0.042614 \*

\* \*

\* Pressure: -0.0018 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000089 | -36259.938127 | <-- min BFGS

| trial step | 1.000000 | 0.000049 | -36259.940173 | <-- min BFGS

| line step | 2.256503 | -8.773E-006 | -36259.941041 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 55 with enthalpy= -3.62599410E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.284176E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.854114E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.611882E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.261448E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 56 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000060 | -36259.941041 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 56 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8757141 -8.2920811 -0.0027560 0.4199287 -0.0043953 0.0000518

0.0353547 3.3778229 0.0001644 1.0308660 1.8493389 0.0000577

-0.0017158 0.0005213 13.9420458 0.0000709 -0.0000227 0.4506645

Lattice parameters(A) Cell Angles

a = 17.030722 alpha = 89.995143

b = 3.378008 beta = 90.016474

c = 13.942046 gamma = 118.536671

Current cell volume = 704.640623 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067305 0.663814 0.122411 x

x Se 2 0.132353 0.342669 0.628569 x

x Se 3 0.132034 0.342048 0.870440 x

x Se 4 0.068257 0.666043 0.377135 x

x Se 5 0.267049 0.665148 0.123128 x

x Se 6 0.332855 0.345104 0.629194 x

x Se 7 0.333764 0.344987 0.872343 x

x Se 8 0.264796 0.660681 0.370373 x

x Se 9 0.467016 0.658015 0.128859 x

x Se 10 0.532262 0.339660 0.620526 x

x Se 11 0.532970 0.341663 0.871214 x

x Se 12 0.467749 0.660802 0.379777 x

x Se 13 0.666151 0.654721 0.127624 x

x Se 14 0.735298 0.339541 0.629776 x

x Se 15 0.732970 0.334864 0.876806 x

x Se 16 0.667173 0.655123 0.371198 x

x Se 17 0.867858 0.657694 0.129523 x

x Se 18 0.931883 0.334272 0.622524 x

x Se 19 0.932688 0.336289 0.877436 x

x Se 20 0.867646 0.657403 0.371531 x

x Nb 1 0.004934 0.010530 0.249419 x

x Nb 2 -0.004983 -0.010634 0.750389 x

x Nb 3 -0.000092 -0.000154 -0.000048 x

x Nb 4 0.000173 0.000867 0.499856 x

x Nb 5 0.194937 -0.008125 0.247523 x

x Nb 6 0.202504 0.011715 0.749707 x

x Nb 7 0.199537 0.003958 -0.002353 x

x Nb 8 0.203744 0.013284 0.500331 x

x Nb 9 0.399937 -0.002079 0.251591 x

x Nb 10 0.402850 0.013136 0.749329 x

x Nb 11 0.402550 0.007163 -0.000983 x

x Nb 12 0.393073 -0.018117 0.501221 x

x Nb 13 0.597110 -0.013194 0.250635 x

x Nb 14 0.600042 0.001641 0.748513 x

x Nb 15 0.597349 -0.007439 0.001079 x

x Nb 16 0.607027 0.018038 0.498844 x

x Nb 17 0.797513 -0.011693 0.250264 x

x Nb 18 0.805212 0.008781 0.752361 x

x Nb 19 0.800507 -0.003957 0.002273 x

x Nb 20 0.796000 -0.014261 0.499662 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599181E+004 39044.56 <-- SCF

1 -3.62599627E+004 1.11565272E-003 39069.69 <-- SCF

2 -3.62599658E+004 7.70304430E-005 39097.84 <-- SCF

3 -3.62599513E+004 -3.61398064E-004 39124.50 <-- SCF

4 -3.62599427E+004 -2.15510492E-004 39150.38 <-- SCF

5 -3.62599425E+004 -6.38459675E-006 39175.73 <-- SCF

6 -3.62599422E+004 -7.58667868E-006 39195.02 <-- SCF

7 -3.62599421E+004 -6.78589114E-007 39213.45 <-- SCF

8 -3.62599422E+004 3.52528954E-007 39230.39 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.94215582 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.05984 -0.02536 -0.02464 \*

\* Se 2 -0.03033 -0.10063 -0.06694 \*

\* Se 3 -0.09280 -0.11111 0.07948 \*

\* Se 4 -0.01829 -0.01350 -0.06099 \*

\* Se 5 -0.00617 0.10405 0.05466 \*

\* Se 6 0.03730 -0.11756 -0.14410 \*

\* Se 7 0.07545 0.04329 -0.09290 \*

\* Se 8 -0.08559 0.03777 0.03752 \*

\* Se 9 -0.06859 -0.07581 -0.02660 \*

\* Se 10 -0.03147 0.07277 -0.03405 \*

\* Se 11 0.06274 0.07686 0.02870 \*

\* Se 12 0.05802 -0.08817 -0.02745 \*

\* Se 13 -0.05995 -0.03391 0.10883 \*

\* Se 14 0.05892 -0.03578 -0.05396 \*

\* Se 15 0.00384 -0.10035 -0.03356 \*

\* Se 16 -0.08617 0.12943 0.02231 \*

\* Se 17 0.10407 0.10852 -0.06508 \*

\* Se 18 0.03655 0.01853 0.03726 \*

\* Se 19 0.05861 0.00535 0.02889 \*

\* Se 20 0.03423 0.09032 0.05988 \*

\* Nb 1 -0.07103 -0.00403 0.01336 \*

\* Nb 2 0.06907 0.00604 -0.00814 \*

\* Nb 3 -0.00196 -0.00005 0.00487 \*

\* Nb 4 0.00407 -0.00710 0.00702 \*

\* Nb 5 0.04201 -0.12299 0.01120 \*

\* Nb 6 -0.05874 0.09540 -0.00354 \*

\* Nb 7 -0.00127 -0.01609 0.00336 \*

\* Nb 8 0.04611 -0.01526 0.01658 \*

\* Nb 9 0.11751 -0.05678 0.06457 \*

\* Nb 10 -0.07475 0.07797 0.11782 \*

\* Nb 11 -0.00824 -0.00001 -0.01429 \*

\* Nb 12 -0.24733 0.05795 -0.10210 \*

\* Nb 13 0.08311 -0.07566 -0.06977 \*

\* Nb 14 -0.10986 0.06915 -0.05374 \*

\* Nb 15 0.01220 -0.00440 0.01565 \*

\* Nb 16 0.24153 -0.04726 0.13065 \*

\* Nb 17 0.04575 -0.09105 0.02963 \*

\* Nb 18 -0.04143 0.11195 0.00772 \*

\* Nb 19 -0.00012 0.01792 0.00471 \*

\* Nb 20 -0.03715 0.01961 -0.00279 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.015509 -0.012954 -0.012401 \*

\* y -0.012954 -0.024352 0.000663 \*

\* z -0.012401 0.000663 0.019636 \*

\* \*

\* Pressure: -0.0036 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000060 | -36259.941041 | <-- min BFGS

| trial step | 1.000000 | 0.000031 | -36259.942300 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 56 with line minimization (lambda= 2.025195)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8788544 -8.2949814 -0.0016084 0.4198781 -0.0043255 0.0000256

0.0347997 3.3780409 0.0001641 1.0310359 1.8493872 -0.0000078

-0.0008438 0.0005291 13.9399005 0.0000363 -0.0000223 0.4507339

Lattice parameters(A) Cell Angles

a = 17.034877 alpha = 89.995078

b = 3.378220 beta = 90.009498

c = 13.939901 gamma = 118.549501

Current cell volume = 704.662542 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067317 0.663907 0.122423 x

x Se 2 0.132276 0.342488 0.628586 x

x Se 3 0.131961 0.341739 0.870451 x

x Se 4 0.068273 0.666270 0.377141 x

x Se 5 0.267031 0.665023 0.123060 x

x Se 6 0.332881 0.345117 0.629149 x

x Se 7 0.333737 0.345205 0.872290 x

x Se 8 0.264839 0.660656 0.370587 x

x Se 9 0.467033 0.657774 0.128834 x

x Se 10 0.532327 0.339926 0.620658 x

x Se 11 0.532952 0.341913 0.871238 x

x Se 12 0.467690 0.660541 0.379629 x

x Se 13 0.666182 0.654516 0.127679 x

x Se 14 0.735248 0.339540 0.629557 x

x Se 15 0.732987 0.334993 0.876873 x

x Se 16 0.667138 0.655075 0.371184 x

x Se 17 0.867936 0.658024 0.129512 x

x Se 18 0.931867 0.334066 0.622525 x

x Se 19 0.932676 0.336178 0.877432 x

x Se 20 0.867723 0.657576 0.371513 x

x Nb 1 0.004940 0.010665 0.249436 x

x Nb 2 -0.004990 -0.010762 0.750378 x

x Nb 3 -0.000090 -0.000157 -0.000044 x

x Nb 4 0.000168 0.000833 0.499860 x

x Nb 5 0.194968 -0.008180 0.247580 x

x Nb 6 0.202538 0.012130 0.749710 x

x Nb 7 0.199530 0.003996 -0.002323 x

x Nb 8 0.203678 0.013259 0.500361 x

x Nb 9 0.399915 -0.002486 0.251584 x

x Nb 10 0.402776 0.013257 0.749378 x

x Nb 11 0.402494 0.007137 -0.000986 x

x Nb 12 0.393174 -0.017788 0.501192 x

x Nb 13 0.597186 -0.013302 0.250603 x

x Nb 14 0.600068 0.002070 0.748519 x

x Nb 15 0.597408 -0.007408 0.001080 x

x Nb 16 0.606920 0.017710 0.498881 x

x Nb 17 0.797474 -0.012128 0.250274 x

x Nb 18 0.805177 0.008800 0.752313 x

x Nb 19 0.800515 -0.003983 0.002249 x

x Nb 20 0.796077 -0.014190 0.499636 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599174E+004 39333.70 <-- SCF

1 -3.62599639E+004 1.16074364E-003 39358.84 <-- SCF

2 -3.62599671E+004 8.06536125E-005 39386.81 <-- SCF

3 -3.62599534E+004 -3.41413563E-004 39413.02 <-- SCF

4 -3.62599434E+004 -2.51009399E-004 39438.72 <-- SCF

5 -3.62599430E+004 -9.33187537E-006 39464.20 <-- SCF

6 -3.62599427E+004 -8.53581419E-006 39483.92 <-- SCF

7 -3.62599427E+004 -6.71519673E-007 39502.48 <-- SCF

8 -3.62599427E+004 1.62277877E-007 39519.41 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.94266570 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.05923 -0.02407 -0.01861 \*

\* Se 2 -0.01953 -0.09766 -0.06415 \*

\* Se 3 -0.07391 -0.09764 0.07219 \*

\* Se 4 -0.02350 -0.02019 -0.06222 \*

\* Se 5 -0.01135 0.10829 0.06650 \*

\* Se 6 0.03693 -0.11547 -0.13891 \*

\* Se 7 0.06281 0.02358 -0.07234 \*

\* Se 8 -0.08588 0.05296 0.00926 \*

\* Se 9 -0.07741 -0.06391 -0.01749 \*

\* Se 10 -0.03793 0.07650 -0.05616 \*

\* Se 11 0.07096 0.06455 0.01910 \*

\* Se 12 0.06963 -0.09522 0.00015 \*

\* Se 13 -0.05009 -0.01492 0.08667 \*

\* Se 14 0.07409 -0.05050 -0.01212 \*

\* Se 15 0.00657 -0.10513 -0.04864 \*

\* Se 16 -0.08043 0.12636 0.03467 \*

\* Se 17 0.08566 0.09458 -0.05796 \*

\* Se 18 0.03797 0.02576 0.03806 \*

\* Se 19 0.05750 0.00574 0.02107 \*

\* Se 20 0.02164 0.08799 0.05667 \*

\* Nb 1 -0.05961 -0.00443 0.01483 \*

\* Nb 2 0.05628 0.00682 -0.01065 \*

\* Nb 3 -0.00221 -0.00018 0.00441 \*

\* Nb 4 0.00353 -0.00632 0.00598 \*

\* Nb 5 0.04184 -0.12227 0.01219 \*

\* Nb 6 -0.06605 0.08731 -0.00733 \*

\* Nb 7 -0.00298 -0.01904 -0.00364 \*

\* Nb 8 0.04550 -0.01830 0.01993 \*

\* Nb 9 0.10741 -0.05480 0.06099 \*

\* Nb 10 -0.06998 0.07555 0.10683 \*

\* Nb 11 -0.00730 0.00086 -0.01442 \*

\* Nb 12 -0.24002 0.05486 -0.09688 \*

\* Nb 13 0.07463 -0.07353 -0.06578 \*

\* Nb 14 -0.10198 0.06761 -0.05204 \*

\* Nb 15 0.00897 -0.00471 0.01503 \*

\* Nb 16 0.23447 -0.04508 0.12048 \*

\* Nb 17 0.05431 -0.08241 0.02895 \*

\* Nb 18 -0.04173 0.11196 0.00422 \*

\* Nb 19 0.00041 0.02140 0.00988 \*

\* Nb 20 -0.03998 0.02308 -0.00873 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.027991 -0.029632 0.002551 \*

\* y -0.029632 -0.016124 0.000750 \*

\* z 0.002551 0.000750 -0.004225 \*

\* \*

\* Pressure: -0.0025 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000060 | -36259.941041 | <-- min BFGS

| trial step | 1.000000 | 0.000031 | -36259.942300 | <-- min BFGS

| line step | 2.025195 | 6.556E-006 | -36259.942833 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 56 with enthalpy= -3.62599428E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 4.480621E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.674370E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.267349E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.963216E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 57 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000156 | -36259.942833 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 57 with trial guess (lambda= 1.000000)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8830032 -8.2920524 0.0012074 0.4197424 -0.0043606 -0.0000452

0.0350869 3.3773811 0.0002680 1.0305398 1.8496660 -0.0002288

0.0015091 0.0008833 13.9380898 -0.0000562 -0.0000352 0.4507924

Lattice parameters(A) Cell Angles

a = 17.037075 alpha = 89.991759

b = 3.377563 beta = 89.992288

c = 13.938090 gamma = 118.529115

Current cell volume = 704.661239 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067288 0.663718 0.122268 x

x Se 2 0.132175 0.342145 0.628522 x

x Se 3 0.131872 0.341453 0.870544 x

x Se 4 0.068297 0.666293 0.377233 x

x Se 5 0.267067 0.664991 0.122879 x

x Se 6 0.332817 0.344787 0.629126 x

x Se 7 0.333739 0.345283 0.872259 x

x Se 8 0.264790 0.660300 0.370606 x

x Se 9 0.467034 0.657595 0.128767 x

x Se 10 0.532203 0.339866 0.620350 x

x Se 11 0.532950 0.342083 0.871310 x

x Se 12 0.467827 0.660665 0.379915 x

x Se 13 0.666179 0.654445 0.127720 x

x Se 14 0.735291 0.339889 0.629534 x

x Se 15 0.732952 0.335033 0.877056 x

x Se 16 0.667188 0.655403 0.371155 x

x Se 17 0.868019 0.658292 0.129421 x

x Se 18 0.931855 0.334053 0.622414 x

x Se 19 0.932703 0.336335 0.877582 x

x Se 20 0.867824 0.657898 0.371584 x

x Nb 1 0.004821 0.010121 0.249396 x

x Nb 2 -0.004872 -0.010210 0.750412 x

x Nb 3 -0.000096 -0.000176 -0.000043 x

x Nb 4 0.000176 0.000849 0.499857 x

x Nb 5 0.194810 -0.008348 0.247489 x

x Nb 6 0.202473 0.012128 0.749701 x

x Nb 7 0.199522 0.003951 -0.002292 x

x Nb 8 0.203775 0.013263 0.500245 x

x Nb 9 0.400032 -0.002340 0.251702 x

x Nb 10 0.402808 0.013067 0.749362 x

x Nb 11 0.402544 0.007273 -0.001049 x

x Nb 12 0.392821 -0.018506 0.501180 x

x Nb 13 0.597156 -0.013094 0.250646 x

x Nb 14 0.599958 0.001947 0.748410 x

x Nb 15 0.597354 -0.007566 0.001151 x

x Nb 16 0.607277 0.018422 0.498910 x

x Nb 17 0.797536 -0.012145 0.250297 x

x Nb 18 0.805340 0.008981 0.752404 x

x Nb 19 0.800524 -0.003929 0.002211 x

x Nb 20 0.795973 -0.014211 0.499765 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598343E+004 39622.66 <-- SCF

1 -3.62602426E+004 1.02074073E-002 39650.05 <-- SCF

2 -3.62602650E+004 5.60243733E-004 39677.77 <-- SCF

3 -3.62601938E+004 -1.77878918E-003 39704.91 <-- SCF

4 -3.62599372E+004 -6.41692349E-003 39730.98 <-- SCF

5 -3.62599549E+004 4.44819205E-004 39757.80 <-- SCF

6 -3.62599490E+004 -1.48698484E-004 39784.27 <-- SCF

7 -3.62599462E+004 -6.91970978E-005 39807.67 <-- SCF

8 -3.62599459E+004 -8.56520595E-006 39828.34 <-- SCF

9 -3.62599460E+004 1.67705851E-006 39846.70 <-- SCF

10 -3.62599460E+004 1.18032172E-006 39864.53 <-- SCF

11 -3.62599460E+004 6.13429425E-007 39881.73 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.94602828 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.05821 -0.03494 -0.00617 \*

\* Se 2 0.00310 -0.08760 -0.05020 \*

\* Se 3 -0.04823 -0.08800 0.04609 \*

\* Se 4 -0.02958 -0.02520 -0.07631 \*

\* Se 5 -0.02976 0.11239 0.09427 \*

\* Se 6 0.04348 -0.10899 -0.11610 \*

\* Se 7 0.05181 0.01379 -0.06999 \*

\* Se 8 -0.07394 0.07462 -0.02563 \*

\* Se 9 -0.08485 -0.05709 0.01592 \*

\* Se 10 -0.03301 0.04358 0.01195 \*

\* Se 11 0.07898 0.05697 -0.01541 \*

\* Se 12 0.04481 -0.05835 -0.06412 \*

\* Se 13 -0.03769 -0.00554 0.07949 \*

\* Se 14 0.06447 -0.07480 0.02244 \*

\* Se 15 0.02481 -0.11000 -0.08381 \*

\* Se 16 -0.07913 0.11646 0.03463 \*

\* Se 17 0.06419 0.08511 -0.03407 \*

\* Se 18 0.04327 0.03173 0.05784 \*

\* Se 19 0.05680 0.01860 0.00866 \*

\* Se 20 -0.00071 0.07978 0.04627 \*

\* Nb 1 -0.03895 0.00090 0.01401 \*

\* Nb 2 0.03561 0.00062 -0.01025 \*

\* Nb 3 -0.00214 -0.00103 0.00344 \*

\* Nb 4 0.00437 -0.00639 0.00528 \*

\* Nb 5 0.05789 -0.13474 0.00920 \*

\* Nb 6 -0.07533 0.07366 -0.00270 \*

\* Nb 7 -0.00296 -0.02077 -0.01706 \*

\* Nb 8 0.04109 -0.01621 0.03112 \*

\* Nb 9 0.09238 -0.05200 0.05610 \*

\* Nb 10 -0.06199 0.08224 0.10787 \*

\* Nb 11 -0.01042 -0.00208 -0.01099 \*

\* Nb 12 -0.23963 0.04252 -0.10559 \*

\* Nb 13 0.06641 -0.08054 -0.07393 \*

\* Nb 14 -0.08838 0.06461 -0.04809 \*

\* Nb 15 0.01376 -0.00189 0.01144 \*

\* Nb 16 0.23498 -0.03226 0.12571 \*

\* Nb 17 0.06632 -0.06886 0.02149 \*

\* Nb 18 -0.05796 0.12437 0.00579 \*

\* Nb 19 0.00122 0.02367 0.02363 \*

\* Nb 20 -0.03685 0.02167 -0.02224 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.033585 -0.007024 0.038530 \*

\* y -0.007024 -0.022720 0.010503 \*

\* z 0.038530 0.010503 -0.036109 \*

\* \*

\* Pressure: 0.0084 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000156 | -36259.942833 | <-- min BFGS

| trial step | 1.000000 | 0.000090 | -36259.946208 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 57 with line minimization (lambda= 2.366391)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8886719 -8.2880501 0.0050548 0.4195571 -0.0044086 -0.0001418

0.0354793 3.3764795 0.0004100 1.0298626 1.8500473 -0.0005306

0.0047241 0.0013673 13.9356156 -0.0001825 -0.0000528 0.4508725

Lattice parameters(A) Cell Angles

a = 17.040081 alpha = 89.987218

b = 3.376666 beta = 89.968767

c = 13.935616 gamma = 118.501262

Current cell volume = 704.659179 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067248 0.663460 0.122056 x

x Se 2 0.132038 0.341676 0.628434 x

x Se 3 0.131750 0.341063 0.870671 x

x Se 4 0.068328 0.666324 0.377360 x

x Se 5 0.267116 0.664947 0.122632 x

x Se 6 0.332729 0.344335 0.629096 x

x Se 7 0.333742 0.345389 0.872217 x

x Se 8 0.264723 0.659815 0.370631 x

x Se 9 0.467035 0.657351 0.128675 x

x Se 10 0.532033 0.339782 0.619929 x

x Se 11 0.532947 0.342315 0.871408 x

x Se 12 0.468013 0.660833 0.380306 x

x Se 13 0.666174 0.654349 0.127776 x

x Se 14 0.735349 0.340366 0.629502 x

x Se 15 0.732905 0.335087 0.877305 x

x Se 16 0.667256 0.655851 0.371115 x

x Se 17 0.868133 0.658657 0.129296 x

x Se 18 0.931837 0.334035 0.622262 x

x Se 19 0.932740 0.336550 0.877788 x

x Se 20 0.867962 0.658340 0.371682 x

x Nb 1 0.004659 0.009378 0.249342 x

x Nb 2 -0.004711 -0.009455 0.750460 x

x Nb 3 -0.000103 -0.000203 -0.000040 x

x Nb 4 0.000187 0.000870 0.499853 x

x Nb 5 0.194594 -0.008578 0.247366 x

x Nb 6 0.202386 0.012124 0.749688 x

x Nb 7 0.199510 0.003891 -0.002248 x

x Nb 8 0.203908 0.013268 0.500087 x

x Nb 9 0.400192 -0.002141 0.251863 x

x Nb 10 0.402851 0.012807 0.749339 x

x Nb 11 0.402612 0.007459 -0.001137 x

x Nb 12 0.392339 -0.019488 0.501165 x

x Nb 13 0.597116 -0.012810 0.250704 x

x Nb 14 0.599808 0.001779 0.748260 x

x Nb 15 0.597280 -0.007782 0.001248 x

x Nb 16 0.607765 0.019394 0.498948 x

x Nb 17 0.797620 -0.012169 0.250330 x

x Nb 18 0.805563 0.009227 0.752529 x

x Nb 19 0.800537 -0.003856 0.002160 x

x Nb 20 0.795830 -0.014239 0.499941 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597388E+004 39985.16 <-- SCF

1 -3.62604976E+004 1.89705372E-002 40012.34 <-- SCF

2 -3.62605384E+004 1.02123442E-003 40039.98 <-- SCF

3 -3.62603856E+004 -3.82081580E-003 40066.88 <-- SCF

4 -3.62599339E+004 -1.12936700E-002 40092.64 <-- SCF

5 -3.62599646E+004 7.67328144E-004 40119.23 <-- SCF

6 -3.62599527E+004 -2.95611191E-004 40145.14 <-- SCF

7 -3.62599482E+004 -1.14428717E-004 40168.75 <-- SCF

8 -3.62599476E+004 -1.29145125E-005 40190.48 <-- SCF

9 -3.62599478E+004 3.90060144E-006 40209.50 <-- SCF

10 -3.62599479E+004 1.56017345E-006 40227.23 <-- SCF

11 -3.62599479E+004 9.69466495E-007 40244.53 <-- SCF

12 -3.62599479E+004 4.73440611E-007 40261.41 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.94791572 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.05818 -0.04811 0.01704 \*

\* Se 2 0.04071 -0.07510 -0.03522 \*

\* Se 3 0.00001 -0.07200 0.00371 \*

\* Se 4 -0.04067 -0.03198 -0.09287 \*

\* Se 5 -0.04642 0.11857 0.11038 \*

\* Se 6 0.04778 -0.10175 -0.08439 \*

\* Se 7 0.04049 0.00007 -0.06643 \*

\* Se 8 -0.05717 0.10487 -0.07676 \*

\* Se 9 -0.09370 -0.04748 0.05806 \*

\* Se 10 -0.00962 -0.01264 0.11742 \*

\* Se 11 0.08796 0.04652 -0.05806 \*

\* Se 12 0.01071 -0.00529 -0.15209 \*

\* Se 13 -0.02547 0.00816 0.06903 \*

\* Se 14 0.04946 -0.10795 0.07141 \*

\* Se 15 0.04331 -0.11657 -0.10623 \*

\* Se 16 -0.07388 0.10499 0.03045 \*

\* Se 17 0.02044 0.06991 0.00442 \*

\* Se 18 0.05318 0.03972 0.08476 \*

\* Se 19 0.05597 0.03520 -0.01175 \*

\* Se 20 -0.03846 0.07039 0.03243 \*

\* Nb 1 -0.01802 0.00711 0.01664 \*

\* Nb 2 0.01409 -0.00698 -0.01484 \*

\* Nb 3 -0.00275 -0.00126 0.00218 \*

\* Nb 4 0.00487 -0.00614 0.00407 \*

\* Nb 5 0.08062 -0.15143 0.00699 \*

\* Nb 6 -0.09125 0.05658 -0.00023 \*

\* Nb 7 -0.00283 -0.02443 -0.03621 \*

\* Nb 8 0.03657 -0.01466 0.04901 \*

\* Nb 9 0.07802 -0.05144 0.04721 \*

\* Nb 10 -0.05446 0.09254 0.11029 \*

\* Nb 11 -0.01071 -0.00371 -0.00781 \*

\* Nb 12 -0.24518 0.03024 -0.11627 \*

\* Nb 13 0.05618 -0.09091 -0.08709 \*

\* Nb 14 -0.07628 0.06422 -0.04241 \*

\* Nb 15 0.01428 0.00007 0.00723 \*

\* Nb 16 0.24064 -0.01727 0.12995 \*

\* Nb 17 0.08438 -0.05082 0.01327 \*

\* Nb 18 -0.08200 0.14165 0.00505 \*

\* Nb 19 0.00131 0.02734 0.04293 \*

\* Nb 20 -0.03394 0.01977 -0.04526 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.043066 0.022334 0.086740 \*

\* y 0.022334 -0.035282 0.016469 \*

\* z 0.086740 0.016469 -0.088001 \*

\* \*

\* Pressure: 0.0267 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000156 | -36259.942833 | <-- min BFGS

| trial step | 1.000000 | 0.000090 | -36259.946208 | <-- min BFGS

| line step | 2.366391 | 1.777E-006 | -36259.948039 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 57 with enthalpy= -3.62599480E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.301552E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.740299E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.274308E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 8.800103E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 58 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000328 | -36259.948039 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 58 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8960881 -8.2929274 0.0045701 0.4194604 -0.0042043 -0.0001242

0.0338351 3.3756635 0.0002959 1.0304804 1.8509899 -0.0004376

0.0041356 0.0009925 13.9372743 -0.0001594 -0.0000379 0.4508189

Lattice parameters(A) Cell Angles

a = 17.048933 alpha = 89.990728

b = 3.375833 beta = 89.971772

c = 13.937275 gamma = 118.531221

Current cell volume = 704.735033 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067217 0.663434 0.121974 x

x Se 2 0.132032 0.341240 0.628494 x

x Se 3 0.131637 0.340413 0.870639 x

x Se 4 0.068353 0.666266 0.377271 x

x Se 5 0.267128 0.665446 0.122722 x

x Se 6 0.332819 0.344219 0.629075 x

x Se 7 0.333866 0.345841 0.872160 x

x Se 8 0.264548 0.659561 0.370445 x

x Se 9 0.466941 0.656991 0.128658 x

x Se 10 0.531974 0.339860 0.619830 x

x Se 11 0.533037 0.342658 0.871423 x

x Se 12 0.468098 0.660744 0.380337 x

x Se 13 0.666063 0.653962 0.127871 x

x Se 14 0.735507 0.340599 0.629673 x

x Se 15 0.732891 0.334578 0.877262 x

x Se 16 0.667121 0.655929 0.371016 x

x Se 17 0.868251 0.659298 0.129341 x

x Se 18 0.931833 0.334149 0.622294 x

x Se 19 0.932770 0.336490 0.877867 x

x Se 20 0.867975 0.658747 0.371619 x

x Nb 1 0.004671 0.009102 0.249351 x

x Nb 2 -0.004723 -0.009199 0.750451 x

x Nb 3 -0.000108 -0.000198 -0.000042 x

x Nb 4 0.000195 0.000883 0.499865 x

x Nb 5 0.194595 -0.009101 0.247325 x

x Nb 6 0.202387 0.012579 0.749648 x

x Nb 7 0.199525 0.003983 -0.002357 x

x Nb 8 0.204073 0.013722 0.500145 x

x Nb 9 0.400325 -0.002050 0.252022 x

x Nb 10 0.402874 0.013643 0.749463 x

x Nb 11 0.402683 0.007535 -0.001116 x

x Nb 12 0.391901 -0.020516 0.500959 x

x Nb 13 0.597104 -0.013602 0.250637 x

x Nb 14 0.599675 0.001737 0.748114 x

x Nb 15 0.597208 -0.007876 0.001221 x

x Nb 16 0.608201 0.020469 0.499191 x

x Nb 17 0.797604 -0.012614 0.250392 x

x Nb 18 0.805564 0.009737 0.752588 x

x Nb 19 0.800520 -0.003963 0.002277 x

x Nb 20 0.795666 -0.014694 0.499892 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597956E+004 40364.58 <-- SCF

1 -3.62601243E+004 8.21746441E-003 40388.69 <-- SCF

2 -3.62601489E+004 6.14840761E-004 40417.52 <-- SCF

3 -3.62600296E+004 -2.98372073E-003 40443.62 <-- SCF

4 -3.62599628E+004 -1.66806139E-003 40469.17 <-- SCF

5 -3.62599570E+004 -1.45991595E-004 40494.81 <-- SCF

6 -3.62599560E+004 -2.41858361E-005 40518.77 <-- SCF

7 -3.62599560E+004 -1.12696062E-006 40539.88 <-- SCF

8 -3.62599560E+004 8.98110218E-007 40557.95 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.95602210 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.04368 -0.05554 0.02447 \*

\* Se 2 0.04138 -0.03714 -0.05314 \*

\* Se 3 0.03947 -0.03047 0.00369 \*

\* Se 4 -0.03007 -0.02369 -0.08136 \*

\* Se 5 -0.04004 0.09531 0.10847 \*

\* Se 6 0.04159 -0.08427 -0.08916 \*

\* Se 7 0.00393 -0.01605 -0.02747 \*

\* Se 8 -0.01823 0.08946 -0.05358 \*

\* Se 9 -0.06714 -0.04527 0.06644 \*

\* Se 10 -0.01113 -0.03443 0.12097 \*

\* Se 11 0.06254 0.04428 -0.06311 \*

\* Se 12 0.00260 0.01626 -0.13763 \*

\* Se 13 0.00972 0.02218 0.01966 \*

\* Se 14 0.00247 -0.09214 0.03759 \*

\* Se 15 0.03941 -0.09279 -0.10347 \*

\* Se 16 -0.05049 0.08007 0.07912 \*

\* Se 17 -0.01954 0.03172 0.00311 \*

\* Se 18 0.04168 0.02805 0.06993 \*

\* Se 19 0.04201 0.04845 -0.01835 \*

\* Se 20 -0.04221 0.03833 0.05020 \*

\* Nb 1 -0.01530 0.00235 0.00659 \*

\* Nb 2 0.01259 -0.00376 -0.00752 \*

\* Nb 3 -0.00370 -0.00247 0.00242 \*

\* Nb 4 0.00727 -0.00503 0.00062 \*

\* Nb 5 0.06088 -0.13690 -0.00520 \*

\* Nb 6 -0.08923 0.03374 0.00966 \*

\* Nb 7 -0.00111 -0.02256 -0.02904 \*

\* Nb 8 0.01810 -0.01807 0.03749 \*

\* Nb 9 0.05967 -0.05521 0.03435 \*

\* Nb 10 -0.04851 0.07487 0.10179 \*

\* Nb 11 -0.01411 -0.00555 -0.00909 \*

\* Nb 12 -0.23513 0.01978 -0.10242 \*

\* Nb 13 0.04568 -0.07202 -0.09292 \*

\* Nb 14 -0.05835 0.06614 -0.03318 \*

\* Nb 15 0.01762 0.00223 0.01271 \*

\* Nb 16 0.23240 -0.00750 0.10559 \*

\* Nb 17 0.08704 -0.02959 -0.00110 \*

\* Nb 18 -0.06234 0.12804 0.01362 \*

\* Nb 19 0.00129 0.02598 0.03793 \*

\* Nb 20 -0.01904 0.02321 -0.03870 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.081742 0.006404 0.071511 \*

\* y 0.006404 -0.053903 0.005780 \*

\* z 0.071511 0.005780 -0.057753 \*

\* \*

\* Pressure: 0.0100 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000328 | -36259.948039 | <-- min BFGS

| trial step | 1.000000 | 0.000245 | -36259.956100 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 58 with line minimization (lambda= 3.969124)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9181077 -8.3074088 0.0031309 0.4191749 -0.0035979 -0.0000718

0.0289532 3.3732407 -0.0000429 1.0323181 1.8537949 -0.0001609

0.0023883 -0.0001200 13.9421991 -0.0000910 0.0000065 0.4506596

Lattice parameters(A) Cell Angles

a = 17.075216 alpha = 90.001137

b = 3.373365 beta = 89.980680

c = 13.942199 gamma = 118.620242

Current cell volume = 704.957907 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067125 0.663357 0.121732 x

x Se 2 0.132014 0.339945 0.628672 x

x Se 3 0.131300 0.338483 0.870545 x

x Se 4 0.068426 0.666094 0.377007 x

x Se 5 0.267165 0.666927 0.122990 x

x Se 6 0.333085 0.343874 0.629013 x

x Se 7 0.334233 0.347182 0.871989 x

x Se 8 0.264029 0.658807 0.369891 x

x Se 9 0.466663 0.655924 0.128607 x

x Se 10 0.531796 0.340092 0.619534 x

x Se 11 0.533305 0.343675 0.871468 x

x Se 12 0.468352 0.660480 0.380433 x

x Se 13 0.665733 0.652815 0.128153 x

x Se 14 0.735977 0.341291 0.630179 x

x Se 15 0.732852 0.333067 0.877133 x

x Se 16 0.666719 0.656161 0.370724 x

x Se 17 0.868603 0.661200 0.129475 x

x Se 18 0.931820 0.334487 0.622390 x

x Se 19 0.932857 0.336310 0.878102 x

x Se 20 0.868012 0.659957 0.371431 x

x Nb 1 0.004708 0.008279 0.249378 x

x Nb 2 -0.004761 -0.008437 0.750425 x

x Nb 3 -0.000123 -0.000184 -0.000047 x

x Nb 4 0.000219 0.000922 0.499902 x

x Nb 5 0.194599 -0.010653 0.247203 x

x Nb 6 0.202392 0.013927 0.749528 x

x Nb 7 0.199569 0.004257 -0.002681 x

x Nb 8 0.204564 0.015068 0.500319 x

x Nb 9 0.400720 -0.001779 0.252495 x

x Nb 10 0.402940 0.016123 0.749832 x

x Nb 11 0.402895 0.007762 -0.001056 x

x Nb 12 0.390600 -0.023568 0.500349 x

x Nb 13 0.597070 -0.015954 0.250436 x

x Nb 14 0.599278 0.001614 0.747679 x

x Nb 15 0.596994 -0.008158 0.001141 x

x Nb 16 0.609496 0.023659 0.499915 x

x Nb 17 0.797555 -0.013936 0.250577 x

x Nb 18 0.805569 0.011252 0.752765 x

x Nb 19 0.800470 -0.004282 0.002625 x

x Nb 20 0.795179 -0.016042 0.499747 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62585504E+004 40661.30 <-- SCF

1 -3.62614761E+004 7.31429375E-002 40686.22 <-- SCF

2 -3.62616868E+004 5.26780294E-003 40715.75 <-- SCF

3 -3.62606116E+004 -2.68807644E-002 40741.98 <-- SCF

4 -3.62600331E+004 -1.44627487E-002 40767.70 <-- SCF

5 -3.62599726E+004 -1.51043696E-003 40793.23 <-- SCF

6 -3.62599668E+004 -1.46754909E-004 40820.83 <-- SCF

7 -3.62599669E+004 2.82601090E-006 40845.86 <-- SCF

8 -3.62599670E+004 3.54748069E-006 40868.53 <-- SCF

9 -3.62599669E+004 -2.42597575E-006 40888.59 <-- SCF

10 -3.62599670E+004 2.62266193E-006 40906.12 <-- SCF

11 -3.62599671E+004 2.57128598E-006 40923.86 <-- SCF

12 -3.62599672E+004 2.12467889E-006 40940.78 <-- SCF

13 -3.62599673E+004 1.57024876E-006 40957.83 <-- SCF

14 -3.62599673E+004 1.32450852E-006 40974.83 <-- SCF

15 -3.62599674E+004 1.09243229E-006 40991.86 <-- SCF

16 -3.62599674E+004 9.60541836E-007 41008.86 <-- SCF

17 -3.62599674E+004 8.05197283E-007 41025.05 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.96744691 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01168 -0.06818 0.04371 \*

\* Se 2 0.04033 0.06879 -0.10225 \*

\* Se 3 0.14611 0.08260 0.02364 \*

\* Se 4 -0.00699 -0.00594 -0.04420 \*

\* Se 5 0.00607 0.03170 0.08636 \*

\* Se 6 0.02664 -0.03522 -0.10023 \*

\* Se 7 -0.08702 -0.04184 0.05320 \*

\* Se 8 0.13737 0.04110 0.06852 \*

\* Se 9 -0.00548 -0.03493 0.09041 \*

\* Se 10 -0.03288 -0.08783 0.10157 \*

\* Se 11 0.00297 0.03366 -0.08356 \*

\* Se 12 -0.01114 0.07821 -0.06403 \*

\* Se 13 0.08421 0.03754 -0.09050 \*

\* Se 14 -0.13187 -0.04911 -0.06632 \*

\* Se 15 0.00493 -0.03098 -0.08970 \*

\* Se 16 0.01979 0.02786 0.20456 \*

\* Se 17 -0.14103 -0.07477 -0.01739 \*

\* Se 18 0.00930 -0.00067 0.01910 \*

\* Se 19 -0.01431 0.07826 -0.03539 \*

\* Se 20 -0.04806 -0.05472 0.10523 \*

\* Nb 1 -0.01089 0.00310 -0.01096 \*

\* Nb 2 0.00679 -0.00588 0.00102 \*

\* Nb 3 -0.00478 -0.00711 0.00326 \*

\* Nb 4 0.01212 -0.00332 -0.01178 \*

\* Nb 5 -0.00195 -0.08377 -0.04640 \*

\* Nb 6 -0.07492 -0.04728 0.04977 \*

\* Nb 7 0.00677 -0.01602 -0.00885 \*

\* Nb 8 -0.01556 -0.02696 0.00144 \*

\* Nb 9 -0.01560 -0.05981 -0.01322 \*

\* Nb 10 -0.02711 0.00740 0.06176 \*

\* Nb 11 -0.03085 -0.01094 -0.01757 \*

\* Nb 12 -0.23712 -0.00852 -0.07510 \*

\* Nb 13 0.00907 -0.00220 -0.10557 \*

\* Nb 14 0.01229 0.06123 0.00296 \*

\* Nb 15 0.03506 0.00955 0.03228 \*

\* Nb 16 0.23923 0.02041 0.04559 \*

\* Nb 17 0.08665 0.04447 -0.05859 \*

\* Nb 18 -0.00262 0.07867 0.04120 \*

\* Nb 19 -0.00268 0.02065 0.02284 \*

\* Nb 20 0.00550 0.03079 -0.01680 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.162498 0.004179 0.007981 \*

\* y 0.004179 -0.146741 -0.029338 \*

\* z 0.007981 -0.029338 -0.000454 \*

\* \*

\* Pressure: -0.0051 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000328 | -36259.948039 | <-- min BFGS

| trial step | 1.000000 | 0.000245 | -36259.956100 | <-- min BFGS

| line step | 3.969124 | 0.000022 | -36259.967558 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 58 with enthalpy= -3.62599676E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 4.879551E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.488798E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.924216E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.624985E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 59 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000370 | -36259.967558 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 59 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9123013 -8.3210872 0.0006452 0.4194378 -0.0034133 -0.0000359

0.0274741 3.3761443 0.0003250 1.0337765 1.8526410 -0.0002295

0.0012025 0.0010556 13.9381364 -0.0000435 -0.0000430 0.4507909

Lattice parameters(A) Cell Angles

a = 17.076804 alpha = 89.990106

b = 3.376256 beta = 89.995633

c = 13.938137 gamma = 118.695338

Current cell volume = 704.917007 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067001 0.663276 0.121930 x

x Se 2 0.132277 0.339982 0.628289 x

x Se 3 0.131505 0.338904 0.870848 x

x Se 4 0.068256 0.665464 0.376697 x

x Se 5 0.267259 0.667936 0.123538 x

x Se 6 0.332823 0.342668 0.628735 x

x Se 7 0.334201 0.345878 0.871933 x

x Se 8 0.263922 0.658838 0.369651 x

x Se 9 0.466555 0.655369 0.128572 x

x Se 10 0.531395 0.339772 0.619485 x

x Se 11 0.533422 0.344209 0.871505 x

x Se 12 0.468750 0.660782 0.380398 x

x Se 13 0.665781 0.654194 0.128222 x

x Se 14 0.736068 0.341257 0.630393 x

x Se 15 0.732757 0.332011 0.876657 x

x Se 16 0.666950 0.657419 0.370985 x

x Se 17 0.868401 0.660716 0.129200 x

x Se 18 0.931996 0.335050 0.622650 x

x Se 19 0.932984 0.336341 0.877892 x

x Se 20 0.867757 0.659903 0.371791 x

x Nb 1 0.004234 0.006899 0.249326 x

x Nb 2 -0.004290 -0.007051 0.750487 x

x Nb 3 -0.000130 -0.000218 -0.000046 x

x Nb 4 0.000220 0.000876 0.499919 x

x Nb 5 0.194753 -0.011080 0.247188 x

x Nb 6 0.202026 0.013273 0.749461 x

x Nb 7 0.199548 0.003505 -0.002526 x

x Nb 8 0.204472 0.013844 0.500222 x

x Nb 9 0.401010 -0.001613 0.252546 x

x Nb 10 0.402803 0.014981 0.749991 x

x Nb 11 0.402782 0.007614 -0.001198 x

x Nb 12 0.390302 -0.023678 0.500215 x

x Nb 13 0.597206 -0.014791 0.250312 x

x Nb 14 0.598994 0.001593 0.747629 x

x Nb 15 0.597107 -0.008045 0.001281 x

x Nb 16 0.609806 0.023842 0.500067 x

x Nb 17 0.797927 -0.013263 0.250651 x

x Nb 18 0.805417 0.011652 0.752790 x

x Nb 19 0.800485 -0.003512 0.002453 x

x Nb 20 0.795268 -0.014798 0.499863 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62595883E+004 41128.11 <-- SCF

1 -3.62604893E+004 2.25259552E-002 41154.55 <-- SCF

2 -3.62605325E+004 1.08092947E-003 41183.83 <-- SCF

3 -3.62603264E+004 -5.15313526E-003 41210.55 <-- SCF

4 -3.62599749E+004 -8.78664061E-003 41236.25 <-- SCF

5 -3.62599913E+004 4.09004398E-004 41263.09 <-- SCF

6 -3.62599766E+004 -3.68749163E-004 41289.30 <-- SCF

7 -3.62599732E+004 -8.43392253E-005 41313.70 <-- SCF

8 -3.62599733E+004 3.38282308E-006 41335.55 <-- SCF

9 -3.62599734E+004 1.20817102E-006 41354.84 <-- SCF

10 -3.62599734E+004 1.30592834E-006 41372.19 <-- SCF

11 -3.62599735E+004 9.32440562E-007 41389.58 <-- SCF

12 -3.62599735E+004 1.12370865E-006 41406.47 <-- SCF

13 -3.62599735E+004 9.88752623E-007 41423.83 <-- SCF

14 -3.62599736E+004 8.28314341E-007 41440.38 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.97357297 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02901 -0.07163 0.01236 \*

\* Se 2 -0.01362 0.08456 -0.07343 \*

\* Se 3 0.11143 0.07946 -0.02089 \*

\* Se 4 -0.00308 0.00119 -0.02916 \*

\* Se 5 0.05627 -0.00912 -0.03439 \*

\* Se 6 0.08694 -0.02629 0.00723 \*

\* Se 7 -0.09884 0.02324 0.06738 \*

\* Se 8 0.15823 -0.00098 0.10229 \*

\* Se 9 0.02246 -0.02689 0.08416 \*

\* Se 10 0.06428 -0.13524 0.07456 \*

\* Se 11 -0.02533 0.02816 -0.07489 \*

\* Se 12 -0.13133 0.12897 -0.01199 \*

\* Se 13 0.09483 -0.02295 -0.10449 \*

\* Se 14 -0.14847 -0.00981 -0.08982 \*

\* Se 15 -0.04445 0.01558 -0.02069 \*

\* Se 16 -0.03126 0.00742 0.11549 \*

\* Se 17 -0.10916 -0.06674 0.02309 \*

\* Se 18 0.00699 -0.01434 0.00528 \*

\* Se 19 -0.03001 0.07994 -0.01375 \*

\* Se 20 0.00905 -0.06898 0.08547 \*

\* Nb 1 -0.01013 0.00262 -0.00123 \*

\* Nb 2 0.00778 -0.00689 -0.01072 \*

\* Nb 3 -0.00529 -0.00739 0.00439 \*

\* Nb 4 0.01398 -0.00234 -0.01444 \*

\* Nb 5 -0.02022 -0.05324 -0.03863 \*

\* Nb 6 -0.04905 -0.06919 0.05816 \*

\* Nb 7 0.02466 0.00221 0.00417 \*

\* Nb 8 -0.01352 -0.01577 -0.01988 \*

\* Nb 9 -0.02828 -0.05403 0.00542 \*

\* Nb 10 -0.03332 0.01674 0.03425 \*

\* Nb 11 -0.03044 -0.02283 -0.00620 \*

\* Nb 12 -0.23107 -0.02290 -0.08152 \*

\* Nb 13 0.01780 -0.00941 -0.08335 \*

\* Nb 14 0.02476 0.05052 -0.01635 \*

\* Nb 15 0.03476 0.02263 0.02458 \*

\* Nb 16 0.23137 0.03634 0.05082 \*

\* Nb 17 0.05993 0.06599 -0.06643 \*

\* Nb 18 0.01434 0.04979 0.03369 \*

\* Nb 19 -0.01668 0.00156 0.01513 \*

\* Nb 20 0.00468 0.02004 0.00434 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.054125 -0.033115 -0.029526 \*

\* y -0.033115 -0.051296 -0.000328 \*

\* z -0.029526 -0.000328 -0.050895 \*

\* \*

\* Pressure: 0.0160 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000370 | -36259.967558 | <-- min BFGS

| trial step | 1.000000 | 0.000046 | -36259.973707 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 59 with enthalpy= -3.62599737E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.537287E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.460918E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 8.206746E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 5.412524E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 60 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000061 | -36259.973707 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 60 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9058055 -8.3215004 0.0017931 0.4196012 -0.0034479 -0.0000679

0.0277473 3.3767476 0.0004218 1.0340457 1.8522242 -0.0003507

0.0022673 0.0013739 13.9421348 -0.0000853 -0.0000556 0.4506617

Lattice parameters(A) Cell Angles

a = 17.071333 alpha = 89.987120

b = 3.376862 beta = 89.988598

c = 13.942135 gamma = 118.702620

Current cell volume = 704.970657 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066973 0.663202 0.121870 x

x Se 2 0.132279 0.339839 0.628136 x

x Se 3 0.131493 0.338741 0.870955 x

x Se 4 0.068254 0.665456 0.376703 x

x Se 5 0.267298 0.668094 0.123550 x

x Se 6 0.332726 0.342326 0.628647 x

x Se 7 0.334171 0.345519 0.871875 x

x Se 8 0.263898 0.658710 0.369645 x

x Se 9 0.466519 0.655301 0.128549 x

x Se 10 0.531278 0.339565 0.619285 x

x Se 11 0.533458 0.344257 0.871535 x

x Se 12 0.468864 0.661003 0.380579 x

x Se 13 0.665812 0.654564 0.128277 x

x Se 14 0.736087 0.341375 0.630395 x

x Se 15 0.732719 0.331858 0.876653 x

x Se 16 0.667039 0.657758 0.371050 x

x Se 17 0.868414 0.660881 0.129099 x

x Se 18 0.932006 0.335051 0.622620 x

x Se 19 0.933010 0.336390 0.877947 x

x Se 20 0.867757 0.660055 0.371944 x

x Nb 1 0.004079 0.006273 0.249287 x

x Nb 2 -0.004137 -0.006433 0.750524 x

x Nb 3 -0.000135 -0.000233 -0.000046 x

x Nb 4 0.000227 0.000887 0.499921 x

x Nb 5 0.194714 -0.011232 0.247115 x

x Nb 6 0.201948 0.013071 0.749475 x

x Nb 7 0.199549 0.003385 -0.002502 x

x Nb 8 0.204523 0.013680 0.500165 x

x Nb 9 0.401121 -0.001386 0.252592 x

x Nb 10 0.402809 0.014813 0.750067 x

x Nb 11 0.402798 0.007635 -0.001213 x

x Nb 12 0.390039 -0.024222 0.500134 x

x Nb 13 0.597201 -0.014605 0.250254 x

x Nb 14 0.598887 0.001394 0.747587 x

x Nb 15 0.597091 -0.008077 0.001301 x

x Nb 16 0.610074 0.024402 0.500158 x

x Nb 17 0.798005 -0.013065 0.250648 x

x Nb 18 0.805459 0.011807 0.752866 x

x Nb 19 0.800483 -0.003392 0.002429 x

x Nb 20 0.795212 -0.014648 0.499927 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599098E+004 41544.28 <-- SCF

1 -3.62600949E+004 4.62645904E-003 41571.00 <-- SCF

2 -3.62601048E+004 2.47932422E-004 41598.88 <-- SCF

3 -3.62600582E+004 -1.16574693E-003 41625.72 <-- SCF

4 -3.62599735E+004 -2.11642508E-003 41651.64 <-- SCF

5 -3.62599786E+004 1.27333595E-004 41678.22 <-- SCF

6 -3.62599757E+004 -7.38771787E-005 41703.72 <-- SCF

7 -3.62599748E+004 -2.12085701E-005 41725.08 <-- SCF

8 -3.62599748E+004 -1.00931238E-006 41744.80 <-- SCF

9 -3.62599748E+004 1.05227504E-006 41762.58 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.97481838 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02442 -0.07996 0.02442 \*

\* Se 2 -0.01517 0.08514 -0.05412 \*

\* Se 3 0.11844 0.08966 -0.03467 \*

\* Se 4 -0.01193 -0.00474 -0.03926 \*

\* Se 5 0.05612 -0.01121 -0.03272 \*

\* Se 6 0.09933 -0.02290 0.04844 \*

\* Se 7 -0.09749 0.04123 0.08023 \*

\* Se 8 0.14997 0.00058 0.08040 \*

\* Se 9 0.02586 -0.02799 0.08647 \*

\* Se 10 0.09625 -0.13415 0.10134 \*

\* Se 11 -0.02664 0.02906 -0.07656 \*

\* Se 12 -0.16594 0.12682 -0.04182 \*

\* Se 13 0.09380 -0.04054 -0.11467 \*

\* Se 14 -0.13815 -0.01138 -0.06646 \*

\* Se 15 -0.04290 0.01839 -0.02460 \*

\* Se 16 -0.05169 0.00054 0.07910 \*

\* Se 17 -0.12077 -0.07886 0.03976 \*

\* Se 18 0.01771 -0.00735 0.01383 \*

\* Se 19 -0.02349 0.09035 -0.02179 \*

\* Se 20 0.00972 -0.06891 0.06624 \*

\* Nb 1 0.00280 0.01058 0.00653 \*

\* Nb 2 -0.00422 -0.01508 -0.01900 \*

\* Nb 3 -0.00519 -0.00737 0.00459 \*

\* Nb 4 0.01491 -0.00205 -0.01541 \*

\* Nb 5 -0.01695 -0.05391 -0.02938 \*

\* Nb 6 -0.06515 -0.07671 0.05081 \*

\* Nb 7 0.02399 0.00216 0.00113 \*

\* Nb 8 -0.02892 -0.01185 -0.02296 \*

\* Nb 9 -0.03431 -0.04957 0.01070 \*

\* Nb 10 -0.04056 0.01677 0.01463 \*

\* Nb 11 -0.03648 -0.02715 -0.00659 \*

\* Nb 12 -0.22492 -0.02654 -0.07568 \*

\* Nb 13 0.02540 -0.00939 -0.06701 \*

\* Nb 14 0.03075 0.04535 -0.02170 \*

\* Nb 15 0.04141 0.02706 0.02609 \*

\* Nb 16 0.22504 0.04048 0.04254 \*

\* Nb 17 0.07725 0.07442 -0.06151 \*

\* Nb 18 0.01191 0.05118 0.02327 \*

\* Nb 19 -0.01489 0.00174 0.01927 \*

\* Nb 20 0.02064 0.01609 0.00615 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.014907 -0.008758 -0.019409 \*

\* y -0.008758 0.011734 0.005034 \*

\* z -0.019409 0.005034 0.007504 \*

\* \*

\* Pressure: -0.0014 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000061 | -36259.973707 | <-- min BFGS

| trial step | 1.000000 | 0.000021 | -36259.974961 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 60 with line minimization (lambda= 1.523905)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9024023 -8.3217169 0.0023944 0.4196868 -0.0034661 -0.0000846

0.0278904 3.3770636 0.0004726 1.0341869 1.8520059 -0.0004142

0.0028252 0.0015406 13.9442296 -0.0001071 -0.0000622 0.4505940

Lattice parameters(A) Cell Angles

a = 17.068467 alpha = 89.985556

b = 3.377179 beta = 89.984913

c = 13.944230 gamma = 118.706439

Current cell volume = 704.998685 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066959 0.663164 0.121839 x

x Se 2 0.132280 0.339764 0.628056 x

x Se 3 0.131487 0.338655 0.871010 x

x Se 4 0.068253 0.665452 0.376707 x

x Se 5 0.267318 0.668177 0.123556 x

x Se 6 0.332675 0.342146 0.628601 x

x Se 7 0.334156 0.345331 0.871844 x

x Se 8 0.263885 0.658643 0.369641 x

x Se 9 0.466500 0.655266 0.128537 x

x Se 10 0.531217 0.339456 0.619179 x

x Se 11 0.533476 0.344282 0.871551 x

x Se 12 0.468924 0.661118 0.380674 x

x Se 13 0.665828 0.654758 0.128306 x

x Se 14 0.736097 0.341436 0.630397 x

x Se 15 0.732700 0.331777 0.876651 x

x Se 16 0.667085 0.657936 0.371084 x

x Se 17 0.868420 0.660967 0.129047 x

x Se 18 0.932011 0.335052 0.622605 x

x Se 19 0.933024 0.336416 0.877976 x

x Se 20 0.867757 0.660135 0.372023 x

x Nb 1 0.003998 0.005946 0.249267 x

x Nb 2 -0.004057 -0.006109 0.750543 x

x Nb 3 -0.000137 -0.000241 -0.000045 x

x Nb 4 0.000231 0.000893 0.499921 x

x Nb 5 0.194693 -0.011311 0.247077 x

x Nb 6 0.201907 0.012966 0.749482 x

x Nb 7 0.199549 0.003322 -0.002490 x

x Nb 8 0.204550 0.013593 0.500135 x

x Nb 9 0.401179 -0.001268 0.252616 x

x Nb 10 0.402812 0.014725 0.750106 x

x Nb 11 0.402806 0.007645 -0.001221 x

x Nb 12 0.389901 -0.024507 0.500092 x

x Nb 13 0.597198 -0.014508 0.250224 x

x Nb 14 0.598831 0.001289 0.747565 x

x Nb 15 0.597082 -0.008094 0.001311 x

x Nb 16 0.610214 0.024695 0.500205 x

x Nb 17 0.798046 -0.012961 0.250646 x

x Nb 18 0.805481 0.011889 0.752905 x

x Nb 19 0.800482 -0.003330 0.002416 x

x Nb 20 0.795183 -0.014569 0.499960 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599568E+004 41866.14 <-- SCF

1 -3.62600185E+004 1.54216865E-003 41893.27 <-- SCF

2 -3.62600218E+004 8.21073805E-005 41919.72 <-- SCF

3 -3.62600124E+004 -2.34404599E-004 41946.52 <-- SCF

4 -3.62599736E+004 -9.69867518E-004 41972.56 <-- SCF

5 -3.62599765E+004 7.07109487E-005 41998.50 <-- SCF

6 -3.62599755E+004 -2.29787364E-005 42021.50 <-- SCF

7 -3.62599751E+004 -1.03181584E-005 42041.28 <-- SCF

8 -3.62599751E+004 -8.05180577E-007 42059.86 <-- SCF

9 -3.62599751E+004 6.15835145E-007 42077.27 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.97512589 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02537 -0.08476 0.03119 \*

\* Se 2 -0.01653 0.08453 -0.04398 \*

\* Se 3 0.12333 0.09411 -0.03845 \*

\* Se 4 -0.01684 -0.00796 -0.04454 \*

\* Se 5 0.05738 -0.01104 -0.03038 \*

\* Se 6 0.10597 -0.02105 0.06902 \*

\* Se 7 -0.09544 0.04984 0.08451 \*

\* Se 8 0.14636 0.00087 0.06498 \*

\* Se 9 0.02684 -0.02879 0.08941 \*

\* Se 10 0.11200 -0.13240 0.10943 \*

\* Se 11 -0.02653 0.02970 -0.07912 \*

\* Se 12 -0.18176 0.12404 -0.05182 \*

\* Se 13 0.09214 -0.04902 -0.11782 \*

\* Se 14 -0.13345 -0.01164 -0.04995 \*

\* Se 15 -0.04336 0.01868 -0.02799 \*

\* Se 16 -0.06358 -0.00261 0.06007 \*

\* Se 17 -0.12800 -0.08424 0.04510 \*

\* Se 18 0.02362 -0.00364 0.01826 \*

\* Se 19 -0.02344 0.09618 -0.02640 \*

\* Se 20 0.01020 -0.06794 0.05552 \*

\* Nb 1 0.00880 0.01631 0.01062 \*

\* Nb 2 -0.00969 -0.02080 -0.02321 \*

\* Nb 3 -0.00505 -0.00735 0.00476 \*

\* Nb 4 0.01535 -0.00191 -0.01572 \*

\* Nb 5 -0.01190 -0.05467 -0.02534 \*

\* Nb 6 -0.07351 -0.08062 0.04856 \*

\* Nb 7 0.02366 0.00328 0.00002 \*

\* Nb 8 -0.03342 -0.01128 -0.02494 \*

\* Nb 9 -0.03533 -0.04617 0.01433 \*

\* Nb 10 -0.04242 0.01745 0.00590 \*

\* Nb 11 -0.03909 -0.02944 -0.00659 \*

\* Nb 12 -0.22583 -0.02625 -0.07326 \*

\* Nb 13 0.02746 -0.01022 -0.05952 \*

\* Nb 14 0.03148 0.04156 -0.02542 \*

\* Nb 15 0.04434 0.02950 0.02639 \*

\* Nb 16 0.22582 0.04048 0.03904 \*

\* Nb 17 0.08620 0.07868 -0.06034 \*

\* Nb 18 0.00724 0.05220 0.01892 \*

\* Nb 19 -0.01375 0.00075 0.02089 \*

\* Nb 20 0.02538 0.01562 0.00788 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.047486 0.003871 -0.012676 \*

\* y 0.003871 0.042818 0.008922 \*

\* z -0.012676 0.008922 0.037663 \*

\* \*

\* Pressure: -0.0110 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000061 | -36259.973707 | <-- min BFGS

| trial step | 1.000000 | 0.000021 | -36259.974961 | <-- min BFGS

| line step | 1.523905 | 4.075E-006 | -36259.975248 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 60 with enthalpy= -3.62599752E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 3.852652E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.388643E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.420360E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.748592E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 61 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000039 | -36259.975248 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 61 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9043005 -8.3217015 0.0032524 0.4196351 -0.0034630 -0.0001034

0.0278686 3.3770271 0.0004553 1.0340688 1.8520335 -0.0004534

0.0034463 0.0014892 13.9432091 -0.0001316 -0.0000597 0.4506270

Lattice parameters(A) Cell Angles

a = 17.070117 alpha = 89.986040

b = 3.377142 beta = 89.979702

c = 13.943210 gamma = 118.703651

Current cell volume = 705.026331 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066946 0.663039 0.121834 x

x Se 2 0.132262 0.339670 0.628005 x

x Se 3 0.131481 0.338707 0.871040 x

x Se 4 0.068246 0.665370 0.376675 x

x Se 5 0.267348 0.668302 0.123545 x

x Se 6 0.332633 0.341858 0.628592 x

x Se 7 0.334137 0.345276 0.871821 x

x Se 8 0.263889 0.658625 0.369634 x

x Se 9 0.466478 0.655065 0.128549 x

x Se 10 0.531189 0.339452 0.619129 x

x Se 11 0.533498 0.344480 0.871542 x

x Se 12 0.468949 0.661098 0.380721 x

x Se 13 0.665849 0.654829 0.128327 x

x Se 14 0.736090 0.341450 0.630402 x

x Se 15 0.732671 0.331662 0.876658 x

x Se 16 0.667127 0.658232 0.371099 x

x Se 17 0.868425 0.660910 0.129023 x

x Se 18 0.932023 0.335132 0.622622 x

x Se 19 0.933037 0.336532 0.877980 x

x Se 20 0.867775 0.660225 0.372075 x

x Nb 1 0.003929 0.005743 0.249261 x

x Nb 2 -0.003989 -0.005902 0.750546 x

x Nb 3 -0.000140 -0.000253 -0.000043 x

x Nb 4 0.000235 0.000898 0.499918 x

x Nb 5 0.194647 -0.011465 0.247057 x

x Nb 6 0.201854 0.012821 0.749482 x

x Nb 7 0.199547 0.003242 -0.002460 x

x Nb 8 0.204567 0.013494 0.500087 x

x Nb 9 0.401234 -0.001132 0.252654 x

x Nb 10 0.402793 0.014507 0.750117 x

x Nb 11 0.402801 0.007633 -0.001251 x

x Nb 12 0.389750 -0.024773 0.500067 x

x Nb 13 0.597215 -0.014291 0.250214 x

x Nb 14 0.598777 0.001171 0.747528 x

x Nb 15 0.597086 -0.008088 0.001347 x

x Nb 16 0.610365 0.024974 0.500230 x

x Nb 17 0.798099 -0.012815 0.250650 x

x Nb 18 0.805528 0.012036 0.752926 x

x Nb 19 0.800485 -0.003240 0.002387 x

x Nb 20 0.795162 -0.014472 0.500011 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599579E+004 42180.20 <-- SCF

1 -3.62600143E+004 1.41171601E-003 42207.38 <-- SCF

2 -3.62600173E+004 7.46258535E-005 42234.50 <-- SCF

3 -3.62600049E+004 -3.09083263E-004 42261.41 <-- SCF

4 -3.62599758E+004 -7.28518842E-004 42287.89 <-- SCF

5 -3.62599774E+004 3.97177832E-005 42314.28 <-- SCF

6 -3.62599765E+004 -2.34730158E-005 42337.50 <-- SCF

7 -3.62599762E+004 -7.33832003E-006 42357.16 <-- SCF

8 -3.62599762E+004 9.01171157E-008 42375.36 <-- SCF

9 -3.62599762E+004 5.48254269E-007 42392.48 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.97618684 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02669 -0.08015 0.03150 \*

\* Se 2 -0.01461 0.08238 -0.04048 \*

\* Se 3 0.12468 0.08715 -0.04013 \*

\* Se 4 -0.01808 -0.00660 -0.04275 \*

\* Se 5 0.05726 -0.01158 -0.02087 \*

\* Se 6 0.10334 -0.01368 0.07744 \*

\* Se 7 -0.09579 0.04623 0.08764 \*

\* Se 8 0.14174 0.00158 0.05402 \*

\* Se 9 0.03159 -0.02684 0.09039 \*

\* Se 10 0.11483 -0.13501 0.10751 \*

\* Se 11 -0.03133 0.02769 -0.08083 \*

\* Se 12 -0.18276 0.12767 -0.05068 \*

\* Se 13 0.09259 -0.04613 -0.11955 \*

\* Se 14 -0.12802 -0.01256 -0.03808 \*

\* Se 15 -0.04232 0.01859 -0.03589 \*

\* Se 16 -0.06547 -0.00877 0.04593 \*

\* Se 17 -0.13033 -0.07738 0.04702 \*

\* Se 18 0.02470 -0.00582 0.01746 \*

\* Se 19 -0.02415 0.09222 -0.02532 \*

\* Se 20 0.00754 -0.06509 0.05093 \*

\* Nb 1 0.01348 0.01562 0.01197 \*

\* Nb 2 -0.01439 -0.02059 -0.02412 \*

\* Nb 3 -0.00508 -0.00729 0.00477 \*

\* Nb 4 0.01558 -0.00187 -0.01575 \*

\* Nb 5 -0.00353 -0.05604 -0.02638 \*

\* Nb 6 -0.07416 -0.08069 0.04817 \*

\* Nb 7 0.02414 0.00523 -0.00189 \*

\* Nb 8 -0.03901 -0.01040 -0.02316 \*

\* Nb 9 -0.04091 -0.04781 0.01223 \*

\* Nb 10 -0.03763 0.02215 0.00405 \*

\* Nb 11 -0.03629 -0.03134 -0.00418 \*

\* Nb 12 -0.22022 -0.02800 -0.07099 \*

\* Nb 13 0.02344 -0.01471 -0.05705 \*

\* Nb 14 0.03646 0.04248 -0.02330 \*

\* Nb 15 0.04191 0.03157 0.02375 \*

\* Nb 16 0.21973 0.04172 0.03730 \*

\* Nb 17 0.08698 0.07886 -0.05955 \*

\* Nb 18 -0.00030 0.05385 0.01915 \*

\* Nb 19 -0.01399 -0.00136 0.02312 \*

\* Nb 20 0.03166 0.01471 0.00657 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.033650 0.001079 -0.004250 \*

\* y 0.001079 0.040795 0.007595 \*

\* z -0.004250 0.007595 0.024391 \*

\* \*

\* Pressure: -0.0105 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000039 | -36259.975248 | <-- min BFGS

| trial step | 1.000000 | 0.000034 | -36259.976319 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 61 with line minimization (lambda= 8.117269)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9178106 -8.3215923 0.0093586 0.4192675 -0.0034410 -0.0002364

0.0277141 3.3767669 0.0003320 1.0332290 1.8522305 -0.0007325

0.0078670 0.0011231 13.9359460 -0.0003062 -0.0000418 0.4508619

Lattice parameters(A) Cell Angles

a = 17.081863 alpha = 89.989484

b = 3.376881 beta = 89.942613

c = 13.935948 gamma = 118.683819

Current cell volume = 705.222611 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066852 0.662150 0.121796 x

x Se 2 0.132133 0.339001 0.627644 x

x Se 3 0.131437 0.339077 0.871250 x

x Se 4 0.068200 0.664786 0.376454 x

x Se 5 0.267562 0.669191 0.123470 x

x Se 6 0.332337 0.339808 0.628529 x

x Se 7 0.334004 0.344884 0.871659 x

x Se 8 0.263916 0.658496 0.369585 x

x Se 9 0.466318 0.653634 0.128636 x

x Se 10 0.530990 0.339420 0.618769 x

x Se 11 0.533651 0.345883 0.871472 x

x Se 12 0.469121 0.660952 0.381054 x

x Se 13 0.666000 0.655340 0.128474 x

x Se 14 0.736042 0.341543 0.630442 x

x Se 15 0.732464 0.330837 0.876708 x

x Se 16 0.667421 0.660340 0.371204 x

x Se 17 0.868461 0.660499 0.128853 x

x Se 18 0.932109 0.335704 0.622740 x

x Se 19 0.933132 0.337355 0.878004 x

x Se 20 0.867905 0.660870 0.372440 x

x Nb 1 0.003439 0.004300 0.249215 x

x Nb 2 -0.003511 -0.004431 0.750571 x

x Nb 3 -0.000157 -0.000342 -0.000025 x

x Nb 4 0.000268 0.000938 0.499895 x

x Nb 5 0.194317 -0.012559 0.246915 x

x Nb 6 0.201480 0.011789 0.749480 x

x Nb 7 0.199537 0.002671 -0.002246 x

x Nb 8 0.204689 0.012791 0.499743 x

x Nb 9 0.401628 -0.000166 0.252924 x

x Nb 10 0.402655 0.012956 0.750191 x

x Nb 11 0.402771 0.007542 -0.001466 x

x Nb 12 0.388681 -0.026667 0.499896 x

x Nb 13 0.597337 -0.012747 0.250147 x

x Nb 14 0.598399 0.000331 0.747267 x

x Nb 15 0.597112 -0.008049 0.001602 x

x Nb 16 0.611443 0.026959 0.500405 x

x Nb 17 0.798480 -0.011781 0.250672 x

x Nb 18 0.805862 0.013085 0.753076 x

x Nb 19 0.800500 -0.002603 0.002178 x

x Nb 20 0.795016 -0.013785 0.500374 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62590482E+004 42495.61 <-- SCF

1 -3.62622637E+004 8.03890879E-002 42523.16 <-- SCF

2 -3.62624308E+004 4.17555338E-003 42552.23 <-- SCF

3 -3.62615905E+004 -2.10061263E-002 42579.33 <-- SCF

4 -3.62599787E+004 -4.02948460E-002 42605.92 <-- SCF

5 -3.62600387E+004 1.49946358E-003 42633.08 <-- SCF

6 -3.62599891E+004 -1.24130026E-003 42659.94 <-- SCF

7 -3.62599777E+004 -2.83298489E-004 42687.22 <-- SCF

8 -3.62599785E+004 2.04459455E-005 42712.20 <-- SCF

9 -3.62599787E+004 5.20645245E-006 42734.77 <-- SCF

10 -3.62599789E+004 3.72823990E-006 42753.94 <-- SCF

11 -3.62599790E+004 3.64503090E-006 42771.61 <-- SCF

12 -3.62599792E+004 3.38485664E-006 42790.06 <-- SCF

13 -3.62599793E+004 2.48226924E-006 42807.41 <-- SCF

14 -3.62599794E+004 1.88341861E-006 42823.64 <-- SCF

15 -3.62599794E+004 1.58693969E-006 42839.98 <-- SCF

16 -3.62599795E+004 1.74321108E-006 42856.30 <-- SCF

17 -3.62599795E+004 6.13486192E-007 42872.78 <-- SCF

18 -3.62599795E+004 9.92004436E-007 42889.08 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.97954875 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.03587 -0.04201 0.03221 \*

\* Se 2 0.02110 0.06134 0.01784 \*

\* Se 3 0.13190 0.03327 -0.04954 \*

\* Se 4 -0.02812 0.00477 -0.02676 \*

\* Se 5 0.06132 -0.02416 0.03820 \*

\* Se 6 0.09961 0.06177 0.13514 \*

\* Se 7 -0.10633 0.02379 0.12143 \*

\* Se 8 0.11583 0.00472 -0.01425 \*

\* Se 9 0.06026 -0.00596 0.08366 \*

\* Se 10 0.14231 -0.15370 0.08847 \*

\* Se 11 -0.05864 0.01211 -0.08158 \*

\* Se 12 -0.19029 0.14982 -0.03375 \*

\* Se 13 0.10040 -0.03000 -0.14490 \*

\* Se 14 -0.09740 -0.01819 0.03555 \*

\* Se 15 -0.04573 0.02564 -0.08172 \*

\* Se 16 -0.07406 -0.07292 -0.04918 \*

\* Se 17 -0.14778 -0.02370 0.05769 \*

\* Se 18 0.02489 -0.01861 0.01548 \*

\* Se 19 -0.03013 0.05921 -0.01761 \*

\* Se 20 -0.03070 -0.04021 -0.01587 \*

\* Nb 1 0.05419 0.00519 0.01689 \*

\* Nb 2 -0.05427 -0.01440 -0.02654 \*

\* Nb 3 -0.00584 -0.00679 0.00397 \*

\* Nb 4 0.01732 -0.00195 -0.01559 \*

\* Nb 5 0.04822 -0.05571 -0.03115 \*

\* Nb 6 -0.07359 -0.08302 0.04963 \*

\* Nb 7 0.03239 0.02566 -0.02353 \*

\* Nb 8 -0.06269 0.00462 -0.01062 \*

\* Nb 9 -0.07282 -0.06598 0.00634 \*

\* Nb 10 -0.00650 0.05073 -0.00842 \*

\* Nb 11 -0.02735 -0.04554 0.01036 \*

\* Nb 12 -0.18138 -0.05855 -0.05723 \*

\* Nb 13 -0.00367 -0.04222 -0.04046 \*

\* Nb 14 0.06681 0.05517 -0.01675 \*

\* Nb 15 0.03478 0.04605 0.00820 \*

\* Nb 16 0.17613 0.06889 0.02591 \*

\* Nb 17 0.08310 0.08128 -0.05999 \*

\* Nb 18 -0.04671 0.05519 0.01754 \*

\* Nb 19 -0.02120 -0.02316 0.04533 \*

\* Nb 20 0.05876 -0.00247 -0.00441 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.052992 -0.017114 0.060942 \*

\* y -0.017114 0.033653 -0.001651 \*

\* z 0.060942 -0.001651 -0.064835 \*

\* \*

\* Pressure: -0.0073 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000039 | -36259.975248 | <-- min BFGS

| trial step | 1.000000 | 0.000034 | -36259.976319 | <-- min BFGS

| line step | 8.117269 | -3.335E-006 | -36259.979649 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 61 with enthalpy= -3.62599796E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.100302E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.445278E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.879026E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 6.483513E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 62 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000225 | -36259.979649 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 62 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9177653 -8.3199143 0.0077889 0.4192666 -0.0034455 -0.0001989

0.0277449 3.3761571 0.0003061 1.0332050 1.8525558 -0.0006280

0.0066196 0.0010334 13.9382707 -0.0002570 -0.0000388 0.4507867

Lattice parameters(A) Cell Angles

a = 17.081006 alpha = 89.990334

b = 3.376271 beta = 89.952178

c = 13.938272 gamma = 118.678372

Current cell volume = 705.214334 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066897 0.662115 0.121773 x

x Se 2 0.132131 0.339377 0.627726 x

x Se 3 0.131493 0.339605 0.871076 x

x Se 4 0.068240 0.664861 0.376439 x

x Se 5 0.267609 0.669300 0.123458 x

x Se 6 0.332439 0.340310 0.628703 x

x Se 7 0.333967 0.344990 0.871695 x

x Se 8 0.263957 0.658655 0.369491 x

x Se 9 0.466307 0.653520 0.128802 x

x Se 10 0.531064 0.339245 0.618803 x

x Se 11 0.533662 0.345991 0.871315 x

x Se 12 0.468998 0.660981 0.381079 x

x Se 13 0.666033 0.655220 0.128411 x

x Se 14 0.736013 0.341383 0.630552 x

x Se 15 0.732427 0.330763 0.876679 x

x Se 16 0.667348 0.659862 0.371157 x

x Se 17 0.868401 0.659992 0.129031 x

x Se 18 0.932074 0.335609 0.622717 x

x Se 19 0.933087 0.337425 0.878027 x

x Se 20 0.867904 0.660540 0.372369 x

x Nb 1 0.003593 0.004586 0.249211 x

x Nb 2 -0.003666 -0.004750 0.750560 x

x Nb 3 -0.000163 -0.000369 -0.000025 x

x Nb 4 0.000282 0.000983 0.499882 x

x Nb 5 0.194247 -0.012929 0.246828 x

x Nb 6 0.201520 0.011803 0.749518 x

x Nb 7 0.199554 0.002890 -0.002352 x

x Nb 8 0.204775 0.013141 0.499784 x

x Nb 9 0.401594 -0.000469 0.252969 x

x Nb 10 0.402708 0.013615 0.750218 x

x Nb 11 0.402819 0.007545 -0.001451 x

x Nb 12 0.388362 -0.027668 0.499796 x

x Nb 13 0.597275 -0.013403 0.250071 x

x Nb 14 0.598426 0.000597 0.747213 x

x Nb 15 0.597067 -0.008046 0.001602 x

x Nb 16 0.611765 0.028012 0.500477 x

x Nb 17 0.798448 -0.011769 0.250621 x

x Nb 18 0.805932 0.013458 0.753155 x

x Nb 19 0.800490 -0.002805 0.002305 x

x Nb 20 0.794920 -0.014165 0.500313 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598951E+004 42992.67 <-- SCF

1 -3.62600981E+004 5.07357334E-003 43018.05 <-- SCF

2 -3.62601133E+004 3.81149623E-004 43046.47 <-- SCF

3 -3.62600288E+004 -2.11456563E-003 43073.06 <-- SCF

4 -3.62599896E+004 -9.78930182E-004 43098.66 <-- SCF

5 -3.62599858E+004 -9.42444211E-005 43123.61 <-- SCF

6 -3.62599851E+004 -1.76663220E-005 43147.27 <-- SCF

7 -3.62599851E+004 -5.94828370E-007 43167.48 <-- SCF

8 -3.62599851E+004 4.07169555E-007 43185.33 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.98511342 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.03048 -0.03396 0.02299 \*

\* Se 2 0.02402 0.04433 0.00573 \*

\* Se 3 0.12647 0.00491 -0.02666 \*

\* Se 4 -0.02187 0.00283 -0.01714 \*

\* Se 5 0.05933 -0.02190 0.03877 \*

\* Se 6 0.08874 0.03611 0.08729 \*

\* Se 7 -0.09514 0.01693 0.11405 \*

\* Se 8 0.08919 -0.00284 -0.00150 \*

\* Se 9 0.06209 -0.01422 0.03968 \*

\* Se 10 0.11733 -0.13237 0.07071 \*

\* Se 11 -0.06392 0.02488 -0.04554 \*

\* Se 12 -0.15002 0.13275 -0.02562 \*

\* Se 13 0.09043 -0.02449 -0.12954 \*

\* Se 14 -0.07516 -0.00739 0.01852 \*

\* Se 15 -0.04714 0.02368 -0.06766 \*

\* Se 16 -0.06910 -0.05451 -0.03594 \*

\* Se 17 -0.13164 0.00622 0.02570 \*

\* Se 18 0.01887 -0.01547 0.00975 \*

\* Se 19 -0.02589 0.05015 -0.00460 \*

\* Se 20 -0.03195 -0.02632 -0.00455 \*

\* Nb 1 0.04062 0.00514 0.01762 \*

\* Nb 2 -0.04313 -0.01272 -0.02577 \*

\* Nb 3 -0.00620 -0.00574 0.00454 \*

\* Nb 4 0.01620 -0.00226 -0.01522 \*

\* Nb 5 0.05700 -0.05277 -0.02304 \*

\* Nb 6 -0.07434 -0.06516 0.04089 \*

\* Nb 7 0.03021 0.02736 -0.01739 \*

\* Nb 8 -0.07429 0.00672 -0.01678 \*

\* Nb 9 -0.07054 -0.05583 0.00131 \*

\* Nb 10 -0.01084 0.04384 -0.00439 \*

\* Nb 11 -0.02640 -0.04595 0.01535 \*

\* Nb 12 -0.16365 -0.04805 -0.03704 \*

\* Nb 13 0.00335 -0.03754 -0.02949 \*

\* Nb 14 0.06429 0.04557 -0.00898 \*

\* Nb 15 0.03381 0.04597 -0.00009 \*

\* Nb 16 0.15379 0.05586 0.01623 \*

\* Nb 17 0.07871 0.06426 -0.04509 \*

\* Nb 18 -0.05424 0.05160 0.00950 \*

\* Nb 19 -0.02180 -0.02469 0.03621 \*

\* Nb 20 0.07233 -0.00494 0.00721 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.037659 -0.006126 0.028705 \*

\* y -0.006126 0.012927 -0.005991 \*

\* z 0.028705 -0.005991 -0.038545 \*

\* \*

\* Pressure: -0.0040 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000225 | -36259.979649 | <-- min BFGS

| trial step | 1.000000 | 0.000170 | -36259.985207 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 62 with line minimization (lambda= 4.101092)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9176248 -8.3147104 0.0029209 0.4192640 -0.0034593 -0.0000825

0.0278404 3.3742661 0.0002258 1.0331309 1.8535653 -0.0003043

0.0027515 0.0007554 13.9454796 -0.0001045 -0.0000293 0.4505536

Lattice parameters(A) Cell Angles

a = 17.078347 alpha = 89.992969

b = 3.374381 beta = 89.981837

c = 13.945480 gamma = 118.661473

Current cell volume = 705.188307 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067038 0.662006 0.121702 x

x Se 2 0.132126 0.340543 0.627981 x

x Se 3 0.131670 0.341245 0.870537 x

x Se 4 0.068364 0.665095 0.376395 x

x Se 5 0.267757 0.669638 0.123421 x

x Se 6 0.332755 0.341869 0.629243 x

x Se 7 0.333851 0.345317 0.871808 x

x Se 8 0.264084 0.659148 0.369200 x

x Se 9 0.466273 0.653164 0.129314 x

x Se 10 0.531294 0.338702 0.618907 x

x Se 11 0.533698 0.346327 0.870827 x

x Se 12 0.468618 0.661073 0.381157 x

x Se 13 0.666137 0.654847 0.128217 x

x Se 14 0.735925 0.340887 0.630894 x

x Se 15 0.732312 0.330533 0.876590 x

x Se 16 0.667120 0.658379 0.371012 x

x Se 17 0.868216 0.658420 0.129585 x

x Se 18 0.931968 0.335313 0.622646 x

x Se 19 0.932950 0.337644 0.878098 x

x Se 20 0.867901 0.659515 0.372148 x

x Nb 1 0.004071 0.005473 0.249198 x

x Nb 2 -0.004146 -0.005741 0.750526 x

x Nb 3 -0.000180 -0.000450 -0.000026 x

x Nb 4 0.000326 0.001122 0.499842 x

x Nb 5 0.194028 -0.014076 0.246559 x

x Nb 6 0.201642 0.011847 0.749635 x

x Nb 7 0.199608 0.003570 -0.002683 x

x Nb 8 0.205039 0.014226 0.499911 x

x Nb 9 0.401488 -0.001406 0.253109 x

x Nb 10 0.402872 0.015656 0.750303 x

x Nb 11 0.402967 0.007556 -0.001406 x

x Nb 12 0.387370 -0.030773 0.499484 x

x Nb 13 0.597082 -0.015437 0.249833 x

x Nb 14 0.598510 0.001420 0.747047 x

x Nb 15 0.596925 -0.008039 0.001603 x

x Nb 16 0.612762 0.031275 0.500701 x

x Nb 17 0.798348 -0.011729 0.250460 x

x Nb 18 0.806151 0.014615 0.753400 x

x Nb 19 0.800458 -0.003431 0.002698 x

x Nb 20 0.794623 -0.015343 0.500124 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62591240E+004 43288.45 <-- SCF

1 -3.62611840E+004 5.15003541E-002 43314.61 <-- SCF

2 -3.62613440E+004 3.99953482E-003 43344.17 <-- SCF

3 -3.62605112E+004 -2.08194378E-002 43371.05 <-- SCF

4 -3.62600319E+004 -1.19822498E-002 43396.88 <-- SCF

5 -3.62600085E+004 -5.87254746E-004 43423.05 <-- SCF

6 -3.62599931E+004 -3.83941910E-004 43449.14 <-- SCF

7 -3.62599915E+004 -4.06617635E-005 43474.94 <-- SCF

8 -3.62599919E+004 1.10230715E-005 43498.25 <-- SCF

9 -3.62599916E+004 -6.68121318E-006 43518.22 <-- SCF

10 -3.62599917E+004 4.46386358E-007 43536.59 <-- SCF

11 -3.62599917E+004 9.51970000E-007 43554.06 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.99170475 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00367 -0.01007 -0.01148 \*

\* Se 2 0.02658 -0.00592 -0.02615 \*

\* Se 3 0.03639 -0.11331 0.10736 \*

\* Se 4 -0.01386 -0.00127 0.02481 \*

\* Se 5 0.05529 -0.02084 0.02398 \*

\* Se 6 0.04957 -0.01094 -0.07514 \*

\* Se 7 -0.05806 0.00202 0.09461 \*

\* Se 8 0.00793 -0.02028 0.03573 \*

\* Se 9 0.05165 -0.03450 -0.12598 \*

\* Se 10 0.02112 -0.05802 -0.00542 \*

\* Se 11 -0.06272 0.05341 0.10685 \*

\* Se 12 0.01169 0.06684 0.02597 \*

\* Se 13 0.05463 -0.01284 -0.08180 \*

\* Se 14 -0.00674 0.01861 -0.03156 \*

\* Se 15 -0.04985 0.02206 -0.00915 \*

\* Se 16 -0.06462 -0.01235 0.01194 \*

\* Se 17 -0.02288 0.12264 -0.13065 \*

\* Se 18 0.00938 -0.00643 -0.01790 \*

\* Se 19 0.00465 0.02260 0.03606 \*

\* Se 20 -0.02964 0.01481 0.02622 \*

\* Nb 1 -0.00265 0.00365 0.01438 \*

\* Nb 2 -0.00478 -0.00617 -0.01993 \*

\* Nb 3 -0.00752 -0.00197 0.00370 \*

\* Nb 4 0.01550 -0.00351 -0.01253 \*

\* Nb 5 0.08608 -0.03710 0.00136 \*

\* Nb 6 -0.07126 -0.01113 0.01513 \*

\* Nb 7 0.02486 0.02824 0.00730 \*

\* Nb 8 -0.09935 0.01084 -0.03767 \*

\* Nb 9 -0.05403 -0.02368 -0.01464 \*

\* Nb 10 -0.03326 0.00721 0.01491 \*

\* Nb 11 -0.02241 -0.04500 0.02303 \*

\* Nb 12 -0.12170 -0.01403 0.02594 \*

\* Nb 13 0.03318 -0.00554 0.00087 \*

\* Nb 14 0.05008 0.01298 0.01413 \*

\* Nb 15 0.02795 0.04415 -0.02034 \*

\* Nb 16 0.10016 0.01313 -0.01759 \*

\* Nb 17 0.05690 0.01203 -0.00008 \*

\* Nb 18 -0.07409 0.03433 -0.01768 \*

\* Nb 19 -0.02282 -0.02445 -0.00390 \*

\* Nb 20 0.10231 -0.01019 0.04531 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.006095 0.033731 -0.069050 \*

\* y 0.033731 -0.054345 -0.028267 \*

\* z -0.069050 -0.028267 0.005425 \*

\* \*

\* Pressure: 0.0143 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000225 | -36259.979649 | <-- min BFGS

| trial step | 1.000000 | 0.000170 | -36259.985207 | <-- min BFGS

| line step | 4.101092 | -0.000025 | -36259.991831 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 62 with enthalpy= -3.62599918E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 3.045524E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.806509E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.070658E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 6.904979E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 63 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000188 | -36259.991831 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 63 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9182645 -8.3231780 0.0062571 0.4193417 -0.0032844 -0.0001814

0.0264358 3.3752491 0.0006135 1.0340736 1.8534481 -0.0007176

0.0060468 0.0020252 13.9437956 -0.0002337 -0.0000801 0.4506081

Lattice parameters(A) Cell Angles

a = 17.083031 alpha = 89.981070

b = 3.375353 beta = 89.961370

c = 13.943797 gamma = 118.709210

Current cell volume = 705.177851 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066983 0.661625 0.121666 x

x Se 2 0.132139 0.340237 0.627768 x

x Se 3 0.131736 0.341015 0.870749 x

x Se 4 0.068307 0.664848 0.376312 x

x Se 5 0.267805 0.670018 0.123495 x

x Se 6 0.332847 0.341565 0.629070 x

x Se 7 0.333841 0.345052 0.871992 x

x Se 8 0.264086 0.659214 0.369221 x

x Se 9 0.466297 0.653383 0.129190 x

x Se 10 0.531149 0.337969 0.618818 x

x Se 11 0.533673 0.346105 0.870958 x

x Se 12 0.468737 0.661722 0.381242 x

x Se 13 0.666150 0.655135 0.128030 x

x Se 14 0.735917 0.340794 0.630869 x

x Se 15 0.732274 0.330189 0.876500 x

x Se 16 0.667024 0.658674 0.371191 x

x Se 17 0.868150 0.658670 0.129383 x

x Se 18 0.932040 0.335540 0.622676 x

x Se 19 0.933004 0.337996 0.878138 x

x Se 20 0.867888 0.659836 0.372373 x

x Nb 1 0.003797 0.004423 0.249188 x

x Nb 2 -0.003870 -0.004720 0.750528 x

x Nb 3 -0.000189 -0.000490 -0.000022 x

x Nb 4 0.000343 0.001139 0.499839 x

x Nb 5 0.194114 -0.014306 0.246499 x

x Nb 6 0.201440 0.011220 0.749663 x

x Nb 7 0.199649 0.003506 -0.002661 x

x Nb 8 0.205058 0.013862 0.499827 x

x Nb 9 0.401615 -0.001469 0.253232 x

x Nb 10 0.402836 0.015573 0.750391 x

x Nb 11 0.402948 0.007304 -0.001405 x

x Nb 12 0.386927 -0.031854 0.499255 x

x Nb 13 0.597117 -0.015312 0.249748 x

x Nb 14 0.598384 0.001508 0.746922 x

x Nb 15 0.596948 -0.007795 0.001617 x

x Nb 16 0.613206 0.032411 0.500930 x

x Nb 17 0.798549 -0.011094 0.250444 x

x Nb 18 0.806063 0.014825 0.753463 x

x Nb 19 0.800420 -0.003344 0.002695 x

x Nb 20 0.794600 -0.014974 0.500207 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598011E+004 43657.55 <-- SCF

1 -3.62602661E+004 1.16252590E-002 43683.45 <-- SCF

2 -3.62602976E+004 7.87065656E-004 43712.41 <-- SCF

3 -3.62601254E+004 -4.30635769E-003 43738.94 <-- SCF

4 -3.62600027E+004 -3.06620614E-003 43764.70 <-- SCF

5 -3.62599980E+004 -1.16527814E-004 43791.19 <-- SCF

6 -3.62599956E+004 -6.24115114E-005 43816.48 <-- SCF

7 -3.62599954E+004 -4.36416829E-006 43838.42 <-- SCF

8 -3.62599954E+004 1.77039789E-006 43858.55 <-- SCF

9 -3.62599954E+004 -3.30735946E-007 43876.09 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.99543570 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00620 0.00843 0.00813 \*

\* Se 2 0.03277 -0.00695 0.01927 \*

\* Se 3 0.03636 -0.07853 0.05846 \*

\* Se 4 -0.01708 0.00384 0.02440 \*

\* Se 5 0.06392 -0.03327 0.01656 \*

\* Se 6 0.03488 0.01011 -0.00748 \*

\* Se 7 -0.05051 0.02500 0.02233 \*

\* Se 8 -0.01041 -0.02866 -0.00590 \*

\* Se 9 0.04915 -0.03521 -0.08229 \*

\* Se 10 0.07268 -0.03620 -0.01215 \*

\* Se 11 -0.05924 0.05389 0.06131 \*

\* Se 12 -0.02900 0.04867 0.03500 \*

\* Se 13 0.04637 -0.03692 -0.00726 \*

\* Se 14 0.01115 0.02874 0.01146 \*

\* Se 15 -0.06195 0.03493 0.00579 \*

\* Se 16 -0.03853 -0.05859 -0.07295 \*

\* Se 17 -0.02348 0.08892 -0.08187 \*

\* Se 18 0.00863 -0.00718 -0.01092 \*

\* Se 19 -0.00452 0.00926 0.01899 \*

\* Se 20 -0.03525 0.01851 -0.02914 \*

\* Nb 1 0.02127 0.00424 0.01343 \*

\* Nb 2 -0.03023 -0.00573 -0.01724 \*

\* Nb 3 -0.00715 -0.00145 0.00387 \*

\* Nb 4 0.01535 -0.00263 -0.01249 \*

\* Nb 5 0.07419 -0.02687 0.00393 \*

\* Nb 6 -0.04426 -0.01646 0.00910 \*

\* Nb 7 0.02829 0.03266 0.01513 \*

\* Nb 8 -0.11213 0.01737 -0.03668 \*

\* Nb 9 -0.05705 -0.00776 -0.03676 \*

\* Nb 10 -0.03694 0.00173 0.01574 \*

\* Nb 11 -0.01718 -0.04289 0.03155 \*

\* Nb 12 -0.08299 -0.01189 0.04411 \*

\* Nb 13 0.03518 0.00011 0.00228 \*

\* Nb 14 0.05008 -0.00234 0.03762 \*

\* Nb 15 0.02025 0.04389 -0.03052 \*

\* Nb 16 0.05701 0.01013 -0.03458 \*

\* Nb 17 0.02949 0.01815 0.00637 \*

\* Nb 18 -0.06214 0.02544 -0.02208 \*

\* Nb 19 -0.02759 -0.02800 -0.01228 \*

\* Nb 20 0.11443 -0.01650 0.04776 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.003643 -0.000280 -0.035848 \*

\* y -0.000280 -0.028160 -0.002928 \*

\* z -0.035848 -0.002928 -0.022160 \*

\* \*

\* Pressure: 0.0180 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000188 | -36259.991831 | <-- min BFGS

| trial step | 1.000000 | 0.000053 | -36259.995565 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 63 with enthalpy= -3.62599956E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 9.335115E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.250872E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.382199E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.584799E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 64 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000081 | -36259.995565 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 64 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9130251 -8.3269967 0.0096512 0.4195002 -0.0032630 -0.0002664

0.0262636 3.3764474 0.0007386 1.0345718 1.8528393 -0.0009838

0.0088749 0.0024480 13.9436567 -0.0003452 -0.0000959 0.4506127

Lattice parameters(A) Cell Angles

a = 17.080319 alpha = 89.977124

b = 3.376550 beta = 89.940689

c = 13.943660 gamma = 118.732034

Current cell volume = 705.154646 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066974 0.661444 0.121705 x

x Se 2 0.132152 0.340323 0.627730 x

x Se 3 0.131831 0.340806 0.870855 x

x Se 4 0.068252 0.664857 0.376345 x

x Se 5 0.267736 0.669737 0.123496 x

x Se 6 0.333073 0.342101 0.628930 x

x Se 7 0.333853 0.345257 0.872173 x

x Se 8 0.264183 0.659483 0.369468 x

x Se 9 0.466443 0.654049 0.129079 x

x Se 10 0.531216 0.337592 0.619037 x

x Se 11 0.533524 0.345467 0.871069 x

x Se 12 0.468659 0.662099 0.381053 x

x Se 13 0.666131 0.654892 0.127836 x

x Se 14 0.735824 0.340499 0.630630 x

x Se 15 0.732349 0.330501 0.876463 x

x Se 16 0.666813 0.658077 0.371316 x

x Se 17 0.868061 0.658943 0.129262 x

x Se 18 0.932086 0.335525 0.622668 x

x Se 19 0.933011 0.338204 0.878117 x

x Se 20 0.867871 0.659777 0.372420 x

x Nb 1 0.003788 0.004545 0.249223 x

x Nb 2 -0.003858 -0.004858 0.750495 x

x Nb 3 -0.000186 -0.000498 -0.000019 x

x Nb 4 0.000341 0.001116 0.499835 x

x Nb 5 0.194325 -0.013910 0.246572 x

x Nb 6 0.201405 0.010972 0.749717 x

x Nb 7 0.199678 0.003664 -0.002641 x

x Nb 8 0.204907 0.013618 0.499856 x

x Nb 9 0.401487 -0.002080 0.253165 x

x Nb 10 0.402786 0.015589 0.750393 x

x Nb 11 0.402877 0.007026 -0.001356 x

x Nb 12 0.387205 -0.031402 0.499244 x

x Nb 13 0.597168 -0.015312 0.249734 x

x Nb 14 0.598511 0.002078 0.746981 x

x Nb 15 0.597025 -0.007493 0.001572 x

x Nb 16 0.612917 0.031942 0.500929 x

x Nb 17 0.798581 -0.010867 0.250396 x

x Nb 18 0.805846 0.014406 0.753388 x

x Nb 19 0.800394 -0.003486 0.002693 x

x Nb 20 0.794763 -0.014683 0.500171 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598992E+004 43979.28 <-- SCF

1 -3.62601548E+004 6.39084304E-003 44005.62 <-- SCF

2 -3.62601689E+004 3.53854806E-004 44033.78 <-- SCF

3 -3.62600867E+004 -2.05736520E-003 44060.38 <-- SCF

4 -3.62599979E+004 -2.21810018E-003 44086.11 <-- SCF

5 -3.62599993E+004 3.33047482E-005 44112.58 <-- SCF

6 -3.62599969E+004 -5.86455642E-005 44137.17 <-- SCF

7 -3.62599965E+004 -9.68731987E-006 44158.52 <-- SCF

8 -3.62599966E+004 2.37686986E-006 44178.52 <-- SCF

9 -3.62599966E+004 3.22523893E-008 44195.91 <-- SCF

10 -3.62599966E+004 3.94072436E-007 44212.52 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.99664191 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01071 0.02194 0.01337 \*

\* Se 2 0.03286 -0.01610 0.04214 \*

\* Se 3 0.01694 -0.03797 0.03715 \*

\* Se 4 -0.01007 -0.00193 0.00593 \*

\* Se 5 0.06492 -0.03058 0.02271 \*

\* Se 6 -0.00273 0.02844 0.02863 \*

\* Se 7 -0.04038 0.01824 -0.04246 \*

\* Se 8 -0.03444 -0.03518 -0.04786 \*

\* Se 9 0.02256 -0.03923 -0.04666 \*

\* Se 10 0.05427 -0.00801 -0.02178 \*

\* Se 11 -0.03043 0.05478 0.02551 \*

\* Se 12 -0.00742 0.02327 0.03769 \*

\* Se 13 0.03662 -0.02744 0.06134 \*

\* Se 14 0.03242 0.03894 0.04788 \*

\* Se 15 -0.06488 0.03121 0.01211 \*

\* Se 16 0.00462 -0.07500 -0.11418 \*

\* Se 17 -0.00959 0.04460 -0.05262 \*

\* Se 18 0.00922 -0.00493 -0.00210 \*

\* Se 19 -0.00974 -0.00570 0.00890 \*

\* Se 20 -0.03351 0.02607 -0.05550 \*

\* Nb 1 0.01274 0.00014 0.00850 \*

\* Nb 2 -0.02370 0.00003 -0.01029 \*

\* Nb 3 -0.00681 -0.00050 0.00414 \*

\* Nb 4 0.01384 -0.00240 -0.01037 \*

\* Nb 5 0.05002 -0.02296 0.00821 \*

\* Nb 6 -0.02772 -0.01375 -0.00651 \*

\* Nb 7 0.01892 0.02623 0.02114 \*

\* Nb 8 -0.08112 0.01315 -0.03187 \*

\* Nb 9 -0.04567 0.01353 -0.04219 \*

\* Nb 10 -0.04169 -0.00041 0.02528 \*

\* Nb 11 -0.01638 -0.03467 0.03325 \*

\* Nb 12 -0.10286 0.00445 0.03625 \*

\* Nb 13 0.03872 -0.00075 -0.00460 \*

\* Nb 14 0.03706 -0.02115 0.04550 \*

\* Nb 15 0.01764 0.03520 -0.03334 \*

\* Nb 16 0.07948 -0.00711 -0.02370 \*

\* Nb 17 0.01452 0.01697 0.02044 \*

\* Nb 18 -0.03771 0.02210 -0.02344 \*

\* Nb 19 -0.02050 -0.02092 -0.02049 \*

\* Nb 20 0.07928 -0.01257 0.04390 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.009218 -0.000872 0.018086 \*

\* y -0.000872 0.013742 0.001066 \*

\* z 0.018086 0.001066 -0.012683 \*

\* \*

\* Pressure: -0.0034 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000081 | -36259.995565 | <-- min BFGS

| trial step | 1.000000 | -0.000016 | -36259.996758 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 64 with enthalpy= -3.62599968E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.981561E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.366843E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.395636E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.808592E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 65 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000030 | -36259.996758 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 65 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.9144905 -8.3276154 0.0102205 0.4194873 -0.0032121 -0.0002816

0.0258509 3.3760048 0.0007742 1.0347526 1.8532073 -0.0010368

0.0093808 0.0025643 13.9457068 -0.0003649 -0.0001005 0.4505465

Lattice parameters(A) Cell Angles

a = 17.081900 alpha = 89.976031

b = 3.376104 beta = 89.937204

c = 13.945710 gamma = 118.738393

Current cell volume = 705.187507 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066957 0.661195 0.121681 x

x Se 2 0.132127 0.340346 0.627724 x

x Se 3 0.131853 0.340812 0.870844 x

x Se 4 0.068253 0.664811 0.376315 x

x Se 5 0.267774 0.669804 0.123518 x

x Se 6 0.333120 0.342229 0.628971 x

x Se 7 0.333834 0.345276 0.872148 x

x Se 8 0.264173 0.659357 0.369395 x

x Se 9 0.466478 0.654042 0.129140 x

x Se 10 0.531123 0.337262 0.618945 x

x Se 11 0.533487 0.345469 0.871014 x

x Se 12 0.468733 0.662413 0.381157 x

x Se 13 0.666147 0.654863 0.127854 x

x Se 14 0.735835 0.340609 0.630707 x

x Se 15 0.732319 0.330462 0.876424 x

x Se 16 0.666769 0.657923 0.371279 x

x Se 17 0.868038 0.658959 0.129273 x

x Se 18 0.932095 0.335559 0.622666 x

x Se 19 0.933027 0.338452 0.878145 x

x Se 20 0.867894 0.659777 0.372436 x

x Nb 1 0.003724 0.004145 0.249195 x

x Nb 2 -0.003796 -0.004480 0.750513 x

x Nb 3 -0.000194 -0.000531 -0.000017 x

x Nb 4 0.000355 0.001142 0.499827 x

x Nb 5 0.194274 -0.014146 0.246475 x

x Nb 6 0.201333 0.010838 0.749744 x

x Nb 7 0.199692 0.003733 -0.002661 x

x Nb 8 0.204969 0.013606 0.499801 x

x Nb 9 0.401548 -0.002292 0.253253 x

x Nb 10 0.402814 0.015752 0.750439 x

x Nb 11 0.402908 0.007017 -0.001379 x

x Nb 12 0.386814 -0.032390 0.499147 x

x Nb 13 0.597137 -0.015449 0.249688 x

x Nb 14 0.598451 0.002288 0.746893 x

x Nb 15 0.596994 -0.007492 0.001608 x

x Nb 16 0.613308 0.032953 0.501026 x

x Nb 17 0.798653 -0.010738 0.250380 x

x Nb 18 0.805900 0.014645 0.753482 x

x Nb 19 0.800385 -0.003536 0.002724 x

x Nb 20 0.794694 -0.014684 0.500226 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599141E+004 44316.55 <-- SCF

1 -3.62600938E+004 4.49204373E-003 44340.67 <-- SCF

2 -3.62601098E+004 4.01332716E-004 44368.91 <-- SCF

3 -3.62600357E+004 -1.85343102E-003 44395.61 <-- SCF

4 -3.62600027E+004 -8.23934980E-004 44421.38 <-- SCF

5 -3.62599987E+004 -9.94621425E-005 44447.02 <-- SCF

6 -3.62599974E+004 -3.33783538E-005 44470.81 <-- SCF

7 -3.62599973E+004 -1.65787849E-006 44491.09 <-- SCF

8 -3.62599974E+004 1.60154493E-006 44509.33 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.99740949 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01207 0.03537 0.01564 \*

\* Se 2 0.04744 -0.02446 0.04645 \*

\* Se 3 0.01301 -0.03508 0.05031 \*

\* Se 4 -0.01137 -0.00133 0.00409 \*

\* Se 5 0.06649 -0.03093 0.01447 \*

\* Se 6 -0.02259 0.02275 0.02039 \*

\* Se 7 -0.04262 0.01162 -0.02982 \*

\* Se 8 -0.04756 -0.02692 -0.05167 \*

\* Se 9 0.00871 -0.03727 -0.07012 \*

\* Se 10 0.09083 -0.00019 -0.02460 \*

\* Se 11 -0.01829 0.05437 0.04623 \*

\* Se 12 -0.03867 0.01302 0.03875 \*

\* Se 13 0.03790 -0.02070 0.05236 \*

\* Se 14 0.04492 0.03167 0.05086 \*

\* Se 15 -0.06852 0.03011 0.02600 \*

\* Se 16 0.02149 -0.06599 -0.10693 \*

\* Se 17 -0.00498 0.03982 -0.06410 \*

\* Se 18 0.01069 -0.00330 0.00121 \*

\* Se 19 -0.00856 -0.01800 0.00835 \*

\* Se 20 -0.04459 0.03328 -0.06283 \*

\* Nb 1 0.01774 -0.00099 0.00706 \*

\* Nb 2 -0.02733 0.00069 -0.00929 \*

\* Nb 3 -0.00615 -0.00044 0.00407 \*

\* Nb 4 0.01541 -0.00296 -0.01096 \*

\* Nb 5 0.05303 -0.02742 0.00772 \*

\* Nb 6 -0.02913 -0.01324 -0.00858 \*

\* Nb 7 0.02376 0.02709 0.01888 \*

\* Nb 8 -0.09702 0.01726 -0.03433 \*

\* Nb 9 -0.04294 0.01944 -0.05103 \*

\* Nb 10 -0.04448 0.00192 0.02750 \*

\* Nb 11 -0.01454 -0.03698 0.03726 \*

\* Nb 12 -0.08029 0.00747 0.04558 \*

\* Nb 13 0.03936 -0.00381 -0.00645 \*

\* Nb 14 0.03183 -0.02629 0.05450 \*

\* Nb 15 0.01411 0.03676 -0.03769 \*

\* Nb 16 0.05319 -0.01083 -0.03410 \*

\* Nb 17 0.01546 0.01700 0.02150 \*

\* Nb 18 -0.03899 0.02573 -0.02538 \*

\* Nb 19 -0.02456 -0.02144 -0.01886 \*

\* Nb 20 0.09578 -0.01677 0.04759 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.036492 -0.018441 0.009454 \*

\* y -0.018441 -0.005403 0.002619 \*

\* z 0.009454 0.002619 -0.007609 \*

\* \*

\* Pressure: -0.0078 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000030 | -36259.996758 | <-- min BFGS

| trial step | 1.000000 | 6.588E-006 | -36259.997525 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 65 with enthalpy= -3.62599975E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.917944E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.274796E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.012084E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.649242E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 66 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000018 | -36259.997525 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 66 with trial guess (lambda= 1.000000)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.9103185 -8.3260253 0.0101709 0.4195815 -0.0032541 -0.0002785

0.0261831 3.3759234 0.0007402 1.0348123 1.8531497 -0.0010140

0.0092776 0.0024517 13.9484913 -0.0003609 -0.0000960 0.4504565

Lattice parameters(A) Cell Angles

a = 17.077482 alpha = 89.977072

b = 3.376025 beta = 89.937513

c = 13.948495 gamma = 118.734912

Current cell volume = 705.152942 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066947 0.661089 0.121695 x

x Se 2 0.132129 0.340327 0.627698 x

x Se 3 0.131869 0.340879 0.870860 x

x Se 4 0.068244 0.664720 0.376267 x

x Se 5 0.267816 0.669943 0.123555 x

x Se 6 0.333093 0.342063 0.628989 x

x Se 7 0.333808 0.345167 0.872115 x

x Se 8 0.264169 0.659322 0.369334 x

x Se 9 0.466470 0.653921 0.129167 x

x Se 10 0.531089 0.337170 0.618899 x

x Se 11 0.533494 0.345592 0.870986 x

x Se 12 0.468766 0.662502 0.381208 x

x Se 13 0.666174 0.654973 0.127886 x

x Se 14 0.735837 0.340641 0.630769 x

x Se 15 0.732280 0.330334 0.876387 x

x Se 16 0.666798 0.658068 0.371262 x

x Se 17 0.868023 0.658898 0.129260 x

x Se 18 0.932109 0.335639 0.622697 x

x Se 19 0.933037 0.338565 0.878134 x

x Se 20 0.867892 0.659809 0.372461 x

x Nb 1 0.003658 0.003888 0.249185 x

x Nb 2 -0.003732 -0.004230 0.750518 x

x Nb 3 -0.000198 -0.000549 -0.000014 x

x Nb 4 0.000363 0.001157 0.499821 x

x Nb 5 0.194244 -0.014301 0.246438 x

x Nb 6 0.201272 0.010637 0.749750 x

x Nb 7 0.199699 0.003707 -0.002644 x

x Nb 8 0.204981 0.013491 0.499752 x

x Nb 9 0.401593 -0.002222 0.253284 x

x Nb 10 0.402806 0.015618 0.750463 x

x Nb 11 0.402910 0.006967 -0.001394 x

x Nb 12 0.386614 -0.032827 0.499113 x

x Nb 13 0.597143 -0.015313 0.249665 x

x Nb 14 0.598405 0.002220 0.746863 x

x Nb 15 0.596992 -0.007447 0.001630 x

x Nb 16 0.613507 0.033394 0.501060 x

x Nb 17 0.798714 -0.010536 0.250378 x

x Nb 18 0.805932 0.014802 0.753515 x

x Nb 19 0.800379 -0.003498 0.002710 x

x Nb 20 0.794677 -0.014577 0.500278 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599719E+004 44612.66 <-- SCF

1 -3.62600974E+004 3.13652317E-003 44639.81 <-- SCF

2 -3.62601050E+004 1.89908856E-004 44666.47 <-- SCF

3 -3.62600933E+004 -2.90562848E-004 44692.98 <-- SCF

4 -3.62599955E+004 -2.44489259E-003 44718.88 <-- SCF

5 -3.62600012E+004 1.41926337E-004 44745.38 <-- SCF

6 -3.62599990E+004 -5.47974586E-005 44769.39 <-- SCF

7 -3.62599983E+004 -1.88334815E-005 44790.20 <-- SCF

8 -3.62599982E+004 -1.67581937E-006 44809.33 <-- SCF

9 -3.62599983E+004 1.57725911E-006 44827.44 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.99827464 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00904 0.03550 0.01084 \*

\* Se 2 0.04940 -0.02580 0.05331 \*

\* Se 3 0.01587 -0.03657 0.05289 \*

\* Se 4 -0.02224 -0.00029 0.00771 \*

\* Se 5 0.06508 -0.03395 0.00737 \*

\* Se 6 -0.01813 0.02558 0.02162 \*

\* Se 7 -0.04393 0.01491 -0.02193 \*

\* Se 8 -0.05939 -0.02809 -0.05256 \*

\* Se 9 0.00619 -0.03608 -0.07762 \*

\* Se 10 0.09962 0.00228 -0.03351 \*

\* Se 11 -0.01611 0.05363 0.05304 \*

\* Se 12 -0.04713 0.00949 0.04912 \*

\* Se 13 0.03863 -0.02435 0.04457 \*

\* Se 14 0.05599 0.03258 0.05220 \*

\* Se 15 -0.06859 0.03285 0.03126 \*

\* Se 16 0.01442 -0.06844 -0.10638 \*

\* Se 17 -0.00830 0.04116 -0.06675 \*

\* Se 18 0.01825 -0.00342 0.00202 \*

\* Se 19 -0.00490 -0.01845 0.01129 \*

\* Se 20 -0.04536 0.03446 -0.06953 \*

\* Nb 1 0.02936 0.00398 0.00742 \*

\* Nb 2 -0.04016 -0.00419 -0.01031 \*

\* Nb 3 -0.00472 -0.00017 0.00379 \*

\* Nb 4 0.01713 -0.00280 -0.01043 \*

\* Nb 5 0.06275 -0.02253 0.01084 \*

\* Nb 6 -0.03061 -0.01348 -0.01190 \*

\* Nb 7 0.02256 0.02715 0.02110 \*

\* Nb 8 -0.09690 0.02249 -0.03590 \*

\* Nb 9 -0.04315 0.02397 -0.05581 \*

\* Nb 10 -0.04647 0.00013 0.02236 \*

\* Nb 11 -0.01639 -0.03643 0.03934 \*

\* Nb 12 -0.07834 0.00910 0.05093 \*

\* Nb 13 0.04125 -0.00280 -0.00091 \*

\* Nb 14 0.03256 -0.03198 0.06047 \*

\* Nb 15 0.01560 0.03724 -0.04169 \*

\* Nb 16 0.05176 -0.01211 -0.03986 \*

\* Nb 17 0.01815 0.01819 0.02259 \*

\* Nb 18 -0.04653 0.02153 -0.02786 \*

\* Nb 19 -0.02372 -0.02168 -0.02214 \*

\* Nb 20 0.09750 -0.02259 0.04900 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.047179 -0.026073 0.001284 \*

\* y -0.026073 -0.031160 0.007400 \*

\* z 0.001284 0.007400 -0.010067 \*

\* \*

\* Pressure: -0.0020 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000018 | -36259.997525 | <-- min BFGS

| trial step | 1.000000 | 0.000016 | -36259.998406 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 66 with line minimization (lambda= 7.027564)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8851712 -8.3164406 0.0098718 0.4201505 -0.0035083 -0.0002600

0.0281852 3.3754330 0.0005356 1.0351730 1.8528021 -0.0008768

0.0086556 0.0017729 13.9652753 -0.0003367 -0.0000686 0.4499151

Lattice parameters(A) Cell Angles

a = 17.050853 alpha = 89.983340

b = 3.375551 beta = 89.939374

c = 13.965278 gamma = 118.713947

Current cell volume = 704.943002 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066886 0.660455 0.121777 x

x Se 2 0.132144 0.340210 0.627545 x

x Se 3 0.131963 0.341282 0.870951 x

x Se 4 0.068192 0.664171 0.375978 x

x Se 5 0.268066 0.670781 0.123781 x

x Se 6 0.332930 0.341061 0.629096 x

x Se 7 0.333650 0.344512 0.871912 x

x Se 8 0.264147 0.659108 0.368967 x

x Se 9 0.466420 0.653188 0.129332 x

x Se 10 0.530881 0.336618 0.618622 x

x Se 11 0.533533 0.346335 0.870818 x

x Se 12 0.468961 0.663039 0.381516 x

x Se 13 0.666332 0.655636 0.128082 x

x Se 14 0.735852 0.340834 0.631140 x

x Se 15 0.732045 0.329565 0.876165 x

x Se 16 0.666973 0.658939 0.371157 x

x Se 17 0.867928 0.658531 0.129178 x

x Se 18 0.932193 0.336119 0.622883 x

x Se 19 0.933101 0.339245 0.878071 x

x Se 20 0.867879 0.660000 0.372611 x

x Nb 1 0.003260 0.002339 0.249126 x

x Nb 2 -0.003350 -0.002728 0.750548 x

x Nb 3 -0.000224 -0.000659 0.000001 x

x Nb 4 0.000415 0.001252 0.499786 x

x Nb 5 0.194069 -0.015233 0.246214 x

x Nb 6 0.200904 0.009422 0.749790 x

x Nb 7 0.199741 0.003550 -0.002541 x

x Nb 8 0.205053 0.012797 0.499452 x

x Nb 9 0.401866 -0.001802 0.253471 x

x Nb 10 0.402755 0.014811 0.750606 x

x Nb 11 0.402921 0.006660 -0.001485 x

x Nb 12 0.385406 -0.035456 0.498911 x

x Nb 13 0.597174 -0.014498 0.249529 x

x Nb 14 0.598130 0.001811 0.746680 x

x Nb 15 0.596979 -0.007176 0.001762 x

x Nb 16 0.614702 0.036055 0.501264 x

x Nb 17 0.799079 -0.009322 0.250366 x

x Nb 18 0.806124 0.015750 0.753716 x

x Nb 19 0.800344 -0.003269 0.002626 x

x Nb 20 0.794576 -0.013933 0.500596 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62591115E+004 44930.97 <-- SCF

1 -3.62617827E+004 6.67803629E-002 44957.86 <-- SCF

2 -3.62619249E+004 3.55605615E-003 44986.56 <-- SCF

3 -3.62611233E+004 -2.00405446E-002 45013.25 <-- SCF

4 -3.62600305E+004 -2.73211088E-002 45039.22 <-- SCF

5 -3.62600584E+004 6.99157940E-004 45066.05 <-- SCF

6 -3.62600065E+004 -1.29764187E-003 45092.17 <-- SCF

7 -3.62599984E+004 -2.03786963E-004 45119.02 <-- SCF

8 -3.62599989E+004 1.36601620E-005 45143.72 <-- SCF

9 -3.62599990E+004 1.42190543E-006 45165.98 <-- SCF

10 -3.62599992E+004 4.63165916E-006 45184.41 <-- SCF

11 -3.62599993E+004 3.75048008E-006 45202.38 <-- SCF

12 -3.62599995E+004 3.62616905E-006 45219.62 <-- SCF

13 -3.62599996E+004 2.95512888E-006 45236.91 <-- SCF

14 -3.62599997E+004 2.47623275E-006 45253.09 <-- SCF

15 -3.62599997E+004 1.94042224E-006 45269.69 <-- SCF

16 -3.62599998E+004 1.61345690E-006 45285.84 <-- SCF

17 -3.62599999E+004 1.28154647E-006 45302.22 <-- SCF

18 -3.62599999E+004 1.07382056E-006 45318.52 <-- SCF

19 -3.62599999E+004 9.40333513E-007 45334.47 <-- SCF

20 -3.62600000E+004 6.97064570E-007 45350.36 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.99997201 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.01593 0.04882 -0.02608 \*

\* Se 2 0.07077 -0.03359 0.08449 \*

\* Se 3 0.01955 -0.04772 0.06686 \*

\* Se 4 -0.06509 0.00639 0.03704 \*

\* Se 5 0.05741 -0.05474 -0.02937 \*

\* Se 6 -0.00891 0.04399 0.01849 \*

\* Se 7 -0.04138 0.04223 0.03115 \*

\* Se 8 -0.10870 -0.04258 -0.05810 \*

\* Se 9 -0.00573 -0.02758 -0.12327 \*

\* Se 10 0.17557 0.01584 -0.05878 \*

\* Se 11 -0.00174 0.04269 0.10302 \*

\* Se 12 -0.11875 -0.01167 0.06894 \*

\* Se 13 0.03643 -0.05055 -0.00497 \*

\* Se 14 0.11177 0.04772 0.06040 \*

\* Se 15 -0.06466 0.05224 0.05799 \*

\* Se 16 -0.00300 -0.07972 -0.09312 \*

\* Se 17 -0.01829 0.04826 -0.08191 \*

\* Se 18 0.03764 -0.00043 0.00220 \*

\* Se 19 0.01872 -0.03328 0.03752 \*

\* Se 20 -0.05974 0.03887 -0.09656 \*

\* Nb 1 0.05965 0.01024 0.00173 \*

\* Nb 2 -0.06737 -0.00940 -0.00292 \*

\* Nb 3 -0.00227 0.00235 0.00088 \*

\* Nb 4 0.01697 -0.00454 -0.00975 \*

\* Nb 5 0.11544 0.01548 0.01741 \*

\* Nb 6 -0.03961 -0.02002 -0.01885 \*

\* Nb 7 0.03199 0.04111 0.01765 \*

\* Nb 8 -0.11711 0.05218 -0.04443 \*

\* Nb 9 -0.02861 0.02905 -0.06735 \*

\* Nb 10 -0.03599 -0.00410 0.01137 \*

\* Nb 11 -0.01313 -0.04455 0.04474 \*

\* Nb 12 -0.01825 -0.01267 0.09418 \*

\* Nb 13 0.03734 -0.00328 0.00952 \*

\* Nb 14 0.01925 -0.03509 0.07039 \*

\* Nb 15 0.01593 0.04575 -0.05369 \*

\* Nb 16 -0.00954 0.00815 -0.08428 \*

\* Nb 17 0.02692 0.02663 0.02184 \*

\* Nb 18 -0.09481 -0.01518 -0.03497 \*

\* Nb 19 -0.03032 -0.03520 -0.02205 \*

\* Nb 20 0.11759 -0.05211 0.05262 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.065746 -0.026418 -0.035977 \*

\* y -0.026418 -0.096132 0.005142 \*

\* z -0.035977 0.005142 0.022478 \*

\* \*

\* Pressure: 0.0465 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000018 | -36259.997525 | <-- min BFGS

| trial step | 1.000000 | 0.000016 | -36259.998406 | <-- min BFGS

| line step | 7.027564 | -0.000019 | -36260.000076 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 66 with quad minimization (lambda= 3.730558)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8989265 -8.3216833 0.0100354 0.4198390 -0.0033692 -0.0002701

0.0270901 3.3757013 0.0006475 1.0349755 1.8529923 -0.0009518

0.0089959 0.0021442 13.9560947 -0.0003499 -0.0000835 0.4502111

Lattice parameters(A) Cell Angles

a = 17.065419 alpha = 89.979911

b = 3.375810 beta = 89.938356

c = 13.956098 gamma = 118.725411

Current cell volume = 705.058177 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066919 0.660802 0.121732 x

x Se 2 0.132136 0.340274 0.627629 x

x Se 3 0.131911 0.341061 0.870901 x

x Se 4 0.068221 0.664471 0.376136 x

x Se 5 0.267929 0.670323 0.123657 x

x Se 6 0.333019 0.341609 0.629038 x

x Se 7 0.333736 0.344870 0.872023 x

x Se 8 0.264159 0.659225 0.369168 x

x Se 9 0.466447 0.653589 0.129242 x

x Se 10 0.530995 0.336920 0.618774 x

x Se 11 0.533512 0.345929 0.870910 x

x Se 12 0.468855 0.662745 0.381348 x

x Se 13 0.666245 0.655273 0.127975 x

x Se 14 0.735844 0.340728 0.630937 x

x Se 15 0.732173 0.329986 0.876286 x

x Se 16 0.666877 0.658463 0.371214 x

x Se 17 0.867980 0.658732 0.129223 x

x Se 18 0.932147 0.335856 0.622781 x

x Se 19 0.933066 0.338873 0.878106 x

x Se 20 0.867886 0.659895 0.372529 x

x Nb 1 0.003478 0.003187 0.249158 x

x Nb 2 -0.003559 -0.003550 0.750532 x

x Nb 3 -0.000210 -0.000599 -0.000007 x

x Nb 4 0.000387 0.001200 0.499805 x

x Nb 5 0.194165 -0.014723 0.246337 x

x Nb 6 0.201105 0.010086 0.749768 x

x Nb 7 0.199718 0.003636 -0.002597 x

x Nb 8 0.205014 0.013176 0.499616 x

x Nb 9 0.401717 -0.002031 0.253369 x

x Nb 10 0.402783 0.015253 0.750527 x

x Nb 11 0.402915 0.006827 -0.001435 x

x Nb 12 0.386067 -0.034018 0.499022 x

x Nb 13 0.597157 -0.014944 0.249603 x

x Nb 14 0.598280 0.002035 0.746780 x

x Nb 15 0.596986 -0.007324 0.001690 x

x Nb 16 0.614048 0.034599 0.501152 x

x Nb 17 0.798880 -0.009986 0.250372 x

x Nb 18 0.806019 0.015232 0.753606 x

x Nb 19 0.800363 -0.003394 0.002672 x

x Nb 20 0.794631 -0.014285 0.500422 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597354E+004 45453.77 <-- SCF

1 -3.62605637E+004 2.07080388E-002 45481.44 <-- SCF

2 -3.62606034E+004 9.90670702E-004 45510.00 <-- SCF

3 -3.62604285E+004 -4.37118494E-003 45536.77 <-- SCF

4 -3.62600006E+004 -1.06989141E-002 45562.88 <-- SCF

5 -3.62600183E+004 4.44234045E-004 45589.86 <-- SCF

6 -3.62600036E+004 -3.69028984E-004 45615.95 <-- SCF

7 -3.62600005E+004 -7.64083910E-005 45639.66 <-- SCF

8 -3.62600003E+004 -5.56310916E-006 45661.31 <-- SCF

9 -3.62600003E+004 1.33715088E-006 45680.50 <-- SCF

10 -3.62600004E+004 1.66077098E-007 45698.12 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.00035093 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00580 0.04106 -0.00975 \*

\* Se 2 0.06087 -0.03091 0.07053 \*

\* Se 3 0.02099 -0.04128 0.05805 \*

\* Se 4 -0.04632 0.00190 0.01907 \*

\* Se 5 0.06415 -0.04795 -0.00911 \*

\* Se 6 -0.00683 0.03821 0.01745 \*

\* Se 7 -0.03852 0.03227 0.00280 \*

\* Se 8 -0.08146 -0.03610 -0.04975 \*

\* Se 9 -0.00105 -0.03222 -0.09336 \*

\* Se 10 0.13563 0.00530 -0.04385 \*

\* Se 11 -0.00665 0.04860 0.07128 \*

\* Se 12 -0.07802 0.00273 0.05745 \*

\* Se 13 0.03309 -0.03985 0.02089 \*

\* Se 14 0.08346 0.04051 0.05107 \*

\* Se 15 -0.06995 0.04559 0.04303 \*

\* Se 16 0.00059 -0.07876 -0.09716 \*

\* Se 17 -0.01692 0.04330 -0.07345 \*

\* Se 18 0.03169 -0.00171 0.00520 \*

\* Se 19 0.00764 -0.02396 0.02598 \*

\* Se 20 -0.05443 0.03753 -0.08522 \*

\* Nb 1 0.04192 0.00145 0.00056 \*

\* Nb 2 -0.05200 -0.00068 -0.00107 \*

\* Nb 3 -0.00336 0.00123 0.00221 \*

\* Nb 4 0.01676 -0.00470 -0.00946 \*

\* Nb 5 0.08751 0.00460 0.01262 \*

\* Nb 6 -0.04391 -0.01954 -0.01321 \*

\* Nb 7 0.02441 0.03345 0.02153 \*

\* Nb 8 -0.09638 0.04249 -0.04853 \*

\* Nb 9 -0.03049 0.02373 -0.06620 \*

\* Nb 10 -0.03962 -0.00593 0.01956 \*

\* Nb 11 -0.01569 -0.04100 0.04182 \*

\* Nb 12 -0.08027 -0.00668 0.07088 \*

\* Nb 13 0.03917 0.00037 0.00100 \*

\* Nb 14 0.01888 -0.02923 0.06829 \*

\* Nb 15 0.01698 0.04232 -0.04659 \*

\* Nb 16 0.05153 0.00399 -0.06009 \*

\* Nb 17 0.03032 0.02506 0.02089 \*

\* Nb 18 -0.06956 -0.00594 -0.02955 \*

\* Nb 19 -0.02378 -0.02758 -0.02396 \*

\* Nb 20 0.09542 -0.04167 0.05816 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.072165 -0.068202 -0.015785 \*

\* y -0.068202 -0.098836 0.018227 \*

\* z -0.015785 0.018227 -0.039692 \*

\* \*

\* Pressure: 0.0221 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000018 | -36259.997525 | <-- min BFGS

| trial step | 1.000000 | 0.000016 | -36259.998406 | <-- min BFGS

| line step | 7.027564 | -0.000019 | -36260.000076 | <-- min BFGS

| quad step | 3.730558 | 0.000012 | -36260.000495 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 66 with enthalpy= -3.62600005E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.426305E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.426426E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.134427E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 9.883561E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 67 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000591 | -36260.000495 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 67 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.7258097 -8.2636162 0.0126457 0.4236868 -0.0053314 -0.0002154

0.0425082 3.3782015 -0.0013724 1.0364047 1.8468791 0.0000643

0.0070870 -0.0044663 14.0537144 -0.0002800 0.0001851 0.4470838

Lattice parameters(A) Cell Angles

a = 16.886000 alpha = 90.041117

b = 3.378469 beta = 89.922984

c = 14.053717 gamma = 118.578725

Current cell volume = 704.063014 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066550 0.656645 0.121864 x

x Se 2 0.132322 0.340008 0.626843 x

x Se 3 0.132535 0.343403 0.871412 x

x Se 4 0.067898 0.660925 0.374833 x

x Se 5 0.269215 0.674947 0.124628 x

x Se 6 0.332474 0.336854 0.629589 x

x Se 7 0.333180 0.342721 0.871092 x

x Se 8 0.263933 0.658294 0.367035 x

x Se 9 0.466216 0.650154 0.130066 x

x Se 10 0.530082 0.333948 0.616948 x

x Se 11 0.533672 0.349430 0.870056 x

x Se 12 0.469733 0.665688 0.383391 x

x Se 13 0.666797 0.657435 0.128863 x

x Se 14 0.736031 0.341550 0.633113 x

x Se 15 0.730966 0.325788 0.875301 x

x Se 16 0.667509 0.662421 0.370647 x

x Se 17 0.867355 0.656625 0.128743 x

x Se 18 0.932645 0.339082 0.623547 x

x Se 19 0.933447 0.343319 0.878092 x

x Se 20 0.867705 0.660583 0.373299 x

x Nb 1 0.001735 -0.003803 0.248892 x

x Nb 2 -0.001908 0.003186 0.750626 x

x Nb 3 -0.000352 -0.001176 0.000080 x

x Nb 4 0.000686 0.001802 0.499586 x

x Nb 5 0.193179 -0.019557 0.245073 x

x Nb 6 0.199136 0.002672 0.750038 x

x Nb 7 0.199970 0.003162 -0.002180 x

x Nb 8 0.205556 0.010182 0.497980 x

x Nb 9 0.403055 0.001085 0.254364 x

x Nb 10 0.402662 0.010875 0.751154 x

x Nb 11 0.403153 0.005093 -0.001916 x

x Nb 12 0.379426 -0.048968 0.498180 x

x Nb 13 0.597168 -0.010566 0.249007 x

x Nb 14 0.596924 -0.001139 0.745822 x

x Nb 15 0.596738 -0.005772 0.002404 x

x Nb 16 0.620602 0.049640 0.502010 x

x Nb 17 0.800828 -0.002579 0.250266 x

x Nb 18 0.807109 0.020204 0.754730 x

x Nb 19 0.800149 -0.002543 0.002367 x

x Nb 20 0.793918 -0.011622 0.502157 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62342191E+004 45801.80 <-- SCF

1 -3.62977468E+004 1.58819118E+000 45828.72 <-- SCF

2 -3.63037349E+004 1.49704097E-001 45858.16 <-- SCF

3 -3.62740408E+004 -7.42352731E-001 45886.16 <-- SCF

4 -3.62611478E+004 -3.22325120E-001 45913.19 <-- SCF

5 -3.62604883E+004 -1.64879038E-002 45939.86 <-- SCF

6 -3.62598112E+004 -1.69268484E-002 45966.41 <-- SCF

7 -3.62598466E+004 8.83765086E-004 45994.12 <-- SCF

8 -3.62598458E+004 -2.10648712E-005 46020.70 <-- SCF

9 -3.62598498E+004 1.02313473E-004 46047.59 <-- SCF

10 -3.62598577E+004 1.97249321E-004 46071.02 <-- SCF

11 -3.62598629E+004 1.29706998E-004 46092.19 <-- SCF

12 -3.62598673E+004 1.09796920E-004 46110.52 <-- SCF

13 -3.62598707E+004 8.45749587E-005 46128.50 <-- SCF

14 -3.62598734E+004 6.86712426E-005 46146.02 <-- SCF

15 -3.62598757E+004 5.55581489E-005 46163.92 <-- SCF

16 -3.62598775E+004 4.52004112E-005 46181.27 <-- SCF

17 -3.62598789E+004 3.66769270E-005 46198.50 <-- SCF

18 -3.62598801E+004 3.02185986E-005 46216.03 <-- SCF

19 -3.62598813E+004 2.79602644E-005 46233.31 <-- SCF

20 -3.62598820E+004 1.87456946E-005 46250.64 <-- SCF

21 -3.62598827E+004 1.68813213E-005 46268.03 <-- SCF

22 -3.62598833E+004 1.42947212E-005 46285.39 <-- SCF

23 -3.62598837E+004 1.17072702E-005 46302.64 <-- SCF

24 -3.62598841E+004 9.92135882E-006 46319.86 <-- SCF

25 -3.62598845E+004 8.31862209E-006 46337.39 <-- SCF

26 -3.62598848E+004 7.51548915E-006 46354.56 <-- SCF

27 -3.62598850E+004 6.09775865E-006 46371.95 <-- SCF

28 -3.62598852E+004 5.63338005E-006 46388.22 <-- SCF

29 -3.62598854E+004 5.01194755E-006 46404.62 <-- SCF

30 -3.62598857E+004 5.54195204E-006 46421.11 <-- SCF

31 -3.62598858E+004 3.62090502E-006 46437.41 <-- SCF

32 -3.62598859E+004 3.54451998E-006 46453.75 <-- SCF

33 -3.62598860E+004 8.50435577E-007 46470.16 <-- SCF

34 -3.62598860E+004 -3.77448484E-007 46486.44 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36259.88595978 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.15993 0.11444 -0.06493 \*

\* Se 2 0.11057 -0.09311 0.13182 \*

\* Se 3 0.05024 -0.09208 0.09514 \*

\* Se 4 -0.17110 -0.03230 -0.01440 \*

\* Se 5 -0.10092 -0.19385 -0.05849 \*

\* Se 6 -0.01341 0.18519 0.00386 \*

\* Se 7 0.05879 0.06477 0.29769 \*

\* Se 8 -0.31740 -0.17326 -0.05105 \*

\* Se 9 -0.04730 0.00262 -0.32442 \*

\* Se 10 0.36111 0.22341 0.05512 \*

\* Se 11 0.07075 0.00308 0.32324 \*

\* Se 12 -0.29657 -0.21926 -0.11601 \*

\* Se 13 -0.05112 -0.07100 -0.22435 \*

\* Se 14 0.34236 0.18751 0.03234 \*

\* Se 15 0.05624 0.19166 0.08067 \*

\* Se 16 -0.01516 -0.14033 -0.04842 \*

\* Se 17 -0.07388 0.07701 -0.11024 \*

\* Se 18 0.08801 0.09154 0.01158 \*

\* Se 19 0.15646 -0.11891 0.04690 \*

\* Se 20 -0.08349 0.07523 -0.06723 \*

\* Nb 1 0.13351 0.05875 0.01552 \*

\* Nb 2 -0.14422 -0.07540 0.02447 \*

\* Nb 3 0.01245 0.00879 -0.01265 \*

\* Nb 4 0.00649 -0.00932 0.00108 \*

\* Nb 5 0.39536 0.16603 0.08400 \*

\* Nb 6 -0.03840 -0.01766 -0.08128 \*

\* Nb 7 0.05360 0.05004 0.03715 \*

\* Nb 8 -0.32570 0.13853 0.01334 \*

\* Nb 9 0.00187 0.06167 -0.07230 \*

\* Nb 10 0.01223 -0.00072 -0.07301 \*

\* Nb 11 -0.01471 -0.05719 0.08532 \*

\* Nb 12 0.53251 -0.08320 0.28197 \*

\* Nb 13 0.00744 -0.03669 0.10450 \*

\* Nb 14 -0.01879 -0.08078 0.08369 \*

\* Nb 15 0.01328 0.06091 -0.13245 \*

\* Nb 16 -0.55885 0.05281 -0.28645 \*

\* Nb 17 0.02579 0.03882 0.05924 \*

\* Nb 18 -0.34051 -0.15597 -0.09530 \*

\* Nb 19 -0.04123 -0.06279 -0.03033 \*

\* Nb 20 0.32360 -0.13899 -0.00531 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -1.356562 0.459729 -0.034232 \*

\* y 0.459729 0.119502 -0.116292 \*

\* z -0.034232 -0.116292 0.313625 \*

\* \*

\* Pressure: 0.3078 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000591 | -36260.000495 | <-- min BFGS

| trial step | 1.000000 | -0.009823 | -36259.885949 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 67 with line minimization (lambda= 0.056753)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8891016 -8.3183878 0.0101836 0.4200551 -0.0034796 -0.0002670

0.0279651 3.3758432 0.0005329 1.0350545 1.8526454 -0.0008936

0.0088875 0.0017690 13.9616349 -0.0003459 -0.0000682 0.4500324

Lattice parameters(A) Cell Angles

a = 17.055235 alpha = 89.983395

b = 3.375959 beta = 89.937490

c = 13.961638 gamma = 118.717010

Current cell volume = 705.004906 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066898 0.660566 0.121740 x

x Se 2 0.132146 0.340258 0.627584 x

x Se 3 0.131947 0.341194 0.870930 x

x Se 4 0.068202 0.664270 0.376062 x

x Se 5 0.268002 0.670585 0.123712 x

x Se 6 0.332988 0.341339 0.629069 x

x Se 7 0.333705 0.344748 0.871970 x

x Se 8 0.264146 0.659172 0.369047 x

x Se 9 0.466434 0.653394 0.129289 x

x Se 10 0.530943 0.336751 0.618670 x

x Se 11 0.533521 0.346127 0.870862 x

x Se 12 0.468904 0.662912 0.381463 x

x Se 13 0.666277 0.655396 0.128025 x

x Se 14 0.735854 0.340775 0.631061 x

x Se 15 0.732105 0.329747 0.876230 x

x Se 16 0.666913 0.658687 0.371182 x

x Se 17 0.867944 0.658612 0.129195 x

x Se 18 0.932175 0.336039 0.622825 x

x Se 19 0.933088 0.339125 0.878105 x

x Se 20 0.867876 0.659934 0.372573 x

x Nb 1 0.003379 0.002790 0.249143 x

x Nb 2 -0.003465 -0.003167 0.750537 x

x Nb 3 -0.000218 -0.000632 -0.000002 x

x Nb 4 0.000404 0.001234 0.499793 x

x Nb 5 0.194109 -0.014998 0.246265 x

x Nb 6 0.200993 0.009666 0.749784 x

x Nb 7 0.199732 0.003609 -0.002574 x

x Nb 8 0.205044 0.013006 0.499523 x

x Nb 9 0.401793 -0.001855 0.253425 x

x Nb 10 0.402776 0.015004 0.750563 x

x Nb 11 0.402928 0.006729 -0.001463 x

x Nb 12 0.385690 -0.034866 0.498974 x

x Nb 13 0.597157 -0.014695 0.249570 x

x Nb 14 0.598203 0.001855 0.746726 x

x Nb 15 0.596972 -0.007236 0.001730 x

x Nb 16 0.614420 0.035453 0.501201 x

x Nb 17 0.798990 -0.009566 0.250366 x

x Nb 18 0.806081 0.015514 0.753670 x

x Nb 19 0.800351 -0.003346 0.002655 x

x Nb 20 0.794591 -0.014134 0.500521 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62371987E+004 46590.19 <-- SCF

1 -3.63045792E+004 1.68451206E+000 46618.78 <-- SCF

2 -3.63088176E+004 1.05961438E-001 46647.70 <-- SCF

3 -3.62887778E+004 -5.00995760E-001 46675.27 <-- SCF

4 -3.62609863E+004 -6.94787977E-001 46705.36 <-- SCF

5 -3.62601031E+004 -2.20791305E-002 46737.22 <-- SCF

6 -3.62601367E+004 8.39867688E-004 46764.50 <-- SCF

7 -3.62599011E+004 -5.89035550E-003 46791.50 <-- SCF

8 -3.62599447E+004 1.08867387E-003 46819.02 <-- SCF

9 -3.62599484E+004 9.24602090E-005 46846.08 <-- SCF

10 -3.62599559E+004 1.89691353E-004 46871.92 <-- SCF

11 -3.62599631E+004 1.79574020E-004 46895.59 <-- SCF

12 -3.62599688E+004 1.41092257E-004 46915.62 <-- SCF

13 -3.62599734E+004 1.16469782E-004 46934.17 <-- SCF

14 -3.62599775E+004 1.01455461E-004 46952.50 <-- SCF

15 -3.62599811E+004 9.08515183E-005 46970.50 <-- SCF

16 -3.62599844E+004 8.13570223E-005 46988.95 <-- SCF

17 -3.62599872E+004 7.17355645E-005 47007.19 <-- SCF

18 -3.62599898E+004 6.27886164E-005 47025.17 <-- SCF

19 -3.62599920E+004 5.50197045E-005 47043.20 <-- SCF

20 -3.62599938E+004 4.55661829E-005 47060.95 <-- SCF

21 -3.62599953E+004 3.78613126E-005 47079.08 <-- SCF

22 -3.62599965E+004 3.03146792E-005 47097.02 <-- SCF

23 -3.62599975E+004 2.47223699E-005 47114.77 <-- SCF

24 -3.62599983E+004 2.01595009E-005 47132.11 <-- SCF

25 -3.62599989E+004 1.61275020E-005 47149.31 <-- SCF

26 -3.62599994E+004 1.25854757E-005 47165.70 <-- SCF

27 -3.62599998E+004 9.50027776E-006 47182.31 <-- SCF

28 -3.62600001E+004 6.22763317E-006 47198.56 <-- SCF

29 -3.62600003E+004 4.90890176E-006 47215.12 <-- SCF

30 -3.62600004E+004 3.70729391E-006 47231.69 <-- SCF

31 -3.62600005E+004 1.87308297E-006 47249.02 <-- SCF

32 -3.62600006E+004 2.88086000E-006 47265.80 <-- SCF

33 -3.62600007E+004 2.47290468E-006 47282.56 <-- SCF

34 -3.62600008E+004 1.63767403E-006 47298.92 <-- SCF

35 -3.62600008E+004 1.42771316E-006 47315.19 <-- SCF

36 -3.62600009E+004 1.51532355E-006 47331.34 <-- SCF

37 -3.62600009E+004 -4.23444087E-008 47347.91 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.00089182 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.02414 0.03661 -0.00649 \*

\* Se 2 0.06448 -0.02613 0.07493 \*

\* Se 3 0.03138 -0.04567 0.04867 \*

\* Se 4 -0.06054 0.01092 0.02193 \*

\* Se 5 0.03996 -0.05627 -0.01844 \*

\* Se 6 -0.00692 0.04050 0.01547 \*

\* Se 7 -0.04397 0.04249 0.02161 \*

\* Se 8 -0.09285 -0.04753 -0.05141 \*

\* Se 9 -0.00446 -0.03146 -0.09903 \*

\* Se 10 0.16674 0.01391 -0.04334 \*

\* Se 11 -0.00661 0.04353 0.07574 \*

\* Se 12 -0.10861 -0.01137 0.05589 \*

\* Se 13 0.03636 -0.05469 0.00638 \*

\* Se 14 0.09512 0.05407 0.04908 \*

\* Se 15 -0.06189 0.05659 0.05642 \*

\* Se 16 -0.00057 -0.08206 -0.09769 \*

\* Se 17 -0.02455 0.04786 -0.06213 \*

\* Se 18 0.04277 -0.00427 0.01287 \*

\* Se 19 0.02699 -0.02246 0.02230 \*

\* Se 20 -0.05823 0.03952 -0.09331 \*

\* Nb 1 0.05714 0.00824 -0.01100 \*

\* Nb 2 -0.08228 -0.00101 0.01062 \*

\* Nb 3 -0.00117 0.00566 0.00844 \*

\* Nb 4 0.01618 -0.01153 -0.00697 \*

\* Nb 5 0.15012 0.02449 0.01718 \*

\* Nb 6 -0.05810 -0.02704 -0.03706 \*

\* Nb 7 0.02294 0.04226 0.02584 \*

\* Nb 8 -0.10437 0.04400 -0.04246 \*

\* Nb 9 -0.02887 0.00899 -0.08052 \*

\* Nb 10 -0.02409 -0.00554 0.01789 \*

\* Nb 11 0.00098 -0.03104 0.03420 \*

\* Nb 12 -0.03945 -0.00500 0.10396 \*

\* Nb 13 0.03085 0.01021 -0.00182 \*

\* Nb 14 0.01480 -0.01975 0.07441 \*

\* Nb 15 0.00559 0.03910 -0.03224 \*

\* Nb 16 0.01073 0.00456 -0.08673 \*

\* Nb 17 0.03570 0.02424 0.04196 \*

\* Nb 18 -0.09849 -0.03031 -0.03491 \*

\* Nb 19 -0.02495 -0.03917 -0.04230 \*

\* Nb 20 0.10626 -0.04544 0.05205 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.020273 0.039305 -0.059933 \*

\* y 0.039305 -0.114311 -0.089084 \*

\* z -0.059933 -0.089084 -0.012716 \*

\* \*

\* Pressure: 0.0491 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000591 | -36260.000495 | <-- min BFGS

| trial step | 1.000000 | -0.009823 | -36259.885949 | <-- min BFGS

| line step | 0.056753 | -0.000262 | -36260.001001 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 67 with enthalpy= -3.62600010E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.263258E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.728385E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 5.681628E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.143109E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 68 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000063 | -36260.001001 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 68 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8843262 -8.3226140 0.0089855 0.4202191 -0.0034257 -0.0002923

0.0275287 3.3767670 0.0014531 1.0357016 1.8522675 -0.0013538

0.0097516 0.0047535 13.9640403 -0.0003782 -0.0001905 0.4499550

Lattice parameters(A) Cell Angles

a = 17.053127 alpha = 89.955515

b = 3.376880 beta = 89.944406

c = 13.964045 gamma = 118.744756

Current cell volume = 705.044045 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066894 0.660567 0.121744 x

x Se 2 0.132195 0.340425 0.627609 x

x Se 3 0.131986 0.341316 0.870937 x

x Se 4 0.068182 0.664187 0.376074 x

x Se 5 0.268018 0.670650 0.123740 x

x Se 6 0.333003 0.341461 0.629081 x

x Se 7 0.333720 0.344871 0.871951 x

x Se 8 0.264114 0.659114 0.369003 x

x Se 9 0.466441 0.653236 0.129285 x

x Se 10 0.530971 0.336930 0.618668 x

x Se 11 0.533511 0.346302 0.870855 x

x Se 12 0.468895 0.662795 0.381472 x

x Se 13 0.666261 0.655257 0.128053 x

x Se 14 0.735886 0.340837 0.631104 x

x Se 15 0.732087 0.329676 0.876221 x

x Se 16 0.666898 0.658502 0.371133 x

x Se 17 0.867908 0.658502 0.129182 x

x Se 18 0.932194 0.336115 0.622818 x

x Se 19 0.933094 0.339154 0.878111 x

x Se 20 0.867828 0.659781 0.372539 x

x Nb 1 0.003445 0.003085 0.249147 x

x Nb 2 -0.003537 -0.003467 0.750533 x

x Nb 3 -0.000220 -0.000638 0.000001 x

x Nb 4 0.000408 0.001237 0.499787 x

x Nb 5 0.194135 -0.015009 0.246272 x

x Nb 6 0.200975 0.009638 0.749771 x

x Nb 7 0.199730 0.003649 -0.002571 x

x Nb 8 0.205007 0.012959 0.499521 x

x Nb 9 0.401765 -0.001949 0.253396 x

x Nb 10 0.402762 0.014921 0.750567 x

x Nb 11 0.402926 0.006692 -0.001481 x

x Nb 12 0.385676 -0.034880 0.499039 x

x Nb 13 0.597169 -0.014620 0.249574 x

x Nb 14 0.598228 0.001933 0.746755 x

x Nb 15 0.596975 -0.007197 0.001749 x

x Nb 16 0.614425 0.035439 0.501141 x

x Nb 17 0.799004 -0.009550 0.250384 x

x Nb 18 0.806062 0.015536 0.753655 x

x Nb 19 0.800353 -0.003375 0.002650 x

x Nb 20 0.794628 -0.014084 0.500530 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599884E+004 47451.19 <-- SCF

1 -3.62600819E+004 2.33943476E-003 47479.55 <-- SCF

2 -3.62600887E+004 1.70516356E-004 47505.91 <-- SCF

3 -3.62600987E+004 2.48765134E-004 47532.83 <-- SCF

4 -3.62599963E+004 -2.55957682E-003 47558.98 <-- SCF

5 -3.62600033E+004 1.75371316E-004 47585.44 <-- SCF

6 -3.62600026E+004 -1.82904778E-005 47608.59 <-- SCF

7 -3.62600017E+004 -2.15350066E-005 47629.92 <-- SCF

8 -3.62600017E+004 -1.22714562E-006 47648.62 <-- SCF

9 -3.62600017E+004 6.20376051E-007 47665.83 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.00171470 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.01801 0.04850 -0.01108 \*

\* Se 2 0.05048 -0.03164 0.07150 \*

\* Se 3 0.01147 -0.04902 0.05631 \*

\* Se 4 -0.05766 0.01225 0.02624 \*

\* Se 5 0.05113 -0.05556 -0.02376 \*

\* Se 6 -0.01223 0.03564 0.00668 \*

\* Se 7 -0.04807 0.02349 0.02277 \*

\* Se 8 -0.09668 -0.04358 -0.03639 \*

\* Se 9 -0.01128 -0.01769 -0.10451 \*

\* Se 10 0.15511 0.00758 -0.04976 \*

\* Se 11 0.00681 0.03028 0.08750 \*

\* Se 12 -0.10357 -0.00315 0.06138 \*

\* Se 13 0.04287 -0.03017 -0.00225 \*

\* Se 14 0.09986 0.04775 0.03862 \*

\* Se 15 -0.06077 0.05449 0.05155 \*

\* Se 16 0.00329 -0.06511 -0.06681 \*

\* Se 17 -0.01236 0.04952 -0.06738 \*

\* Se 18 0.04148 -0.00569 0.00074 \*

\* Se 19 0.01919 -0.03485 0.02325 \*

\* Se 20 -0.04363 0.03705 -0.08434 \*

\* Nb 1 0.03874 -0.00729 0.00017 \*

\* Nb 2 -0.04910 0.00779 -0.00067 \*

\* Nb 3 -0.00152 0.00342 0.00194 \*

\* Nb 4 0.01619 -0.00521 -0.00888 \*

\* Nb 5 0.10449 0.01960 0.01284 \*

\* Nb 6 -0.04073 -0.01904 -0.01611 \*

\* Nb 7 0.03336 0.03996 0.01923 \*

\* Nb 8 -0.10307 0.05135 -0.04527 \*

\* Nb 9 -0.01984 0.01712 -0.06250 \*

\* Nb 10 -0.03507 0.00051 0.01278 \*

\* Nb 11 -0.01437 -0.04389 0.04653 \*

\* Nb 12 -0.04658 -0.01079 0.07497 \*

\* Nb 13 0.03654 -0.00771 0.00263 \*

\* Nb 14 0.01031 -0.02338 0.06499 \*

\* Nb 15 0.01751 0.04608 -0.05309 \*

\* Nb 16 0.01961 0.00723 -0.06654 \*

\* Nb 17 0.03052 0.02241 0.01716 \*

\* Nb 18 -0.08346 -0.02089 -0.02728 \*

\* Nb 19 -0.03248 -0.03639 -0.02483 \*

\* Nb 20 0.10150 -0.05099 0.05168 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.044817 -0.082678 -0.006777 \*

\* y -0.082678 -0.044208 0.073040 \*

\* z -0.006777 0.073040 0.021934 \*

\* \*

\* Pressure: 0.0224 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000063 | -36260.001001 | <-- min BFGS

| trial step | 1.000000 | 0.000027 | -36260.001813 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 68 with line minimization (lambda= 1.759038)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8807015 -8.3258219 0.0080761 0.4203436 -0.0033847 -0.0003115

0.0271974 3.3774682 0.0021516 1.0361930 1.8519811 -0.0017029

0.0104074 0.0070188 13.9658661 -0.0004027 -0.0002834 0.4498963

Lattice parameters(A) Cell Angles

a = 17.051529 alpha = 89.934363

b = 3.377578 beta = 89.949662

c = 13.965872 gamma = 118.765817

Current cell volume = 705.073558 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066890 0.660568 0.121746 x

x Se 2 0.132232 0.340552 0.627629 x

x Se 3 0.132015 0.341409 0.870942 x

x Se 4 0.068167 0.664124 0.376084 x

x Se 5 0.268030 0.670699 0.123761 x

x Se 6 0.333014 0.341554 0.629090 x

x Se 7 0.333731 0.344965 0.871937 x

x Se 8 0.264089 0.659070 0.368969 x

x Se 9 0.466446 0.653116 0.129282 x

x Se 10 0.530992 0.337065 0.618667 x

x Se 11 0.533503 0.346435 0.870849 x

x Se 12 0.468887 0.662707 0.381479 x

x Se 13 0.666248 0.655152 0.128075 x

x Se 14 0.735910 0.340885 0.631138 x

x Se 15 0.732073 0.329622 0.876213 x

x Se 16 0.666887 0.658361 0.371096 x

x Se 17 0.867880 0.658419 0.129172 x

x Se 18 0.932208 0.336172 0.622813 x

x Se 19 0.933099 0.339176 0.878116 x

x Se 20 0.867791 0.659664 0.372513 x

x Nb 1 0.003495 0.003308 0.249150 x

x Nb 2 -0.003591 -0.003695 0.750529 x

x Nb 3 -0.000221 -0.000643 0.000003 x

x Nb 4 0.000411 0.001239 0.499783 x

x Nb 5 0.194154 -0.015017 0.246278 x

x Nb 6 0.200960 0.009618 0.749761 x

x Nb 7 0.199729 0.003679 -0.002569 x

x Nb 8 0.204978 0.012924 0.499519 x

x Nb 9 0.401743 -0.002021 0.253374 x

x Nb 10 0.402752 0.014857 0.750571 x

x Nb 11 0.402924 0.006663 -0.001494 x

x Nb 12 0.385666 -0.034890 0.499089 x

x Nb 13 0.597178 -0.014562 0.249577 x

x Nb 14 0.598247 0.001993 0.746777 x

x Nb 15 0.596977 -0.007167 0.001763 x

x Nb 16 0.614429 0.035429 0.501096 x

x Nb 17 0.799015 -0.009538 0.250398 x

x Nb 18 0.806049 0.015553 0.753643 x

x Nb 19 0.800354 -0.003397 0.002646 x

x Nb 20 0.794657 -0.014045 0.500536 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599959E+004 47769.06 <-- SCF

1 -3.62600104E+004 3.61509412E-004 47796.05 <-- SCF

2 -3.62600112E+004 2.01982854E-005 47820.30 <-- SCF

3 -3.62600083E+004 -7.13423193E-005 47846.84 <-- SCF

4 -3.62600022E+004 -1.53406737E-004 47872.34 <-- SCF

5 -3.62600024E+004 5.76660445E-006 47894.86 <-- SCF

6 -3.62600023E+004 -4.08116591E-006 47913.42 <-- SCF

7 -3.62600022E+004 -1.35839926E-006 47930.97 <-- SCF

8 -3.62600022E+004 -5.90839048E-008 47948.41 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.00219982 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.01522 0.05097 -0.01566 \*

\* Se 2 0.04038 -0.03177 0.07090 \*

\* Se 3 0.00554 -0.05339 0.05986 \*

\* Se 4 -0.05163 0.01710 0.02149 \*

\* Se 5 0.05268 -0.05344 -0.03068 \*

\* Se 6 -0.01040 0.03007 0.00722 \*

\* Se 7 -0.04820 0.01318 0.03192 \*

\* Se 8 -0.09287 -0.04341 -0.03330 \*

\* Se 9 -0.01771 -0.00567 -0.10560 \*

\* Se 10 0.14974 0.00264 -0.04044 \*

\* Se 11 0.01178 0.01738 0.09203 \*

\* Se 12 -0.10590 0.00117 0.05121 \*

\* Se 13 0.04393 -0.01879 -0.01477 \*

\* Se 14 0.09664 0.04631 0.03429 \*

\* Se 15 -0.06095 0.05263 0.05491 \*

\* Se 16 0.00246 -0.05209 -0.05387 \*

\* Se 17 -0.00796 0.05315 -0.07041 \*

\* Se 18 0.03861 -0.00806 0.00166 \*

\* Se 19 0.01720 -0.03895 0.02560 \*

\* Se 20 -0.03362 0.03495 -0.08105 \*

\* Nb 1 0.03445 -0.01076 -0.00384 \*

\* Nb 2 -0.04365 0.01067 0.00283 \*

\* Nb 3 -0.00111 0.00290 0.00136 \*

\* Nb 4 0.01591 -0.00508 -0.00850 \*

\* Nb 5 0.10416 0.01992 0.00839 \*

\* Nb 6 -0.03565 -0.01556 -0.01139 \*

\* Nb 7 0.03728 0.03970 0.02032 \*

\* Nb 8 -0.10363 0.05009 -0.04954 \*

\* Nb 9 -0.01448 0.01333 -0.06660 \*

\* Nb 10 -0.03419 0.00649 0.01537 \*

\* Nb 11 -0.01365 -0.04489 0.04921 \*

\* Nb 12 -0.04898 -0.01113 0.07108 \*

\* Nb 13 0.03354 -0.01507 -0.00087 \*

\* Nb 14 0.00508 -0.01896 0.06908 \*

\* Nb 15 0.01608 0.04583 -0.05650 \*

\* Nb 16 0.02360 0.00635 -0.06516 \*

\* Nb 17 0.02645 0.01936 0.01072 \*

\* Nb 18 -0.08302 -0.02133 -0.02129 \*

\* Nb 19 -0.03560 -0.03602 -0.02441 \*

\* Nb 20 0.10289 -0.04984 0.05445 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.086595 -0.097528 0.008271 \*

\* y -0.097528 -0.002699 0.122799 \*

\* z 0.008271 0.122799 0.046648 \*

\* \*

\* Pressure: 0.0142 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000063 | -36260.001001 | <-- min BFGS

| trial step | 1.000000 | 0.000027 | -36260.001813 | <-- min BFGS

| line step | 1.759038 | 0.000013 | -36260.002278 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 68 with enthalpy= -3.62600023E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 3.192296E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.551232E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.028515E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.227988E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 69 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000146 | -36260.002278 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 69 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8804986 -8.3250660 0.0071043 0.4202887 -0.0034932 -0.0002822

0.0280832 3.3786588 0.0020309 1.0355984 1.8510616 -0.0015779

0.0094293 0.0066259 13.9617834 -0.0003645 -0.0002675 0.4500278

Lattice parameters(A) Cell Angles

a = 17.050983 alpha = 89.938050

b = 3.378776 beta = 89.955634

c = 13.961788 gamma = 118.749081

Current cell volume = 705.208012 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066911 0.660936 0.121750 x

x Se 2 0.132326 0.340750 0.627740 x

x Se 3 0.132039 0.341368 0.870978 x

x Se 4 0.068146 0.664121 0.376194 x

x Se 5 0.268009 0.670498 0.123728 x

x Se 6 0.333010 0.341833 0.629086 x

x Se 7 0.333764 0.345112 0.871962 x

x Se 8 0.264035 0.658950 0.368965 x

x Se 9 0.466454 0.653189 0.129141 x

x Se 10 0.531175 0.337623 0.618712 x

x Se 11 0.533489 0.346409 0.870956 x

x Se 12 0.468771 0.662360 0.381447 x

x Se 13 0.666211 0.654948 0.128082 x

x Se 14 0.735966 0.341040 0.631141 x

x Se 15 0.732081 0.329781 0.876303 x

x Se 16 0.666888 0.657943 0.370998 x

x Se 17 0.867864 0.658475 0.129112 x

x Se 18 0.932212 0.336170 0.622764 x

x Se 19 0.933080 0.338887 0.878135 x

x Se 20 0.867699 0.659482 0.372377 x

x Nb 1 0.003691 0.004139 0.249185 x

x Nb 2 -0.003795 -0.004524 0.750502 x

x Nb 3 -0.000217 -0.000611 0.000004 x

x Nb 4 0.000407 0.001233 0.499779 x

x Nb 5 0.194272 -0.014537 0.246385 x

x Nb 6 0.201043 0.009702 0.749722 x

x Nb 7 0.199729 0.003842 -0.002557 x

x Nb 8 0.204837 0.012932 0.499560 x

x Nb 9 0.401591 -0.001934 0.253198 x

x Nb 10 0.402729 0.014694 0.750507 x

x Nb 11 0.402908 0.006575 -0.001436 x

x Nb 12 0.386106 -0.033865 0.499331 x

x Nb 13 0.597202 -0.014440 0.249661 x

x Nb 14 0.598390 0.001834 0.746956 x

x Nb 15 0.596993 -0.007060 0.001688 x

x Nb 16 0.613965 0.034292 0.500868 x

x Nb 17 0.798920 -0.009645 0.250438 x

x Nb 18 0.805946 0.015118 0.753517 x

x Nb 19 0.800349 -0.003570 0.002616 x

x Nb 20 0.794805 -0.014048 0.500508 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598253E+004 48051.83 <-- SCF

1 -3.62602474E+004 1.05526886E-002 48077.61 <-- SCF

2 -3.62602775E+004 7.52043040E-004 48106.77 <-- SCF

3 -3.62601109E+004 -4.16434589E-003 48133.48 <-- SCF

4 -3.62600120E+004 -2.47286470E-003 48159.33 <-- SCF

5 -3.62600095E+004 -6.30627858E-005 48186.12 <-- SCF

6 -3.62600054E+004 -1.00514219E-004 48211.56 <-- SCF

7 -3.62600048E+004 -1.68439081E-005 48233.66 <-- SCF

8 -3.62600048E+004 1.12337068E-006 48254.00 <-- SCF

9 -3.62600048E+004 -5.27085081E-007 48271.59 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.00478532 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00953 0.02819 -0.00834 \*

\* Se 2 0.00007 -0.01557 0.04033 \*

\* Se 3 -0.00443 -0.04179 0.04026 \*

\* Se 4 -0.04050 0.01421 0.00265 \*

\* Se 5 0.05065 -0.04508 -0.02818 \*

\* Se 6 -0.00085 0.01792 -0.00439 \*

\* Se 7 -0.04421 0.00768 0.02540 \*

\* Se 8 -0.06034 -0.04217 0.00447 \*

\* Se 9 -0.01119 -0.00183 -0.05875 \*

\* Se 10 0.08467 -0.00901 -0.02619 \*

\* Se 11 0.00791 0.01067 0.05398 \*

\* Se 12 -0.06775 0.00940 0.03717 \*

\* Se 13 0.04315 -0.00880 -0.02200 \*

\* Se 14 0.06446 0.04173 -0.00332 \*

\* Se 15 -0.05436 0.04711 0.03690 \*

\* Se 16 -0.00333 -0.01981 0.00173 \*

\* Se 17 -0.00080 0.04068 -0.04521 \*

\* Se 18 0.03901 -0.00858 -0.00213 \*

\* Se 19 0.00939 -0.02235 0.01233 \*

\* Se 20 0.00468 0.01422 -0.03884 \*

\* Nb 1 0.00153 -0.01332 -0.01168 \*

\* Nb 2 -0.01048 0.01291 0.01022 \*

\* Nb 3 -0.00042 0.00241 0.00116 \*

\* Nb 4 0.01295 -0.00553 -0.00621 \*

\* Nb 5 0.08144 0.01732 -0.00486 \*

\* Nb 6 -0.03661 -0.01571 0.00220 \*

\* Nb 7 0.03552 0.03386 0.02106 \*

\* Nb 8 -0.07309 0.03914 -0.04598 \*

\* Nb 9 0.00242 0.00086 -0.04635 \*

\* Nb 10 -0.02273 0.01230 0.02016 \*

\* Nb 11 -0.01508 -0.04285 0.04182 \*

\* Nb 12 -0.09532 -0.00516 0.03254 \*

\* Nb 13 0.01952 -0.02290 -0.01517 \*

\* Nb 14 -0.00758 -0.00351 0.04798 \*

\* Nb 15 0.01722 0.04295 -0.04665 \*

\* Nb 16 0.07867 0.00031 -0.03393 \*

\* Nb 17 0.03453 0.01843 -0.00859 \*

\* Nb 18 -0.06562 -0.01901 0.00099 \*

\* Nb 19 -0.03326 -0.03083 -0.02163 \*

\* Nb 20 0.06965 -0.03847 0.04506 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.008519 -0.077490 0.009911 \*

\* y -0.077490 0.045433 0.118116 \*

\* z 0.009911 0.118116 0.032278 \*

\* \*

\* Pressure: -0.0231 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000146 | -36260.002278 | <-- min BFGS

| trial step | 1.000000 | 0.000040 | -36260.004850 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 69 with enthalpy= -3.62600048E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 6.429939E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.008494E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.636185E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.181160E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 70 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000115 | -36260.004850 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 70 with trial guess (lambda= 1.000000)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8749977 -8.3246753 0.0098226 0.4203974 -0.0035771 -0.0003345

0.0287585 3.3796237 0.0018553 1.0355219 1.8503268 -0.0016321

0.0111610 0.0060695 13.9621507 -0.0004334 -0.0002434 0.4500160

Lattice parameters(A) Cell Angles

a = 17.045993 alpha = 89.943251

b = 3.379747 beta = 89.939180

c = 13.962156 gamma = 118.745643

Current cell volume = 705.245668 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066909 0.660910 0.121709 x

x Se 2 0.132397 0.340860 0.627758 x

x Se 3 0.132121 0.341274 0.871110 x

x Se 4 0.068102 0.663967 0.376254 x

x Se 5 0.268087 0.670526 0.123696 x

x Se 6 0.333087 0.342082 0.629071 x

x Se 7 0.333728 0.345156 0.872038 x

x Se 8 0.263995 0.658736 0.368925 x

x Se 9 0.466499 0.653268 0.128989 x

x Se 10 0.531314 0.337650 0.618623 x

x Se 11 0.533430 0.346389 0.871074 x

x Se 12 0.468681 0.662518 0.381588 x

x Se 13 0.666238 0.654826 0.128029 x

x Se 14 0.736008 0.341266 0.631186 x

x Se 15 0.732002 0.329768 0.876371 x

x Se 16 0.666821 0.657455 0.370909 x

x Se 17 0.867791 0.658640 0.128952 x

x Se 18 0.932254 0.336295 0.622712 x

x Se 19 0.933086 0.339023 0.878217 x

x Se 20 0.867628 0.659448 0.372341 x

x Nb 1 0.003733 0.004251 0.249198 x

x Nb 2 -0.003854 -0.004684 0.750480 x

x Nb 3 -0.000226 -0.000636 0.000014 x

x Nb 4 0.000433 0.001279 0.499753 x

x Nb 5 0.194384 -0.014366 0.246374 x

x Nb 6 0.200959 0.009160 0.749736 x

x Nb 7 0.199777 0.004161 -0.002538 x

x Nb 8 0.204720 0.012736 0.499481 x

x Nb 9 0.401516 -0.001981 0.253116 x

x Nb 10 0.402694 0.014549 0.750537 x

x Nb 11 0.402905 0.006233 -0.001368 x

x Nb 12 0.385924 -0.034431 0.499409 x

x Nb 13 0.597230 -0.014310 0.249647 x

x Nb 14 0.598450 0.001779 0.747039 x

x Nb 15 0.596999 -0.006701 0.001628 x

x Nb 16 0.614112 0.034760 0.500800 x

x Nb 17 0.798986 -0.009137 0.250442 x

x Nb 18 0.805858 0.015002 0.753495 x

x Nb 19 0.800302 -0.003858 0.002603 x

x Nb 20 0.794918 -0.013863 0.500601 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599523E+004 48375.69 <-- SCF

1 -3.62601866E+004 5.85910669E-003 48403.09 <-- SCF

2 -3.62601993E+004 3.16176832E-004 48430.75 <-- SCF

3 -3.62601706E+004 -7.16286056E-004 48457.48 <-- SCF

4 -3.62600035E+004 -4.17815046E-003 48483.19 <-- SCF

5 -3.62600111E+004 1.89750075E-004 48509.97 <-- SCF

6 -3.62600082E+004 -7.32372921E-005 48534.86 <-- SCF

7 -3.62600072E+004 -2.44492336E-005 48556.98 <-- SCF

8 -3.62600071E+004 -1.14841272E-006 48577.86 <-- SCF

9 -3.62600072E+004 2.97583481E-007 48595.67 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.00716130 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00625 0.02959 0.01042 \*

\* Se 2 -0.02001 -0.01056 0.03934 \*

\* Se 3 -0.01958 -0.01623 0.01310 \*

\* Se 4 -0.02775 0.01418 -0.02047 \*

\* Se 5 0.03976 -0.04271 -0.02108 \*

\* Se 6 -0.03022 0.01832 0.00768 \*

\* Se 7 -0.03353 -0.00090 -0.00861 \*

\* Se 8 -0.06298 -0.03624 0.01138 \*

\* Se 9 -0.01453 0.00520 -0.00922 \*

\* Se 10 0.04276 -0.00213 -0.01125 \*

\* Se 11 0.01486 -0.00034 0.01562 \*

\* Se 12 -0.04978 -0.00622 0.01362 \*

\* Se 13 0.03542 0.00597 0.00146 \*

\* Se 14 0.06622 0.03500 -0.01186 \*

\* Se 15 -0.04310 0.04554 0.01824 \*

\* Se 16 0.02682 0.00295 0.03241 \*

\* Se 17 0.00722 0.01101 -0.00835 \*

\* Se 18 0.03799 -0.00642 -0.00139 \*

\* Se 19 0.00479 -0.03100 -0.01493 \*

\* Se 20 0.02677 0.00246 -0.02873 \*

\* Nb 1 -0.01024 -0.01262 -0.02020 \*

\* Nb 2 0.00140 0.01348 0.02021 \*

\* Nb 3 0.00155 0.00360 0.00058 \*

\* Nb 4 0.00969 -0.00568 -0.00250 \*

\* Nb 5 0.06483 0.01927 -0.01236 \*

\* Nb 6 -0.02549 -0.01206 0.00152 \*

\* Nb 7 0.03382 0.02606 0.02345 \*

\* Nb 8 -0.07272 0.03532 -0.03417 \*

\* Nb 9 0.02260 -0.00054 -0.04403 \*

\* Nb 10 -0.01180 0.01489 0.02191 \*

\* Nb 11 -0.01411 -0.03838 0.03879 \*

\* Nb 12 -0.08201 0.00232 0.01926 \*

\* Nb 13 0.00557 -0.03078 -0.02294 \*

\* Nb 14 -0.02301 0.00176 0.04831 \*

\* Nb 15 0.01595 0.03702 -0.04528 \*

\* Nb 16 0.07348 -0.00941 -0.02675 \*

\* Nb 17 0.03048 0.01604 -0.01716 \*

\* Nb 18 -0.05075 -0.02038 0.01760 \*

\* Nb 19 -0.03301 -0.02313 -0.02341 \*

\* Nb 20 0.06890 -0.03425 0.02975 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.023802 -0.050688 0.043882 \*

\* y -0.050688 0.083722 0.105276 \*

\* z 0.043882 0.105276 0.037794 \*

\* \*

\* Pressure: -0.0326 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000115 | -36260.004850 | <-- min BFGS

| trial step | 1.000000 | 0.000061 | -36260.007209 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 70 with line minimization (lambda= 2.146705)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8686898 -8.3242274 0.0129398 0.4205221 -0.0036734 -0.0003945

0.0295330 3.3807300 0.0016541 1.0354344 1.8494848 -0.0016944

0.0131468 0.0054316 13.9625718 -0.0005124 -0.0002157 0.4500026

Lattice parameters(A) Cell Angles

a = 17.040272 alpha = 89.949210

b = 3.380859 beta = 89.920306

c = 13.962579 gamma = 118.741715

Current cell volume = 705.288620 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066907 0.660881 0.121663 x

x Se 2 0.132479 0.340986 0.627779 x

x Se 3 0.132214 0.341166 0.871262 x

x Se 4 0.068052 0.663789 0.376323 x

x Se 5 0.268176 0.670557 0.123659 x

x Se 6 0.333175 0.342368 0.629054 x

x Se 7 0.333686 0.345206 0.872125 x

x Se 8 0.263950 0.658490 0.368880 x

x Se 9 0.466551 0.653359 0.128816 x

x Se 10 0.531474 0.337682 0.618521 x

x Se 11 0.533363 0.346366 0.871208 x

x Se 12 0.468578 0.662699 0.381749 x

x Se 13 0.666269 0.654686 0.127968 x

x Se 14 0.736055 0.341525 0.631239 x

x Se 15 0.731912 0.329754 0.876448 x

x Se 16 0.666744 0.656895 0.370808 x

x Se 17 0.867708 0.658830 0.128770 x

x Se 18 0.932302 0.336437 0.622653 x

x Se 19 0.933092 0.339179 0.878311 x

x Se 20 0.867547 0.659409 0.372301 x

x Nb 1 0.003783 0.004380 0.249213 x

x Nb 2 -0.003922 -0.004866 0.750454 x

x Nb 3 -0.000236 -0.000666 0.000025 x

x Nb 4 0.000463 0.001332 0.499724 x

x Nb 5 0.194514 -0.014170 0.246363 x

x Nb 6 0.200863 0.008540 0.749753 x

x Nb 7 0.199832 0.004527 -0.002517 x

x Nb 8 0.204586 0.012512 0.499390 x

x Nb 9 0.401431 -0.002036 0.253023 x

x Nb 10 0.402654 0.014383 0.750571 x

x Nb 11 0.402901 0.005841 -0.001289 x

x Nb 12 0.385715 -0.035080 0.499498 x

x Nb 13 0.597263 -0.014161 0.249631 x

x Nb 14 0.598519 0.001715 0.747133 x

x Nb 15 0.597007 -0.006290 0.001559 x

x Nb 16 0.614280 0.035298 0.500722 x

x Nb 17 0.799063 -0.008553 0.250446 x

x Nb 18 0.805757 0.014869 0.753471 x

x Nb 19 0.800249 -0.004189 0.002588 x

x Nb 20 0.795047 -0.013650 0.500708 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599348E+004 48698.92 <-- SCF

1 -3.62602712E+004 8.41223223E-003 48726.55 <-- SCF

2 -3.62602892E+004 4.49599318E-004 48754.31 <-- SCF

3 -3.62602517E+004 -9.37796385E-004 48781.28 <-- SCF

4 -3.62600033E+004 -6.21066507E-003 48807.19 <-- SCF

5 -3.62600142E+004 2.73349917E-004 48834.19 <-- SCF

6 -3.62600094E+004 -1.19613330E-004 48860.14 <-- SCF

7 -3.62600082E+004 -3.10394150E-005 48883.38 <-- SCF

8 -3.62600081E+004 -2.44591385E-006 48905.42 <-- SCF

9 -3.62600081E+004 3.48941797E-007 48923.67 <-- SCF

10 -3.62600081E+004 6.35740143E-007 48940.69 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.00814300 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00509 0.02953 0.03389 \*

\* Se 2 -0.04073 -0.00481 0.04120 \*

\* Se 3 -0.03310 0.00798 -0.01905 \*

\* Se 4 -0.01744 0.01423 -0.04628 \*

\* Se 5 0.02806 -0.04191 -0.00976 \*

\* Se 6 -0.05993 0.01809 0.02202 \*

\* Se 7 -0.02093 -0.00921 -0.05231 \*

\* Se 8 -0.06194 -0.03034 0.01762 \*

\* Se 9 -0.01865 0.00958 0.05112 \*

\* Se 10 0.00003 0.00180 0.00180 \*

\* Se 11 0.02294 -0.00979 -0.03093 \*

\* Se 12 -0.03074 -0.02632 -0.01341 \*

\* Se 13 0.02629 0.02222 0.03267 \*

\* Se 14 0.06434 0.02845 -0.01992 \*

\* Se 15 -0.03254 0.04569 -0.00717 \*

\* Se 16 0.05564 0.02517 0.06431 \*

\* Se 17 0.01386 -0.01642 0.03493 \*

\* Se 18 0.03925 -0.00278 0.00103 \*

\* Se 19 0.00214 -0.03930 -0.04934 \*

\* Se 20 0.04941 -0.01003 -0.01945 \*

\* Nb 1 -0.02913 -0.01149 -0.02904 \*

\* Nb 2 0.02058 0.01465 0.03197 \*

\* Nb 3 0.00398 0.00529 0.00031 \*

\* Nb 4 0.00589 -0.00574 0.00234 \*

\* Nb 5 0.04700 0.02461 -0.01779 \*

\* Nb 6 -0.01133 -0.00572 0.00282 \*

\* Nb 7 0.03062 0.01870 0.02526 \*

\* Nb 8 -0.05924 0.03255 -0.02106 \*

\* Nb 9 0.04401 -0.00191 -0.03526 \*

\* Nb 10 0.00241 0.01774 0.02143 \*

\* Nb 11 -0.01602 -0.03246 0.03410 \*

\* Nb 12 -0.07241 0.01057 0.00345 \*

\* Nb 13 -0.01114 -0.03905 -0.02844 \*

\* Nb 14 -0.04036 0.00862 0.04191 \*

\* Nb 15 0.01765 0.03077 -0.04202 \*

\* Nb 16 0.07276 -0.01974 -0.01696 \*

\* Nb 17 0.02430 0.01071 -0.02810 \*

\* Nb 18 -0.03305 -0.02465 0.03456 \*

\* Nb 19 -0.03009 -0.01519 -0.02369 \*

\* Nb 20 0.05270 -0.03010 0.01121 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.037180 -0.024053 0.087092 \*

\* y -0.024053 0.124876 0.089767 \*

\* z 0.087092 0.089767 0.047915 \*

\* \*

\* Pressure: -0.0452 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000115 | -36260.004850 | <-- min BFGS

| trial step | 1.000000 | 0.000061 | -36260.007209 | <-- min BFGS

| line step | 2.146705 | -3.072E-007 | -36260.008232 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 70 with enthalpy= -3.62600082E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 8.455521E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 8.868283E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.357045E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.248757E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 71 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000068 | -36260.008232 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 71 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8678148 -8.3192765 0.0122017 0.4204883 -0.0037801 -0.0003472

0.0303884 3.3802108 0.0011253 1.0348940 1.8495113 -0.0013478

0.0115631 0.0037061 13.9638868 -0.0004508 -0.0001457 0.4499600

Lattice parameters(A) Cell Angles

a = 17.037090 alpha = 89.965294

b = 3.380348 beta = 89.924987

c = 13.963892 gamma = 118.714062

Current cell volume = 705.303508 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066908 0.660896 0.121707 x

x Se 2 0.132476 0.340978 0.627761 x

x Se 3 0.132230 0.341256 0.871302 x

x Se 4 0.068042 0.663750 0.376267 x

x Se 5 0.268273 0.670624 0.123687 x

x Se 6 0.333063 0.342108 0.629108 x

x Se 7 0.333569 0.344811 0.872036 x

x Se 8 0.263955 0.658278 0.368818 x

x Se 9 0.466537 0.653108 0.128834 x

x Se 10 0.531480 0.337681 0.618445 x

x Se 11 0.533372 0.346636 0.871180 x

x Se 12 0.468582 0.662754 0.381848 x

x Se 13 0.666384 0.655054 0.128058 x

x Se 14 0.736051 0.341744 0.631304 x

x Se 15 0.731815 0.329695 0.876434 x

x Se 16 0.666864 0.657067 0.370739 x

x Se 17 0.867692 0.658759 0.128725 x

x Se 18 0.932315 0.336448 0.622694 x

x Se 19 0.933092 0.339215 0.878280 x

x Se 20 0.867551 0.659460 0.372311 x

x Nb 1 0.003674 0.003963 0.249187 x

x Nb 2 -0.003823 -0.004471 0.750472 x

x Nb 3 -0.000243 -0.000693 0.000031 x

x Nb 4 0.000481 0.001358 0.499709 x

x Nb 5 0.194487 -0.014257 0.246311 x

x Nb 6 0.200777 0.008205 0.749764 x

x Nb 7 0.199850 0.004566 -0.002456 x

x Nb 8 0.204536 0.012221 0.499287 x

x Nb 9 0.401478 -0.001949 0.253005 x

x Nb 10 0.402618 0.014081 0.750622 x

x Nb 11 0.402883 0.005694 -0.001279 x

x Nb 12 0.385438 -0.035655 0.499490 x

x Nb 13 0.597292 -0.013871 0.249584 x

x Nb 14 0.598467 0.001605 0.747150 x

x Nb 15 0.597026 -0.006142 0.001558 x

x Nb 16 0.614544 0.035841 0.500730 x

x Nb 17 0.799146 -0.008228 0.250442 x

x Nb 18 0.805799 0.014985 0.753507 x

x Nb 19 0.800232 -0.004201 0.002528 x

x Nb 20 0.795089 -0.013373 0.500819 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599548E+004 49044.38 <-- SCF

1 -3.62602212E+004 6.65989702E-003 49071.91 <-- SCF

2 -3.62602362E+004 3.75321506E-004 49099.97 <-- SCF

3 -3.62602196E+004 -4.15556443E-004 49126.91 <-- SCF

4 -3.62600082E+004 -5.28490238E-003 49152.81 <-- SCF

5 -3.62600173E+004 2.26845128E-004 49179.73 <-- SCF

6 -3.62600114E+004 -1.48031701E-004 49205.62 <-- SCF

7 -3.62600099E+004 -3.73589961E-005 49228.58 <-- SCF

8 -3.62600098E+004 -1.85731826E-006 49249.20 <-- SCF

9 -3.62600098E+004 7.61480718E-007 49267.17 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.00984468 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.01001 0.02107 0.02100 \*

\* Se 2 -0.04119 -0.00529 0.04038 \*

\* Se 3 -0.03452 0.00331 -0.01798 \*

\* Se 4 -0.02662 0.00806 -0.04227 \*

\* Se 5 0.01473 -0.04138 -0.01546 \*

\* Se 6 -0.04855 0.01185 0.01281 \*

\* Se 7 -0.01527 0.00044 -0.02937 \*

\* Se 8 -0.07209 -0.01886 0.01096 \*

\* Se 9 -0.01322 0.01571 0.03740 \*

\* Se 10 -0.00232 0.00916 -0.00139 \*

\* Se 11 0.01828 -0.01719 -0.01378 \*

\* Se 12 -0.03247 -0.04043 -0.01859 \*

\* Se 13 0.02094 0.01531 0.00939 \*

\* Se 14 0.07439 0.01786 -0.01405 \*

\* Se 15 -0.02019 0.04531 -0.00264 \*

\* Se 16 0.04329 0.03119 0.07708 \*

\* Se 17 0.01455 -0.01184 0.03544 \*

\* Se 18 0.04400 0.00231 0.00175 \*

\* Se 19 0.00717 -0.03347 -0.04007 \*

\* Se 20 0.05024 -0.01096 -0.01557 \*

\* Nb 1 -0.01807 -0.00426 -0.02391 \*

\* Nb 2 0.01004 0.00883 0.02738 \*

\* Nb 3 0.00502 0.00652 -0.00044 \*

\* Nb 4 0.00637 -0.00574 0.00286 \*

\* Nb 5 0.05964 0.02504 -0.01247 \*

\* Nb 6 -0.02010 -0.00575 0.00074 \*

\* Nb 7 0.03252 0.02085 0.01896 \*

\* Nb 8 -0.06881 0.03855 -0.01733 \*

\* Nb 9 0.03824 -0.00227 -0.02820 \*

\* Nb 10 0.00713 0.01922 0.01467 \*

\* Nb 11 -0.01192 -0.03684 0.03218 \*

\* Nb 12 -0.05489 0.00713 0.01207 \*

\* Nb 13 -0.01401 -0.04157 -0.02178 \*

\* Nb 14 -0.03341 0.01072 0.03568 \*

\* Nb 15 0.01383 0.03603 -0.04075 \*

\* Nb 16 0.05574 -0.01572 -0.02592 \*

\* Nb 17 0.03385 0.01227 -0.02844 \*

\* Nb 18 -0.04393 -0.02379 0.03182 \*

\* Nb 19 -0.03128 -0.01669 -0.01785 \*

\* Nb 20 0.06289 -0.03468 0.00571 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.021884 -0.004095 0.059172 \*

\* y -0.004095 0.110184 0.055953 \*

\* z 0.059172 0.055953 0.060037 \*

\* \*

\* Pressure: -0.0494 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000068 | -36260.008232 | <-- min BFGS

| trial step | 1.000000 | 0.000046 | -36260.009893 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 71 with line minimization (lambda= 3.089135)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8659869 -8.3089334 0.0106596 0.4204178 -0.0040031 -0.0002484

0.0321754 3.3791260 0.0000207 1.0337655 1.8495681 -0.0006244

0.0082545 0.0001015 13.9666341 -0.0003224 0.0000003 0.4498713

Lattice parameters(A) Cell Angles

a = 17.030445 alpha = 89.998911

b = 3.379279 beta = 89.934782

c = 13.966637 gamma = 118.656255

Current cell volume = 705.334080 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066911 0.660927 0.121800 x

x Se 2 0.132470 0.340963 0.627725 x

x Se 3 0.132264 0.341444 0.871385 x

x Se 4 0.068021 0.663668 0.376150 x

x Se 5 0.268477 0.670765 0.123746 x

x Se 6 0.332827 0.341565 0.629223 x

x Se 7 0.333323 0.343986 0.871849 x

x Se 8 0.263966 0.657834 0.368690 x

x Se 9 0.466507 0.652583 0.128874 x

x Se 10 0.531493 0.337679 0.618285 x

x Se 11 0.533392 0.347199 0.871122 x

x Se 12 0.468589 0.662869 0.382056 x

x Se 13 0.666622 0.655824 0.128245 x

x Se 14 0.736042 0.342201 0.631439 x

x Se 15 0.731613 0.329574 0.876404 x

x Se 16 0.667115 0.657428 0.370595 x

x Se 17 0.867661 0.658611 0.128631 x

x Se 18 0.932343 0.336470 0.622780 x

x Se 19 0.933093 0.339289 0.878215 x

x Se 20 0.867560 0.659566 0.372332 x

x Nb 1 0.003447 0.003091 0.249133 x

x Nb 2 -0.003618 -0.003647 0.750511 x

x Nb 3 -0.000259 -0.000749 0.000044 x

x Nb 4 0.000518 0.001413 0.499680 x

x Nb 5 0.194430 -0.014438 0.246202 x

x Nb 6 0.200597 0.007506 0.749787 x

x Nb 7 0.199888 0.004648 -0.002329 x

x Nb 8 0.204432 0.011612 0.499071 x

x Nb 9 0.401575 -0.001767 0.252969 x

x Nb 10 0.402543 0.013449 0.750728 x

x Nb 11 0.402844 0.005386 -0.001257 x

x Nb 12 0.384860 -0.036856 0.499475 x

x Nb 13 0.597351 -0.013266 0.249485 x

x Nb 14 0.598359 0.001374 0.747187 x

x Nb 15 0.597068 -0.005833 0.001556 x

x Nb 16 0.615096 0.036976 0.500746 x

x Nb 17 0.799320 -0.007549 0.250432 x

x Nb 18 0.805887 0.015228 0.753584 x

x Nb 19 0.800197 -0.004228 0.002402 x

x Nb 20 0.795176 -0.012795 0.501051 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597712E+004 49370.56 <-- SCF

1 -3.62609678E+004 2.99152689E-002 49398.05 <-- SCF

2 -3.62610350E+004 1.68161976E-003 49425.61 <-- SCF

3 -3.62608976E+004 -3.43503562E-003 49452.47 <-- SCF

4 -3.62600032E+004 -2.23612999E-002 49478.64 <-- SCF

5 -3.62600446E+004 1.03571652E-003 49505.53 <-- SCF

6 -3.62600175E+004 -6.78534353E-004 49531.98 <-- SCF

7 -3.62600107E+004 -1.69976224E-004 49557.17 <-- SCF

8 -3.62600111E+004 1.15655725E-005 49580.45 <-- SCF

9 -3.62600111E+004 -6.33373557E-007 49600.88 <-- SCF

10 -3.62600112E+004 2.35645257E-006 49618.84 <-- SCF

11 -3.62600112E+004 8.06488541E-007 49636.41 <-- SCF

12 -3.62600113E+004 1.02849564E-006 49653.34 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01128043 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.01664 0.00567 -0.00827 \*

\* Se 2 -0.04219 -0.00623 0.03932 \*

\* Se 3 -0.03885 -0.00468 -0.01287 \*

\* Se 4 -0.04327 -0.00605 -0.03301 \*

\* Se 5 -0.00718 -0.04604 -0.01763 \*

\* Se 6 -0.02826 0.00384 -0.00021 \*

\* Se 7 0.02799 0.02097 0.02781 \*

\* Se 8 -0.07973 0.00308 -0.00348 \*

\* Se 9 -0.00275 0.02877 0.02131 \*

\* Se 10 -0.01196 0.02883 -0.00393 \*

\* Se 11 0.00915 -0.03279 0.00898 \*

\* Se 12 -0.03073 -0.07338 -0.03846 \*

\* Se 13 -0.02355 -0.00035 -0.04675 \*

\* Se 14 0.08171 -0.00313 -0.00304 \*

\* Se 15 0.00147 0.04889 0.00184 \*

\* Se 16 0.02660 0.03440 0.09304 \*

\* Se 17 0.01737 -0.00368 0.03369 \*

\* Se 18 0.04852 0.01405 0.00463 \*

\* Se 19 0.01298 -0.02281 -0.01794 \*

\* Se 20 0.05165 -0.01276 -0.00702 \*

\* Nb 1 -0.00528 0.01490 -0.02055 \*

\* Nb 2 -0.00227 -0.00641 0.02545 \*

\* Nb 3 0.00711 0.00958 -0.00140 \*

\* Nb 4 0.00522 -0.00519 0.00528 \*

\* Nb 5 0.08844 0.02585 -0.00360 \*

\* Nb 6 -0.03027 -0.00427 -0.00195 \*

\* Nb 7 0.03450 0.02422 0.00833 \*

\* Nb 8 -0.06579 0.04865 -0.00467 \*

\* Nb 9 0.04225 0.00010 -0.00596 \*

\* Nb 10 0.02398 0.02636 0.00043 \*

\* Nb 11 -0.00769 -0.04207 0.02321 \*

\* Nb 12 -0.02750 -0.00132 0.02751 \*

\* Nb 13 -0.02810 -0.05004 -0.00840 \*

\* Nb 14 -0.03425 0.01303 0.01486 \*

\* Nb 15 0.01039 0.04308 -0.03434 \*

\* Nb 16 0.03309 -0.00606 -0.04244 \*

\* Nb 17 0.04636 0.01466 -0.03122 \*

\* Nb 18 -0.07097 -0.02147 0.02910 \*

\* Nb 19 -0.03162 -0.01822 -0.00774 \*

\* Nb 20 0.06005 -0.04199 -0.00991 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.001426 0.042326 0.003141 \*

\* y 0.042326 0.065544 -0.017871 \*

\* z 0.003141 -0.017871 0.065103 \*

\* \*

\* Pressure: -0.0440 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000068 | -36260.008232 | <-- min BFGS

| trial step | 1.000000 | 0.000046 | -36260.009893 | <-- min BFGS

| line step | 3.089135 | -7.102E-007 | -36260.011325 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 71 with enthalpy= -3.62600113E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.731710E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.027063E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.281899E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 6.554433E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 72 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000024 | -36260.011325 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 72 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8680905 -8.3097834 0.0105614 0.4203972 -0.0039333 -0.0002350

0.0316097 3.3785153 -0.0001750 1.0340072 1.8500732 -0.0005063

0.0078023 -0.0005391 13.9649655 -0.0003050 0.0000262 0.4499250

Lattice parameters(A) Cell Angles

a = 17.032696 alpha = 90.004879

b = 3.378663 beta = 89.935450

c = 13.964968 gamma = 118.664794

Current cell volume = 705.157045 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066910 0.660994 0.121805 x

x Se 2 0.132472 0.340786 0.627759 x

x Se 3 0.132248 0.341162 0.871418 x

x Se 4 0.068013 0.663646 0.376112 x

x Se 5 0.268500 0.670824 0.123783 x

x Se 6 0.332869 0.341598 0.629214 x

x Se 7 0.333319 0.343966 0.871903 x

x Se 8 0.263923 0.657708 0.368643 x

x Se 9 0.466510 0.652701 0.128804 x

x Se 10 0.531506 0.337568 0.618289 x

x Se 11 0.533387 0.347096 0.871185 x

x Se 12 0.468587 0.662991 0.382046 x

x Se 13 0.666626 0.655843 0.128205 x

x Se 14 0.736084 0.342330 0.631482 x

x Se 15 0.731590 0.329513 0.876385 x

x Se 16 0.667065 0.657346 0.370571 x

x Se 17 0.867678 0.658899 0.128595 x

x Se 18 0.932353 0.336495 0.622804 x

x Se 19 0.933094 0.339224 0.878217 x

x Se 20 0.867561 0.659752 0.372297 x

x Nb 1 0.003407 0.002828 0.249139 x

x Nb 2 -0.003581 -0.003405 0.750504 x

x Nb 3 -0.000261 -0.000746 0.000045 x

x Nb 4 0.000526 0.001424 0.499679 x

x Nb 5 0.194504 -0.014398 0.246202 x

x Nb 6 0.200576 0.007449 0.749780 x

x Nb 7 0.199918 0.004788 -0.002345 x

x Nb 8 0.204416 0.011620 0.499067 x

x Nb 9 0.401587 -0.001794 0.252980 x

x Nb 10 0.402537 0.013699 0.750764 x

x Nb 11 0.402844 0.005246 -0.001199 x

x Nb 12 0.384750 -0.037183 0.499410 x

x Nb 13 0.597359 -0.013516 0.249461 x

x Nb 14 0.598343 0.001389 0.747178 x

x Nb 15 0.597069 -0.005689 0.001495 x

x Nb 16 0.615197 0.037290 0.500818 x

x Nb 17 0.799335 -0.007485 0.250440 x

x Nb 18 0.805820 0.015206 0.753582 x

x Nb 19 0.800167 -0.004363 0.002423 x

x Nb 20 0.795192 -0.012802 0.501056 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599952E+004 49756.78 <-- SCF

1 -3.62600520E+004 1.41947213E-003 49784.20 <-- SCF

2 -3.62600547E+004 6.84452304E-005 49810.89 <-- SCF

3 -3.62600472E+004 -1.88546515E-004 49837.80 <-- SCF

4 -3.62600117E+004 -8.86650725E-004 49863.62 <-- SCF

5 -3.62600128E+004 2.73351965E-005 49889.64 <-- SCF

6 -3.62600120E+004 -2.07531711E-005 49912.59 <-- SCF

7 -3.62600118E+004 -3.94357632E-006 49931.28 <-- SCF

8 -3.62600118E+004 -5.92032086E-007 49950.61 <-- SCF

9 -3.62600118E+004 3.56436605E-007 49967.56 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01182222 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.01096 0.00038 -0.00698 \*

\* Se 2 -0.04391 0.00510 0.02394 \*

\* Se 3 -0.03391 0.01453 -0.01639 \*

\* Se 4 -0.04422 -0.00632 -0.02905 \*

\* Se 5 -0.00774 -0.04706 -0.02002 \*

\* Se 6 -0.03938 0.00826 0.00095 \*

\* Se 7 0.02353 0.02652 0.00715 \*

\* Se 8 -0.07628 0.00402 -0.00050 \*

\* Se 9 0.00572 0.02212 0.04191 \*

\* Se 10 -0.01776 0.03188 -0.00728 \*

\* Se 11 0.00192 -0.02732 -0.00913 \*

\* Se 12 -0.02903 -0.07882 -0.03491 \*

\* Se 13 -0.02074 -0.00470 -0.03161 \*

\* Se 14 0.07836 -0.00477 -0.00670 \*

\* Se 15 0.00315 0.05000 0.00398 \*

\* Se 16 0.04082 0.03370 0.10315 \*

\* Se 17 0.01224 -0.02233 0.03831 \*

\* Se 18 0.04565 0.01335 0.00307 \*

\* Se 19 0.00787 -0.01768 -0.02111 \*

\* Se 20 0.05313 -0.02368 0.00928 \*

\* Nb 1 -0.00311 0.01893 -0.02504 \*

\* Nb 2 -0.00442 -0.00981 0.02959 \*

\* Nb 3 0.00746 0.00943 -0.00107 \*

\* Nb 4 0.00592 -0.00536 0.00472 \*

\* Nb 5 0.07372 0.02906 -0.00962 \*

\* Nb 6 -0.02808 -0.01064 0.00111 \*

\* Nb 7 0.02811 0.02066 0.01571 \*

\* Nb 8 -0.07757 0.04598 -0.00502 \*

\* Nb 9 0.03918 0.00387 -0.01284 \*

\* Nb 10 0.02651 0.01654 0.00262 \*

\* Nb 11 -0.01036 -0.04107 0.02048 \*

\* Nb 12 -0.01954 0.00129 0.03251 \*

\* Nb 13 -0.03195 -0.04060 -0.01498 \*

\* Nb 14 -0.03090 0.00953 0.02093 \*

\* Nb 15 0.01280 0.04245 -0.03051 \*

\* Nb 16 0.02692 -0.00891 -0.05105 \*

\* Nb 17 0.04630 0.01999 -0.03549 \*

\* Nb 18 -0.05636 -0.02466 0.03543 \*

\* Nb 19 -0.02484 -0.01466 -0.01436 \*

\* Nb 20 0.07174 -0.03920 -0.01117 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.015220 0.030573 -0.007004 \*

\* y 0.030573 0.005307 -0.032218 \*

\* z -0.007004 -0.032218 0.013976 \*

\* \*

\* Pressure: -0.0014 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000024 | -36260.011325 | <-- min BFGS

| trial step | 1.000000 | 9.644E-006 | -36260.011892 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 72 with line minimization (lambda= 1.685922)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8695334 -8.3103664 0.0104940 0.4203830 -0.0038854 -0.0002258

0.0312217 3.3780964 -0.0003092 1.0341731 1.8504198 -0.0004252

0.0074922 -0.0009786 13.9638210 -0.0002930 0.0000439 0.4499619

Lattice parameters(A) Cell Angles

a = 17.034240 alpha = 90.008974

b = 3.378241 beta = 89.935909

c = 13.963823 gamma = 118.670654

Current cell volume = 705.035594 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066909 0.661040 0.121809 x

x Se 2 0.132474 0.340665 0.627783 x

x Se 3 0.132236 0.340969 0.871442 x

x Se 4 0.068008 0.663630 0.376086 x

x Se 5 0.268516 0.670864 0.123809 x

x Se 6 0.332898 0.341621 0.629208 x

x Se 7 0.333317 0.343952 0.871940 x

x Se 8 0.263894 0.657623 0.368611 x

x Se 9 0.466512 0.652782 0.128755 x

x Se 10 0.531514 0.337492 0.618292 x

x Se 11 0.533383 0.347025 0.871229 x

x Se 12 0.468586 0.663074 0.382040 x

x Se 13 0.666629 0.655856 0.128178 x

x Se 14 0.736112 0.342417 0.631512 x

x Se 15 0.731574 0.329471 0.876373 x

x Se 16 0.667031 0.657290 0.370554 x

x Se 17 0.867691 0.659097 0.128570 x

x Se 18 0.932359 0.336513 0.622820 x

x Se 19 0.933095 0.339180 0.878218 x

x Se 20 0.867561 0.659879 0.372274 x

x Nb 1 0.003379 0.002648 0.249142 x

x Nb 2 -0.003555 -0.003239 0.750500 x

x Nb 3 -0.000262 -0.000744 0.000045 x

x Nb 4 0.000532 0.001432 0.499679 x

x Nb 5 0.194555 -0.014371 0.246202 x

x Nb 6 0.200562 0.007410 0.749776 x

x Nb 7 0.199939 0.004883 -0.002356 x

x Nb 8 0.204405 0.011625 0.499063 x

x Nb 9 0.401596 -0.001812 0.252988 x

x Nb 10 0.402533 0.013870 0.750789 x

x Nb 11 0.402844 0.005150 -0.001159 x

x Nb 12 0.384674 -0.037408 0.499365 x

x Nb 13 0.597363 -0.013687 0.249444 x

x Nb 14 0.598331 0.001399 0.747172 x

x Nb 15 0.597070 -0.005590 0.001452 x

x Nb 16 0.615266 0.037506 0.500867 x

x Nb 17 0.799345 -0.007441 0.250446 x

x Nb 18 0.805774 0.015191 0.753581 x

x Nb 19 0.800146 -0.004456 0.002437 x

x Nb 20 0.795203 -0.012807 0.501060 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600040E+004 50071.42 <-- SCF

1 -3.62600331E+004 7.27897027E-004 50099.02 <-- SCF

2 -3.62600346E+004 3.77394183E-005 50124.73 <-- SCF

3 -3.62600304E+004 -1.05394849E-004 50151.09 <-- SCF

4 -3.62600117E+004 -4.67377512E-004 50176.59 <-- SCF

5 -3.62600124E+004 1.82116105E-005 50201.47 <-- SCF

6 -3.62600120E+004 -1.03842418E-005 50222.44 <-- SCF

7 -3.62600119E+004 -2.50242915E-006 50240.59 <-- SCF

8 -3.62600119E+004 -2.49881462E-007 50259.38 <-- SCF

9 -3.62600119E+004 1.81430672E-007 50275.34 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01192751 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00626 -0.00242 -0.00705 \*

\* Se 2 -0.04448 0.01283 0.01545 \*

\* Se 3 -0.03033 0.02651 -0.01750 \*

\* Se 4 -0.04345 -0.00630 -0.02668 \*

\* Se 5 -0.00600 -0.04748 -0.02117 \*

\* Se 6 -0.04402 0.01161 0.00154 \*

\* Se 7 0.02221 0.02995 -0.00645 \*

\* Se 8 -0.07013 0.00507 0.00212 \*

\* Se 9 0.01093 0.01785 0.05616 \*

\* Se 10 -0.02182 0.03359 -0.00875 \*

\* Se 11 -0.00281 -0.02381 -0.02235 \*

\* Se 12 -0.02800 -0.08212 -0.03289 \*

\* Se 13 -0.02050 -0.00719 -0.02145 \*

\* Se 14 0.07272 -0.00614 -0.00923 \*

\* Se 15 0.00284 0.05042 0.00440 \*

\* Se 16 0.04752 0.03340 0.11016 \*

\* Se 17 0.00873 -0.03394 0.03985 \*

\* Se 18 0.04192 0.01278 0.00238 \*

\* Se 19 0.00334 -0.01499 -0.02271 \*

\* Se 20 0.05376 -0.03122 0.01878 \*

\* Nb 1 -0.00234 0.02326 -0.02905 \*

\* Nb 2 -0.00553 -0.01374 0.03331 \*

\* Nb 3 0.00778 0.00929 -0.00118 \*

\* Nb 4 0.00593 -0.00543 0.00459 \*

\* Nb 5 0.06581 0.03125 -0.01281 \*

\* Nb 6 -0.02379 -0.01428 0.00387 \*

\* Nb 7 0.02537 0.01775 0.01882 \*

\* Nb 8 -0.07912 0.04351 -0.00594 \*

\* Nb 9 0.03786 0.00642 -0.01642 \*

\* Nb 10 0.02984 0.01074 0.00360 \*

\* Nb 11 -0.01157 -0.03956 0.01732 \*

\* Nb 12 -0.01595 0.00235 0.03469 \*

\* Nb 13 -0.03577 -0.03518 -0.01879 \*

\* Nb 14 -0.02931 0.00708 0.02394 \*

\* Nb 15 0.01387 0.04113 -0.02697 \*

\* Nb 16 0.02456 -0.01020 -0.05520 \*

\* Nb 17 0.04328 0.02270 -0.03909 \*

\* Nb 18 -0.04834 -0.02695 0.03889 \*

\* Nb 19 -0.02194 -0.01184 -0.01740 \*

\* Nb 20 0.07318 -0.03671 -0.01077 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.026087 0.027186 -0.013543 \*

\* y 0.027186 -0.033628 -0.042002 \*

\* z -0.013543 -0.042002 -0.017229 \*

\* \*

\* Pressure: 0.0256 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000024 | -36260.011325 | <-- min BFGS

| trial step | 1.000000 | 9.644E-006 | -36260.011892 | <-- min BFGS

| line step | 1.685922 | 9.432E-007 | -36260.012008 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 72 with enthalpy= -3.62600120E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.709924E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.245322E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.193566E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.200209E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 73 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000016 | -36260.012008 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 73 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8704827 -8.3104364 0.0103366 0.4203558 -0.0038859 -0.0002282

0.0312288 3.3781389 -0.0002048 1.0341020 1.8503951 -0.0004757

0.0075745 -0.0006433 13.9627817 -0.0002960 0.0000300 0.4499954

Lattice parameters(A) Cell Angles

a = 17.035102 alpha = 90.005826

b = 3.378283 beta = 89.936814

c = 13.962784 gamma = 118.669187

Current cell volume = 705.037562 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066896 0.661006 0.121867 x

x Se 2 0.132487 0.340601 0.627774 x

x Se 3 0.132259 0.340936 0.871504 x

x Se 4 0.067971 0.663498 0.376025 x

x Se 5 0.268558 0.670886 0.123862 x

x Se 6 0.332856 0.341434 0.629199 x

x Se 7 0.333271 0.343783 0.871931 x

x Se 8 0.263881 0.657502 0.368582 x

x Se 9 0.466524 0.652756 0.128725 x

x Se 10 0.531515 0.337484 0.618300 x

x Se 11 0.533368 0.347072 0.871255 x

x Se 12 0.468594 0.663096 0.382032 x

x Se 13 0.666674 0.656024 0.128191 x

x Se 14 0.736124 0.342543 0.631540 x

x Se 15 0.731530 0.329451 0.876332 x

x Se 16 0.667074 0.657433 0.370548 x

x Se 17 0.867667 0.659131 0.128506 x

x Se 18 0.932397 0.336632 0.622877 x

x Se 19 0.933109 0.339234 0.878167 x

x Se 20 0.867550 0.659955 0.372282 x

x Nb 1 0.003287 0.002399 0.249136 x

x Nb 2 -0.003470 -0.002998 0.750505 x

x Nb 3 -0.000264 -0.000748 0.000049 x

x Nb 4 0.000541 0.001437 0.499673 x

x Nb 5 0.194611 -0.014266 0.246207 x

x Nb 6 0.200485 0.007106 0.749775 x

x Nb 7 0.199958 0.004909 -0.002297 x

x Nb 8 0.204324 0.011345 0.498999 x

x Nb 9 0.401615 -0.001751 0.252961 x

x Nb 10 0.402494 0.013581 0.750808 x

x Nb 11 0.402811 0.004963 -0.001143 x

x Nb 12 0.384603 -0.037517 0.499381 x

x Nb 13 0.597400 -0.013422 0.249432 x

x Nb 14 0.598310 0.001334 0.747201 x

x Nb 15 0.597106 -0.005400 0.001437 x

x Nb 16 0.615328 0.037583 0.500851 x

x Nb 17 0.799421 -0.007135 0.250446 x

x Nb 18 0.805729 0.015108 0.753572 x

x Nb 19 0.800127 -0.004462 0.002379 x

x Nb 20 0.795282 -0.012521 0.501129 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599946E+004 50379.05 <-- SCF

1 -3.62600788E+004 2.10597222E-003 50406.58 <-- SCF

2 -3.62600836E+004 1.18286864E-004 50433.52 <-- SCF

3 -3.62600832E+004 -1.02676426E-005 50460.47 <-- SCF

4 -3.62600115E+004 -1.79028563E-003 50486.44 <-- SCF

5 -3.62600140E+004 6.16402555E-005 50513.28 <-- SCF

6 -3.62600126E+004 -3.49188586E-005 50537.05 <-- SCF

7 -3.62600123E+004 -8.35669149E-006 50557.00 <-- SCF

8 -3.62600123E+004 -7.03566494E-007 50576.59 <-- SCF

9 -3.62600123E+004 2.98923154E-007 50593.42 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01226785 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00476 -0.00292 -0.01719 \*

\* Se 2 -0.04952 0.01616 0.01209 \*

\* Se 3 -0.03249 0.02953 -0.02188 \*

\* Se 4 -0.04749 -0.00442 -0.02400 \*

\* Se 5 -0.00823 -0.04773 -0.02091 \*

\* Se 6 -0.04651 0.01206 0.00975 \*

\* Se 7 0.02723 0.03099 -0.00544 \*

\* Se 8 -0.06647 0.01137 0.00636 \*

\* Se 9 0.01569 0.02127 0.06069 \*

\* Se 10 -0.02280 0.03206 -0.01282 \*

\* Se 11 -0.00661 -0.02876 -0.02644 \*

\* Se 12 -0.02937 -0.08059 -0.02848 \*

\* Se 13 -0.02700 -0.00822 -0.02414 \*

\* Se 14 0.06932 -0.01301 -0.01398 \*

\* Se 15 0.00811 0.04950 0.00651 \*

\* Se 16 0.05168 0.03429 0.10706 \*

\* Se 17 0.01100 -0.03648 0.04463 \*

\* Se 18 0.03758 0.01079 0.00162 \*

\* Se 19 0.00199 -0.01496 -0.01392 \*

\* Se 20 0.05879 -0.03432 0.02281 \*

\* Nb 1 -0.00030 0.02570 -0.02982 \*

\* Nb 2 -0.00722 -0.01581 0.03356 \*

\* Nb 3 0.00821 0.00945 -0.00167 \*

\* Nb 4 0.00555 -0.00532 0.00514 \*

\* Nb 5 0.05851 0.03038 -0.01459 \*

\* Nb 6 -0.01925 -0.01481 0.00394 \*

\* Nb 7 0.02271 0.01665 0.01626 \*

\* Nb 8 -0.07479 0.04316 -0.00041 \*

\* Nb 9 0.03830 0.00551 -0.01166 \*

\* Nb 10 0.03581 0.01433 0.00225 \*

\* Nb 11 -0.00860 -0.03829 0.01447 \*

\* Nb 12 -0.01256 0.00087 0.02951 \*

\* Nb 13 -0.04023 -0.03877 -0.01933 \*

\* Nb 14 -0.02906 0.00847 0.01835 \*

\* Nb 15 0.01147 0.04004 -0.02435 \*

\* Nb 16 0.02298 -0.00892 -0.05162 \*

\* Nb 17 0.04012 0.02305 -0.04032 \*

\* Nb 18 -0.04138 -0.02575 0.04163 \*

\* Nb 19 -0.01877 -0.01065 -0.01564 \*

\* Nb 20 0.06835 -0.03591 -0.01802 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.012885 0.020037 -0.010663 \*

\* y 0.020037 -0.036472 -0.035403 \*

\* z -0.010663 -0.035403 -0.025090 \*

\* \*

\* Pressure: 0.0248 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000016 | -36260.012008 | <-- min BFGS

| trial step | 1.000000 | 0.000010 | -36260.012350 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 73 with line minimization (lambda= 2.895182)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8722816 -8.3105692 0.0100385 0.4203043 -0.0038870 -0.0002327

0.0312422 3.3782194 -0.0000070 1.0339672 1.8503481 -0.0005715

0.0077304 -0.0000080 13.9608119 -0.0003017 0.0000037 0.4500589

Lattice parameters(A) Cell Angles

a = 17.036737 alpha = 89.999858

b = 3.378364 beta = 89.938529

c = 13.960814 gamma = 118.666409

Current cell volume = 705.041269 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066870 0.660942 0.121976 x

x Se 2 0.132513 0.340479 0.627757 x

x Se 3 0.132302 0.340873 0.871623 x

x Se 4 0.067899 0.663248 0.375910 x

x Se 5 0.268639 0.670927 0.123962 x

x Se 6 0.332776 0.341081 0.629183 x

x Se 7 0.333183 0.343461 0.871914 x

x Se 8 0.263858 0.657272 0.368526 x

x Se 9 0.466548 0.652706 0.128667 x

x Se 10 0.531518 0.337467 0.618317 x

x Se 11 0.533339 0.347160 0.871304 x

x Se 12 0.468610 0.663139 0.382016 x

x Se 13 0.666760 0.656343 0.128215 x

x Se 14 0.736146 0.342780 0.631592 x

x Se 15 0.731447 0.329413 0.876256 x

x Se 16 0.667155 0.657702 0.370535 x

x Se 17 0.867623 0.659196 0.128384 x

x Se 18 0.932468 0.336858 0.622984 x

x Se 19 0.933136 0.339336 0.878071 x

x Se 20 0.867529 0.660099 0.372298 x

x Nb 1 0.003113 0.001926 0.249125 x

x Nb 2 -0.003309 -0.002540 0.750515 x

x Nb 3 -0.000268 -0.000756 0.000056 x

x Nb 4 0.000558 0.001446 0.499660 x

x Nb 5 0.194716 -0.014069 0.246217 x

x Nb 6 0.200337 0.006530 0.749773 x

x Nb 7 0.199996 0.004958 -0.002187 x

x Nb 8 0.204170 0.010815 0.498877 x

x Nb 9 0.401651 -0.001635 0.252909 x

x Nb 10 0.402419 0.013033 0.750843 x

x Nb 11 0.402746 0.004609 -0.001113 x

x Nb 12 0.384467 -0.037724 0.499412 x

x Nb 13 0.597468 -0.012920 0.249408 x

x Nb 14 0.598270 0.001210 0.747256 x

x Nb 15 0.597172 -0.005039 0.001408 x

x Nb 16 0.615445 0.037730 0.500821 x

x Nb 17 0.799564 -0.006554 0.250448 x

x Nb 18 0.805643 0.014952 0.753553 x

x Nb 19 0.800090 -0.004472 0.002268 x

x Nb 20 0.795432 -0.011981 0.501259 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599493E+004 50696.95 <-- SCF

1 -3.62602488E+004 7.48810069E-003 50724.34 <-- SCF

2 -3.62602658E+004 4.24908009E-004 50752.52 <-- SCF

3 -3.62602601E+004 -1.43326840E-004 50779.67 <-- SCF

4 -3.62600092E+004 -6.27157764E-003 50805.62 <-- SCF

5 -3.62600192E+004 2.47874594E-004 50832.39 <-- SCF

6 -3.62600139E+004 -1.32192108E-004 50858.33 <-- SCF

7 -3.62600125E+004 -3.44798923E-005 50881.06 <-- SCF

8 -3.62600125E+004 1.02028344E-006 50901.89 <-- SCF

9 -3.62600125E+004 1.30514582E-007 50919.81 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01253957 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00058 -0.00367 -0.03434 \*

\* Se 2 -0.05951 0.02247 0.00583 \*

\* Se 3 -0.03688 0.03390 -0.02840 \*

\* Se 4 -0.05351 -0.00149 -0.01987 \*

\* Se 5 -0.01037 -0.05024 -0.01624 \*

\* Se 6 -0.04949 0.01380 0.02391 \*

\* Se 7 0.03807 0.03246 0.00182 \*

\* Se 8 -0.05825 0.02355 0.01184 \*

\* Se 9 0.02243 0.02735 0.06848 \*

\* Se 10 -0.02416 0.02894 -0.01949 \*

\* Se 11 -0.01206 -0.03789 -0.03276 \*

\* Se 12 -0.03376 -0.07747 -0.02125 \*

\* Se 13 -0.04190 -0.00977 -0.03356 \*

\* Se 14 0.06187 -0.02608 -0.02038 \*

\* Se 15 0.01613 0.04968 0.00506 \*

\* Se 16 0.05775 0.03553 0.10117 \*

\* Se 17 0.01644 -0.04026 0.05212 \*

\* Se 18 0.02720 0.00791 -0.00066 \*

\* Se 19 -0.00145 -0.01486 0.00176 \*

\* Se 20 0.06933 -0.04031 0.03021 \*

\* Nb 1 0.00699 0.02881 -0.03146 \*

\* Nb 2 -0.01412 -0.01875 0.03431 \*

\* Nb 3 0.00920 0.01002 -0.00282 \*

\* Nb 4 0.00488 -0.00488 0.00656 \*

\* Nb 5 0.04818 0.02849 -0.01842 \*

\* Nb 6 -0.00831 -0.01431 0.00520 \*

\* Nb 7 0.02023 0.01540 0.01183 \*

\* Nb 8 -0.06628 0.04301 0.00841 \*

\* Nb 9 0.03960 0.00281 -0.00183 \*

\* Nb 10 0.04713 0.02302 -0.00216 \*

\* Nb 11 -0.00496 -0.03666 0.01061 \*

\* Nb 12 -0.00679 -0.00178 0.02023 \*

\* Nb 13 -0.04986 -0.04739 -0.01906 \*

\* Nb 14 -0.02798 0.01193 0.00737 \*

\* Nb 15 0.00858 0.03905 -0.02118 \*

\* Nb 16 0.02104 -0.00656 -0.04495 \*

\* Nb 17 0.03188 0.02254 -0.04375 \*

\* Nb 18 -0.03118 -0.02306 0.04735 \*

\* Nb 19 -0.01532 -0.00968 -0.01172 \*

\* Nb 20 0.05977 -0.03555 -0.02979 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.014596 0.007086 -0.003763 \*

\* y 0.007086 -0.045666 -0.022682 \*

\* z -0.003763 -0.022682 -0.042435 \*

\* \*

\* Pressure: 0.0245 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000016 | -36260.012008 | <-- min BFGS

| trial step | 1.000000 | 0.000010 | -36260.012350 | <-- min BFGS

| line step | 2.895182 | 4.957E-008 | -36260.012618 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 73 with enthalpy= -3.62600126E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.523660E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.217920E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.501650E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.566569E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 74 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000020 | -36260.012618 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 74 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8743890 -8.3131034 0.0092031 0.4202780 -0.0038264 -0.0002393

0.0307592 3.3784150 0.0004429 1.0341579 1.8503872 -0.0007823

0.0079636 0.0014517 13.9606287 -0.0003099 -0.0000562 0.4500648

Lattice parameters(A) Cell Angles

a = 17.039813 alpha = 89.986234

b = 3.378555 beta = 89.943432

c = 13.960631 gamma = 118.678608

Current cell volume = 705.117049 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066874 0.660985 0.121978 x

x Se 2 0.132500 0.340551 0.627756 x

x Se 3 0.132296 0.340982 0.871598 x

x Se 4 0.067893 0.663283 0.375916 x

x Se 5 0.268629 0.670837 0.123951 x

x Se 6 0.332747 0.341112 0.629188 x

x Se 7 0.333180 0.343489 0.871891 x

x Se 8 0.263858 0.657266 0.368569 x

x Se 9 0.466549 0.652628 0.128712 x

x Se 10 0.531507 0.337577 0.618343 x

x Se 11 0.533342 0.347233 0.871273 x

x Se 12 0.468602 0.662942 0.381976 x

x Se 13 0.666764 0.656340 0.128224 x

x Se 14 0.736147 0.342784 0.631547 x

x Se 15 0.731458 0.329499 0.876258 x

x Se 16 0.667186 0.657740 0.370577 x

x Se 17 0.867623 0.659063 0.128418 x

x Se 18 0.932471 0.336823 0.622975 x

x Se 19 0.933132 0.339271 0.878056 x

x Se 20 0.867543 0.660010 0.372310 x

x Nb 1 0.003136 0.002081 0.249112 x

x Nb 2 -0.003332 -0.002683 0.750531 x

x Nb 3 -0.000265 -0.000743 0.000054 x

x Nb 4 0.000555 0.001432 0.499665 x

x Nb 5 0.194717 -0.014032 0.246220 x

x Nb 6 0.200350 0.006662 0.749772 x

x Nb 7 0.199988 0.004942 -0.002179 x

x Nb 8 0.204145 0.010806 0.498896 x

x Nb 9 0.401653 -0.001744 0.252898 x

x Nb 10 0.402418 0.013060 0.750845 x

x Nb 11 0.402732 0.004627 -0.001132 x

x Nb 12 0.384525 -0.037546 0.499434 x

x Nb 13 0.597468 -0.012973 0.249398 x

x Nb 14 0.598273 0.001351 0.747268 x

x Nb 15 0.597187 -0.005055 0.001423 x

x Nb 16 0.615393 0.037559 0.500790 x

x Nb 17 0.799559 -0.006666 0.250437 x

x Nb 18 0.805642 0.014917 0.753560 x

x Nb 19 0.800099 -0.004447 0.002258 x

x Nb 20 0.795458 -0.011961 0.501233 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600078E+004 51023.08 <-- SCF

1 -3.62600370E+004 7.30335540E-004 51050.25 <-- SCF

2 -3.62600388E+004 4.51607866E-005 51073.64 <-- SCF

3 -3.62600434E+004 1.14567100E-004 51100.42 <-- SCF

4 -3.62600116E+004 -7.94763012E-004 51126.39 <-- SCF

5 -3.62600134E+004 4.59109175E-005 51150.52 <-- SCF

6 -3.62600132E+004 -4.85426966E-006 51170.36 <-- SCF

7 -3.62600130E+004 -5.04165702E-006 51188.88 <-- SCF

8 -3.62600130E+004 -9.01387398E-007 51206.31 <-- SCF

9 -3.62600130E+004 1.11572398E-006 51225.02 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01302713 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00198 -0.00318 -0.03572 \*

\* Se 2 -0.06075 0.01661 0.01067 \*

\* Se 3 -0.03802 0.02523 -0.02441 \*

\* Se 4 -0.05339 -0.00011 -0.02277 \*

\* Se 5 -0.01010 -0.04624 -0.01713 \*

\* Se 6 -0.04167 0.00846 0.02142 \*

\* Se 7 0.03952 0.02712 0.01133 \*

\* Se 8 -0.05660 0.02711 0.00677 \*

\* Se 9 0.02129 0.03337 0.05406 \*

\* Se 10 -0.02348 0.02210 -0.02410 \*

\* Se 11 -0.01222 -0.04262 -0.02282 \*

\* Se 12 -0.02806 -0.06324 -0.00913 \*

\* Se 13 -0.04242 -0.00780 -0.03761 \*

\* Se 14 0.06076 -0.02928 -0.01447 \*

\* Se 15 0.01554 0.04576 0.00696 \*

\* Se 16 0.04763 0.03482 0.08773 \*

\* Se 17 0.01871 -0.03139 0.04533 \*

\* Se 18 0.02745 0.00610 0.00265 \*

\* Se 19 0.00044 -0.01358 0.00611 \*

\* Se 20 0.06986 -0.03240 0.02173 \*

\* Nb 1 0.00007 0.02400 -0.02840 \*

\* Nb 2 -0.00745 -0.01508 0.03067 \*

\* Nb 3 0.00828 0.00944 -0.00271 \*

\* Nb 4 0.00610 -0.00519 0.00552 \*

\* Nb 5 0.05097 0.02418 -0.01600 \*

\* Nb 6 -0.01450 -0.01200 0.00495 \*

\* Nb 7 0.01941 0.01516 0.00973 \*

\* Nb 8 -0.06492 0.04221 0.00580 \*

\* Nb 9 0.03195 0.00230 0.00218 \*

\* Nb 10 0.04470 0.02749 -0.00521 \*

\* Nb 11 -0.00680 -0.03635 0.01282 \*

\* Nb 12 -0.01664 -0.00286 0.01786 \*

\* Nb 13 -0.04465 -0.04935 -0.01160 \*

\* Nb 14 -0.02253 0.01116 0.00205 \*

\* Nb 15 0.00994 0.03892 -0.02284 \*

\* Nb 16 0.02826 -0.00493 -0.03891 \*

\* Nb 17 0.03467 0.01920 -0.03820 \*

\* Nb 18 -0.03421 -0.01979 0.04105 \*

\* Nb 19 -0.01379 -0.01006 -0.01034 \*

\* Nb 20 0.05861 -0.03526 -0.02501 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.035080 -0.018246 0.001174 \*

\* y -0.018246 -0.024892 0.007273 \*

\* z 0.001174 0.007273 -0.036636 \*

\* \*

\* Pressure: 0.0088 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000020 | -36260.012618 | <-- min BFGS

| trial step | 1.000000 | 0.000013 | -36260.013120 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 74 with line minimization (lambda= 2.803120)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8781889 -8.3176728 0.0076969 0.4202305 -0.0037172 -0.0002513

0.0298884 3.3787676 0.0012540 1.0345017 1.8504579 -0.0011626

0.0083841 0.0040839 13.9602983 -0.0003246 -0.0001642 0.4500755

Lattice parameters(A) Cell Angles

a = 17.045358 alpha = 89.961672

b = 3.378900 beta = 89.952272

c = 13.960301 gamma = 118.700598

Current cell volume = 705.253576 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066880 0.661063 0.121983 x

x Se 2 0.132477 0.340680 0.627753 x

x Se 3 0.132286 0.341176 0.871552 x

x Se 4 0.067881 0.663346 0.375925 x

x Se 5 0.268610 0.670675 0.123931 x

x Se 6 0.332695 0.341169 0.629198 x

x Se 7 0.333175 0.343540 0.871851 x

x Se 8 0.263858 0.657254 0.368648 x

x Se 9 0.466551 0.652486 0.128793 x

x Se 10 0.531487 0.337775 0.618390 x

x Se 11 0.533347 0.347365 0.871216 x

x Se 12 0.468589 0.662588 0.381904 x

x Se 13 0.666771 0.656334 0.128241 x

x Se 14 0.736149 0.342792 0.631464 x

x Se 15 0.731476 0.329656 0.876261 x

x Se 16 0.667242 0.657808 0.370653 x

x Se 17 0.867623 0.658824 0.128480 x

x Se 18 0.932475 0.336760 0.622961 x

x Se 19 0.933124 0.339153 0.878029 x

x Se 20 0.867569 0.659848 0.372331 x

x Nb 1 0.003178 0.002360 0.249089 x

x Nb 2 -0.003375 -0.002940 0.750560 x

x Nb 3 -0.000260 -0.000720 0.000052 x

x Nb 4 0.000549 0.001405 0.499672 x

x Nb 5 0.194719 -0.013965 0.246227 x

x Nb 6 0.200373 0.006900 0.749769 x

x Nb 7 0.199973 0.004913 -0.002163 x

x Nb 8 0.204099 0.010792 0.498930 x

x Nb 9 0.401656 -0.001939 0.252877 x

x Nb 10 0.402416 0.013107 0.750849 x

x Nb 11 0.402706 0.004658 -0.001166 x

x Nb 12 0.384630 -0.037227 0.499473 x

x Nb 13 0.597467 -0.013068 0.249379 x

x Nb 14 0.598277 0.001606 0.747289 x

x Nb 15 0.597214 -0.005084 0.001449 x

x Nb 16 0.615299 0.037252 0.500734 x

x Nb 17 0.799550 -0.006867 0.250416 x

x Nb 18 0.805641 0.014854 0.753572 x

x Nb 19 0.800116 -0.004400 0.002240 x

x Nb 20 0.795504 -0.011926 0.501187 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599971E+004 51328.69 <-- SCF

1 -3.62600694E+004 1.80853879E-003 51356.14 <-- SCF

2 -3.62600739E+004 1.13218722E-004 51382.80 <-- SCF

3 -3.62600820E+004 2.01289218E-004 51409.56 <-- SCF

4 -3.62600101E+004 -1.79589446E-003 51435.66 <-- SCF

5 -3.62600145E+004 1.07896937E-004 51461.78 <-- SCF

6 -3.62600139E+004 -1.33904504E-005 51485.08 <-- SCF

7 -3.62600134E+004 -1.20212209E-005 51504.56 <-- SCF

8 -3.62600133E+004 -2.40015645E-006 51522.89 <-- SCF

9 -3.62600133E+004 4.59219750E-008 51541.19 <-- SCF

10 -3.62600134E+004 5.33734259E-007 51557.62 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01336943 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00129 -0.00150 -0.03899 \*

\* Se 2 -0.05869 0.00592 0.01716 \*

\* Se 3 -0.03704 0.00909 -0.01869 \*

\* Se 4 -0.04974 0.00293 -0.02538 \*

\* Se 5 -0.00693 -0.03948 -0.01773 \*

\* Se 6 -0.03183 0.00012 0.01836 \*

\* Se 7 0.04393 0.01683 0.02963 \*

\* Se 8 -0.05493 0.03457 -0.00089 \*

\* Se 9 0.01798 0.04422 0.02560 \*

\* Se 10 -0.01964 0.01113 -0.02772 \*

\* Se 11 -0.00975 -0.05132 -0.00228 \*

\* Se 12 -0.01958 -0.03966 0.00769 \*

\* Se 13 -0.04544 -0.00371 -0.04571 \*

\* Se 14 0.05820 -0.03609 -0.00470 \*

\* Se 15 0.01106 0.03917 0.01003 \*

\* Se 16 0.03125 0.03418 0.06116 \*

\* Se 17 0.01992 -0.01457 0.03481 \*

\* Se 18 0.02603 0.00221 0.00533 \*

\* Se 19 0.00110 -0.01253 0.01526 \*

\* Se 20 0.06714 -0.01836 0.00794 \*

\* Nb 1 0.00028 0.01520 -0.02254 \*

\* Nb 2 -0.00760 -0.00803 0.02380 \*

\* Nb 3 0.00677 0.00839 -0.00261 \*

\* Nb 4 0.00690 -0.00525 0.00512 \*

\* Nb 5 0.04983 0.01672 -0.01116 \*

\* Nb 6 -0.01763 -0.00703 0.00302 \*

\* Nb 7 0.02067 0.01557 0.00511 \*

\* Nb 8 -0.06049 0.04042 0.00505 \*

\* Nb 9 0.02523 -0.00226 0.00756 \*

\* Nb 10 0.03953 0.03473 -0.01072 \*

\* Nb 11 -0.00364 -0.03695 0.01593 \*

\* Nb 12 -0.02538 -0.00302 0.01567 \*

\* Nb 13 -0.03578 -0.05324 -0.00105 \*

\* Nb 14 -0.01745 0.01263 -0.00437 \*

\* Nb 15 0.00670 0.03961 -0.02531 \*

\* Nb 16 0.03377 -0.00419 -0.03035 \*

\* Nb 17 0.03271 0.01331 -0.02842 \*

\* Nb 18 -0.03535 -0.01337 0.03177 \*

\* Nb 19 -0.01565 -0.01165 -0.00623 \*

\* Nb 20 0.05482 -0.03472 -0.02113 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.065079 -0.066463 0.009340 \*

\* y -0.066463 0.010658 0.063107 \*

\* z 0.009340 0.063107 -0.018545 \*

\* \*

\* Pressure: -0.0191 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000020 | -36260.012618 | <-- min BFGS

| trial step | 1.000000 | 0.000013 | -36260.013120 | <-- min BFGS

| line step | 2.803120 | 1.142E-006 | -36260.013458 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 74 with enthalpy= -3.62600135E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.099209E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 7.671661E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.595977E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 6.646307E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 75 ...

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Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000028 | -36260.013458 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 75 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8780497 -8.3177546 0.0070607 0.4202536 -0.0036829 -0.0002511

0.0296068 3.3783265 0.0015041 1.0347040 1.8507841 -0.0012699

0.0083850 0.0048926 13.9623348 -0.0003240 -0.0001975 0.4500099

Lattice parameters(A) Cell Angles

a = 17.045277 alpha = 89.954113

b = 3.378457 beta = 89.956030

c = 13.962338 gamma = 118.705774

Current cell volume = 705.225557 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066886 0.661143 0.121967 x

x Se 2 0.132456 0.340709 0.627803 x

x Se 3 0.132282 0.341155 0.871548 x

x Se 4 0.067860 0.663345 0.375921 x

x Se 5 0.268652 0.670528 0.123921 x

x Se 6 0.332673 0.341319 0.629248 x

x Se 7 0.333140 0.343525 0.871840 x

x Se 8 0.263806 0.657002 0.368618 x

x Se 9 0.466577 0.652504 0.128810 x

x Se 10 0.531483 0.337788 0.618341 x

x Se 11 0.533323 0.347361 0.871211 x

x Se 12 0.468578 0.662485 0.381946 x

x Se 13 0.666802 0.656360 0.128241 x

x Se 14 0.736205 0.343049 0.631492 x

x Se 15 0.731436 0.329806 0.876276 x

x Se 16 0.667268 0.657677 0.370645 x

x Se 17 0.867619 0.658825 0.128489 x

x Se 18 0.932492 0.336746 0.622943 x

x Se 19 0.933118 0.339072 0.878038 x

x Se 20 0.867595 0.659826 0.372300 x

x Nb 1 0.003177 0.002287 0.249055 x

x Nb 2 -0.003382 -0.002881 0.750592 x

x Nb 3 -0.000261 -0.000707 0.000053 x

x Nb 4 0.000562 0.001416 0.499668 x

x Nb 5 0.194763 -0.013844 0.246182 x

x Nb 6 0.200340 0.006846 0.749774 x

x Nb 7 0.200001 0.005120 -0.002157 x

x Nb 8 0.204036 0.010737 0.498902 x

x Nb 9 0.401669 -0.002119 0.252863 x

x Nb 10 0.402431 0.013322 0.750883 x

x Nb 11 0.402704 0.004498 -0.001136 x

x Nb 12 0.384461 -0.037667 0.499481 x

x Nb 13 0.597448 -0.013335 0.249341 x

x Nb 14 0.598264 0.001797 0.747307 x

x Nb 15 0.597219 -0.004915 0.001416 x

x Nb 16 0.615463 0.037660 0.500715 x

x Nb 17 0.799588 -0.006781 0.250394 x

x Nb 18 0.805615 0.014785 0.753622 x

x Nb 19 0.800092 -0.004573 0.002237 x

x Nb 20 0.795562 -0.011870 0.501208 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599931E+004 51661.11 <-- SCF

1 -3.62600987E+004 2.63876421E-003 51688.50 <-- SCF

2 -3.62601045E+004 1.47050277E-004 51715.05 <-- SCF

3 -3.62601057E+004 2.91030573E-005 51741.92 <-- SCF

4 -3.62600123E+004 -2.33470708E-003 51767.59 <-- SCF

5 -3.62600167E+004 1.10046174E-004 51794.14 <-- SCF

6 -3.62600147E+004 -5.05430979E-005 51817.78 <-- SCF

7 -3.62600140E+004 -1.60211572E-005 51838.38 <-- SCF

8 -3.62600140E+004 -7.18608700E-007 51857.33 <-- SCF

9 -3.62600140E+004 3.64221435E-007 51874.66 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01403392 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00226 -0.00510 -0.03917 \*

\* Se 2 -0.05434 0.00484 0.00827 \*

\* Se 3 -0.03608 0.01046 -0.01114 \*

\* Se 4 -0.04439 0.00115 -0.03137 \*

\* Se 5 -0.00938 -0.03343 -0.01611 \*

\* Se 6 -0.03885 -0.00549 0.00969 \*

\* Se 7 0.05301 0.01000 0.03866 \*

\* Se 8 -0.05077 0.04829 -0.00091 \*

\* Se 9 0.01387 0.04643 0.01331 \*

\* Se 10 -0.01568 0.01591 -0.02643 \*

\* Se 11 -0.00696 -0.05333 0.00690 \*

\* Se 12 -0.01898 -0.04188 0.00725 \*

\* Se 13 -0.05406 0.00037 -0.04789 \*

\* Se 14 0.05260 -0.04886 -0.00476 \*

\* Se 15 0.01426 0.03381 0.01015 \*

\* Se 16 0.03600 0.03373 0.05312 \*

\* Se 17 0.02008 -0.01513 0.02659 \*

\* Se 18 0.02252 0.00314 0.00881 \*

\* Se 19 -0.00163 -0.00834 0.01814 \*

\* Se 20 0.06229 -0.01542 0.01261 \*

\* Nb 1 0.00358 0.01777 -0.02184 \*

\* Nb 2 -0.01108 -0.01006 0.02274 \*

\* Nb 3 0.00613 0.00822 -0.00252 \*

\* Nb 4 0.00697 -0.00473 0.00577 \*

\* Nb 5 0.04205 0.01012 -0.01178 \*

\* Nb 6 -0.01765 -0.00515 0.00467 \*

\* Nb 7 0.01839 0.01196 0.00359 \*

\* Nb 8 -0.06407 0.03926 0.00886 \*

\* Nb 9 0.02629 0.00070 0.01091 \*

\* Nb 10 0.03903 0.03457 -0.01415 \*

\* Nb 11 -0.00311 -0.03598 0.01590 \*

\* Nb 12 -0.01582 -0.00003 0.01686 \*

\* Nb 13 -0.03320 -0.05096 0.00574 \*

\* Nb 14 -0.01862 0.00881 -0.00782 \*

\* Nb 15 0.00545 0.03904 -0.02406 \*

\* Nb 16 0.02484 -0.00667 -0.02768 \*

\* Nb 17 0.03058 0.01099 -0.02485 \*

\* Nb 18 -0.02949 -0.00680 0.03166 \*

\* Nb 19 -0.01393 -0.00830 -0.00492 \*

\* Nb 20 0.05787 -0.03392 -0.02281 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.050673 -0.074824 0.008257 \*

\* y -0.074824 -0.006952 0.082134 \*

\* z 0.008257 0.082134 -0.003063 \*

\* \*

\* Pressure: -0.0136 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000028 | -36260.013458 | <-- min BFGS

| trial step | 1.000000 | 0.000021 | -36260.014106 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 75 with line minimization (lambda= 3.979168)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8776352 -8.3179984 0.0051653 0.4203225 -0.0035804 -0.0002505

0.0287678 3.3770124 0.0022495 1.0353068 1.8517567 -0.0015897

0.0083879 0.0073019 13.9684017 -0.0003222 -0.0002969 0.4498145

Lattice parameters(A) Cell Angles

a = 17.045033 alpha = 89.931593

b = 3.377136 beta = 89.967223

c = 13.968406 gamma = 118.721203

Current cell volume = 705.141828 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066902 0.661383 0.121920 x

x Se 2 0.132395 0.340794 0.627949 x

x Se 3 0.132268 0.341091 0.871536 x

x Se 4 0.067796 0.663345 0.375907 x

x Se 5 0.268777 0.670090 0.123890 x

x Se 6 0.332607 0.341765 0.629398 x

x Se 7 0.333036 0.343482 0.871809 x

x Se 8 0.263650 0.656252 0.368530 x

x Se 9 0.466654 0.652559 0.128860 x

x Se 10 0.531471 0.337824 0.618196 x

x Se 11 0.533250 0.347349 0.871196 x

x Se 12 0.468545 0.662181 0.382071 x

x Se 13 0.666894 0.656436 0.128242 x

x Se 14 0.736372 0.343815 0.631574 x

x Se 15 0.731315 0.330255 0.876318 x

x Se 16 0.667345 0.657286 0.370624 x

x Se 17 0.867606 0.658828 0.128518 x

x Se 18 0.932542 0.336704 0.622892 x

x Se 19 0.933101 0.338831 0.878065 x

x Se 20 0.867672 0.659759 0.372208 x

x Nb 1 0.003173 0.002069 0.248954 x

x Nb 2 -0.003405 -0.002706 0.750688 x

x Nb 3 -0.000263 -0.000668 0.000055 x

x Nb 4 0.000602 0.001449 0.499657 x

x Nb 5 0.194893 -0.013483 0.246050 x

x Nb 6 0.200244 0.006688 0.749789 x

x Nb 7 0.200082 0.005735 -0.002140 x

x Nb 8 0.203847 0.010572 0.498817 x

x Nb 9 0.401706 -0.002657 0.252821 x

x Nb 10 0.402475 0.013965 0.750986 x

x Nb 11 0.402697 0.004020 -0.001049 x

x Nb 12 0.383959 -0.038979 0.499507 x

x Nb 13 0.597391 -0.014131 0.249228 x

x Nb 14 0.598225 0.002368 0.747360 x

x Nb 15 0.597233 -0.004411 0.001318 x

x Nb 16 0.615949 0.038878 0.500659 x

x Nb 17 0.799700 -0.006526 0.250329 x

x Nb 18 0.805539 0.014581 0.753771 x

x Nb 19 0.800021 -0.005090 0.002227 x

x Nb 20 0.795733 -0.011704 0.501271 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598323E+004 51978.06 <-- SCF

1 -3.62606323E+004 1.99995761E-002 52005.33 <-- SCF

2 -3.62606774E+004 1.12802867E-003 52033.16 <-- SCF

3 -3.62605845E+004 -2.32318474E-003 52059.98 <-- SCF

4 -3.62600178E+004 -1.41665186E-002 52085.53 <-- SCF

5 -3.62600381E+004 5.07047770E-004 52112.20 <-- SCF

6 -3.62600187E+004 -4.85224087E-004 52138.06 <-- SCF

7 -3.62600150E+004 -9.27124125E-005 52162.31 <-- SCF

8 -3.62600148E+004 -5.32699411E-006 52185.50 <-- SCF

9 -3.62600148E+004 4.42865559E-007 52204.61 <-- SCF

10 -3.62600148E+004 6.29007129E-007 52221.89 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01480559 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00967 -0.01706 -0.03392 \*

\* Se 2 -0.04341 -0.00113 -0.01583 \*

\* Se 3 -0.03455 0.01202 0.00392 \*

\* Se 4 -0.03069 -0.00490 -0.04586 \*

\* Se 5 -0.03006 -0.00655 -0.00260 \*

\* Se 6 -0.05823 -0.01151 -0.01265 \*

\* Se 7 0.08044 -0.00988 0.05813 \*

\* Se 8 -0.03116 0.08822 0.00128 \*

\* Se 9 0.00182 0.05165 -0.01306 \*

\* Se 10 -0.00455 0.02975 -0.02357 \*

\* Se 11 0.00291 -0.05890 0.02234 \*

\* Se 12 -0.01602 -0.04584 0.00629 \*

\* Se 13 -0.07897 0.01175 -0.04892 \*

\* Se 14 0.02850 -0.08548 -0.00562 \*

\* Se 15 0.03534 0.00987 0.00077 \*

\* Se 16 0.04610 0.03157 0.03159 \*

\* Se 17 0.02251 -0.01503 0.00840 \*

\* Se 18 0.01532 0.00725 0.01746 \*

\* Se 19 -0.00609 0.00429 0.02017 \*

\* Se 20 0.04999 -0.00547 0.02683 \*

\* Nb 1 0.00940 0.02605 -0.01040 \*

\* Nb 2 -0.01661 -0.01838 0.01002 \*

\* Nb 3 0.00425 0.00693 -0.00224 \*

\* Nb 4 0.00842 -0.00398 0.00746 \*

\* Nb 5 0.01680 -0.00998 -0.00148 \*

\* Nb 6 -0.01478 -0.00001 0.00720 \*

\* Nb 7 0.01117 -0.00256 -0.00547 \*

\* Nb 8 -0.06150 0.03373 0.02177 \*

\* Nb 9 0.02736 0.00816 0.02852 \*

\* Nb 10 0.03873 0.03470 -0.02762 \*

\* Nb 11 0.00014 -0.03032 0.01242 \*

\* Nb 12 0.00964 0.00691 0.01734 \*

\* Nb 13 -0.02453 -0.04540 0.02889 \*

\* Nb 14 -0.02039 -0.00214 -0.02677 \*

\* Nb 15 0.00060 0.03429 -0.01894 \*

\* Nb 16 -0.00334 -0.01316 -0.01691 \*

\* Nb 17 0.02094 0.00342 -0.01020 \*

\* Nb 18 -0.01226 0.01220 0.01755 \*

\* Nb 19 -0.00683 0.00510 0.00326 \*

\* Nb 20 0.05391 -0.03019 -0.02958 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.014662 -0.095878 0.004721 \*

\* y -0.095878 -0.073161 0.132897 \*

\* z 0.004721 0.132897 0.031869 \*

\* \*

\* Pressure: 0.0089 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000028 | -36260.013458 | <-- min BFGS

| trial step | 1.000000 | 0.000021 | -36260.014106 | <-- min BFGS

| line step | 3.979168 | -3.448E-006 | -36260.014868 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 75 with enthalpy= -3.62600149E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 3.525603E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 9.973777E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.004775E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.328967E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 76 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000051 | -36260.014868 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 76 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8774576 -8.3192025 0.0071602 0.4203216 -0.0035905 -0.0002539

0.0288531 3.3776310 0.0015094 1.0352648 1.8513913 -0.0012794

0.0084781 0.0049109 13.9662540 -0.0003274 -0.0001982 0.4498836

Lattice parameters(A) Cell Angles

a = 17.045466 alpha = 89.953953

b = 3.377755 beta = 89.955408

c = 13.966257 gamma = 118.723672

Current cell volume = 705.164083 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066905 0.661448 0.121848 x

x Se 2 0.132381 0.340719 0.627993 x

x Se 3 0.132226 0.340973 0.871502 x

x Se 4 0.067788 0.663303 0.375935 x

x Se 5 0.268731 0.669986 0.123848 x

x Se 6 0.332639 0.341873 0.629388 x

x Se 7 0.333130 0.343793 0.871871 x

x Se 8 0.263580 0.656259 0.368513 x

x Se 9 0.466646 0.652772 0.128850 x

x Se 10 0.531476 0.337905 0.618168 x

x Se 11 0.533263 0.347123 0.871225 x

x Se 12 0.468523 0.661953 0.382063 x

x Se 13 0.666802 0.656175 0.128175 x

x Se 14 0.736443 0.343814 0.631584 x

x Se 15 0.731359 0.330351 0.876359 x

x Se 16 0.667306 0.657297 0.370691 x

x Se 17 0.867638 0.658892 0.128565 x

x Se 18 0.932544 0.336765 0.622852 x

x Se 19 0.933097 0.338706 0.878114 x

x Se 20 0.867692 0.659792 0.372185 x

x Nb 1 0.003262 0.002357 0.248950 x

x Nb 2 -0.003494 -0.002980 0.750697 x

x Nb 3 -0.000256 -0.000617 0.000050 x

x Nb 4 0.000599 0.001442 0.499667 x

x Nb 5 0.194931 -0.013314 0.246060 x

x Nb 6 0.200297 0.006847 0.749775 x

x Nb 7 0.200090 0.005840 -0.002186 x

x Nb 8 0.203858 0.010827 0.498876 x

x Nb 9 0.401702 -0.002539 0.252826 x

x Nb 10 0.402532 0.014344 0.750955 x

x Nb 11 0.402727 0.004014 -0.001023 x

x Nb 12 0.384055 -0.038814 0.499536 x

x Nb 13 0.597339 -0.014555 0.249254 x

x Nb 14 0.598233 0.002288 0.747361 x

x Nb 15 0.597203 -0.004396 0.001278 x

x Nb 16 0.615860 0.038711 0.500624 x

x Nb 17 0.799654 -0.006640 0.250319 x

x Nb 18 0.805506 0.014443 0.753782 x

x Nb 19 0.800013 -0.005198 0.002270 x

x Nb 20 0.795721 -0.011958 0.501199 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599969E+004 52324.73 <-- SCF

1 -3.62600467E+004 1.24617799E-003 52351.55 <-- SCF

2 -3.62600493E+004 6.59504896E-005 52378.66 <-- SCF

3 -3.62600349E+004 -3.62182276E-004 52405.19 <-- SCF

4 -3.62600157E+004 -4.77801119E-004 52430.84 <-- SCF

5 -3.62600167E+004 2.47193676E-005 52456.55 <-- SCF

6 -3.62600161E+004 -1.68750271E-005 52477.95 <-- SCF

7 -3.62600159E+004 -3.94344330E-006 52496.56 <-- SCF

8 -3.62600159E+004 -1.32768716E-007 52514.88 <-- SCF

9 -3.62600159E+004 3.81195269E-007 52530.86 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01591188 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01457 -0.02079 -0.02097 \*

\* Se 2 -0.04088 0.00374 -0.02039 \*

\* Se 3 -0.02707 0.01609 0.00758 \*

\* Se 4 -0.02507 -0.00414 -0.05099 \*

\* Se 5 -0.01910 -0.00537 -0.00823 \*

\* Se 6 -0.05343 -0.00975 -0.01285 \*

\* Se 7 0.05789 -0.00907 0.03135 \*

\* Se 8 -0.01026 0.07412 0.01231 \*

\* Se 9 0.00323 0.03699 -0.00724 \*

\* Se 10 -0.00396 0.02881 -0.01995 \*

\* Se 11 0.00069 -0.04229 0.01092 \*

\* Se 12 -0.01012 -0.03635 0.01141 \*

\* Se 13 -0.05575 0.00640 -0.02035 \*

\* Se 14 0.00771 -0.07158 -0.01452 \*

\* Se 15 0.02400 0.00773 0.00436 \*

\* Se 16 0.03667 0.02670 0.01675 \*

\* Se 17 0.01870 -0.01757 0.00040 \*

\* Se 18 0.01315 0.00608 0.01974 \*

\* Se 19 -0.00974 0.01144 0.01345 \*

\* Se 20 0.04557 -0.00603 0.02864 \*

\* Nb 1 0.00088 0.02430 -0.01856 \*

\* Nb 2 -0.00806 -0.01847 0.01693 \*

\* Nb 3 0.00298 0.00499 -0.00193 \*

\* Nb 4 0.01035 -0.00430 0.00682 \*

\* Nb 5 0.00697 -0.00891 -0.01039 \*

\* Nb 6 -0.01737 -0.00188 0.01716 \*

\* Nb 7 0.00794 -0.00515 -0.00185 \*

\* Nb 8 -0.06306 0.03030 0.01661 \*

\* Nb 9 0.02281 0.00692 0.02184 \*

\* Nb 10 0.03463 0.02672 -0.01941 \*

\* Nb 11 -0.00249 -0.02752 0.01460 \*

\* Nb 12 -0.01044 0.00711 0.00993 \*

\* Nb 13 -0.01944 -0.03426 0.02356 \*

\* Nb 14 -0.01818 -0.00360 -0.02156 \*

\* Nb 15 0.00321 0.03127 -0.01808 \*

\* Nb 16 0.01513 -0.01319 -0.00687 \*

\* Nb 17 0.02033 0.00239 -0.01160 \*

\* Nb 18 -0.00411 0.00973 0.02194 \*

\* Nb 19 -0.00351 0.00673 0.00068 \*

\* Nb 20 0.05465 -0.02830 -0.02124 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.021212 -0.087310 0.011074 \*

\* y -0.087310 -0.049984 0.084293 \*

\* z 0.011074 0.084293 0.017505 \*

\* \*

\* Pressure: 0.0038 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000051 | -36260.014868 | <-- min BFGS

| trial step | 1.000000 | 0.000031 | -36260.015998 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 76 with line minimization (lambda= 2.521826)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8771873 -8.3210350 0.0101963 0.4203204 -0.0036057 -0.0002590

0.0289830 3.3785724 0.0003832 1.0352009 1.8508357 -0.0008073

0.0086152 0.0012721 13.9629855 -0.0003353 -0.0000482 0.4499889

Lattice parameters(A) Cell Angles

a = 17.046127 alpha = 89.987979

b = 3.378697 beta = 89.937423

c = 13.962988 gamma = 118.727434

Current cell volume = 705.197772 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066908 0.661548 0.121739 x

x Se 2 0.132359 0.340604 0.628059 x

x Se 3 0.132162 0.340795 0.871451 x

x Se 4 0.067775 0.663240 0.375977 x

x Se 5 0.268660 0.669828 0.123784 x

x Se 6 0.332687 0.342037 0.629372 x

x Se 7 0.333272 0.344265 0.871964 x

x Se 8 0.263472 0.656270 0.368488 x

x Se 9 0.466635 0.653096 0.128835 x

x Se 10 0.531484 0.338029 0.618125 x

x Se 11 0.533282 0.346779 0.871269 x

x Se 12 0.468490 0.661605 0.382051 x

x Se 13 0.666662 0.655777 0.128073 x

x Se 14 0.736552 0.343814 0.631598 x

x Se 15 0.731427 0.330497 0.876422 x

x Se 16 0.667247 0.657313 0.370792 x

x Se 17 0.867686 0.658989 0.128638 x

x Se 18 0.932548 0.336858 0.622791 x

x Se 19 0.933091 0.338515 0.878188 x

x Se 20 0.867722 0.659842 0.372150 x

x Nb 1 0.003396 0.002794 0.248943 x

x Nb 2 -0.003630 -0.003396 0.750711 x

x Nb 3 -0.000246 -0.000540 0.000043 x

x Nb 4 0.000594 0.001433 0.499684 x

x Nb 5 0.194990 -0.013057 0.246075 x

x Nb 6 0.200378 0.007088 0.749754 x

x Nb 7 0.200103 0.005998 -0.002255 x

x Nb 8 0.203876 0.011215 0.498966 x

x Nb 9 0.401696 -0.002360 0.252833 x

x Nb 10 0.402618 0.014922 0.750909 x

x Nb 11 0.402772 0.004005 -0.000983 x

x Nb 12 0.384203 -0.038563 0.499581 x

x Nb 13 0.597260 -0.015200 0.249294 x

x Nb 14 0.598246 0.002165 0.747363 x

x Nb 15 0.597158 -0.004374 0.001217 x

x Nb 16 0.615725 0.038458 0.500570 x

x Nb 17 0.799585 -0.006814 0.250304 x

x Nb 18 0.805456 0.014234 0.753801 x

x Nb 19 0.800001 -0.005363 0.002335 x

x Nb 20 0.795702 -0.012346 0.501088 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599723E+004 52634.30 <-- SCF

1 -3.62601170E+004 3.61662259E-003 52661.55 <-- SCF

2 -3.62601244E+004 1.84972035E-004 52689.41 <-- SCF

3 -3.62600966E+004 -6.93182711E-004 52716.28 <-- SCF

4 -3.62600157E+004 -2.02381813E-003 52742.39 <-- SCF

5 -3.62600199E+004 1.05400607E-004 52769.31 <-- SCF

6 -3.62600173E+004 -6.44408096E-005 52794.14 <-- SCF

7 -3.62600166E+004 -1.87529587E-005 52815.08 <-- SCF

8 -3.62600165E+004 -1.50965627E-006 52834.56 <-- SCF

9 -3.62600165E+004 4.62673109E-007 52852.23 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01652757 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02267 -0.02654 0.00710 \*

\* Se 2 -0.03419 0.01045 -0.02845 \*

\* Se 3 -0.01139 0.02141 0.00442 \*

\* Se 4 -0.01438 -0.00342 -0.05494 \*

\* Se 5 -0.00122 -0.00289 -0.01042 \*

\* Se 6 -0.04816 -0.00786 -0.01457 \*

\* Se 7 0.02816 -0.01042 -0.01268 \*

\* Se 8 0.02461 0.05300 0.03506 \*

\* Se 9 0.00421 0.01549 0.00717 \*

\* Se 10 -0.00151 0.02668 -0.01161 \*

\* Se 11 -0.00054 -0.01798 -0.01307 \*

\* Se 12 -0.00236 -0.02141 0.01695 \*

\* Se 13 -0.02685 0.00086 0.02501 \*

\* Se 14 -0.02841 -0.05099 -0.03411 \*

\* Se 15 0.00499 0.00380 0.00198 \*

\* Se 16 0.02479 0.01942 -0.00484 \*

\* Se 17 0.00975 -0.02069 -0.00322 \*

\* Se 18 0.00795 0.00485 0.01893 \*

\* Se 19 -0.01637 0.02258 -0.00253 \*

\* Se 20 0.03695 -0.00630 0.03227 \*

\* Nb 1 -0.00818 0.02124 -0.02160 \*

\* Nb 2 0.00122 -0.01834 0.01804 \*

\* Nb 3 0.00041 0.00167 -0.00108 \*

\* Nb 4 0.01248 -0.00441 0.00544 \*

\* Nb 5 -0.00879 -0.00839 -0.01561 \*

\* Nb 6 -0.01497 -0.00382 0.02657 \*

\* Nb 7 0.00582 -0.00796 -0.00048 \*

\* Nb 8 -0.06368 0.02394 0.01220 \*

\* Nb 9 0.01981 0.00292 0.01850 \*

\* Nb 10 0.02839 0.01265 -0.01344 \*

\* Nb 11 -0.00039 -0.02269 0.01628 \*

\* Nb 12 -0.03065 0.00793 0.00056 \*

\* Nb 13 -0.00949 -0.01458 0.02224 \*

\* Nb 14 -0.01823 -0.00471 -0.02050 \*

\* Nb 15 0.00154 0.02590 -0.01538 \*

\* Nb 16 0.03253 -0.01353 0.00859 \*

\* Nb 17 0.01242 0.00020 -0.00752 \*

\* Nb 18 0.00660 0.00730 0.02039 \*

\* Nb 19 -0.00077 0.00846 -0.00021 \*

\* Nb 20 0.05523 -0.02384 -0.01146 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.029059 -0.071543 0.018965 \*

\* y -0.071543 -0.020029 0.011042 \*

\* z 0.018965 0.011042 -0.011998 \*

\* \*

\* Pressure: 0.0010 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000051 | -36260.014868 | <-- min BFGS

| trial step | 1.000000 | 0.000031 | -36260.015998 | <-- min BFGS

| line step | 2.521826 | 1.454E-006 | -36260.016632 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 76 with enthalpy= -3.62600166E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 4.410087E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 6.911395E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.214842E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 7.154314E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 77 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000042 | -36260.016632 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 77 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8730985 -8.3171632 0.0099285 0.4203487 -0.0037633 -0.0002347

0.0302531 3.3791668 0.0000664 1.0346068 1.8501263 -0.0006098

0.0077989 0.0002408 13.9621964 -0.0003038 -0.0000061 0.4500143

Lattice parameters(A) Cell Angles

a = 17.040668 alpha = 89.997599

b = 3.379302 beta = 89.939167

c = 13.962199 gamma = 118.701340

Current cell volume = 705.234478 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066888 0.661398 0.121727 x

x Se 2 0.132306 0.340402 0.628044 x

x Se 3 0.132131 0.340769 0.871491 x

x Se 4 0.067708 0.662962 0.375887 x

x Se 5 0.268711 0.669781 0.123763 x

x Se 6 0.332587 0.341587 0.629378 x

x Se 7 0.333269 0.344370 0.871919 x

x Se 8 0.263403 0.656113 0.368463 x

x Se 9 0.466621 0.652995 0.128876 x

x Se 10 0.531496 0.338196 0.618041 x

x Se 11 0.533297 0.346886 0.871257 x

x Se 12 0.468449 0.661191 0.382095 x

x Se 13 0.666667 0.655748 0.128097 x

x Se 14 0.736619 0.343969 0.631614 x

x Se 15 0.731374 0.330564 0.876438 x

x Se 16 0.667347 0.657866 0.370873 x

x Se 17 0.867700 0.658951 0.128623 x

x Se 18 0.932611 0.337137 0.622834 x

x Se 19 0.933111 0.338612 0.878177 x

x Se 20 0.867784 0.660019 0.372197 x

x Nb 1 0.003318 0.002671 0.248908 x

x Nb 2 -0.003568 -0.003263 0.750746 x

x Nb 3 -0.000243 -0.000500 0.000047 x

x Nb 4 0.000613 0.001445 0.499680 x

x Nb 5 0.195031 -0.012913 0.246043 x

x Nb 6 0.200274 0.006644 0.749765 x

x Nb 7 0.200141 0.006123 -0.002185 x

x Nb 8 0.203775 0.011019 0.498882 x

x Nb 9 0.401777 -0.002003 0.252830 x

x Nb 10 0.402610 0.014736 0.750932 x

x Nb 11 0.402752 0.003684 -0.000965 x

x Nb 12 0.383985 -0.038976 0.499625 x

x Nb 13 0.597261 -0.015121 0.249267 x

x Nb 14 0.598172 0.001870 0.747377 x

x Nb 15 0.597182 -0.004037 0.001195 x

x Nb 16 0.615940 0.038834 0.500510 x

x Nb 17 0.799701 -0.006307 0.250265 x

x Nb 18 0.805441 0.014160 0.753857 x

x Nb 19 0.799968 -0.005438 0.002265 x

x Nb 20 0.795791 -0.012145 0.501161 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599701E+004 52956.17 <-- SCF

1 -3.62601526E+004 4.56444913E-003 52983.58 <-- SCF

2 -3.62601624E+004 2.44456708E-004 53011.14 <-- SCF

3 -3.62601477E+004 -3.68530245E-004 53038.14 <-- SCF

4 -3.62600170E+004 -3.26739222E-003 53064.19 <-- SCF

5 -3.62600221E+004 1.27991843E-004 53090.91 <-- SCF

6 -3.62600184E+004 -9.24446373E-005 53115.97 <-- SCF

7 -3.62600174E+004 -2.37703169E-005 53137.98 <-- SCF

8 -3.62600175E+004 6.66158815E-007 53157.89 <-- SCF

9 -3.62600175E+004 -7.46000462E-009 53175.50 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01747613 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02473 -0.02538 0.01313 \*

\* Se 2 -0.02236 0.01276 -0.03093 \*

\* Se 3 0.00275 0.01679 0.00314 \*

\* Se 4 -0.01387 -0.00297 -0.05288 \*

\* Se 5 -0.01679 0.00014 -0.00097 \*

\* Se 6 -0.05221 0.00187 -0.00168 \*

\* Se 7 0.02220 -0.02253 0.00493 \*

\* Se 8 0.03098 0.04508 0.03417 \*

\* Se 9 0.00743 0.01388 -0.00980 \*

\* Se 10 -0.00304 0.02821 -0.00748 \*

\* Se 11 -0.00499 -0.01711 -0.00546 \*

\* Se 12 0.00820 -0.00787 0.02068 \*

\* Se 13 -0.01986 0.00389 0.01814 \*

\* Se 14 -0.03453 -0.04337 -0.02980 \*

\* Se 15 0.02129 -0.00042 -0.00304 \*

\* Se 16 0.02587 0.00716 -0.04540 \*

\* Se 17 0.00088 -0.01582 -0.00670 \*

\* Se 18 -0.00150 0.00287 0.01827 \*

\* Se 19 -0.01629 0.02547 0.00048 \*

\* Se 20 0.02131 -0.00147 0.02382 \*

\* Nb 1 0.00208 0.02106 -0.02096 \*

\* Nb 2 -0.00650 -0.02083 0.01552 \*

\* Nb 3 -0.00179 -0.00091 -0.00104 \*

\* Nb 4 0.01373 -0.00398 0.00535 \*

\* Nb 5 -0.01408 -0.00660 -0.01722 \*

\* Nb 6 -0.01947 -0.00341 0.02320 \*

\* Nb 7 0.00099 -0.00797 -0.00929 \*

\* Nb 8 -0.07184 0.02235 0.02347 \*

\* Nb 9 0.00679 -0.00463 0.02514 \*

\* Nb 10 0.03080 0.00815 -0.02171 \*

\* Nb 11 0.00423 -0.01765 0.01444 \*

\* Nb 12 -0.01265 0.00203 0.00311 \*

\* Nb 13 -0.00621 -0.00505 0.03572 \*

\* Nb 14 -0.00662 -0.00132 -0.02895 \*

\* Nb 15 -0.00330 0.02072 -0.01185 \*

\* Nb 16 0.01340 -0.00843 0.01292 \*

\* Nb 17 0.01278 -0.00296 0.00590 \*

\* Nb 18 0.00801 0.00541 0.01510 \*

\* Nb 19 0.00485 0.00737 0.00793 \*

\* Nb 20 0.06463 -0.02453 -0.01940 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.024863 -0.038164 0.008063 \*

\* y -0.038164 0.004167 -0.008114 \*

\* z 0.008063 -0.008114 -0.021373 \*

\* \*

\* Pressure: -0.0026 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000042 | -36260.016632 | <-- min BFGS

| trial step | 1.000000 | 0.000021 | -36260.017555 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 77 with line minimization (lambda= 1.953976)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8691978 -8.3134696 0.0096730 0.4203758 -0.0039136 -0.0002116

0.0314648 3.3797339 -0.0002358 1.0340404 1.8494501 -0.0004215

0.0070201 -0.0007430 13.9614437 -0.0002738 0.0000339 0.4500385

Lattice parameters(A) Cell Angles

a = 17.035461 alpha = 90.006778

b = 3.379880 beta = 89.940832

c = 13.961445 gamma = 118.676451

Current cell volume = 705.269281 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066869 0.661255 0.121716 x

x Se 2 0.132256 0.340209 0.628029 x

x Se 3 0.132100 0.340744 0.871528 x

x Se 4 0.067645 0.662696 0.375801 x

x Se 5 0.268761 0.669737 0.123743 x

x Se 6 0.332492 0.341159 0.629384 x

x Se 7 0.333265 0.344471 0.871875 x

x Se 8 0.263336 0.655964 0.368439 x

x Se 9 0.466609 0.652898 0.128916 x

x Se 10 0.531508 0.338356 0.617961 x

x Se 11 0.533312 0.346988 0.871245 x

x Se 12 0.468411 0.660796 0.382138 x

x Se 13 0.666673 0.655721 0.128121 x

x Se 14 0.736683 0.344118 0.631629 x

x Se 15 0.731323 0.330628 0.876453 x

x Se 16 0.667443 0.658394 0.370950 x

x Se 17 0.867713 0.658915 0.128610 x

x Se 18 0.932671 0.337402 0.622875 x

x Se 19 0.933129 0.338706 0.878167 x

x Se 20 0.867844 0.660188 0.372243 x

x Nb 1 0.003243 0.002553 0.248873 x

x Nb 2 -0.003509 -0.003136 0.750779 x

x Nb 3 -0.000241 -0.000462 0.000052 x

x Nb 4 0.000632 0.001457 0.499676 x

x Nb 5 0.195071 -0.012776 0.246013 x

x Nb 6 0.200174 0.006219 0.749775 x

x Nb 7 0.200177 0.006243 -0.002118 x

x Nb 8 0.203679 0.010832 0.498802 x

x Nb 9 0.401855 -0.001662 0.252826 x

x Nb 10 0.402604 0.014558 0.750953 x

x Nb 11 0.402733 0.003377 -0.000948 x

x Nb 12 0.383777 -0.039371 0.499667 x

x Nb 13 0.597263 -0.015045 0.249241 x

x Nb 14 0.598101 0.001588 0.747391 x

x Nb 15 0.597204 -0.003716 0.001173 x

x Nb 16 0.616144 0.039193 0.500454 x

x Nb 17 0.799811 -0.005823 0.250228 x

x Nb 18 0.805427 0.014089 0.753911 x

x Nb 19 0.799936 -0.005510 0.002199 x

x Nb 20 0.795876 -0.011954 0.501231 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599721E+004 53278.56 <-- SCF

1 -3.62602398E+004 6.69249672E-003 53306.00 <-- SCF

2 -3.62602560E+004 4.04082146E-004 53333.55 <-- SCF

3 -3.62602693E+004 3.32150200E-004 53360.48 <-- SCF

4 -3.62600114E+004 -6.44710456E-003 53386.39 <-- SCF

5 -3.62600240E+004 3.13735339E-004 53413.09 <-- SCF

6 -3.62600194E+004 -1.12657403E-004 53438.78 <-- SCF

7 -3.62600178E+004 -4.20136289E-005 53461.38 <-- SCF

8 -3.62600178E+004 4.24130242E-007 53481.27 <-- SCF

9 -3.62600178E+004 9.75616679E-007 53499.16 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01782296 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02732 -0.02474 0.01787 \*

\* Se 2 -0.01217 0.01462 -0.03132 \*

\* Se 3 0.01523 0.01187 0.00302 \*

\* Se 4 -0.01068 -0.00340 -0.05201 \*

\* Se 5 -0.03031 0.00421 0.00846 \*

\* Se 6 -0.04805 0.01293 0.00741 \*

\* Se 7 0.02020 -0.03294 0.02176 \*

\* Se 8 0.04368 0.03694 0.03225 \*

\* Se 9 0.01010 0.01162 -0.02384 \*

\* Se 10 -0.00550 0.02766 -0.00067 \*

\* Se 11 -0.00894 -0.01553 0.00095 \*

\* Se 12 0.01771 0.00683 0.02170 \*

\* Se 13 -0.01787 0.00593 0.01060 \*

\* Se 14 -0.04606 -0.03595 -0.02533 \*

\* Se 15 0.03477 -0.00583 -0.00911 \*

\* Se 16 0.02510 -0.00698 -0.08053 \*

\* Se 17 -0.00621 -0.01076 -0.01029 \*

\* Se 18 -0.01164 0.00228 0.01883 \*

\* Se 19 -0.01591 0.02848 0.00253 \*

\* Se 20 0.00573 0.00340 0.01384 \*

\* Nb 1 0.00712 0.02070 -0.02166 \*

\* Nb 2 -0.01099 -0.02287 0.01414 \*

\* Nb 3 -0.00295 -0.00283 -0.00106 \*

\* Nb 4 0.01521 -0.00371 0.00581 \*

\* Nb 5 -0.01566 -0.00471 -0.01853 \*

\* Nb 6 -0.02329 -0.00265 0.02325 \*

\* Nb 7 -0.00250 -0.00754 -0.01775 \*

\* Nb 8 -0.07139 0.02114 0.03239 \*

\* Nb 9 -0.00154 -0.01180 0.03275 \*

\* Nb 10 0.03709 0.00584 -0.02866 \*

\* Nb 11 0.00952 -0.01294 0.01421 \*

\* Nb 12 -0.00115 -0.00466 0.00411 \*

\* Nb 13 -0.00725 0.00227 0.04685 \*

\* Nb 14 0.00044 0.00173 -0.03815 \*

\* Nb 15 -0.00874 0.01655 -0.00991 \*

\* Nb 16 0.00034 -0.00200 0.01794 \*

\* Nb 17 0.01215 -0.00613 0.01715 \*

\* Nb 18 0.00645 0.00315 0.00954 \*

\* Nb 19 0.00780 0.00532 0.01641 \*

\* Nb 20 0.06284 -0.02551 -0.02496 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.022975 -0.005731 -0.000187 \*

\* y -0.005731 0.016984 -0.027015 \*

\* z -0.000187 -0.027015 -0.037790 \*

\* \*

\* Pressure: -0.0007 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000042 | -36260.016632 | <-- min BFGS

| trial step | 1.000000 | 0.000021 | -36260.017555 | <-- min BFGS

| line step | 1.953976 | 1.110E-007 | -36260.017860 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 77 with enthalpy= -3.62600179E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 3.071310E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 8.464321E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.537205E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.778952E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 78 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000014 | -36260.017860 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 78 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8635504 -8.3094230 0.0087616 0.4204834 -0.0040089 -0.0002122

0.0322190 3.3793861 0.0001414 1.0339080 1.8494111 -0.0005853

0.0070534 0.0004764 13.9652482 -0.0002743 -0.0000162 0.4499159

Lattice parameters(A) Cell Angles

a = 17.028556 alpha = 89.995373

b = 3.379540 beta = 89.946215

c = 13.965250 gamma = 118.660996

Current cell volume = 705.208450 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066863 0.661184 0.121769 x

x Se 2 0.132235 0.340215 0.628012 x

x Se 3 0.132119 0.340860 0.871542 x

x Se 4 0.067616 0.662639 0.375765 x

x Se 5 0.268746 0.669604 0.123755 x

x Se 6 0.332458 0.341027 0.629380 x

x Se 7 0.333251 0.344399 0.871873 x

x Se 8 0.263376 0.656055 0.368494 x

x Se 9 0.466648 0.652994 0.128934 x

x Se 10 0.531474 0.338325 0.618022 x

x Se 11 0.533275 0.346892 0.871233 x

x Se 12 0.468432 0.660790 0.382075 x

x Se 13 0.666686 0.655794 0.128113 x

x Se 14 0.736644 0.344025 0.631573 x

x Se 15 0.731339 0.330765 0.876425 x

x Se 16 0.667482 0.658575 0.370986 x

x Se 17 0.867690 0.658783 0.128599 x

x Se 18 0.932693 0.337444 0.622914 x

x Se 19 0.933136 0.338773 0.878108 x

x Se 20 0.867865 0.660172 0.372267 x

x Nb 1 0.003177 0.002478 0.248865 x

x Nb 2 -0.003444 -0.003046 0.750789 x

x Nb 3 -0.000238 -0.000458 0.000052 x

x Nb 4 0.000630 0.001442 0.499677 x

x Nb 5 0.195082 -0.012637 0.246029 x

x Nb 6 0.200133 0.006079 0.749782 x

x Nb 7 0.200173 0.006163 -0.002063 x

x Nb 8 0.203610 0.010598 0.498773 x

x Nb 9 0.401853 -0.001729 0.252815 x

x Nb 10 0.402588 0.014255 0.750912 x

x Nb 11 0.402697 0.003318 -0.000973 x

x Nb 12 0.383885 -0.039045 0.499715 x

x Nb 13 0.597279 -0.014754 0.249274 x

x Nb 14 0.598107 0.001673 0.747401 x

x Nb 15 0.597240 -0.003654 0.001199 x

x Nb 16 0.616041 0.038859 0.500399 x

x Nb 17 0.799859 -0.005681 0.250216 x

x Nb 18 0.805414 0.013948 0.753899 x

x Nb 19 0.799941 -0.005417 0.002141 x

x Nb 20 0.795946 -0.011709 0.501258 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600001E+004 53602.27 <-- SCF

1 -3.62600642E+004 1.60065467E-003 53629.42 <-- SCF

2 -3.62600680E+004 9.67498255E-005 53656.34 <-- SCF

3 -3.62600623E+004 -1.42240116E-004 53683.34 <-- SCF

4 -3.62600168E+004 -1.13956450E-003 53709.67 <-- SCF

5 -3.62600193E+004 6.23943990E-005 53735.55 <-- SCF

6 -3.62600185E+004 -1.84986113E-005 53758.81 <-- SCF

7 -3.62600182E+004 -8.66302267E-006 53778.64 <-- SCF

8 -3.62600181E+004 -1.20472725E-006 53797.05 <-- SCF

9 -3.62600181E+004 3.68246951E-007 53814.81 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01814069 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02255 -0.02490 0.00751 \*

\* Se 2 -0.00568 0.01044 -0.02778 \*

\* Se 3 0.01442 0.00746 0.00289 \*

\* Se 4 -0.01088 -0.00577 -0.04952 \*

\* Se 5 -0.02933 0.00557 0.01121 \*

\* Se 6 -0.04583 0.01657 0.00723 \*

\* Se 7 0.02287 -0.02968 0.01643 \*

\* Se 8 0.03386 0.03584 0.02053 \*

\* Se 9 0.00317 0.00788 -0.02702 \*

\* Se 10 0.00520 0.02704 -0.01028 \*

\* Se 11 -0.00267 -0.01071 0.00103 \*

\* Se 12 0.01350 0.00627 0.03319 \*

\* Se 13 -0.01925 0.00165 0.02010 \*

\* Se 14 -0.03573 -0.03462 -0.01283 \*

\* Se 15 0.03460 -0.00636 -0.01014 \*

\* Se 16 0.02385 -0.01147 -0.09051 \*

\* Se 17 -0.00597 -0.00588 -0.01142 \*

\* Se 18 -0.01359 0.00272 0.01992 \*

\* Se 19 -0.01109 0.02918 0.01297 \*

\* Se 20 -0.00253 0.00892 0.00615 \*

\* Nb 1 0.00262 0.02160 -0.02112 \*

\* Nb 2 -0.00635 -0.02440 0.01406 \*

\* Nb 3 -0.00254 -0.00315 -0.00135 \*

\* Nb 4 0.01494 -0.00365 0.00593 \*

\* Nb 5 -0.00562 -0.00521 -0.01542 \*

\* Nb 6 -0.02673 -0.00327 0.01880 \*

\* Nb 7 -0.00659 -0.00723 -0.01799 \*

\* Nb 8 -0.06485 0.02245 0.03781 \*

\* Nb 9 -0.00176 -0.00658 0.03373 \*

\* Nb 10 0.03671 0.01153 -0.02146 \*

\* Nb 11 0.00677 -0.01112 0.01539 \*

\* Nb 12 -0.00979 -0.00759 0.00127 \*

\* Nb 13 -0.00716 -0.00198 0.04297 \*

\* Nb 14 -0.00103 -0.00411 -0.03903 \*

\* Nb 15 -0.00646 0.01444 -0.01115 \*

\* Nb 16 0.00779 0.00236 0.02251 \*

\* Nb 17 0.01380 -0.00522 0.02371 \*

\* Nb 18 -0.00358 0.00331 0.00561 \*

\* Nb 19 0.01205 0.00469 0.01575 \*

\* Nb 20 0.05630 -0.02701 -0.02970 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.007271 0.005409 0.005179 \*

\* y 0.005409 0.003544 -0.002616 \*

\* z 0.005179 -0.002616 -0.006268 \*

\* \*

\* Pressure: -0.0015 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000014 | -36260.017860 | <-- min BFGS

| trial step | 1.000000 | 4.205E-006 | -36260.018192 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 78 with line minimization (lambda= 1.442842)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8610494 -8.3076309 0.0083579 0.4205310 -0.0040511 -0.0002125

0.0325529 3.3792320 0.0003084 1.0338494 1.8493938 -0.0006578

0.0070681 0.0010164 13.9669331 -0.0002745 -0.0000384 0.4498616

Lattice parameters(A) Cell Angles

a = 17.025498 alpha = 89.990322

b = 3.379389 beta = 89.948599

c = 13.966935 gamma = 118.654151

Current cell volume = 705.181453 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066860 0.661152 0.121793 x

x Se 2 0.132225 0.340218 0.628005 x

x Se 3 0.132127 0.340912 0.871548 x

x Se 4 0.067603 0.662613 0.375749 x

x Se 5 0.268739 0.669546 0.123760 x

x Se 6 0.332443 0.340969 0.629378 x

x Se 7 0.333244 0.344367 0.871873 x

x Se 8 0.263394 0.656095 0.368519 x

x Se 9 0.466665 0.653037 0.128942 x

x Se 10 0.531459 0.338311 0.618050 x

x Se 11 0.533259 0.346850 0.871228 x

x Se 12 0.468441 0.660788 0.382047 x

x Se 13 0.666692 0.655827 0.128110 x

x Se 14 0.736627 0.343985 0.631549 x

x Se 15 0.731346 0.330826 0.876413 x

x Se 16 0.667499 0.658656 0.371002 x

x Se 17 0.867680 0.658725 0.128594 x

x Se 18 0.932702 0.337463 0.622932 x

x Se 19 0.933139 0.338802 0.878082 x

x Se 20 0.867874 0.660165 0.372278 x

x Nb 1 0.003148 0.002445 0.248861 x

x Nb 2 -0.003415 -0.003007 0.750794 x

x Nb 3 -0.000237 -0.000457 0.000053 x

x Nb 4 0.000629 0.001435 0.499678 x

x Nb 5 0.195087 -0.012575 0.246036 x

x Nb 6 0.200114 0.006017 0.749786 x

x Nb 7 0.200171 0.006127 -0.002039 x

x Nb 8 0.203579 0.010494 0.498760 x

x Nb 9 0.401853 -0.001759 0.252809 x

x Nb 10 0.402582 0.014121 0.750894 x

x Nb 11 0.402681 0.003292 -0.000984 x

x Nb 12 0.383932 -0.038901 0.499736 x

x Nb 13 0.597286 -0.014625 0.249288 x

x Nb 14 0.598110 0.001710 0.747406 x

x Nb 15 0.597256 -0.003626 0.001210 x

x Nb 16 0.615996 0.038711 0.500374 x

x Nb 17 0.799880 -0.005619 0.250211 x

x Nb 18 0.805408 0.013885 0.753894 x

x Nb 19 0.799944 -0.005375 0.002116 x

x Nb 20 0.795976 -0.011601 0.501269 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600147E+004 53917.95 <-- SCF

1 -3.62600230E+004 2.08164037E-004 53944.14 <-- SCF

2 -3.62600235E+004 1.20211090E-005 53966.55 <-- SCF

3 -3.62600210E+004 -6.29165716E-005 53992.92 <-- SCF

4 -3.62600183E+004 -6.85319990E-005 54017.47 <-- SCF

5 -3.62600183E+004 7.02370209E-007 54038.86 <-- SCF

6 -3.62600182E+004 -1.84689383E-006 54056.38 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01822298 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02200 -0.02430 -0.00099 \*

\* Se 2 -0.00101 0.00803 -0.02773 \*

\* Se 3 0.01247 0.00499 0.00114 \*

\* Se 4 -0.00624 -0.00668 -0.04432 \*

\* Se 5 -0.02643 0.00715 0.01036 \*

\* Se 6 -0.04048 0.01892 0.00726 \*

\* Se 7 0.02787 -0.02741 0.01867 \*

\* Se 8 0.02619 0.03530 0.01378 \*

\* Se 9 -0.00202 0.00662 -0.03214 \*

\* Se 10 0.00946 0.02598 -0.01880 \*

\* Se 11 0.00235 -0.00889 0.00483 \*

\* Se 12 0.01217 0.00691 0.04302 \*

\* Se 13 -0.02375 -0.00111 0.02005 \*

\* Se 14 -0.02843 -0.03388 -0.00522 \*

\* Se 15 0.03180 -0.00745 -0.00772 \*

\* Se 16 0.01866 -0.01447 -0.09551 \*

\* Se 17 -0.00428 -0.00301 -0.00994 \*

\* Se 18 -0.01802 0.00285 0.01619 \*

\* Se 19 -0.01045 0.02895 0.02198 \*

\* Se 20 -0.00723 0.01194 0.00338 \*

\* Nb 1 -0.00924 0.02243 -0.02035 \*

\* Nb 2 0.00524 -0.02516 0.01387 \*

\* Nb 3 -0.00219 -0.00318 -0.00187 \*

\* Nb 4 0.01436 -0.00372 0.00622 \*

\* Nb 5 0.00094 -0.00317 -0.01552 \*

\* Nb 6 -0.03518 -0.00356 0.01580 \*

\* Nb 7 -0.00661 -0.00698 -0.01475 \*

\* Nb 8 -0.07241 0.02315 0.04046 \*

\* Nb 9 0.00281 -0.00704 0.03718 \*

\* Nb 10 0.03884 0.00803 -0.03210 \*

\* Nb 11 -0.00076 -0.00990 0.01187 \*

\* Nb 12 0.00232 -0.00830 0.00543 \*

\* Nb 13 -0.01096 0.00088 0.05218 \*

\* Nb 14 -0.00513 -0.00374 -0.04231 \*

\* Nb 15 0.00021 0.01339 -0.00763 \*

\* Nb 16 -0.00387 0.00318 0.01922 \*

\* Nb 17 0.02239 -0.00487 0.02728 \*

\* Nb 18 -0.01076 0.00147 0.00639 \*

\* Nb 19 0.01213 0.00420 0.01270 \*

\* Nb 20 0.06323 -0.02754 -0.03237 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.001552 0.014053 0.005112 \*

\* y 0.014053 0.002287 0.011132 \*

\* z 0.005112 0.011132 0.021475 \*

\* \*

\* Pressure: -0.0074 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000014 | -36260.017860 | <-- min BFGS

| trial step | 1.000000 | 4.205E-006 | -36260.018192 | <-- min BFGS

| line step | 1.442842 | 2.603E-006 | -36260.018275 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 78 with enthalpy= -3.62600183E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.035557E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 9.838510E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.527841E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.147511E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 79 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000011 | -36260.018275 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 79 with trial guess (lambda= 1.000000)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8558265 -8.3048725 0.0076857 0.4206307 -0.0041385 -0.0001999

0.0332485 3.3792972 0.0003577 1.0337312 1.8491465 -0.0006470

0.0066507 0.0011693 13.9683594 -0.0002579 -0.0000451 0.4498157

Lattice parameters(A) Cell Angles

a = 17.019593 alpha = 89.988871

b = 3.379461 beta = 89.952655

c = 13.968361 gamma = 118.642843

Current cell volume = 705.099919 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066838 0.661033 0.121859 x

x Se 2 0.132224 0.340181 0.627984 x

x Se 3 0.132162 0.340975 0.871614 x

x Se 4 0.067541 0.662405 0.375687 x

x Se 5 0.268736 0.669391 0.123806 x

x Se 6 0.332378 0.340740 0.629359 x

x Se 7 0.333238 0.344240 0.871881 x

x Se 8 0.263394 0.656080 0.368518 x

x Se 9 0.466721 0.653226 0.128919 x

x Se 10 0.531396 0.338269 0.618064 x

x Se 11 0.533206 0.346672 0.871253 x

x Se 12 0.468502 0.660827 0.382023 x

x Se 13 0.666696 0.655946 0.128103 x

x Se 14 0.736627 0.344005 0.631547 x

x Se 15 0.731348 0.330981 0.876365 x

x Se 16 0.667563 0.658920 0.371029 x

x Se 17 0.867638 0.658636 0.128529 x

x Se 18 0.932754 0.337641 0.622993 x

x Se 19 0.933163 0.338924 0.878013 x

x Se 20 0.867877 0.660195 0.372307 x

x Nb 1 0.003032 0.002242 0.248839 x

x Nb 2 -0.003304 -0.002791 0.750817 x

x Nb 3 -0.000235 -0.000446 0.000054 x

x Nb 4 0.000634 0.001425 0.499678 x

x Nb 5 0.195138 -0.012284 0.246047 x

x Nb 6 0.200020 0.005655 0.749786 x

x Nb 7 0.200178 0.006060 -0.001954 x

x Nb 8 0.203460 0.010097 0.498692 x

x Nb 9 0.401869 -0.001708 0.252786 x

x Nb 10 0.402570 0.013635 0.750839 x

x Nb 11 0.402640 0.003132 -0.001002 x

x Nb 12 0.384015 -0.038603 0.499827 x

x Nb 13 0.597301 -0.014163 0.249344 x

x Nb 14 0.598098 0.001673 0.747430 x

x Nb 15 0.597297 -0.003459 0.001226 x

x Nb 16 0.615913 0.038372 0.500281 x

x Nb 17 0.799979 -0.005257 0.250208 x

x Nb 18 0.805365 0.013619 0.753885 x

x Nb 19 0.799938 -0.005286 0.002023 x

x Nb 20 0.796091 -0.011199 0.501339 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599844E+004 54159.73 <-- SCF

1 -3.62600620E+004 1.93950752E-003 54185.94 <-- SCF

2 -3.62600663E+004 1.07480174E-004 54213.92 <-- SCF

3 -3.62600394E+004 -6.71589351E-004 54240.80 <-- SCF

4 -3.62600186E+004 -5.20751980E-004 54266.73 <-- SCF

5 -3.62600189E+004 7.18873340E-006 54292.67 <-- SCF

6 -3.62600184E+004 -1.18176096E-005 54313.19 <-- SCF

7 -3.62600182E+004 -4.24384766E-006 54332.23 <-- SCF

8 -3.62600182E+004 2.41245589E-007 54349.75 <-- SCF

9 -3.62600182E+004 4.32510121E-007 54365.78 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01823921 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01996 -0.02274 -0.01049 \*

\* Se 2 -0.00133 0.00806 -0.02736 \*

\* Se 3 0.01328 0.00418 0.00314 \*

\* Se 4 0.00111 -0.00635 -0.04728 \*

\* Se 5 -0.01999 0.01154 0.01236 \*

\* Se 6 -0.04198 0.02174 0.01589 \*

\* Se 7 0.02769 -0.02364 0.01051 \*

\* Se 8 0.03535 0.03365 0.01740 \*

\* Se 9 -0.00582 0.00179 -0.02942 \*

\* Se 10 0.03417 0.02279 -0.01092 \*

\* Se 11 0.00672 -0.00324 0.00100 \*

\* Se 12 -0.01017 0.01112 0.03566 \*

\* Se 13 -0.02276 -0.00625 0.02780 \*

\* Se 14 -0.03743 -0.03290 -0.00849 \*

\* Se 15 0.02842 -0.01093 -0.00803 \*

\* Se 16 0.02564 -0.01812 -0.10724 \*

\* Se 17 -0.00757 -0.00251 -0.01012 \*

\* Se 18 -0.02661 0.00111 0.02043 \*

\* Se 19 -0.00892 0.02772 0.03091 \*

\* Se 20 -0.00839 0.01312 -0.00069 \*

\* Nb 1 -0.00087 0.02250 -0.02268 \*

\* Nb 2 -0.00368 -0.02658 0.01546 \*

\* Nb 3 -0.00318 -0.00329 -0.00185 \*

\* Nb 4 0.01445 -0.00350 0.00597 \*

\* Nb 5 0.00372 -0.01002 -0.01552 \*

\* Nb 6 -0.02156 -0.00343 0.01642 \*

\* Nb 7 -0.00673 -0.00634 -0.02165 \*

\* Nb 8 -0.05300 0.02535 0.04696 \*

\* Nb 9 0.00488 -0.00105 0.03364 \*

\* Nb 10 0.03902 0.02242 -0.01345 \*

\* Nb 11 0.00913 -0.00888 0.01884 \*

\* Nb 12 -0.01876 -0.01236 -0.01106 \*

\* Nb 13 -0.00931 -0.01151 0.03510 \*

\* Nb 14 -0.00996 -0.01000 -0.03939 \*

\* Nb 15 -0.00904 0.01221 -0.01370 \*

\* Nb 16 0.01623 0.00925 0.03679 \*

\* Nb 17 0.00694 -0.00471 0.02853 \*

\* Nb 18 -0.01513 0.00758 0.00516 \*

\* Nb 19 0.01149 0.00269 0.02046 \*

\* Nb 20 0.04398 -0.03047 -0.03911 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.021335 0.019497 0.006065 \*

\* y 0.019497 0.000840 0.012264 \*

\* z 0.006065 0.012264 0.026211 \*

\* \*

\* Pressure: -0.0019 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000011 | -36260.018275 | <-- min BFGS

| trial step | 1.000000 | -6.438E-006 | -36260.018276 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 79 with enthalpy= -3.62600183E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 4.504402E-008 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 1.117442E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.045273E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.621132E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 80 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 9.804E-006 | -36260.018276 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 80 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8573841 -8.3068453 0.0078420 0.4206124 -0.0040914 -0.0001931

0.0328730 3.3794500 0.0001756 1.0338849 1.8491762 -0.0005517

0.0064187 0.0005786 13.9673769 -0.0002492 -0.0000210 0.4498473

Lattice parameters(A) Cell Angles

a = 17.021915 alpha = 89.994393

b = 3.379610 beta = 89.951780

c = 13.967378 gamma = 118.652475

Current cell volume = 705.112918 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066845 0.661081 0.121832 x

x Se 2 0.132241 0.340207 0.627991 x

x Se 3 0.132163 0.340924 0.871609 x

x Se 4 0.067549 0.662426 0.375693 x

x Se 5 0.268747 0.669449 0.123816 x

x Se 6 0.332392 0.340851 0.629367 x

x Se 7 0.333244 0.344243 0.871886 x

x Se 8 0.263370 0.656042 0.368481 x

x Se 9 0.466705 0.653213 0.128908 x

x Se 10 0.531414 0.338276 0.618025 x

x Se 11 0.533220 0.346686 0.871258 x

x Se 12 0.468490 0.660853 0.382069 x

x Se 13 0.666690 0.655926 0.128108 x

x Se 14 0.736651 0.344044 0.631586 x

x Se 15 0.731338 0.330924 0.876366 x

x Se 16 0.667545 0.658775 0.370996 x

x Se 17 0.867641 0.658699 0.128532 x

x Se 18 0.932744 0.337614 0.622976 x

x Se 19 0.933157 0.338887 0.878046 x

x Se 20 0.867860 0.660188 0.372294 x

x Nb 1 0.003066 0.002270 0.248835 x

x Nb 2 -0.003340 -0.002835 0.750819 x

x Nb 3 -0.000237 -0.000450 0.000054 x

x Nb 4 0.000639 0.001440 0.499678 x

x Nb 5 0.195148 -0.012345 0.246027 x

x Nb 6 0.200030 0.005686 0.749789 x

x Nb 7 0.200186 0.006134 -0.001990 x

x Nb 8 0.203477 0.010195 0.498714 x

x Nb 9 0.401870 -0.001711 0.252793 x

x Nb 10 0.402587 0.013870 0.750869 x

x Nb 11 0.402660 0.003122 -0.000976 x

x Nb 12 0.383927 -0.038875 0.499796 x

x Nb 13 0.597287 -0.014382 0.249322 x

x Nb 14 0.598093 0.001658 0.747423 x

x Nb 15 0.597278 -0.003446 0.001200 x

x Nb 16 0.615997 0.038640 0.500318 x

x Nb 17 0.799964 -0.005292 0.250213 x

x Nb 18 0.805357 0.013684 0.753902 x

x Nb 19 0.799931 -0.005362 0.002060 x

x Nb 20 0.796073 -0.011309 0.501318 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600114E+004 54469.83 <-- SCF

1 -3.62600301E+004 4.67121426E-004 54496.53 <-- SCF

2 -3.62600312E+004 2.75569058E-005 54521.31 <-- SCF

3 -3.62600257E+004 -1.37381113E-004 54547.69 <-- SCF

4 -3.62600186E+004 -1.77893294E-004 54573.33 <-- SCF

5 -3.62600187E+004 4.10874639E-006 54597.08 <-- SCF

6 -3.62600185E+004 -5.36566985E-006 54616.14 <-- SCF

7 -3.62600185E+004 -1.70306574E-006 54633.73 <-- SCF

8 -3.62600185E+004 -1.08626292E-007 54650.84 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01845149 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02160 -0.02454 -0.00684 \*

\* Se 2 -0.00479 0.00906 -0.02792 \*

\* Se 3 0.01296 0.00724 0.00451 \*

\* Se 4 0.00170 -0.00626 -0.04907 \*

\* Se 5 -0.02064 0.00999 0.01155 \*

\* Se 6 -0.04344 0.01992 0.01448 \*

\* Se 7 0.02726 -0.02119 0.00952 \*

\* Se 8 0.04065 0.03051 0.02242 \*

\* Se 9 -0.00264 0.00077 -0.02433 \*

\* Se 10 0.02944 0.02552 -0.00549 \*

\* Se 11 0.00409 -0.00258 -0.00165 \*

\* Se 12 -0.00919 0.00819 0.02806 \*

\* Se 13 -0.02268 -0.00663 0.02451 \*

\* Se 14 -0.04319 -0.02959 -0.01401 \*

\* Se 15 0.02955 -0.00970 -0.00779 \*

\* Se 16 0.02614 -0.01431 -0.09731 \*

\* Se 17 -0.00780 -0.00589 -0.01036 \*

\* Se 18 -0.02561 0.00161 0.02129 \*

\* Se 19 -0.01040 0.02892 0.02633 \*

\* Se 20 -0.00347 0.01031 0.00300 \*

\* Nb 1 0.00013 0.02129 -0.02523 \*

\* Nb 2 -0.00446 -0.02523 0.01712 \*

\* Nb 3 -0.00283 -0.00336 -0.00147 \*

\* Nb 4 0.01559 -0.00329 0.00569 \*

\* Nb 5 0.00426 -0.00882 -0.01666 \*

\* Nb 6 -0.02018 -0.00219 0.01844 \*

\* Nb 7 -0.00480 -0.00549 -0.02042 \*

\* Nb 8 -0.05407 0.02686 0.04437 \*

\* Nb 9 0.00525 -0.00165 0.03151 \*

\* Nb 10 0.04165 0.02177 -0.01316 \*

\* Nb 11 0.01058 -0.01035 0.01967 \*

\* Nb 12 -0.01895 -0.01192 -0.01001 \*

\* Nb 13 -0.01333 -0.01144 0.03323 \*

\* Nb 14 -0.01007 -0.00922 -0.03734 \*

\* Nb 15 -0.01050 0.01310 -0.01451 \*

\* Nb 16 0.01668 0.00859 0.03370 \*

\* Nb 17 0.00610 -0.00596 0.02461 \*

\* Nb 18 -0.01508 0.00624 0.00680 \*

\* Nb 19 0.00977 0.00167 0.02028 \*

\* Nb 20 0.04474 -0.03195 -0.03754 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.018651 0.008130 0.002217 \*

\* y 0.008130 -0.000176 0.000361 \*

\* z 0.002217 0.000361 0.009096 \*

\* \*

\* Pressure: 0.0032 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 9.804E-006 | -36260.018276 | <-- min BFGS

| trial step | 1.000000 | 7.652E-006 | -36260.018490 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 80 with line minimization (lambda= 4.555898)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8629224 -8.3138605 0.0083977 0.4205474 -0.0039240 -0.0001689

0.0315376 3.3799935 -0.0004719 1.0344315 1.8492822 -0.0002128

0.0055937 -0.0015218 13.9638832 -0.0002180 0.0000649 0.4499598

Lattice parameters(A) Cell Angles

a = 17.030174 alpha = 90.014029

b = 3.380141 beta = 89.948668

c = 13.963884 gamma = 118.686712

Current cell volume = 705.158926 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066871 0.661253 0.121737 x

x Se 2 0.132302 0.340302 0.628015 x

x Se 3 0.132164 0.340743 0.871591 x

x Se 4 0.067580 0.662498 0.375713 x

x Se 5 0.268789 0.669658 0.123848 x

x Se 6 0.332441 0.341246 0.629395 x

x Se 7 0.333264 0.344254 0.871904 x

x Se 8 0.263283 0.655909 0.368348 x

x Se 9 0.466650 0.653166 0.128866 x

x Se 10 0.531480 0.338301 0.617886 x

x Se 11 0.533271 0.346734 0.871277 x

x Se 12 0.468449 0.660945 0.382229 x

x Se 13 0.666670 0.655855 0.128122 x

x Se 14 0.736738 0.344182 0.631724 x

x Se 15 0.731300 0.330718 0.876369 x

x Se 16 0.667480 0.658257 0.370877 x

x Se 17 0.867648 0.658923 0.128541 x

x Se 18 0.932712 0.337519 0.622916 x

x Se 19 0.933136 0.338756 0.878164 x

x Se 20 0.867800 0.660162 0.372249 x

x Nb 1 0.003187 0.002369 0.248819 x

x Nb 2 -0.003468 -0.002992 0.750825 x

x Nb 3 -0.000245 -0.000461 0.000052 x

x Nb 4 0.000660 0.001491 0.499677 x

x Nb 5 0.195186 -0.012559 0.245953 x

x Nb 6 0.200067 0.005796 0.749800 x

x Nb 7 0.200214 0.006398 -0.002115 x

x Nb 8 0.203534 0.010542 0.498791 x

x Nb 9 0.401873 -0.001721 0.252817 x

x Nb 10 0.402647 0.014705 0.750973 x

x Nb 11 0.402731 0.003086 -0.000884 x

x Nb 12 0.383613 -0.039843 0.499688 x

x Nb 13 0.597238 -0.015161 0.249244 x

x Nb 14 0.598077 0.001607 0.747400 x

x Nb 15 0.597209 -0.003402 0.001108 x

x Nb 16 0.616298 0.039596 0.500451 x

x Nb 17 0.799911 -0.005418 0.250230 x

x Nb 18 0.805327 0.013918 0.753962 x

x Nb 19 0.799904 -0.005633 0.002195 x

x Nb 20 0.796008 -0.011699 0.501245 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599306E+004 54754.31 <-- SCF

1 -3.62601260E+004 4.88365296E-003 54780.42 <-- SCF

2 -3.62601401E+004 3.53823317E-004 54808.89 <-- SCF

3 -3.62600717E+004 -1.71148730E-003 54835.50 <-- SCF

4 -3.62600222E+004 -1.23761859E-003 54861.47 <-- SCF

5 -3.62600200E+004 -5.50755168E-005 54887.16 <-- SCF

6 -3.62600187E+004 -3.14580033E-005 54911.06 <-- SCF

7 -3.62600184E+004 -6.98981288E-006 54931.92 <-- SCF

8 -3.62600185E+004 1.20159856E-006 54951.31 <-- SCF

9 -3.62600185E+004 -7.71679621E-007 54968.53 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01845332 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02403 -0.02770 0.01098 \*

\* Se 2 -0.02398 0.01361 -0.02737 \*

\* Se 3 0.00611 0.01876 0.00325 \*

\* Se 4 -0.00161 -0.00495 -0.05107 \*

\* Se 5 -0.02514 0.00735 0.00709 \*

\* Se 6 -0.04954 0.01470 0.01177 \*

\* Se 7 0.02337 -0.01280 0.00280 \*

\* Se 8 0.05759 0.02054 0.05003 \*

\* Se 9 0.00920 -0.00126 -0.00593 \*

\* Se 10 0.01031 0.03437 0.01200 \*

\* Se 11 -0.00507 -0.00250 -0.01083 \*

\* Se 12 -0.00178 -0.00197 0.00125 \*

\* Se 13 -0.01956 -0.00755 0.01665 \*

\* Se 14 -0.06077 -0.01954 -0.04462 \*

\* Se 15 0.03654 -0.00790 -0.00459 \*

\* Se 16 0.03110 -0.00511 -0.06307 \*

\* Se 17 -0.00421 -0.01858 -0.00548 \*

\* Se 18 -0.01918 0.00252 0.02036 \*

\* Se 19 -0.01442 0.02984 0.00394 \*

\* Se 20 0.02046 -0.00049 0.01653 \*

\* Nb 1 -0.01021 0.02260 -0.02484 \*

\* Nb 2 0.00518 -0.02440 0.01608 \*

\* Nb 3 -0.00144 -0.00311 -0.00081 \*

\* Nb 4 0.01446 -0.00343 0.00510 \*

\* Nb 5 -0.01443 0.00037 -0.01215 \*

\* Nb 6 -0.02134 -0.00033 0.01757 \*

\* Nb 7 -0.00624 -0.00983 -0.00831 \*

\* Nb 8 -0.07005 0.02271 0.02897 \*

\* Nb 9 0.00779 -0.00412 0.03416 \*

\* Nb 10 0.03763 0.00508 -0.03080 \*

\* Nb 11 0.00358 -0.01082 0.01070 \*

\* Nb 12 0.00480 -0.00180 0.00730 \*

\* Nb 13 -0.01528 0.00140 0.04270 \*

\* Nb 14 -0.01004 -0.00503 -0.03921 \*

\* Nb 15 -0.00300 0.01249 -0.00587 \*

\* Nb 16 -0.00361 -0.00278 0.00825 \*

\* Nb 17 0.01315 -0.00790 0.01648 \*

\* Nb 18 0.00509 -0.00249 0.00706 \*

\* Nb 19 0.01139 0.00660 0.00828 \*

\* Nb 20 0.05915 -0.02654 -0.02435 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.021862 -0.017244 -0.020004 \*

\* y -0.017244 0.015520 -0.042536 \*

\* z -0.020004 -0.042536 -0.035006 \*

\* \*

\* Pressure: 0.0138 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 9.804E-006 | -36260.018276 | <-- min BFGS

| trial step | 1.000000 | 7.652E-006 | -36260.018490 | <-- min BFGS

| line step | 4.555898 | -6.922E-006 | -36260.018489 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 80 with enthalpy= -3.62600185E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 5.317136E-006 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 7.912938E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.384965E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.253619E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 81 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000025 | -36260.018489 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 81 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8598072 -8.3095992 0.0081127 0.4205762 -0.0040322 -0.0001818

0.0324027 3.3797545 -0.0001317 1.0340453 1.8491519 -0.0003914

0.0060330 -0.0004177 13.9655736 -0.0002346 0.0000198 0.4499054

Lattice parameters(A) Cell Angles

a = 17.025374 alpha = 90.003709

b = 3.379910 beta = 89.950259

c = 13.965575 gamma = 118.664609

Current cell volume = 705.146148 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066865 0.661151 0.121798 x

x Se 2 0.132257 0.340241 0.627993 x

x Se 3 0.132162 0.340827 0.871603 x

x Se 4 0.067552 0.662440 0.375659 x

x Se 5 0.268771 0.669511 0.123843 x

x Se 6 0.332389 0.341002 0.629386 x

x Se 7 0.333247 0.344231 0.871881 x

x Se 8 0.263336 0.656023 0.368441 x

x Se 9 0.466681 0.653181 0.128892 x

x Se 10 0.531465 0.338365 0.617968 x

x Se 11 0.533243 0.346719 0.871258 x

x Se 12 0.468451 0.660830 0.382140 x

x Se 13 0.666688 0.655887 0.128136 x

x Se 14 0.736684 0.344062 0.631630 x

x Se 15 0.731319 0.330874 0.876355 x

x Se 16 0.667536 0.658564 0.370914 x

x Se 17 0.867645 0.658820 0.128534 x

x Se 18 0.932733 0.337565 0.622969 x

x Se 19 0.933143 0.338845 0.878097 x

x Se 20 0.867844 0.660208 0.372279 x

x Nb 1 0.003110 0.002319 0.248812 x

x Nb 2 -0.003392 -0.002921 0.750834 x

x Nb 3 -0.000241 -0.000455 0.000053 x

x Nb 4 0.000658 0.001471 0.499679 x

x Nb 5 0.195190 -0.012430 0.245982 x

x Nb 6 0.200025 0.005668 0.749810 x

x Nb 7 0.200207 0.006295 -0.002045 x

x Nb 8 0.203452 0.010294 0.498760 x

x Nb 9 0.401880 -0.001737 0.252808 x

x Nb 10 0.402618 0.014345 0.750932 x

x Nb 11 0.402683 0.003014 -0.000912 x

x Nb 12 0.383739 -0.039433 0.499737 x

x Nb 13 0.597269 -0.014814 0.249278 x

x Nb 14 0.598077 0.001649 0.747408 x

x Nb 15 0.597257 -0.003325 0.001137 x

x Nb 16 0.616176 0.039179 0.500395 x

x Nb 17 0.799959 -0.005291 0.250218 x

x Nb 18 0.805321 0.013778 0.753941 x

x Nb 19 0.799913 -0.005515 0.002122 x

x Nb 20 0.796091 -0.011437 0.501274 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599976E+004 55072.11 <-- SCF

1 -3.62600387E+004 1.02873481E-003 55096.95 <-- SCF

2 -3.62600418E+004 7.79329837E-005 55123.81 <-- SCF

3 -3.62600260E+004 -3.96051923E-004 55150.14 <-- SCF

4 -3.62600196E+004 -1.58816196E-004 55175.98 <-- SCF

5 -3.62600191E+004 -1.30457566E-005 55200.83 <-- SCF

6 -3.62600189E+004 -5.42235314E-006 55220.08 <-- SCF

7 -3.62600189E+004 -1.96221215E-007 55238.02 <-- SCF

8 -3.62600189E+004 1.96809613E-007 55254.11 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01889086 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02058 -0.02361 -0.00331 \*

\* Se 2 -0.01516 0.00917 -0.02317 \*

\* Se 3 0.00896 0.01254 0.00478 \*

\* Se 4 -0.00054 -0.00588 -0.04729 \*

\* Se 5 -0.02220 0.01021 0.00891 \*

\* Se 6 -0.04477 0.02077 0.01552 \*

\* Se 7 0.02514 -0.01697 0.01183 \*

\* Se 8 0.04117 0.02373 0.02708 \*

\* Se 9 0.00297 -0.00039 -0.01816 \*

\* Se 10 0.01179 0.02777 -0.00524 \*

\* Se 11 -0.00010 -0.00252 -0.00142 \*

\* Se 12 0.00241 0.00407 0.02278 \*

\* Se 13 -0.02076 -0.00512 0.01261 \*

\* Se 14 -0.04386 -0.02295 -0.02146 \*

\* Se 15 0.03209 -0.01026 -0.00442 \*

\* Se 16 0.02843 -0.01210 -0.07707 \*

\* Se 17 -0.00546 -0.01229 -0.00843 \*

\* Se 18 -0.02162 0.00076 0.01974 \*

\* Se 19 -0.01032 0.02717 0.01924 \*

\* Se 20 0.00875 0.00591 0.00597 \*

\* Nb 1 -0.00685 0.02295 -0.02391 \*

\* Nb 2 0.00226 -0.02552 0.01501 \*

\* Nb 3 -0.00168 -0.00346 -0.00048 \*

\* Nb 4 0.01434 -0.00334 0.00500 \*

\* Nb 5 -0.00777 -0.00048 -0.00988 \*

\* Nb 6 -0.02267 -0.00132 0.01347 \*

\* Nb 7 -0.00939 -0.01013 -0.01343 \*

\* Nb 8 -0.06075 0.02344 0.03593 \*

\* Nb 9 0.00389 -0.00247 0.03352 \*

\* Nb 10 0.03676 0.00629 -0.02627 \*

\* Nb 11 0.00720 -0.00908 0.01205 \*

\* Nb 12 -0.00350 -0.00522 0.00326 \*

\* Nb 13 -0.01299 0.00157 0.04067 \*

\* Nb 14 -0.00822 -0.00698 -0.03914 \*

\* Nb 15 -0.00690 0.01096 -0.00687 \*

\* Nb 16 0.00374 0.00168 0.01472 \*

\* Nb 17 0.01189 -0.00679 0.02266 \*

\* Nb 18 -0.00105 -0.00173 0.00248 \*

\* Nb 19 0.01454 0.00691 0.01349 \*

\* Nb 20 0.04966 -0.02728 -0.03078 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.019820 0.006003 -0.009968 \*

\* y 0.006003 0.010240 -0.020651 \*

\* z -0.009968 -0.020651 -0.010217 \*

\* \*

\* Pressure: 0.0066 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000025 | -36260.018489 | <-- min BFGS

| trial step | 1.000000 | 9.258E-006 | -36260.018937 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 81 with line minimization (lambda= 1.604824)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8579231 -8.3070218 0.0079403 0.4205936 -0.0040976 -0.0001896

0.0329259 3.3796100 0.0000741 1.0338117 1.8490732 -0.0004993

0.0062987 0.0002500 13.9665960 -0.0002446 -0.0000075 0.4498725

Lattice parameters(A) Cell Angles

a = 17.022472 alpha = 89.997467

b = 3.379770 beta = 89.951220

c = 13.966597 gamma = 118.651238

Current cell volume = 705.138362 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066861 0.661089 0.121835 x

x Se 2 0.132230 0.340204 0.627979 x

x Se 3 0.132161 0.340877 0.871611 x

x Se 4 0.067535 0.662405 0.375627 x

x Se 5 0.268760 0.669423 0.123840 x

x Se 6 0.332357 0.340854 0.629380 x

x Se 7 0.333236 0.344218 0.871867 x

x Se 8 0.263368 0.656092 0.368498 x

x Se 9 0.466699 0.653190 0.128908 x

x Se 10 0.531456 0.338404 0.618017 x

x Se 11 0.533226 0.346710 0.871247 x

x Se 12 0.468451 0.660761 0.382086 x

x Se 13 0.666699 0.655906 0.128145 x

x Se 14 0.736652 0.343990 0.631573 x

x Se 15 0.731330 0.330968 0.876346 x

x Se 16 0.667569 0.658749 0.370936 x

x Se 17 0.867644 0.658758 0.128530 x

x Se 18 0.932745 0.337592 0.623002 x

x Se 19 0.933147 0.338899 0.878057 x

x Se 20 0.867870 0.660235 0.372297 x

x Nb 1 0.003063 0.002288 0.248808 x

x Nb 2 -0.003346 -0.002879 0.750840 x

x Nb 3 -0.000239 -0.000452 0.000054 x

x Nb 4 0.000657 0.001460 0.499680 x

x Nb 5 0.195192 -0.012351 0.245999 x

x Nb 6 0.200000 0.005590 0.749816 x

x Nb 7 0.200203 0.006232 -0.002002 x

x Nb 8 0.203402 0.010145 0.498741 x

x Nb 9 0.401883 -0.001746 0.252803 x

x Nb 10 0.402600 0.014126 0.750908 x

x Nb 11 0.402654 0.002971 -0.000929 x

x Nb 12 0.383815 -0.039185 0.499767 x

x Nb 13 0.597288 -0.014604 0.249299 x

x Nb 14 0.598078 0.001674 0.747412 x

x Nb 15 0.597286 -0.003278 0.001155 x

x Nb 16 0.616103 0.038927 0.500361 x

x Nb 17 0.799988 -0.005214 0.250211 x

x Nb 18 0.805317 0.013694 0.753929 x

x Nb 19 0.799918 -0.005443 0.002078 x

x Nb 20 0.796140 -0.011278 0.501292 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600110E+004 55357.31 <-- SCF

1 -3.62600323E+004 5.32773380E-004 55383.62 <-- SCF

2 -3.62600334E+004 2.90609134E-005 55408.47 <-- SCF

3 -3.62600276E+004 -1.46071031E-004 55435.02 <-- SCF

4 -3.62600190E+004 -2.14688468E-004 55460.67 <-- SCF

5 -3.62600193E+004 8.30553441E-006 55484.31 <-- SCF

6 -3.62600191E+004 -7.11711324E-006 55503.83 <-- SCF

7 -3.62600190E+004 -1.99436060E-006 55521.72 <-- SCF

8 -3.62600190E+004 -3.04473494E-007 55539.03 <-- SCF

9 -3.62600190E+004 5.27696371E-007 55555.91 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01898139 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01770 -0.02234 -0.00935 \*

\* Se 2 -0.00771 0.00658 -0.02168 \*

\* Se 3 0.01093 0.00945 0.00480 \*

\* Se 4 0.00241 -0.00720 -0.04617 \*

\* Se 5 -0.02364 0.01055 0.01171 \*

\* Se 6 -0.04370 0.02427 0.01404 \*

\* Se 7 0.02522 -0.01907 0.01583 \*

\* Se 8 0.03129 0.02470 0.01771 \*

\* Se 9 0.00054 -0.00099 -0.02481 \*

\* Se 10 0.01308 0.02498 -0.01458 \*

\* Se 11 0.00202 -0.00150 0.00300 \*

\* Se 12 0.00465 0.00625 0.03453 \*

\* Se 13 -0.02006 -0.00374 0.01044 \*

\* Se 14 -0.03337 -0.02407 -0.01038 \*

\* Se 15 0.03307 -0.01014 -0.00701 \*

\* Se 16 0.02886 -0.01619 -0.08028 \*

\* Se 17 -0.00697 -0.00919 -0.00998 \*

\* Se 18 -0.02495 0.00047 0.02206 \*

\* Se 19 -0.00761 0.02668 0.02483 \*

\* Se 20 -0.00035 0.00949 0.00146 \*

\* Nb 1 -0.00303 0.02157 -0.02303 \*

\* Nb 2 -0.00185 -0.02472 0.01400 \*

\* Nb 3 -0.00221 -0.00350 -0.00098 \*

\* Nb 4 0.01446 -0.00305 0.00518 \*

\* Nb 5 -0.00181 -0.00284 -0.00873 \*

\* Nb 6 -0.02468 -0.00182 0.00984 \*

\* Nb 7 -0.01025 -0.00816 -0.01706 \*

\* Nb 8 -0.05586 0.02449 0.03992 \*

\* Nb 9 -0.00046 -0.00028 0.03510 \*

\* Nb 10 0.03787 0.01176 -0.02446 \*

\* Nb 11 0.00775 -0.00796 0.01266 \*

\* Nb 12 -0.00882 -0.00822 0.00161 \*

\* Nb 13 -0.01365 -0.00251 0.04032 \*

\* Nb 14 -0.00485 -0.00975 -0.04085 \*

\* Nb 15 -0.00737 0.00986 -0.00760 \*

\* Nb 16 0.00785 0.00543 0.01831 \*

\* Nb 17 0.01256 -0.00579 0.02740 \*

\* Nb 18 -0.00691 0.00055 -0.00031 \*

\* Nb 19 0.01536 0.00463 0.01647 \*

\* Nb 20 0.04448 -0.02867 -0.03395 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.010856 0.014202 -0.002131 \*

\* y 0.014202 0.004395 -0.008639 \*

\* z -0.002131 -0.008639 -0.000859 \*

\* \*

\* Pressure: 0.0024 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000025 | -36260.018489 | <-- min BFGS

| trial step | 1.000000 | 9.258E-006 | -36260.018937 | <-- min BFGS

| line step | 1.604824 | 1.357E-006 | -36260.019037 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 81 with enthalpy= -3.62600190E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.368682E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 8.682987E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.273675E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.420232E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 82 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000017 | -36260.019037 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 82 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8562733 -8.3058893 0.0076637 0.4206229 -0.0041293 -0.0001906

0.0331781 3.3795826 0.0002016 1.0337512 1.8490116 -0.0005567

0.0063358 0.0006631 13.9677655 -0.0002457 -0.0000244 0.4498348

Lattice parameters(A) Cell Angles

a = 17.020479 alpha = 89.993606

b = 3.379745 beta = 89.952845

c = 13.967767 gamma = 118.646339

Current cell volume = 705.142584 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066869 0.661065 0.121839 x

x Se 2 0.132214 0.340210 0.627970 x

x Se 3 0.132167 0.340933 0.871622 x

x Se 4 0.067506 0.662318 0.375568 x

x Se 5 0.268767 0.669329 0.123855 x

x Se 6 0.332295 0.340785 0.629404 x

x Se 7 0.333238 0.344176 0.871863 x

x Se 8 0.263357 0.656113 0.368496 x

x Se 9 0.466712 0.653220 0.128909 x

x Se 10 0.531449 0.338511 0.617986 x

x Se 11 0.533216 0.346681 0.871240 x

x Se 12 0.468455 0.660669 0.382120 x

x Se 13 0.666699 0.655913 0.128163 x

x Se 14 0.736663 0.343970 0.631577 x

x Se 15 0.731327 0.331075 0.876333 x

x Se 16 0.667623 0.658842 0.370896 x

x Se 17 0.867633 0.658688 0.128522 x

x Se 18 0.932758 0.337629 0.623027 x

x Se 19 0.933145 0.338935 0.878057 x

x Se 20 0.867886 0.660256 0.372305 x

x Nb 1 0.003035 0.002272 0.248770 x

x Nb 2 -0.003327 -0.002874 0.750872 x

x Nb 3 -0.000240 -0.000447 0.000054 x

x Nb 4 0.000672 0.001474 0.499683 x

x Nb 5 0.195219 -0.012264 0.245971 x

x Nb 6 0.199949 0.005428 0.749830 x

x Nb 7 0.200215 0.006277 -0.001989 x

x Nb 8 0.203314 0.010005 0.498740 x

x Nb 9 0.401905 -0.001755 0.252815 x

x Nb 10 0.402624 0.014187 0.750899 x

x Nb 11 0.402647 0.002835 -0.000911 x

x Nb 12 0.383744 -0.039350 0.499792 x

x Nb 13 0.597276 -0.014649 0.249317 x

x Nb 14 0.598056 0.001676 0.747399 x

x Nb 15 0.597295 -0.003129 0.001136 x

x Nb 16 0.616172 0.039060 0.500344 x

x Nb 17 0.800039 -0.005061 0.250212 x

x Nb 18 0.805296 0.013622 0.753959 x

x Nb 19 0.799911 -0.005465 0.002063 x

x Nb 20 0.796219 -0.011159 0.501293 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600105E+004 55659.38 <-- SCF

1 -3.62600618E+004 1.28151920E-003 55686.52 <-- SCF

2 -3.62600649E+004 7.73891308E-005 55711.50 <-- SCF

3 -3.62600703E+004 1.36213075E-004 55738.03 <-- SCF

4 -3.62600177E+004 -1.31420253E-003 55764.00 <-- SCF

5 -3.62600206E+004 7.17298021E-005 55789.53 <-- SCF

6 -3.62600198E+004 -2.03646060E-005 55811.44 <-- SCF

7 -3.62600194E+004 -9.69590284E-006 55831.27 <-- SCF

8 -3.62600194E+004 2.42963297E-008 55848.94 <-- SCF

9 -3.62600194E+004 1.64542684E-007 55865.92 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01940954 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.01499 -0.02138 -0.01145 \*

\* Se 2 -0.00725 0.00352 -0.01918 \*

\* Se 3 0.01084 0.00564 0.00736 \*

\* Se 4 0.00737 -0.00728 -0.04621 \*

\* Se 5 -0.02411 0.01366 0.01256 \*

\* Se 6 -0.04211 0.02869 0.01228 \*

\* Se 7 0.02464 -0.01549 0.01462 \*

\* Se 8 0.02950 0.01987 0.01707 \*

\* Se 9 -0.00113 -0.00423 -0.02521 \*

\* Se 10 0.01744 0.02094 -0.01198 \*

\* Se 11 0.00427 0.00163 0.00566 \*

\* Se 12 0.00043 0.01036 0.02964 \*

\* Se 13 -0.01891 -0.00439 0.00588 \*

\* Se 14 -0.03247 -0.01983 -0.01024 \*

\* Se 15 0.03309 -0.01287 -0.00666 \*

\* Se 16 0.03057 -0.01972 -0.07213 \*

\* Se 17 -0.00742 -0.00568 -0.01163 \*

\* Se 18 -0.02580 -0.00045 0.02387 \*

\* Se 19 -0.00571 0.02588 0.02606 \*

\* Se 20 -0.00127 0.01056 0.00037 \*

\* Nb 1 -0.00025 0.01958 -0.02001 \*

\* Nb 2 -0.00525 -0.02315 0.00985 \*

\* Nb 3 -0.00221 -0.00376 -0.00007 \*

\* Nb 4 0.01458 -0.00302 0.00450 \*

\* Nb 5 -0.00055 -0.00303 -0.00381 \*

\* Nb 6 -0.02430 -0.00074 0.00795 \*

\* Nb 7 -0.00963 -0.00781 -0.01713 \*

\* Nb 8 -0.05388 0.02472 0.03889 \*

\* Nb 9 -0.00174 0.00084 0.03525 \*

\* Nb 10 0.03584 0.01054 -0.02437 \*

\* Nb 11 0.01010 -0.00599 0.01220 \*

\* Nb 12 -0.00791 -0.00734 0.00301 \*

\* Nb 13 -0.01464 -0.00081 0.03801 \*

\* Nb 14 -0.00416 -0.01071 -0.04075 \*

\* Nb 15 -0.00933 0.00660 -0.00627 \*

\* Nb 16 0.00624 0.00591 0.01587 \*

\* Nb 17 0.01298 -0.00643 0.02693 \*

\* Nb 18 -0.00766 0.00038 -0.00519 \*

\* Nb 19 0.01398 0.00375 0.01819 \*

\* Nb 20 0.04084 -0.02897 -0.03374 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.015339 0.013843 -0.000525 \*

\* y 0.013843 0.003460 0.000667 \*

\* z -0.000525 0.000667 0.009287 \*

\* \*

\* Pressure: 0.0009 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000017 | -36260.019037 | <-- min BFGS

| trial step | 1.000000 | 0.000015 | -36260.019451 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 82 with line minimization (lambda= 8.731239)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8435177 -8.2971339 0.0055247 0.4208497 -0.0043746 -0.0001982

0.0351285 3.3793709 0.0011878 1.0332831 1.8485360 -0.0009997

0.0066223 0.0038570 13.9768069 -0.0002542 -0.0001554 0.4495438

Lattice parameters(A) Cell Angles

a = 17.005072 alpha = 89.963770

b = 3.379554 beta = 89.965404

c = 13.976809 gamma = 118.608459

Current cell volume = 705.174631 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066927 0.660887 0.121874 x

x Se 2 0.132092 0.340250 0.627899 x

x Se 3 0.132217 0.341369 0.871705 x

x Se 4 0.067278 0.661646 0.375110 x

x Se 5 0.268825 0.668602 0.123970 x

x Se 6 0.331811 0.340251 0.629588 x

x Se 7 0.333248 0.343847 0.871830 x

x Se 8 0.263275 0.656279 0.368486 x

x Se 9 0.466813 0.653455 0.128911 x

x Se 10 0.531398 0.339336 0.617748 x

x Se 11 0.533135 0.346458 0.871192 x

x Se 12 0.468484 0.659963 0.382382 x

x Se 13 0.666692 0.655967 0.128305 x

x Se 14 0.736744 0.343822 0.631605 x

x Se 15 0.731300 0.331898 0.876233 x

x Se 16 0.668041 0.659560 0.370586 x

x Se 17 0.867552 0.658150 0.128459 x

x Se 18 0.932856 0.337914 0.623217 x

x Se 19 0.933131 0.339209 0.878057 x

x Se 20 0.868010 0.660414 0.372366 x

x Nb 1 0.002818 0.002143 0.248484 x

x Nb 2 -0.003175 -0.002839 0.751119 x

x Nb 3 -0.000243 -0.000412 0.000051 x

x Nb 4 0.000788 0.001582 0.499707 x

x Nb 5 0.195425 -0.011589 0.245749 x

x Nb 6 0.199550 0.004174 0.749943 x

x Nb 7 0.200302 0.006624 -0.001892 x

x Nb 8 0.202636 0.008926 0.498732 x

x Nb 9 0.402073 -0.001824 0.252911 x

x Nb 10 0.402811 0.014656 0.750832 x

x Nb 11 0.402589 0.001788 -0.000770 x

x Nb 12 0.383192 -0.040624 0.499981 x

x Nb 13 0.597186 -0.014997 0.249458 x

x Nb 14 0.597891 0.001694 0.747298 x

x Nb 15 0.597364 -0.001979 0.000995 x

x Nb 16 0.616711 0.040089 0.500217 x

x Nb 17 0.800430 -0.003881 0.250218 x

x Nb 18 0.805136 0.013067 0.754191 x

x Nb 19 0.799860 -0.005640 0.001954 x

x Nb 20 0.796826 -0.010236 0.501299 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62595082E+004 55968.98 <-- SCF

1 -3.62617822E+004 5.68492539E-002 55996.50 <-- SCF

2 -3.62619113E+004 3.22885527E-003 56024.89 <-- SCF

3 -3.62616542E+004 -6.42755914E-003 56051.84 <-- SCF

4 -3.62600208E+004 -4.08351172E-002 56077.94 <-- SCF

5 -3.62600660E+004 1.12882790E-003 56104.67 <-- SCF

6 -3.62600257E+004 -1.00709809E-003 56130.73 <-- SCF

7 -3.62600183E+004 -1.86121770E-004 56156.75 <-- SCF

8 -3.62600196E+004 3.43387348E-005 56180.02 <-- SCF

9 -3.62600198E+004 5.03872972E-006 56200.27 <-- SCF

10 -3.62600201E+004 5.48945234E-006 56218.39 <-- SCF

11 -3.62600202E+004 3.83745011E-006 56236.05 <-- SCF

12 -3.62600203E+004 3.37977359E-006 56254.33 <-- SCF

13 -3.62600204E+004 2.48176066E-006 56270.81 <-- SCF

14 -3.62600205E+004 1.77376803E-006 56287.20 <-- SCF

15 -3.62600206E+004 1.33935583E-006 56303.34 <-- SCF

16 -3.62600206E+004 1.00226877E-006 56319.64 <-- SCF

17 -3.62600206E+004 8.11726739E-007 56335.77 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02063675 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00101 -0.00722 -0.03366 \*

\* Se 2 0.00527 -0.02064 0.01363 \*

\* Se 3 0.00822 -0.02356 0.02465 \*

\* Se 4 0.07706 -0.00801 -0.07219 \*

\* Se 5 -0.02472 0.03823 0.02194 \*

\* Se 6 0.00525 0.05035 -0.00705 \*

\* Se 7 0.02446 0.01318 0.00596 \*

\* Se 8 0.02428 -0.01618 0.00956 \*

\* Se 9 -0.01265 -0.02551 -0.03167 \*

\* Se 10 0.04749 -0.03129 0.01861 \*

\* Se 11 0.01752 0.02425 0.03165 \*

\* Se 12 -0.03078 0.04983 -0.00891 \*

\* Se 13 -0.01638 -0.00824 -0.03276 \*

\* Se 14 -0.03239 0.01329 -0.00630 \*

\* Se 15 0.03287 -0.03302 -0.00860 \*

\* Se 16 -0.00201 -0.05640 -0.00689 \*

\* Se 17 -0.00904 0.02251 -0.02557 \*

\* Se 18 -0.04266 -0.00584 0.04525 \*

\* Se 19 0.00205 0.01423 0.04183 \*

\* Se 20 -0.01233 0.02034 -0.01424 \*

\* Nb 1 -0.01031 0.01028 -0.00678 \*

\* Nb 2 -0.00056 -0.01393 -0.01027 \*

\* Nb 3 -0.00365 -0.00553 0.00673 \*

\* Nb 4 0.01488 -0.00079 0.00005 \*

\* Nb 5 0.01329 -0.00739 0.02716 \*

\* Nb 6 -0.02883 0.01171 -0.00469 \*

\* Nb 7 -0.01410 -0.01098 -0.02156 \*

\* Nb 8 -0.02564 0.02318 0.03573 \*

\* Nb 9 -0.00902 0.01013 0.03988 \*

\* Nb 10 0.02197 0.00789 -0.02590 \*

\* Nb 11 0.01364 0.00471 0.00396 \*

\* Nb 12 0.00703 -0.00451 0.01387 \*

\* Nb 13 -0.02430 0.00762 0.03070 \*

\* Nb 14 -0.00199 -0.01854 -0.04369 \*

\* Nb 15 -0.00959 -0.00981 0.00857 \*

\* Nb 16 -0.01297 0.01521 -0.00412 \*

\* Nb 17 0.01079 -0.01286 0.02335 \*

\* Nb 18 -0.01341 0.00331 -0.03488 \*

\* Nb 19 0.01371 0.00495 0.02912 \*

\* Nb 20 -0.00144 -0.02498 -0.03246 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.033392 0.052201 0.012469 \*

\* y 0.052201 0.011111 0.057547 \*

\* z 0.012469 0.057547 0.108978 \*

\* \*

\* Pressure: -0.0289 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000017 | -36260.019037 | <-- min BFGS

| trial step | 1.000000 | 0.000015 | -36260.019451 | <-- min BFGS

| line step | 8.731239 | -4.180E-006 | -36260.020606 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 82 with enthalpy= -3.62600206E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 3.923959E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.058968E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.163741E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.089779E-001 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 83 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000063 | -36260.020606 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 83 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8514961 -8.3040502 0.0066901 0.4207199 -0.0041988 -0.0001917

0.0337304 3.3797740 0.0006063 1.0337021 1.8487386 -0.0007338

0.0063854 0.0019746 13.9699839 -0.0002463 -0.0000782 0.4497634

Lattice parameters(A) Cell Angles

a = 17.015412 alpha = 89.981362

b = 3.379942 beta = 89.958567

c = 13.969986 gamma = 118.639452

Current cell volume = 705.131929 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066964 0.660902 0.121877 x

x Se 2 0.132112 0.340260 0.627875 x

x Se 3 0.132222 0.341225 0.871683 x

x Se 4 0.067332 0.661809 0.375080 x

x Se 5 0.268755 0.668722 0.123998 x

x Se 6 0.331910 0.340527 0.629549 x

x Se 7 0.333299 0.343950 0.871905 x

x Se 8 0.263364 0.656712 0.368576 x

x Se 9 0.466797 0.653544 0.128835 x

x Se 10 0.531488 0.339378 0.617867 x

x Se 11 0.533148 0.346358 0.871221 x

x Se 12 0.468430 0.660205 0.382309 x

x Se 13 0.666648 0.655748 0.128281 x

x Se 14 0.736651 0.343373 0.631529 x

x Se 15 0.731379 0.331794 0.876210 x

x Se 16 0.667920 0.659172 0.370460 x

x Se 17 0.867568 0.658372 0.128461 x

x Se 18 0.932792 0.337714 0.623237 x

x Se 19 0.933103 0.339250 0.878095 x

x Se 20 0.867977 0.660471 0.372343 x

x Nb 1 0.002900 0.002422 0.248512 x

x Nb 2 -0.003251 -0.003154 0.751082 x

x Nb 3 -0.000246 -0.000450 0.000048 x

x Nb 4 0.000788 0.001596 0.499717 x

x Nb 5 0.195443 -0.011781 0.245792 x

x Nb 6 0.199628 0.004436 0.749967 x

x Nb 7 0.200284 0.006557 -0.001987 x

x Nb 8 0.202659 0.009162 0.498879 x

x Nb 9 0.402007 -0.001970 0.252958 x

x Nb 10 0.402828 0.015143 0.750829 x

x Nb 11 0.402603 0.001907 -0.000720 x

x Nb 12 0.383351 -0.040406 0.499882 x

x Nb 13 0.597197 -0.015310 0.249489 x

x Nb 14 0.597947 0.001750 0.747239 x

x Nb 15 0.597351 -0.002089 0.000954 x

x Nb 16 0.616548 0.039897 0.500354 x

x Nb 17 0.800328 -0.004238 0.250264 x

x Nb 18 0.805088 0.013163 0.754129 x

x Nb 19 0.799880 -0.005615 0.002057 x

x Nb 20 0.796805 -0.010504 0.501164 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599678E+004 56439.16 <-- SCF

1 -3.62601447E+004 4.42251205E-003 56466.59 <-- SCF

2 -3.62601535E+004 2.22018492E-004 56494.36 <-- SCF

3 -3.62601306E+004 -5.72420948E-004 56521.48 <-- SCF

4 -3.62600211E+004 -2.73885824E-003 56547.55 <-- SCF

5 -3.62600254E+004 1.07361468E-004 56574.27 <-- SCF

6 -3.62600225E+004 -7.27757585E-005 56599.55 <-- SCF

7 -3.62600217E+004 -2.00163120E-005 56620.95 <-- SCF

8 -3.62600216E+004 -7.30842557E-007 56640.50 <-- SCF

9 -3.62600216E+004 2.41330662E-007 56658.03 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02164998 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00078 0.00681 -0.03703 \*

\* Se 2 -0.00141 -0.02211 0.02327 \*

\* Se 3 0.00261 -0.01357 0.02257 \*

\* Se 4 0.06545 -0.00134 -0.06506 \*

\* Se 5 0.00359 0.02526 0.01013 \*

\* Se 6 -0.00250 0.04709 -0.00131 \*

\* Se 7 0.01461 0.02254 -0.02223 \*

\* Se 8 0.00159 -0.03194 -0.00541 \*

\* Se 9 -0.00665 -0.02641 0.00377 \*

\* Se 10 0.00981 -0.01914 -0.01667 \*

\* Se 11 0.01700 0.02498 0.01338 \*

\* Se 12 -0.00379 0.02792 0.01158 \*

\* Se 13 -0.00503 -0.00125 -0.02671 \*

\* Se 14 -0.00689 0.02747 0.00639 \*

\* Se 15 0.00321 -0.01960 0.00064 \*

\* Se 16 0.00859 -0.05187 0.03864 \*

\* Se 17 -0.00798 0.01012 -0.01581 \*

\* Se 18 -0.03848 -0.01146 0.04317 \*

\* Se 19 -0.00202 -0.00274 0.03245 \*

\* Se 20 -0.00167 0.01248 -0.00891 \*

\* Nb 1 -0.02118 -0.00014 -0.01512 \*

\* Nb 2 0.00660 -0.00162 -0.00060 \*

\* Nb 3 0.00007 -0.00448 0.00730 \*

\* Nb 4 0.01403 -0.00146 -0.00260 \*

\* Nb 5 0.01694 0.00383 0.03105 \*

\* Nb 6 -0.02115 0.01193 -0.01186 \*

\* Nb 7 -0.01480 -0.01200 -0.00426 \*

\* Nb 8 -0.02172 0.02288 0.01736 \*

\* Nb 9 -0.00659 0.01372 0.02144 \*

\* Nb 10 0.02055 -0.00271 -0.02202 \*

\* Nb 11 0.01105 0.00319 0.00134 \*

\* Nb 12 -0.00000 0.00205 0.02900 \*

\* Nb 13 -0.03492 0.01218 0.01408 \*

\* Nb 14 -0.00313 -0.01696 -0.02317 \*

\* Nb 15 -0.00701 -0.00980 0.00939 \*

\* Nb 16 -0.00288 0.00984 -0.03275 \*

\* Nb 17 0.01496 -0.01083 0.01032 \*

\* Nb 18 -0.00870 -0.00823 -0.03127 \*

\* Nb 19 0.01532 0.00689 0.01515 \*

\* Nb 20 -0.00669 -0.02154 -0.01965 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.016927 0.007800 0.000946 \*

\* y 0.007800 0.011943 0.019691 \*

\* z 0.000946 0.019691 0.027712 \*

\* \*

\* Pressure: -0.0076 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000063 | -36260.020606 | <-- min BFGS

| trial step | 1.000000 | 0.000010 | -36260.021668 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 83 with enthalpy= -3.62600217E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.654427E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 9.229319E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.178600E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.771237E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 84 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000010 | -36260.021668 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 84 with trial guess (lambda= 1.000000)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8539703 -8.3047985 0.0073418 0.4206628 -0.0041751 -0.0001899

0.0335444 3.3797652 0.0003123 1.0336577 1.8488006 -0.0006027

0.0063156 0.0010224 13.9676522 -0.0002442 -0.0000391 0.4498384

Lattice parameters(A) Cell Angles

a = 17.017937 alpha = 89.990255

b = 3.379932 beta = 89.954716

c = 13.967654 gamma = 118.640739

Current cell volume = 705.108020 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066985 0.660909 0.121873 x

x Se 2 0.132106 0.340243 0.627872 x

x Se 3 0.132227 0.341234 0.871700 x

x Se 4 0.067319 0.661742 0.375004 x

x Se 5 0.268750 0.668644 0.124015 x

x Se 6 0.331849 0.340519 0.629577 x

x Se 7 0.333317 0.343910 0.871931 x

x Se 8 0.263363 0.656800 0.368566 x

x Se 9 0.466803 0.653625 0.128790 x

x Se 10 0.531513 0.339529 0.617831 x

x Se 11 0.533145 0.346282 0.871242 x

x Se 12 0.468423 0.660193 0.382365 x

x Se 13 0.666633 0.655714 0.128288 x

x Se 14 0.736651 0.343290 0.631546 x

x Se 15 0.731389 0.331890 0.876206 x

x Se 16 0.667966 0.659161 0.370359 x

x Se 17 0.867563 0.658364 0.128438 x

x Se 18 0.932783 0.337708 0.623270 x

x Se 19 0.933091 0.339285 0.878117 x

x Se 20 0.867980 0.660535 0.372329 x

x Nb 1 0.002892 0.002473 0.248474 x

x Nb 2 -0.003253 -0.003234 0.751109 x

x Nb 3 -0.000248 -0.000454 0.000048 x

x Nb 4 0.000808 0.001626 0.499723 x

x Nb 5 0.195476 -0.011672 0.245773 x

x Nb 6 0.199592 0.004273 0.749982 x

x Nb 7 0.200293 0.006598 -0.001999 x

x Nb 8 0.202561 0.009077 0.498911 x

x Nb 9 0.402010 -0.001911 0.252980 x

x Nb 10 0.402873 0.015316 0.750798 x

x Nb 11 0.402608 0.001785 -0.000674 x

x Nb 12 0.383320 -0.040526 0.499910 x

x Nb 13 0.597175 -0.015417 0.249540 x

x Nb 14 0.597939 0.001642 0.747213 x

x Nb 15 0.597347 -0.001950 0.000910 x

x Nb 16 0.616574 0.039976 0.500349 x

x Nb 17 0.800354 -0.004118 0.250287 x

x Nb 18 0.805057 0.013057 0.754139 x

x Nb 19 0.799876 -0.005647 0.002068 x

x Nb 20 0.796889 -0.010468 0.501137 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600121E+004 56761.67 <-- SCF

1 -3.62600315E+004 4.84466336E-004 56787.36 <-- SCF

2 -3.62600327E+004 3.17124487E-005 56813.28 <-- SCF

3 -3.62600267E+004 -1.50767361E-004 56839.47 <-- SCF

4 -3.62600221E+004 -1.15041245E-004 56864.75 <-- SCF

5 -3.62600220E+004 -1.19281219E-006 56888.23 <-- SCF

6 -3.62600219E+004 -4.34808293E-006 56906.89 <-- SCF

7 -3.62600218E+004 -8.63493253E-007 56924.19 <-- SCF

8 -3.62600219E+004 5.62746436E-007 56942.02 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02185577 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00438 0.01221 -0.03660 \*

\* Se 2 -0.00769 -0.02389 0.02520 \*

\* Se 3 -0.00058 -0.01573 0.02303 \*

\* Se 4 0.06946 0.00342 -0.07014 \*

\* Se 5 0.00665 0.02910 0.00651 \*

\* Se 6 0.00484 0.04314 -0.00388 \*

\* Se 7 0.00940 0.03051 -0.03280 \*

\* Se 8 -0.00149 -0.03821 -0.00236 \*

\* Se 9 -0.00314 -0.02973 0.01620 \*

\* Se 10 0.00343 -0.02795 -0.00976 \*

\* Se 11 0.01662 0.02769 0.00917 \*

\* Se 12 -0.00415 0.02939 -0.00125 \*

\* Se 13 0.00221 0.00044 -0.03021 \*

\* Se 14 -0.00468 0.03301 0.00192 \*

\* Se 15 -0.00021 -0.02295 0.00229 \*

\* Se 16 0.00530 -0.05243 0.06487 \*

\* Se 17 -0.00769 0.01167 -0.01215 \*

\* Se 18 -0.03771 -0.01461 0.04595 \*

\* Se 19 -0.00196 -0.00919 0.02765 \*

\* Se 20 0.00509 0.00907 -0.00436 \*

\* Nb 1 -0.02107 -0.00214 -0.01708 \*

\* Nb 2 0.00589 0.00108 0.00019 \*

\* Nb 3 -0.00016 -0.00391 0.00793 \*

\* Nb 4 0.01452 -0.00115 -0.00300 \*

\* Nb 5 0.01631 0.00430 0.02879 \*

\* Nb 6 -0.02163 0.01423 -0.01137 \*

\* Nb 7 -0.01290 -0.01219 -0.00163 \*

\* Nb 8 -0.02649 0.02228 0.01512 \*

\* Nb 9 -0.00993 0.01292 0.01739 \*

\* Nb 10 0.02030 -0.00455 -0.01697 \*

\* Nb 11 0.01332 0.00288 0.00036 \*

\* Nb 12 -0.00508 0.00620 0.02889 \*

\* Nb 13 -0.03615 0.01285 0.00546 \*

\* Nb 14 -0.00116 -0.01358 -0.01947 \*

\* Nb 15 -0.00825 -0.00977 0.01172 \*

\* Nb 16 0.00278 0.00787 -0.03644 \*

\* Nb 17 0.01773 -0.01196 0.00416 \*

\* Nb 18 -0.00759 -0.00830 -0.02775 \*

\* Nb 19 0.01438 0.00756 0.01424 \*

\* Nb 20 -0.00415 -0.01958 -0.01981 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.013802 -0.001523 -0.000935 \*

\* y -0.001523 0.007672 0.000202 \*

\* z -0.000935 0.000202 0.003921 \*

\* \*

\* Pressure: 0.0007 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000010 | -36260.021668 | <-- min BFGS

| trial step | 1.000000 | 5.265E-006 | -36260.021907 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 84 with line minimization (lambda= 2.044572)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8565548 -8.3055801 0.0080225 0.4206033 -0.0041503 -0.0001880

0.0333501 3.3797561 0.0000051 1.0336114 1.8488655 -0.0004657

0.0062426 0.0000278 13.9652166 -0.0002420 0.0000017 0.4499169

Lattice parameters(A) Cell Angles

a = 17.020574 alpha = 89.999546

b = 3.379921 beta = 89.950694

c = 13.965218 gamma = 118.642083

Current cell volume = 705.082999 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067008 0.660918 0.121869 x

x Se 2 0.132099 0.340225 0.627870 x

x Se 3 0.132233 0.341243 0.871717 x

x Se 4 0.067306 0.661673 0.374924 x

x Se 5 0.268745 0.668561 0.124033 x

x Se 6 0.331784 0.340511 0.629606 x

x Se 7 0.333334 0.343867 0.871957 x

x Se 8 0.263362 0.656891 0.368555 x

x Se 9 0.466810 0.653710 0.128743 x

x Se 10 0.531539 0.339687 0.617793 x

x Se 11 0.533140 0.346202 0.871264 x

x Se 12 0.468415 0.660180 0.382423 x

x Se 13 0.666618 0.655677 0.128295 x

x Se 14 0.736651 0.343203 0.631564 x

x Se 15 0.731400 0.331990 0.876202 x

x Se 16 0.668013 0.659150 0.370254 x

x Se 17 0.867558 0.658356 0.128415 x

x Se 18 0.932773 0.337702 0.623305 x

x Se 19 0.933079 0.339321 0.878141 x

x Se 20 0.867983 0.660602 0.372314 x

x Nb 1 0.002884 0.002527 0.248434 x

x Nb 2 -0.003255 -0.003318 0.751138 x

x Nb 3 -0.000249 -0.000458 0.000047 x

x Nb 4 0.000829 0.001656 0.499728 x

x Nb 5 0.195511 -0.011559 0.245754 x

x Nb 6 0.199555 0.004103 0.749998 x

x Nb 7 0.200303 0.006640 -0.002011 x

x Nb 8 0.202459 0.008990 0.498945 x

x Nb 9 0.402014 -0.001850 0.253003 x

x Nb 10 0.402920 0.015496 0.750766 x

x Nb 11 0.402614 0.001657 -0.000626 x

x Nb 12 0.383287 -0.040652 0.499939 x

x Nb 13 0.597152 -0.015529 0.249594 x

x Nb 14 0.597930 0.001528 0.747186 x

x Nb 15 0.597343 -0.001805 0.000865 x

x Nb 16 0.616601 0.040059 0.500344 x

x Nb 17 0.800381 -0.003992 0.250312 x

x Nb 18 0.805024 0.012946 0.754150 x

x Nb 19 0.799871 -0.005680 0.002079 x

x Nb 20 0.796976 -0.010430 0.501109 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600107E+004 57045.52 <-- SCF

1 -3.62600493E+004 9.64216471E-004 57072.73 <-- SCF

2 -3.62600515E+004 5.51407880E-005 57098.95 <-- SCF

3 -3.62600465E+004 -1.25556139E-004 57125.73 <-- SCF

4 -3.62600211E+004 -6.34524365E-004 57151.34 <-- SCF

5 -3.62600228E+004 4.19363887E-005 57176.72 <-- SCF

6 -3.62600221E+004 -1.71255044E-005 57198.73 <-- SCF

7 -3.62600219E+004 -4.79944314E-006 57217.41 <-- SCF

8 -3.62600219E+004 -8.77545051E-007 57235.41 <-- SCF

9 -3.62600219E+004 2.56104964E-007 57253.00 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02188428 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00878 0.01761 -0.03899 \*

\* Se 2 -0.01441 -0.02554 0.02965 \*

\* Se 3 -0.00564 -0.01800 0.02420 \*

\* Se 4 0.07244 0.00845 -0.07756 \*

\* Se 5 0.01060 0.03219 0.00478 \*

\* Se 6 0.00907 0.03934 -0.00528 \*

\* Se 7 0.00474 0.03742 -0.04640 \*

\* Se 8 -0.00263 -0.04364 0.00463 \*

\* Se 9 0.00119 -0.03260 0.03452 \*

\* Se 10 -0.00102 -0.03620 -0.00751 \*

\* Se 11 0.01542 0.02964 0.00123 \*

\* Se 12 -0.00540 0.03024 -0.01009 \*

\* Se 13 0.00888 0.00268 -0.03026 \*

\* Se 14 -0.00292 0.03752 -0.00546 \*

\* Se 15 -0.00337 -0.02560 0.00258 \*

\* Se 16 0.00225 -0.05297 0.09305 \*

\* Se 17 -0.00524 0.01320 -0.01030 \*

\* Se 18 -0.03756 -0.01800 0.05136 \*

\* Se 19 -0.00125 -0.01598 0.02425 \*

\* Se 20 0.01330 0.00615 0.00189 \*

\* Nb 1 -0.02198 -0.00754 -0.01657 \*

\* Nb 2 0.00632 0.00709 0.00066 \*

\* Nb 3 0.00103 -0.00380 0.00910 \*

\* Nb 4 0.01266 -0.00123 -0.00484 \*

\* Nb 5 0.01118 0.00231 0.03209 \*

\* Nb 6 -0.01572 0.01842 -0.01024 \*

\* Nb 7 -0.01453 -0.01363 0.00092 \*

\* Nb 8 -0.01901 0.01832 0.00735 \*

\* Nb 9 -0.00974 0.01048 0.01156 \*

\* Nb 10 0.01422 -0.00570 -0.00933 \*

\* Nb 11 0.01253 0.00634 -0.00634 \*

\* Nb 12 -0.00938 0.01121 0.02764 \*

\* Nb 13 -0.03868 0.01264 -0.00995 \*

\* Nb 14 0.00029 -0.00769 -0.01209 \*

\* Nb 15 -0.00629 -0.01362 0.01853 \*

\* Nb 16 0.00863 0.00609 -0.04296 \*

\* Nb 17 0.01714 -0.01523 -0.00925 \*

\* Nb 18 -0.00007 -0.00663 -0.02564 \*

\* Nb 19 0.01546 0.01035 0.01373 \*

\* Nb 20 -0.01372 -0.01408 -0.01464 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.007971 -0.006618 -0.000546 \*

\* y -0.006618 0.005367 -0.019481 \*

\* z -0.000546 -0.019481 -0.019148 \*

\* \*

\* Pressure: 0.0073 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000010 | -36260.021668 | <-- min BFGS

| trial step | 1.000000 | 5.265E-006 | -36260.021907 | <-- min BFGS

| line step | 2.044572 | -2.566E-006 | -36260.021929 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 84 with enthalpy= -3.62600219E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 6.535469E-006 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.070933E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.296956E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.948066E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 85 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 5.357E-006 | -36260.021929 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 85 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8571722 -8.3053029 0.0077700 0.4205860 -0.0041501 -0.0001879

0.0333483 3.3796451 0.0001051 1.0335684 1.8489271 -0.0005086

0.0062433 0.0003515 13.9654722 -0.0002418 -0.0000116 0.4499087

Lattice parameters(A) Cell Angles

a = 17.020978 alpha = 89.996523

b = 3.379810 beta = 89.952190

c = 13.965474 gamma = 118.640266

Current cell volume = 705.101681 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067001 0.660942 0.121868 x

x Se 2 0.132087 0.340196 0.627883 x

x Se 3 0.132226 0.341244 0.871720 x

x Se 4 0.067306 0.661698 0.374924 x

x Se 5 0.268758 0.668557 0.124023 x

x Se 6 0.331782 0.340499 0.629607 x

x Se 7 0.333319 0.343885 0.871944 x

x Se 8 0.263352 0.656793 0.368565 x

x Se 9 0.466813 0.653635 0.128761 x

x Se 10 0.531528 0.339676 0.617802 x

x Se 11 0.533140 0.346281 0.871260 x

x Se 12 0.468415 0.660115 0.382401 x

x Se 13 0.666634 0.655707 0.128289 x

x Se 14 0.736661 0.343297 0.631551 x

x Se 15 0.731387 0.331994 0.876209 x

x Se 16 0.668020 0.659185 0.370298 x

x Se 17 0.867561 0.658338 0.128419 x

x Se 18 0.932780 0.337695 0.623308 x

x Se 19 0.933082 0.339279 0.878131 x

x Se 20 0.867998 0.660606 0.372315 x

x Nb 1 0.002870 0.002479 0.248433 x

x Nb 2 -0.003243 -0.003265 0.751140 x

x Nb 3 -0.000249 -0.000453 0.000048 x

x Nb 4 0.000828 0.001649 0.499726 x

x Nb 5 0.195513 -0.011552 0.245760 x

x Nb 6 0.199547 0.004145 0.749989 x

x Nb 7 0.200304 0.006647 -0.001994 x

x Nb 8 0.202454 0.008962 0.498926 x

x Nb 9 0.402022 -0.001912 0.252997 x

x Nb 10 0.402904 0.015449 0.750775 x

x Nb 11 0.402604 0.001647 -0.000640 x

x Nb 12 0.383268 -0.040655 0.499944 x

x Nb 13 0.597159 -0.015519 0.249577 x

x Nb 14 0.597923 0.001615 0.747193 x

x Nb 15 0.597354 -0.001799 0.000877 x

x Nb 16 0.616621 0.040073 0.500329 x

x Nb 17 0.800394 -0.004011 0.250302 x

x Nb 18 0.805027 0.012950 0.754150 x

x Nb 19 0.799870 -0.005679 0.002063 x

x Nb 20 0.796980 -0.010392 0.501124 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600206E+004 57356.84 <-- SCF

1 -3.62600250E+004 1.10084989E-004 57383.53 <-- SCF

2 -3.62600252E+004 4.94010248E-006 57403.67 <-- SCF

3 -3.62600241E+004 -2.65573051E-005 57430.12 <-- SCF

4 -3.62600221E+004 -5.07958030E-005 57454.23 <-- SCF

5 -3.62600221E+004 9.46315252E-007 57474.34 <-- SCF

6 -3.62600220E+004 -1.78883004E-006 57491.66 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02203112 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00493 0.01412 -0.03896 \*

\* Se 2 -0.01011 -0.02485 0.02643 \*

\* Se 3 -0.00325 -0.01904 0.02135 \*

\* Se 4 0.07502 0.00620 -0.07472 \*

\* Se 5 0.00604 0.03515 0.00819 \*

\* Se 6 0.00884 0.03996 -0.00688 \*

\* Se 7 0.00956 0.03076 -0.04127 \*

\* Se 8 0.00140 -0.03590 0.00452 \*

\* Se 9 -0.00038 -0.02685 0.03032 \*

\* Se 10 0.00163 -0.03702 -0.00926 \*

\* Se 11 0.01434 0.02403 0.00053 \*

\* Se 12 -0.00702 0.03558 -0.00197 \*

\* Se 13 0.00135 0.00314 -0.02580 \*

\* Se 14 -0.00609 0.03052 -0.00368 \*

\* Se 15 0.00183 -0.02869 0.00019 \*

\* Se 16 -0.00001 -0.05367 0.07999 \*

\* Se 17 -0.00502 0.01481 -0.00987 \*

\* Se 18 -0.04023 -0.01742 0.05026 \*

\* Se 19 -0.00213 -0.01149 0.02624 \*

\* Se 20 0.01008 0.00865 0.00219 \*

\* Nb 1 -0.02983 -0.00838 -0.01509 \*

\* Nb 2 0.01525 0.00753 -0.00026 \*

\* Nb 3 0.00269 -0.00363 0.01017 \*

\* Nb 4 0.01327 -0.00149 -0.00413 \*

\* Nb 5 0.01213 0.00213 0.03655 \*

\* Nb 6 -0.01995 0.02164 -0.01303 \*

\* Nb 7 -0.01392 -0.01340 0.00465 \*

\* Nb 8 -0.01821 0.01708 0.00244 \*

\* Nb 9 -0.00771 0.00582 0.01114 \*

\* Nb 10 0.00509 -0.00588 -0.00699 \*

\* Nb 11 0.00408 0.00806 -0.00957 \*

\* Nb 12 -0.02061 0.01287 0.03014 \*

\* Nb 13 -0.03817 0.01187 -0.01512 \*

\* Nb 14 -0.00193 -0.00301 -0.00822 \*

\* Nb 15 0.00211 -0.01645 0.02317 \*

\* Nb 16 0.01940 0.00449 -0.04647 \*

\* Nb 17 0.02408 -0.01758 -0.01135 \*

\* Nb 18 0.00277 -0.00663 -0.02636 \*

\* Nb 19 0.01319 0.00969 0.01026 \*

\* Nb 20 -0.01466 -0.01269 -0.00972 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.002897 -0.005917 -0.000103 \*

\* y -0.005917 0.000792 -0.012636 \*

\* z -0.000103 -0.012636 -0.011284 \*

\* \*

\* Pressure: 0.0045 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 5.357E-006 | -36260.021929 | <-- min BFGS

| trial step | 1.000000 | 5.050E-006 | -36260.022082 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 85 with line minimization (lambda= 17.437904)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8673199 -8.3007451 0.0036189 0.4203026 -0.0041457 -0.0001865

0.0333182 3.3778217 0.0017486 1.0328628 1.8499420 -0.0012137

0.0062552 0.0056726 13.9696728 -0.0002382 -0.0002305 0.4497735

Lattice parameters(A) Cell Angles

a = 17.027612 alpha = 89.946823

b = 3.377986 beta = 89.976764

c = 13.969675 gamma = 118.610415

Current cell volume = 705.408391 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066898 0.661337 0.121858 x

x Se 2 0.131888 0.339722 0.628091 x

x Se 3 0.132097 0.341262 0.871761 x

x Se 4 0.067305 0.662119 0.374915 x

x Se 5 0.268965 0.668483 0.123864 x

x Se 6 0.331748 0.340298 0.629624 x

x Se 7 0.333067 0.344176 0.871716 x

x Se 8 0.263183 0.655186 0.368730 x

x Se 9 0.466852 0.652413 0.129058 x

x Se 10 0.531351 0.339497 0.617944 x

x Se 11 0.533128 0.347588 0.871201 x

x Se 12 0.468420 0.659047 0.382042 x

x Se 13 0.666893 0.656190 0.128187 x

x Se 14 0.736834 0.344846 0.631327 x

x Se 15 0.731165 0.332060 0.876333 x

x Se 16 0.668146 0.659768 0.371026 x

x Se 17 0.867615 0.658029 0.128485 x

x Se 18 0.932899 0.337580 0.623343 x

x Se 19 0.933131 0.338586 0.877973 x

x Se 20 0.868236 0.660672 0.372330 x

x Nb 1 0.002646 0.001690 0.248422 x

x Nb 2 -0.003039 -0.002395 0.751171 x

x Nb 3 -0.000234 -0.000374 0.000075 x

x Nb 4 0.000803 0.001524 0.499694 x

x Nb 5 0.195555 -0.011440 0.245854 x

x Nb 6 0.199422 0.004828 0.749852 x

x Nb 7 0.200320 0.006763 -0.001707 x

x Nb 8 0.202384 0.008504 0.498609 x

x Nb 9 0.402167 -0.002945 0.252910 x

x Nb 10 0.402641 0.014673 0.750923 x

x Nb 11 0.402429 0.001483 -0.000863 x

x Nb 12 0.382949 -0.040711 0.500017 x

x Nb 13 0.597275 -0.015355 0.249282 x

x Nb 14 0.597803 0.003036 0.747313 x

x Nb 15 0.597541 -0.001705 0.001088 x

x Nb 16 0.616956 0.040292 0.500074 x

x Nb 17 0.800602 -0.004325 0.250145 x

x Nb 18 0.805065 0.013021 0.754159 x

x Nb 19 0.799850 -0.005667 0.001802 x

x Nb 20 0.797043 -0.009756 0.501371 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62596297E+004 57595.31 <-- SCF

1 -3.62607743E+004 2.86144705E-002 57622.66 <-- SCF

2 -3.62608328E+004 1.46108256E-003 57651.80 <-- SCF

3 -3.62605564E+004 -6.90971174E-003 57678.75 <-- SCF

4 -3.62600305E+004 -1.31479211E-002 57704.81 <-- SCF

5 -3.62600393E+004 2.19836802E-004 57731.80 <-- SCF

6 -3.62600205E+004 -4.69655608E-004 57758.05 <-- SCF

7 -3.62600169E+004 -8.79889896E-005 57782.89 <-- SCF

8 -3.62600171E+004 3.69135612E-006 57806.14 <-- SCF

9 -3.62600170E+004 -1.47005556E-006 57825.92 <-- SCF

10 -3.62600171E+004 7.97787858E-007 57843.55 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.01706995 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.02806 -0.03686 -0.01863 \*

\* Se 2 0.04012 0.00021 -0.03135 \*

\* Se 3 0.03144 -0.02707 0.02664 \*

\* Se 4 0.07291 -0.02633 -0.08868 \*

\* Se 5 -0.06716 0.06169 0.05776 \*

\* Se 6 -0.01814 0.04986 -0.01246 \*

\* Se 7 0.05372 -0.04983 0.06675 \*

\* Se 8 0.04193 0.06626 -0.04724 \*

\* Se 9 -0.01596 0.02616 -0.09149 \*

\* Se 10 0.04873 -0.03570 -0.03753 \*

\* Se 11 0.00402 -0.02954 0.03975 \*

\* Se 12 -0.00164 0.07064 0.08557 \*

\* Se 13 -0.04878 0.00968 0.00796 \*

\* Se 14 -0.04687 -0.06238 0.06433 \*

\* Se 15 0.07290 -0.05904 -0.04139 \*

\* Se 16 -0.00013 -0.03865 -0.15790 \*

\* Se 17 -0.01013 0.03410 -0.05020 \*

\* Se 18 -0.06303 -0.00981 0.05658 \*

\* Se 19 -0.01543 0.04971 0.04993 \*

\* Se 20 -0.04607 0.03326 -0.00499 \*

\* Nb 1 0.02411 0.01918 -0.00801 \*

\* Nb 2 -0.03197 -0.02760 -0.00640 \*

\* Nb 3 -0.01096 -0.00709 -0.00049 \*

\* Nb 4 0.02267 0.00046 0.00154 \*

\* Nb 5 -0.00048 -0.02622 -0.00447 \*

\* Nb 6 -0.01400 -0.01475 0.01413 \*

\* Nb 7 -0.02037 -0.01589 -0.04474 \*

\* Nb 8 -0.02298 0.01382 0.07129 \*

\* Nb 9 -0.04513 0.01738 0.04337 \*

\* Nb 10 0.05241 0.01987 -0.03151 \*

\* Nb 11 0.03713 0.00745 0.01541 \*

\* Nb 12 0.03281 -0.01708 0.00746 \*

\* Nb 13 -0.01150 0.01064 0.06482 \*

\* Nb 14 0.02730 -0.03810 -0.05397 \*

\* Nb 15 -0.03870 -0.00403 -0.00329 \*

\* Nb 16 -0.04842 0.02411 0.04062 \*

\* Nb 17 -0.02692 0.00295 0.06019 \*

\* Nb 18 -0.01532 0.02300 -0.02826 \*

\* Nb 19 0.02616 0.00817 0.04151 \*

\* Nb 20 0.00364 -0.02263 -0.05260 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.139357 -0.017323 0.009173 \*

\* y -0.017323 -0.067823 0.100840 \*

\* z 0.009173 0.100840 0.052347 \*

\* \*

\* Pressure: -0.0413 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 5.357E-006 | -36260.021929 | <-- min BFGS

| trial step | 1.000000 | 5.050E-006 | -36260.022082 | <-- min BFGS

| line step | 17.437904 | -0.000026 | -36260.017112 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 85 with quad minimization (lambda= 3.697197)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8588372 -8.3045550 0.0070889 0.4205395 -0.0041494 -0.0001877

0.0333434 3.3793459 0.0003748 1.0334526 1.8490935 -0.0006243

0.0062453 0.0012246 13.9661614 -0.0002412 -0.0000475 0.4498865

Lattice parameters(A) Cell Angles

a = 17.022066 alpha = 89.988369

b = 3.379510 beta = 89.956225

c = 13.966163 gamma = 118.635366

Current cell volume = 705.152056 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066985 0.661007 0.121866 x

x Se 2 0.132054 0.340118 0.627917 x

x Se 3 0.132204 0.341247 0.871726 x

x Se 4 0.067306 0.661767 0.374922 x

x Se 5 0.268792 0.668545 0.123997 x

x Se 6 0.331776 0.340466 0.629610 x

x Se 7 0.333278 0.343933 0.871906 x

x Se 8 0.263324 0.656530 0.368592 x

x Se 9 0.466819 0.653435 0.128810 x

x Se 10 0.531499 0.339647 0.617825 x

x Se 11 0.533138 0.346496 0.871251 x

x Se 12 0.468416 0.659940 0.382342 x

x Se 13 0.666676 0.655786 0.128272 x

x Se 14 0.736689 0.343551 0.631514 x

x Se 15 0.731350 0.332005 0.876230 x

x Se 16 0.668041 0.659281 0.370418 x

x Se 17 0.867570 0.658287 0.128430 x

x Se 18 0.932800 0.337676 0.623313 x

x Se 19 0.933090 0.339165 0.878105 x

x Se 20 0.868037 0.660617 0.372318 x

x Nb 1 0.002833 0.002349 0.248431 x

x Nb 2 -0.003209 -0.003122 0.751145 x

x Nb 3 -0.000246 -0.000440 0.000053 x

x Nb 4 0.000823 0.001628 0.499721 x

x Nb 5 0.195520 -0.011534 0.245775 x

x Nb 6 0.199527 0.004257 0.749967 x

x Nb 7 0.200306 0.006666 -0.001946 x

x Nb 8 0.202443 0.008887 0.498874 x

x Nb 9 0.402046 -0.002082 0.252983 x

x Nb 10 0.402861 0.015322 0.750799 x

x Nb 11 0.402575 0.001620 -0.000676 x

x Nb 12 0.383216 -0.040664 0.499956 x

x Nb 13 0.597178 -0.015492 0.249528 x

x Nb 14 0.597903 0.001848 0.747213 x

x Nb 15 0.597385 -0.001783 0.000912 x

x Nb 16 0.616676 0.040109 0.500287 x

x Nb 17 0.800428 -0.004063 0.250276 x

x Nb 18 0.805033 0.012962 0.754152 x

x Nb 19 0.799867 -0.005677 0.002020 x

x Nb 20 0.796990 -0.010288 0.501165 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597520E+004 57946.94 <-- SCF

1 -3.62605118E+004 1.89953410E-002 57973.67 <-- SCF

2 -3.62605485E+004 9.17047260E-004 58002.83 <-- SCF

3 -3.62603519E+004 -4.91393826E-003 58029.48 <-- SCF

4 -3.62600330E+004 -7.97381309E-003 58055.38 <-- SCF

5 -3.62600350E+004 5.12201826E-005 58082.11 <-- SCF

6 -3.62600240E+004 -2.76850011E-004 58108.05 <-- SCF

7 -3.62600222E+004 -4.48229924E-005 58131.77 <-- SCF

8 -3.62600222E+004 3.11948657E-007 58153.55 <-- SCF

9 -3.62600221E+004 -1.67004923E-006 58172.62 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02210712 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00433 0.00867 -0.03614 \*

\* Se 2 -0.00065 -0.01992 0.01613 \*

\* Se 3 0.00113 -0.01654 0.02634 \*

\* Se 4 0.07671 0.00359 -0.07861 \*

\* Se 5 0.00065 0.04001 0.01539 \*

\* Se 6 0.00931 0.04092 -0.00949 \*

\* Se 7 0.01333 0.01968 -0.02473 \*

\* Se 8 0.01367 -0.02367 -0.00479 \*

\* Se 9 -0.00240 -0.02013 0.01090 \*

\* Se 10 0.00636 -0.03567 -0.01700 \*

\* Se 11 0.01141 0.01914 0.00589 \*

\* Se 12 -0.00047 0.04066 0.01598 \*

\* Se 13 -0.00683 0.00172 -0.01910 \*

\* Se 14 -0.01966 0.01950 0.00858 \*

\* Se 15 0.00577 -0.03348 -0.00914 \*

\* Se 16 0.00134 -0.05360 0.04579 \*

\* Se 17 -0.00464 0.01426 -0.01879 \*

\* Se 18 -0.04565 -0.01854 0.05245 \*

\* Se 19 -0.00695 -0.00403 0.03011 \*

\* Se 20 -0.00317 0.01187 0.00084 \*

\* Nb 1 -0.02657 -0.00219 -0.01697 \*

\* Nb 2 0.00750 -0.00000 0.00084 \*

\* Nb 3 0.00098 -0.00435 0.00739 \*

\* Nb 4 0.01387 -0.00112 -0.00366 \*

\* Nb 5 0.01185 -0.00352 0.02781 \*

\* Nb 6 -0.01522 0.00977 -0.00478 \*

\* Nb 7 -0.01414 -0.01796 -0.00406 \*

\* Nb 8 -0.00970 0.01888 0.01494 \*

\* Nb 9 -0.01061 0.01751 0.01955 \*

\* Nb 10 0.02406 0.00067 -0.01601 \*

\* Nb 11 0.00543 0.00493 -0.00148 \*

\* Nb 12 -0.00713 0.00281 0.02331 \*

\* Nb 13 -0.04183 0.01189 0.00469 \*

\* Nb 14 0.00299 -0.01702 -0.02055 \*

\* Nb 15 -0.00284 -0.01031 0.01457 \*

\* Nb 16 0.00567 0.01184 -0.02909 \*

\* Nb 17 0.01309 -0.00857 0.00301 \*

\* Nb 18 -0.00375 -0.00210 -0.02708 \*

\* Nb 19 0.01373 0.01234 0.01570 \*

\* Nb 20 -0.02092 -0.01796 -0.01875 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.010121 -0.002085 -0.001198 \*

\* y -0.002085 -0.004439 0.007859 \*

\* z -0.001198 0.007859 0.005612 \*

\* \*

\* Pressure: -0.0038 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 5.357E-006 | -36260.021929 | <-- min BFGS

| trial step | 1.000000 | 5.050E-006 | -36260.022082 | <-- min BFGS

| line step | 17.437904 | -0.000026 | -36260.017112 | <-- min BFGS

| quad step | 3.697197 | -4.782E-007 | -36260.022156 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 85 with enthalpy= -3.62600222E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 5.655259E-006 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.098930E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.334884E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.012070E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 86 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000012 | -36260.022156 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 86 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8610297 -8.3044080 0.0073264 0.4204801 -0.0041447 -0.0001920

0.0333098 3.3792387 0.0003533 1.0333211 1.8491638 -0.0006252

0.0063865 0.0011531 13.9650032 -0.0002467 -0.0000446 0.4499238

Lattice parameters(A) Cell Angles

a = 17.023908 alpha = 89.989021

b = 3.379403 beta = 89.954776

c = 13.965005 gamma = 118.631885

Current cell volume = 705.170823 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066983 0.660931 0.121876 x

x Se 2 0.132042 0.340006 0.627901 x

x Se 3 0.132208 0.341202 0.871759 x

x Se 4 0.067313 0.661732 0.374826 x

x Se 5 0.268807 0.668597 0.124033 x

x Se 6 0.331737 0.340365 0.629614 x

x Se 7 0.333268 0.343863 0.871896 x

x Se 8 0.263333 0.656520 0.368568 x

x Se 9 0.466820 0.653462 0.128810 x

x Se 10 0.531491 0.339562 0.617802 x

x Se 11 0.533141 0.346475 0.871255 x

x Se 12 0.468426 0.660055 0.382369 x

x Se 13 0.666691 0.655878 0.128269 x

x Se 14 0.736678 0.343550 0.631541 x

x Se 15 0.731341 0.331979 0.876197 x

x Se 16 0.668079 0.659371 0.370417 x

x Se 17 0.867564 0.658323 0.128402 x

x Se 18 0.932796 0.337692 0.623378 x

x Se 19 0.933093 0.339252 0.878098 x

x Se 20 0.868048 0.660731 0.372338 x

x Nb 1 0.002757 0.002117 0.248408 x

x Nb 2 -0.003141 -0.002915 0.751157 x

x Nb 3 -0.000248 -0.000450 0.000056 x

x Nb 4 0.000838 0.001653 0.499720 x

x Nb 5 0.195535 -0.011490 0.245769 x

x Nb 6 0.199474 0.004020 0.749977 x

x Nb 7 0.200314 0.006629 -0.001932 x

x Nb 8 0.202403 0.008779 0.498858 x

x Nb 9 0.402072 -0.001925 0.253008 x

x Nb 10 0.402875 0.015270 0.750793 x

x Nb 11 0.402574 0.001536 -0.000655 x

x Nb 12 0.383134 -0.040856 0.499947 x

x Nb 13 0.597165 -0.015422 0.249536 x

x Nb 14 0.597873 0.001672 0.747187 x

x Nb 15 0.597387 -0.001698 0.000898 x

x Nb 16 0.616756 0.040307 0.500299 x

x Nb 17 0.800477 -0.003836 0.250276 x

x Nb 18 0.805022 0.012921 0.754156 x

x Nb 19 0.799862 -0.005638 0.002012 x

x Nb 20 0.797015 -0.010219 0.501180 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600137E+004 58275.75 <-- SCF

1 -3.62600420E+004 7.07286915E-004 58303.22 <-- SCF

2 -3.62600435E+004 3.64285863E-005 58328.16 <-- SCF

3 -3.62600421E+004 -3.52015091E-005 58355.12 <-- SCF

4 -3.62600217E+004 -5.10598991E-004 58381.25 <-- SCF

5 -3.62600227E+004 2.68418112E-005 58405.72 <-- SCF

6 -3.62600225E+004 -5.67695447E-006 58425.80 <-- SCF

7 -3.62600224E+004 -2.92455723E-006 58444.08 <-- SCF

8 -3.62600223E+004 -1.01631051E-006 58461.64 <-- SCF

9 -3.62600224E+004 1.35137360E-006 58480.67 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02239756 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00502 0.01256 -0.03879 \*

\* Se 2 0.00269 -0.01883 0.01413 \*

\* Se 3 0.00158 -0.01692 0.02458 \*

\* Se 4 0.07107 0.00519 -0.08110 \*

\* Se 5 0.00280 0.04160 0.01701 \*

\* Se 6 0.00924 0.04067 -0.00663 \*

\* Se 7 0.01736 0.01957 -0.02241 \*

\* Se 8 0.00904 -0.01855 -0.00421 \*

\* Se 9 0.00009 -0.01795 0.00905 \*

\* Se 10 0.00871 -0.03443 -0.01368 \*

\* Se 11 0.00878 0.01696 0.00547 \*

\* Se 12 -0.00372 0.03891 0.01275 \*

\* Se 13 -0.01191 -0.00002 -0.01529 \*

\* Se 14 -0.01475 0.01547 0.00620 \*

\* Se 15 0.00509 -0.03416 -0.00740 \*

\* Se 16 -0.00039 -0.05357 0.03930 \*

\* Se 17 -0.00611 0.01375 -0.01802 \*

\* Se 18 -0.04793 -0.01720 0.05364 \*

\* Se 19 -0.00796 -0.00815 0.03336 \*

\* Se 20 -0.00438 0.01093 0.00098 \*

\* Nb 1 -0.01508 -0.00180 -0.01540 \*

\* Nb 2 0.00034 -0.00060 0.00081 \*

\* Nb 3 -0.00081 -0.00400 0.00631 \*

\* Nb 4 0.01429 -0.00112 -0.00362 \*

\* Nb 5 0.01373 -0.00468 0.02310 \*

\* Nb 6 -0.00984 0.01277 -0.00692 \*

\* Nb 7 -0.01466 -0.01626 -0.00448 \*

\* Nb 8 -0.01789 0.01711 0.01893 \*

\* Nb 9 -0.01698 0.01132 0.01597 \*

\* Nb 10 0.02418 0.00270 -0.01567 \*

\* Nb 11 0.01542 0.00706 -0.00422 \*

\* Nb 12 0.00783 0.00482 0.02509 \*

\* Nb 13 -0.03382 0.00856 0.00672 \*

\* Nb 14 0.00637 -0.01249 -0.01889 \*

\* Nb 15 -0.01125 -0.01261 0.01496 \*

\* Nb 16 -0.01101 0.00998 -0.02810 \*

\* Nb 17 0.00289 -0.01222 0.00659 \*

\* Nb 18 -0.00559 0.00004 -0.02557 \*

\* Nb 19 0.01737 0.01139 0.01555 \*

\* Nb 20 -0.00983 -0.01581 -0.02009 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.022579 -0.003253 0.001885 \*

\* y -0.003253 -0.005339 0.005491 \*

\* z 0.001885 0.005491 0.002861 \*

\* \*

\* Pressure: -0.0067 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000012 | -36260.022156 | <-- min BFGS

| trial step | 1.000000 | 7.856E-006 | -36260.022442 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 86 with line minimization (lambda= 3.123027)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8656844 -8.3040960 0.0078307 0.4203540 -0.0041349 -0.0002010

0.0332386 3.3790111 0.0003077 1.0330420 1.8493129 -0.0006273

0.0066864 0.0010011 13.9625441 -0.0002585 -0.0000384 0.4500030

Lattice parameters(A) Cell Angles

a = 17.027820 alpha = 89.990404

b = 3.379175 beta = 89.951701

c = 13.962546 gamma = 118.624498

Current cell volume = 705.210602 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066979 0.660770 0.121898 x

x Se 2 0.132016 0.339768 0.627868 x

x Se 3 0.132216 0.341107 0.871827 x

x Se 4 0.067327 0.661658 0.374621 x

x Se 5 0.268838 0.668707 0.124109 x

x Se 6 0.331652 0.340151 0.629623 x

x Se 7 0.333246 0.343716 0.871875 x

x Se 8 0.263351 0.656500 0.368516 x

x Se 9 0.466822 0.653519 0.128809 x

x Se 10 0.531473 0.339381 0.617751 x

x Se 11 0.533148 0.346433 0.871263 x

x Se 12 0.468448 0.660300 0.382427 x

x Se 13 0.666722 0.656072 0.128261 x

x Se 14 0.736654 0.343547 0.631598 x

x Se 15 0.731320 0.331924 0.876128 x

x Se 16 0.668159 0.659562 0.370416 x

x Se 17 0.867551 0.658399 0.128343 x

x Se 18 0.932789 0.337726 0.623515 x

x Se 19 0.933100 0.339436 0.878082 x

x Se 20 0.868070 0.660973 0.372380 x

x Nb 1 0.002593 0.001624 0.248359 x

x Nb 2 -0.002996 -0.002476 0.751183 x

x Nb 3 -0.000251 -0.000471 0.000065 x

x Nb 4 0.000868 0.001705 0.499717 x

x Nb 5 0.195567 -0.011397 0.245757 x

x Nb 6 0.199363 0.003517 0.750000 x

x Nb 7 0.200330 0.006550 -0.001901 x

x Nb 8 0.202318 0.008551 0.498825 x

x Nb 9 0.402128 -0.001594 0.253062 x

x Nb 10 0.402906 0.015159 0.750780 x

x Nb 11 0.402573 0.001358 -0.000609 x

x Nb 12 0.382959 -0.041263 0.499929 x

x Nb 13 0.597137 -0.015272 0.249551 x

x Nb 14 0.597810 0.001299 0.747130 x

x Nb 15 0.597393 -0.001518 0.000869 x

x Nb 16 0.616925 0.040726 0.500324 x

x Nb 17 0.800582 -0.003354 0.250276 x

x Nb 18 0.804999 0.012836 0.754167 x

x Nb 19 0.799850 -0.005555 0.001994 x

x Nb 20 0.797067 -0.010073 0.501213 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599858E+004 58584.22 <-- SCF

1 -3.62600601E+004 1.85689341E-003 58609.08 <-- SCF

2 -3.62600655E+004 1.36600751E-004 58636.95 <-- SCF

3 -3.62600393E+004 -6.56048451E-004 58663.58 <-- SCF

4 -3.62600244E+004 -3.70896107E-004 58689.22 <-- SCF

5 -3.62600231E+004 -3.44716189E-005 58714.28 <-- SCF

6 -3.62600228E+004 -6.77392828E-006 58734.34 <-- SCF

7 -3.62600228E+004 -5.11422613E-007 58752.83 <-- SCF

8 -3.62600228E+004 2.10247954E-007 58769.23 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02277530 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00363 0.02169 -0.04068 \*

\* Se 2 0.00584 -0.01528 0.01569 \*

\* Se 3 -0.00170 -0.01569 0.02511 \*

\* Se 4 0.05072 0.00957 -0.08951 \*

\* Se 5 0.00817 0.04272 0.01752 \*

\* Se 6 0.01168 0.03858 -0.00589 \*

\* Se 7 0.01752 0.02313 -0.01539 \*

\* Se 8 0.00340 -0.01257 -0.00258 \*

\* Se 9 0.00462 -0.01815 0.00836 \*

\* Se 10 0.01191 -0.02939 -0.01186 \*

\* Se 11 0.00339 0.01747 0.00452 \*

\* Se 12 -0.00788 0.02982 0.00639 \*

\* Se 13 -0.01466 -0.00590 -0.00992 \*

\* Se 14 -0.00725 0.01036 0.00242 \*

\* Se 15 0.00239 -0.03367 -0.00477 \*

\* Se 16 -0.00266 -0.05198 0.03582 \*

\* Se 17 -0.00385 0.01040 -0.01542 \*

\* Se 18 -0.04458 -0.01383 0.06219 \*

\* Se 19 -0.00613 -0.01869 0.03549 \*

\* Se 20 -0.00303 0.00715 -0.00152 \*

\* Nb 1 -0.00669 -0.00086 -0.01590 \*

\* Nb 2 -0.00467 -0.00158 0.00282 \*

\* Nb 3 -0.00103 -0.00391 0.00581 \*

\* Nb 4 0.01623 -0.00175 -0.00538 \*

\* Nb 5 0.01594 -0.00630 0.01775 \*

\* Nb 6 -0.00963 0.01371 -0.00893 \*

\* Nb 7 -0.01567 -0.01533 -0.00180 \*

\* Nb 8 -0.02271 0.01490 0.01594 \*

\* Nb 9 -0.02115 0.00845 0.01320 \*

\* Nb 10 0.02594 0.00471 -0.01353 \*

\* Nb 11 0.01720 0.00740 -0.00587 \*

\* Nb 12 0.01476 0.00748 0.02869 \*

\* Nb 13 -0.03355 0.00566 0.00376 \*

\* Nb 14 0.01011 -0.00902 -0.01475 \*

\* Nb 15 -0.01179 -0.01335 0.01620 \*

\* Nb 16 -0.01832 0.00819 -0.03195 \*

\* Nb 17 0.00350 -0.01362 0.00521 \*

\* Nb 18 -0.00556 0.00177 -0.02108 \*

\* Nb 19 0.02044 0.01177 0.01216 \*

\* Nb 20 -0.00490 -0.01405 -0.01831 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.052636 -0.013323 0.003640 \*

\* y -0.013323 -0.012700 0.000084 \*

\* z 0.003640 0.000084 -0.016449 \*

\* \*

\* Pressure: -0.0078 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000012 | -36260.022156 | <-- min BFGS

| trial step | 1.000000 | 7.856E-006 | -36260.022442 | <-- min BFGS

| line step | 3.123027 | 5.000E-006 | -36260.022812 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 86 with enthalpy= -3.62600228E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.640055E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.033223E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.255407E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 5.263649E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 87 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000062 | -36260.022812 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 87 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8676352 -8.3021004 0.0080769 0.4202723 -0.0041834 -0.0001967

0.0336337 3.3788967 0.0001292 1.0326280 1.8492588 -0.0005375

0.0065367 0.0004074 13.9594465 -0.0002527 -0.0000147 0.4501029

Lattice parameters(A) Cell Angles

a = 17.028550 alpha = 89.995871

b = 3.379064 beta = 89.950214

c = 13.959448 gamma = 118.608718

Current cell volume = 705.167301 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067000 0.660461 0.121954 x

x Se 2 0.131965 0.339262 0.627803 x

x Se 3 0.132267 0.340904 0.872015 x

x Se 4 0.067338 0.661452 0.373953 x

x Se 5 0.268855 0.668848 0.124375 x

x Se 6 0.331386 0.339838 0.629647 x

x Se 7 0.333278 0.343525 0.871823 x

x Se 8 0.263401 0.656713 0.368452 x

x Se 9 0.466863 0.653787 0.128769 x

x Se 10 0.531481 0.339300 0.617683 x

x Se 11 0.533139 0.346215 0.871298 x

x Se 12 0.468473 0.660736 0.382521 x

x Se 13 0.666722 0.656316 0.128268 x

x Se 14 0.736584 0.343263 0.631685 x

x Se 15 0.731341 0.331960 0.875901 x

x Se 16 0.668386 0.659808 0.370314 x

x Se 17 0.867485 0.658539 0.128177 x

x Se 18 0.932759 0.337725 0.623944 x

x Se 19 0.933101 0.339850 0.878061 x

x Se 20 0.868107 0.661532 0.372455 x

x Nb 1 0.002240 0.000857 0.248177 x

x Nb 2 -0.002710 -0.001889 0.751288 x

x Nb 3 -0.000256 -0.000519 0.000086 x

x Nb 4 0.000972 0.001862 0.499724 x

x Nb 5 0.195771 -0.010903 0.245753 x

x Nb 6 0.199042 0.002227 0.750075 x

x Nb 7 0.200364 0.006353 -0.001844 x

x Nb 8 0.201878 0.007815 0.498865 x

x Nb 9 0.402221 -0.000961 0.253199 x

x Nb 10 0.403043 0.015230 0.750692 x

x Nb 11 0.402554 0.000737 -0.000446 x

x Nb 12 0.382704 -0.041880 0.499994 x

x Nb 13 0.597041 -0.015144 0.249677 x

x Nb 14 0.597691 0.000499 0.746979 x

x Nb 15 0.597430 -0.000861 0.000751 x

x Nb 16 0.617161 0.041329 0.500309 x

x Nb 17 0.800870 -0.002187 0.250312 x

x Nb 18 0.804817 0.012351 0.754161 x

x Nb 19 0.799837 -0.005335 0.001972 x

x Nb 20 0.797398 -0.009614 0.501177 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62597769E+004 58872.27 <-- SCF

1 -3.62605544E+004 1.94386197E-002 58899.09 <-- SCF

2 -3.62605972E+004 1.06910238E-003 58927.67 <-- SCF

3 -3.62604288E+004 -4.20921878E-003 58954.58 <-- SCF

4 -3.62600203E+004 -1.02124976E-002 58980.91 <-- SCF

5 -3.62600406E+004 5.07088175E-004 59007.92 <-- SCF

6 -3.62600273E+004 -3.31125484E-004 59033.94 <-- SCF

7 -3.62600238E+004 -8.92464062E-005 59058.47 <-- SCF

8 -3.62600233E+004 -1.28839599E-005 59080.67 <-- SCF

9 -3.62600233E+004 2.04966833E-006 59100.36 <-- SCF

10 -3.62600234E+004 1.42594162E-006 59118.05 <-- SCF

11 -3.62600234E+004 4.47712110E-007 59135.05 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02340897 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00236 0.04178 -0.05501 \*

\* Se 2 0.00358 -0.00476 0.02150 \*

\* Se 3 -0.01095 -0.01169 0.02379 \*

\* Se 4 0.01249 0.00847 -0.01264 \*

\* Se 5 0.04356 0.03884 -0.00047 \*

\* Se 6 0.03337 0.01948 -0.00126 \*

\* Se 7 0.00452 0.03832 -0.01139 \*

\* Se 8 -0.00912 -0.02089 0.01208 \*

\* Se 9 0.01087 -0.02510 0.01869 \*

\* Se 10 0.00440 -0.02784 -0.02305 \*

\* Se 11 -0.00694 0.02563 -0.00510 \*

\* Se 12 -0.01142 0.00704 0.00431 \*

\* Se 13 -0.00898 -0.01783 0.00166 \*

\* Se 14 0.00986 0.01841 -0.01485 \*

\* Se 15 -0.02925 -0.02586 0.00578 \*

\* Se 16 -0.02541 -0.03912 0.06099 \*

\* Se 17 -0.00208 -0.00050 -0.00822 \*

\* Se 18 -0.02116 0.00632 0.02143 \*

\* Se 19 -0.00552 -0.04434 0.03455 \*

\* Se 20 0.01209 -0.01100 0.00472 \*

\* Nb 1 -0.00142 -0.00422 -0.01559 \*

\* Nb 2 -0.00942 0.00361 0.00287 \*

\* Nb 3 0.00015 -0.00243 0.00335 \*

\* Nb 4 0.01943 -0.00106 -0.01160 \*

\* Nb 5 0.02879 -0.00173 0.00731 \*

\* Nb 6 0.00613 0.01856 -0.01701 \*

\* Nb 7 -0.01131 -0.00771 0.00549 \*

\* Nb 8 -0.00114 0.00726 0.00231 \*

\* Nb 9 -0.02430 0.00227 0.00174 \*

\* Nb 10 0.02021 0.01267 -0.00591 \*

\* Nb 11 0.01844 0.01842 -0.02353 \*

\* Nb 12 0.02165 0.01704 0.03511 \*

\* Nb 13 -0.03113 -0.00484 -0.01405 \*

\* Nb 14 0.01560 0.00368 -0.00189 \*

\* Nb 15 -0.01216 -0.02582 0.03076 \*

\* Nb 16 -0.02338 0.00233 -0.05014 \*

\* Nb 17 -0.01061 -0.01597 -0.00861 \*

\* Nb 18 -0.00295 -0.00085 -0.01020 \*

\* Nb 19 0.02048 0.00734 -0.00105 \*

\* Nb 20 -0.02933 -0.00390 -0.00686 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.077543 -0.015633 0.007003 \*

\* y -0.015633 -0.030442 -0.015209 \*

\* z 0.007003 -0.015209 -0.059981 \*

\* \*

\* Pressure: 0.0043 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000062 | -36260.022812 | <-- min BFGS

| trial step | 1.000000 | -0.000028 | -36260.023444 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 87 with enthalpy= -3.62600234E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.579702E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 7.678125E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 9.356573E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 7.754347E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 88 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000044 | -36260.023444 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 88 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8617925 -8.3022172 0.0075956 0.4204288 -0.0041990 -0.0001854

0.0337486 3.3791179 0.0001270 1.0329594 1.8490993 -0.0005090

0.0061615 0.0004016 13.9631721 -0.0002381 -0.0000145 0.4499828

Lattice parameters(A) Cell Angles

a = 17.023506 alpha = 89.995946

b = 3.379286 beta = 89.953167

c = 13.963174 gamma = 118.616738

Current cell volume = 705.139153 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066983 0.660581 0.121855 x

x Se 2 0.132005 0.339398 0.627840 x

x Se 3 0.132259 0.340892 0.871975 x

x Se 4 0.067419 0.661747 0.374130 x

x Se 5 0.268818 0.669025 0.124296 x

x Se 6 0.331532 0.340252 0.629597 x

x Se 7 0.333329 0.343862 0.871793 x

x Se 8 0.263393 0.656613 0.368480 x

x Se 9 0.466845 0.653624 0.128808 x

x Se 10 0.531473 0.339182 0.617683 x

x Se 11 0.533158 0.346373 0.871291 x

x Se 12 0.468479 0.660793 0.382499 x

x Se 13 0.666671 0.656106 0.128240 x

x Se 14 0.736591 0.343347 0.631652 x

x Se 15 0.731372 0.331769 0.875977 x

x Se 16 0.668261 0.659376 0.370441 x

x Se 17 0.867495 0.658549 0.128218 x

x Se 18 0.932717 0.337547 0.623834 x

x Se 19 0.933103 0.339688 0.878136 x

x Se 20 0.868068 0.661310 0.372438 x

x Nb 1 0.002395 0.001236 0.248234 x

x Nb 2 -0.002852 -0.002246 0.751239 x

x Nb 3 -0.000253 -0.000524 0.000088 x

x Nb 4 0.000941 0.001833 0.499719 x

x Nb 5 0.195693 -0.011089 0.245805 x

x Nb 6 0.199173 0.002810 0.750035 x

x Nb 7 0.200318 0.006242 -0.001895 x

x Nb 8 0.202069 0.008230 0.498904 x

x Nb 9 0.402156 -0.001125 0.253177 x

x Nb 10 0.403030 0.015246 0.750688 x

x Nb 11 0.402594 0.001148 -0.000531 x

x Nb 12 0.382890 -0.041427 0.500021 x

x Nb 13 0.597023 -0.015209 0.249653 x

x Nb 14 0.597756 0.000691 0.747004 x

x Nb 15 0.597387 -0.001306 0.000838 x

x Nb 16 0.616984 0.040960 0.500258 x

x Nb 17 0.800745 -0.002743 0.250309 x

x Nb 18 0.804889 0.012517 0.754113 x

x Nb 19 0.799875 -0.005270 0.002026 x

x Nb 20 0.797216 -0.010005 0.501134 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599629E+004 59238.08 <-- SCF

1 -3.62601728E+004 5.24838507E-003 59265.38 <-- SCF

2 -3.62601831E+004 2.57081029E-004 59293.39 <-- SCF

3 -3.62601619E+004 -5.31399291E-004 59319.89 <-- SCF

4 -3.62600238E+004 -3.45028964E-003 59345.55 <-- SCF

5 -3.62600275E+004 9.11492215E-005 59372.12 <-- SCF

6 -3.62600249E+004 -6.46424228E-005 59397.38 <-- SCF

7 -3.62600243E+004 -1.55457001E-005 59418.31 <-- SCF

8 -3.62600242E+004 -1.77486842E-006 59438.98 <-- SCF

9 -3.62600242E+004 1.30714272E-007 59456.55 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02421498 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00708 0.03322 -0.03288 \*

\* Se 2 -0.00135 0.00012 0.01646 \*

\* Se 3 -0.00993 -0.00488 0.01619 \*

\* Se 4 -0.00732 0.00925 -0.04362 \*

\* Se 5 0.04491 0.02570 0.00336 \*

\* Se 6 0.02177 0.01873 0.01112 \*

\* Se 7 -0.00294 0.02134 0.00360 \*

\* Se 8 -0.00119 -0.01396 0.01299 \*

\* Se 9 0.00200 -0.01577 0.01075 \*

\* Se 10 0.01000 -0.01882 -0.01204 \*

\* Se 11 -0.00120 0.01807 -0.00859 \*

\* Se 12 -0.01523 0.00397 0.00136 \*

\* Se 13 -0.00074 -0.01468 0.01231 \*

\* Se 14 0.00333 0.01273 -0.01412 \*

\* Se 15 -0.02973 -0.01642 0.00558 \*

\* Se 16 -0.01565 -0.03078 0.02020 \*

\* Se 17 -0.00235 -0.00516 -0.00375 \*

\* Se 18 -0.01558 0.00323 0.03502 \*

\* Se 19 -0.00692 -0.03505 0.01881 \*

\* Se 20 0.01381 -0.00801 -0.00069 \*

\* Nb 1 -0.01498 -0.00192 -0.02280 \*

\* Nb 2 0.00455 0.00117 0.01299 \*

\* Nb 3 -0.00099 -0.00249 0.00183 \*

\* Nb 4 0.02084 -0.00139 -0.00952 \*

\* Nb 5 0.03176 0.00052 -0.00269 \*

\* Nb 6 -0.00166 0.01007 -0.00933 \*

\* Nb 7 -0.00791 -0.00801 0.00792 \*

\* Nb 8 -0.01035 0.00943 0.00245 \*

\* Nb 9 -0.01880 0.00404 0.00353 \*

\* Nb 10 0.02438 0.01622 -0.00955 \*

\* Nb 11 0.01149 0.01410 -0.01539 \*

\* Nb 12 0.01348 0.01480 0.02239 \*

\* Nb 13 -0.02304 -0.00885 -0.00386 \*

\* Nb 14 0.01015 0.00035 -0.00399 \*

\* Nb 15 -0.00584 -0.01995 0.02123 \*

\* Nb 16 -0.01437 0.00107 -0.03078 \*

\* Nb 17 -0.00523 -0.00915 -0.00477 \*

\* Nb 18 -0.00859 -0.00282 -0.00213 \*

\* Nb 19 0.01842 0.00747 -0.00633 \*

\* Nb 20 -0.01609 -0.00745 -0.00324 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.021196 -0.000361 0.001176 \*

\* y -0.000361 -0.013462 -0.012052 \*

\* z 0.001176 -0.012052 -0.020361 \*

\* \*

\* Pressure: 0.0042 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000044 | -36260.023444 | <-- min BFGS

| trial step | 1.000000 | 0.000012 | -36260.024252 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 88 with enthalpy= -3.62600243E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.021533E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 5.185668E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.910790E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.119636E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 89 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000030 | -36260.024252 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 89 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8585563 -8.3030389 0.0068613 0.4205249 -0.0041904 -0.0001697

0.0336736 3.3793076 0.0001468 1.0332398 1.8490156 -0.0004784

0.0056396 0.0004622 13.9656036 -0.0002175 -0.0000174 0.4499044

Lattice parameters(A) Cell Angles

a = 17.021081 alpha = 89.995384

b = 3.379475 beta = 89.957631

c = 13.965605 gamma = 118.625770

Current cell volume = 705.140296 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066993 0.660807 0.121751 x

x Se 2 0.131986 0.339344 0.627916 x

x Se 3 0.132259 0.340857 0.872018 x

x Se 4 0.067496 0.662075 0.373998 x

x Se 5 0.268828 0.669138 0.124295 x

x Se 6 0.331530 0.340733 0.629605 x

x Se 7 0.333356 0.344178 0.871735 x

x Se 8 0.263367 0.656356 0.368532 x

x Se 9 0.466867 0.653357 0.128838 x

x Se 10 0.531477 0.339223 0.617662 x

x Se 11 0.533157 0.346682 0.871306 x

x Se 12 0.468470 0.660740 0.382492 x

x Se 13 0.666657 0.655989 0.128200 x

x Se 14 0.736611 0.343555 0.631599 x

x Se 15 0.731376 0.331727 0.876002 x

x Se 16 0.668269 0.658886 0.370542 x

x Se 17 0.867479 0.658504 0.128199 x

x Se 18 0.932666 0.337229 0.623900 x

x Se 19 0.933089 0.339459 0.878220 x

x Se 20 0.868087 0.661282 0.372409 x

x Nb 1 0.002419 0.001382 0.248172 x

x Nb 2 -0.002906 -0.002465 0.751270 x

x Nb 3 -0.000251 -0.000539 0.000102 x

x Nb 4 0.000969 0.001870 0.499715 x

x Nb 5 0.195753 -0.010978 0.245850 x

x Nb 6 0.199141 0.003059 0.750010 x

x Nb 7 0.200296 0.006186 -0.001903 x

x Nb 8 0.201956 0.008230 0.498961 x

x Nb 9 0.402129 -0.001477 0.253205 x

x Nb 10 0.403070 0.015558 0.750661 x

x Nb 11 0.402596 0.001175 -0.000550 x

x Nb 12 0.382885 -0.041367 0.500121 x

x Nb 13 0.596965 -0.015532 0.249661 x

x Nb 14 0.597769 0.001025 0.746973 x

x Nb 15 0.597393 -0.001348 0.000875 x

x Nb 16 0.616986 0.040968 0.500143 x

x Nb 17 0.800774 -0.002990 0.250316 x

x Nb 18 0.804852 0.012433 0.754078 x

x Nb 19 0.799903 -0.005209 0.002054 x

x Nb 20 0.797280 -0.010102 0.501066 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600007E+004 59560.08 <-- SCF

1 -3.62600557E+004 1.37342440E-003 59587.12 <-- SCF

2 -3.62600582E+004 6.21113607E-005 59615.02 <-- SCF

3 -3.62600504E+004 -1.94664087E-004 59641.48 <-- SCF

4 -3.62600243E+004 -6.51832961E-004 59667.11 <-- SCF

5 -3.62600253E+004 2.60362285E-005 59692.97 <-- SCF

6 -3.62600249E+004 -1.17819796E-005 59714.25 <-- SCF

7 -3.62600247E+004 -4.23664396E-006 59732.69 <-- SCF

8 -3.62600247E+004 -4.65170399E-007 59752.02 <-- SCF

9 -3.62600247E+004 2.45627485E-007 59768.17 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02469836 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00723 0.02143 -0.00508 \*

\* Se 2 -0.00271 0.01221 0.00238 \*

\* Se 3 -0.01187 -0.00033 0.00518 \*

\* Se 4 -0.03092 0.00359 -0.02168 \*

\* Se 5 0.04382 0.02201 0.00505 \*

\* Se 6 0.02036 -0.00287 0.01316 \*

\* Se 7 -0.01115 -0.00013 0.02218 \*

\* Se 8 0.00289 0.00537 0.01296 \*

\* Se 9 -0.01113 0.00057 0.00010 \*

\* Se 10 0.01570 -0.01790 -0.00698 \*

\* Se 11 0.00477 0.00419 -0.01373 \*

\* Se 12 -0.01904 0.00332 0.00522 \*

\* Se 13 0.00171 -0.01010 0.03545 \*

\* Se 14 0.00119 -0.00331 -0.01362 \*

\* Se 15 -0.02678 -0.01408 0.00448 \*

\* Se 16 -0.01732 -0.00616 -0.02273 \*

\* Se 17 -0.00079 -0.00907 0.00351 \*

\* Se 18 0.00498 0.01238 0.01547 \*

\* Se 19 -0.00562 -0.02419 -0.00227 \*

\* Se 20 0.01500 -0.01186 0.00252 \*

\* Nb 1 -0.01005 0.00006 -0.02407 \*

\* Nb 2 0.00274 -0.00126 0.01831 \*

\* Nb 3 -0.00337 -0.00193 -0.00171 \*

\* Nb 4 0.02158 -0.00152 -0.01161 \*

\* Nb 5 0.03071 0.00018 -0.01664 \*

\* Nb 6 0.00490 -0.00098 -0.00178 \*

\* Nb 7 -0.00193 -0.00600 0.00864 \*

\* Nb 8 -0.00404 0.00368 0.00214 \*

\* Nb 9 -0.01444 0.00593 0.00086 \*

\* Nb 10 0.01990 0.02162 -0.00858 \*

\* Nb 11 0.01363 0.01368 -0.01253 \*

\* Nb 12 0.01524 0.01998 0.01383 \*

\* Nb 13 -0.00807 -0.01403 -0.00017 \*

\* Nb 14 0.00756 -0.00237 -0.00010 \*

\* Nb 15 -0.00837 -0.01785 0.01683 \*

\* Nb 16 -0.01808 -0.00523 -0.01731 \*

\* Nb 17 -0.01575 -0.00062 -0.00516 \*

\* Nb 18 -0.00928 -0.00171 0.00768 \*

\* Nb 19 0.01621 0.00654 -0.01048 \*

\* Nb 20 -0.01941 -0.00326 0.00027 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.004370 -0.005463 -0.002211 \*

\* y -0.005463 0.007570 -0.007767 \*

\* z -0.002211 -0.007767 0.005638 \*

\* \*

\* Pressure: -0.0029 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000030 | -36260.024252 | <-- min BFGS

| trial step | 1.000000 | 5.929E-006 | -36260.024744 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 89 with enthalpy= -3.62600247E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.229564E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 4.929500E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.229364E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 7.767028E-003 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 90 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 7.212E-006 | -36260.024744 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 90 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8584259 -8.3025961 0.0065551 0.4205245 -0.0041979 -0.0001657

0.0337337 3.3792332 0.0002010 1.0332064 1.8490383 -0.0004924

0.0055100 0.0006402 13.9655263 -0.0002123 -0.0000246 0.4499069

Lattice parameters(A) Cell Angles

a = 17.020751 alpha = 89.993740

b = 3.379402 beta = 89.959482

c = 13.965527 gamma = 118.623650

Current cell volume = 705.121581 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067018 0.661017 0.121704 x

x Se 2 0.131975 0.339400 0.627971 x

x Se 3 0.132243 0.340889 0.871995 x

x Se 4 0.067533 0.662269 0.373989 x

x Se 5 0.268823 0.669132 0.124257 x

x Se 6 0.331534 0.341007 0.629633 x

x Se 7 0.333369 0.344341 0.871724 x

x Se 8 0.263369 0.656331 0.368588 x

x Se 9 0.466862 0.653200 0.128842 x

x Se 10 0.531530 0.339419 0.617684 x

x Se 11 0.533168 0.346853 0.871305 x

x Se 12 0.468421 0.660572 0.382470 x

x Se 13 0.666648 0.655854 0.128200 x

x Se 14 0.736609 0.343572 0.631546 x

x Se 15 0.731388 0.331755 0.876052 x

x Se 16 0.668265 0.658601 0.370527 x

x Se 17 0.867490 0.658447 0.128227 x

x Se 18 0.932627 0.337030 0.623894 x

x Se 19 0.933064 0.339262 0.878266 x

x Se 20 0.868097 0.661214 0.372362 x

x Nb 1 0.002505 0.001703 0.248154 x

x Nb 2 -0.003002 -0.002811 0.751278 x

x Nb 3 -0.000250 -0.000542 0.000104 x

x Nb 4 0.000978 0.001883 0.499714 x

x Nb 5 0.195767 -0.010951 0.245876 x

x Nb 6 0.199182 0.003349 0.749999 x

x Nb 7 0.200281 0.006205 -0.001928 x

x Nb 8 0.201911 0.008344 0.499024 x

x Nb 9 0.402085 -0.001697 0.253200 x

x Nb 10 0.403088 0.015849 0.750640 x

x Nb 11 0.402599 0.001236 -0.000550 x

x Nb 12 0.382969 -0.041159 0.500174 x

x Nb 13 0.596946 -0.015807 0.249676 x

x Nb 14 0.597807 0.001226 0.746975 x

x Nb 15 0.597393 -0.001409 0.000878 x

x Nb 16 0.616900 0.040778 0.500089 x

x Nb 17 0.800729 -0.003294 0.250328 x

x Nb 18 0.804845 0.012410 0.754051 x

x Nb 19 0.799922 -0.005226 0.002083 x

x Nb 20 0.797310 -0.010252 0.501000 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600103E+004 59872.08 <-- SCF

1 -3.62600431E+004 8.19549238E-004 59898.47 <-- SCF

2 -3.62600448E+004 4.28361614E-005 59925.27 <-- SCF

3 -3.62600364E+004 -2.12018223E-004 59952.08 <-- SCF

4 -3.62600251E+004 -2.82072608E-004 59977.94 <-- SCF

5 -3.62600252E+004 3.40637618E-006 60003.19 <-- SCF

6 -3.62600249E+004 -8.47102465E-006 60022.89 <-- SCF

7 -3.62600248E+004 -1.84047745E-006 60041.02 <-- SCF

8 -3.62600248E+004 -2.41460592E-007 60057.98 <-- SCF

9 -3.62600248E+004 3.14424910E-007 60074.17 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02479730 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00506 0.01194 0.00562 \*

\* Se 2 -0.00553 0.01564 -0.00380 \*

\* Se 3 -0.01022 -0.00079 0.00595 \*

\* Se 4 -0.03813 0.00168 -0.01859 \*

\* Se 5 0.04167 0.02102 0.00614 \*

\* Se 6 0.02447 -0.01295 0.00579 \*

\* Se 7 -0.01184 -0.00741 0.02695 \*

\* Se 8 0.00279 0.00996 0.01168 \*

\* Se 9 -0.01201 0.00702 0.00001 \*

\* Se 10 0.00036 -0.01966 -0.01173 \*

\* Se 11 0.00572 -0.00219 -0.01476 \*

\* Se 12 -0.00516 0.00436 0.01171 \*

\* Se 13 0.00105 -0.00389 0.03563 \*

\* Se 14 0.00177 -0.00764 -0.01132 \*

\* Se 15 -0.02472 -0.01383 0.00258 \*

\* Se 16 -0.02083 0.00346 -0.02201 \*

\* Se 17 -0.00203 -0.00686 0.00320 \*

\* Se 18 0.01365 0.01361 0.01104 \*

\* Se 19 -0.00521 -0.01576 -0.01221 \*

\* Se 20 0.01551 -0.01415 0.00973 \*

\* Nb 1 -0.01529 -0.00037 -0.02611 \*

\* Nb 2 0.00729 -0.00050 0.02034 \*

\* Nb 3 -0.00329 -0.00166 -0.00196 \*

\* Nb 4 0.02251 -0.00148 -0.01142 \*

\* Nb 5 0.03192 0.00110 -0.02020 \*

\* Nb 6 0.00403 -0.00456 0.00237 \*

\* Nb 7 0.00011 -0.00557 0.00899 \*

\* Nb 8 0.00187 0.00044 0.00046 \*

\* Nb 9 -0.01204 0.00655 -0.00118 \*

\* Nb 10 0.02088 0.01920 -0.00598 \*

\* Nb 11 0.01500 0.01304 -0.01356 \*

\* Nb 12 0.00877 0.02234 0.01105 \*

\* Nb 13 -0.00691 -0.01154 -0.00256 \*

\* Nb 14 0.00634 -0.00267 0.00214 \*

\* Nb 15 -0.00970 -0.01674 0.01746 \*

\* Nb 16 -0.01084 -0.00777 -0.01459 \*

\* Nb 17 -0.01380 0.00265 -0.00838 \*

\* Nb 18 -0.01142 -0.00233 0.01174 \*

\* Nb 19 0.01346 0.00671 -0.01126 \*

\* Nb 20 -0.02526 -0.00039 0.00104 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.006902 -0.002041 -0.001245 \*

\* y -0.002041 0.000835 -0.002251 \*

\* z -0.001245 -0.002251 -0.001670 \*

\* \*

\* Pressure: 0.0026 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 7.212E-006 | -36260.024744 | <-- min BFGS

| trial step | 1.000000 | 7.700E-007 | -36260.024842 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 90 with enthalpy= -3.62600248E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.452050E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 4.707186E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.489635E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 6.901631E-003 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 91 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.635E-006 | -36260.024842 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 91 with trial guess (lambda= 1.000000)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8579571 -8.3018696 0.0063462 0.4205270 -0.0042176 -0.0001649

0.0338917 3.3792104 0.0002712 1.0331291 1.8490033 -0.0005207

0.0054864 0.0008673 13.9657652 -0.0002112 -0.0000340 0.4498992

Lattice parameters(A) Cell Angles

a = 17.019987 alpha = 89.991619

b = 3.379380 beta = 89.960723

c = 13.965766 gamma = 118.619604

Current cell volume = 705.124741 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067022 0.661023 0.121708 x

x Se 2 0.131974 0.339406 0.627973 x

x Se 3 0.132243 0.340887 0.871991 x

x Se 4 0.067533 0.662270 0.373970 x

x Se 5 0.268819 0.669147 0.124265 x

x Se 6 0.331535 0.341023 0.629635 x

x Se 7 0.333375 0.344354 0.871725 x

x Se 8 0.263378 0.656381 0.368597 x

x Se 9 0.466861 0.653225 0.128845 x

x Se 10 0.531541 0.339424 0.617697 x

x Se 11 0.533169 0.346828 0.871299 x

x Se 12 0.468410 0.660571 0.382459 x

x Se 13 0.666642 0.655834 0.128205 x

x Se 14 0.736600 0.343522 0.631538 x

x Se 15 0.731395 0.331754 0.876045 x

x Se 16 0.668264 0.658582 0.370522 x

x Se 17 0.867489 0.658442 0.128232 x

x Se 18 0.932623 0.337026 0.623908 x

x Se 19 0.933061 0.339257 0.878262 x

x Se 20 0.868098 0.661212 0.372360 x

x Nb 1 0.002508 0.001739 0.248149 x

x Nb 2 -0.003007 -0.002853 0.751280 x

x Nb 3 -0.000250 -0.000544 0.000104 x

x Nb 4 0.000982 0.001892 0.499714 x

x Nb 5 0.195777 -0.010916 0.245881 x

x Nb 6 0.199186 0.003336 0.750003 x

x Nb 7 0.200279 0.006190 -0.001930 x

x Nb 8 0.201900 0.008351 0.499037 x

x Nb 9 0.402075 -0.001672 0.253199 x

x Nb 10 0.403096 0.015880 0.750631 x

x Nb 11 0.402600 0.001243 -0.000545 x

x Nb 12 0.383005 -0.041073 0.500183 x

x Nb 13 0.596941 -0.015823 0.249684 x

x Nb 14 0.597815 0.001194 0.746976 x

x Nb 15 0.597393 -0.001414 0.000875 x

x Nb 16 0.616864 0.040700 0.500081 x

x Nb 17 0.800723 -0.003289 0.250327 x

x Nb 18 0.804836 0.012376 0.754044 x

x Nb 19 0.799926 -0.005209 0.002085 x

x Nb 20 0.797316 -0.010274 0.500987 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600239E+004 60177.42 <-- SCF

1 -3.62600271E+004 8.00725133E-005 60204.16 <-- SCF

2 -3.62600272E+004 3.60025215E-006 60222.98 <-- SCF

3 -3.62600264E+004 -1.92269795E-005 60248.53 <-- SCF

4 -3.62600249E+004 -3.95900912E-005 60272.36 <-- SCF

5 -3.62600249E+004 1.34165265E-006 60291.89 <-- SCF

6 -3.62600249E+004 -1.27147874E-006 60308.72 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02485594 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00436 0.01168 0.00691 \*

\* Se 2 -0.00585 0.01550 -0.00569 \*

\* Se 3 -0.00959 -0.00004 0.00512 \*

\* Se 4 -0.03858 0.00170 -0.01207 \*

\* Se 5 0.04399 0.01905 0.00428 \*

\* Se 6 0.02371 -0.01347 0.00543 \*

\* Se 7 -0.01427 -0.00670 0.02876 \*

\* Se 8 -0.00245 0.00702 0.00865 \*

\* Se 9 -0.01267 0.00460 -0.00417 \*

\* Se 10 -0.00658 -0.01694 -0.01843 \*

\* Se 11 0.00492 0.00021 -0.01084 \*

\* Se 12 0.00064 0.00158 0.01867 \*

\* Se 13 0.00325 -0.00348 0.03128 \*

\* Se 14 0.00670 -0.00484 -0.00830 \*

\* Se 15 -0.02795 -0.01215 0.00328 \*

\* Se 16 -0.01984 0.00415 -0.02001 \*

\* Se 17 -0.00197 -0.00712 0.00358 \*

\* Se 18 0.01654 0.01434 0.00653 \*

\* Se 19 -0.00412 -0.01545 -0.01413 \*

\* Se 20 0.01596 -0.01432 0.01211 \*

\* Nb 1 -0.01356 0.00236 -0.02764 \*

\* Nb 2 0.00372 -0.00289 0.01986 \*

\* Nb 3 -0.00350 -0.00204 -0.00151 \*

\* Nb 4 0.02432 -0.00141 -0.01157 \*

\* Nb 5 0.03891 0.00235 -0.02033 \*

\* Nb 6 0.00604 -0.00739 0.00233 \*

\* Nb 7 0.00164 -0.00799 0.01045 \*

\* Nb 8 -0.00681 0.00067 0.00547 \*

\* Nb 9 -0.01478 0.01003 -0.00227 \*

\* Nb 10 0.02677 0.01935 -0.01020 \*

\* Nb 11 0.01915 0.01340 -0.00869 \*

\* Nb 12 0.02289 0.02228 0.01130 \*

\* Nb 13 -0.01109 -0.01177 0.00188 \*

\* Nb 14 0.00775 -0.00617 0.00162 \*

\* Nb 15 -0.01427 -0.01738 0.01443 \*

\* Nb 16 -0.02304 -0.00796 -0.01490 \*

\* Nb 17 -0.01829 0.00498 -0.00667 \*

\* Nb 18 -0.01644 -0.00361 0.01082 \*

\* Nb 19 0.01396 0.00838 -0.01156 \*

\* Nb 20 -0.01955 -0.00048 -0.00379 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.006308 0.006053 -0.001560 \*

\* y 0.006053 -0.002735 0.001896 \*

\* z -0.001560 0.001896 0.001749 \*

\* \*

\* Pressure: 0.0024 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.635E-006 | -36260.024842 | <-- min BFGS

| trial step | 1.000000 | 1.961E-006 | -36260.024894 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 91 with line minimization (lambda= -5.021955)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8607804 -8.3062444 0.0076039 0.4205122 -0.0040990 -0.0001696

0.0329406 3.3793480 -0.0001515 1.0335949 1.8492141 -0.0003504

0.0056288 -0.0004999 13.9643266 -0.0002178 0.0000223 0.4499455

Lattice parameters(A) Cell Angles

a = 17.024587 alpha = 90.004395

b = 3.379509 beta = 89.953249

c = 13.964328 gamma = 118.643971

Current cell volume = 705.105656 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066998 0.660983 0.121683 x

x Se 2 0.131980 0.339369 0.627963 x

x Se 3 0.132243 0.340899 0.872012 x

x Se 4 0.067531 0.662265 0.374086 x

x Se 5 0.268843 0.669057 0.124221 x

x Se 6 0.331531 0.340925 0.629623 x

x Se 7 0.333340 0.344275 0.871719 x

x Se 8 0.263321 0.656085 0.368540 x

x Se 9 0.466866 0.653075 0.128823 x

x Se 10 0.531472 0.339391 0.617621 x

x Se 11 0.533161 0.346975 0.871335 x

x Se 12 0.468476 0.660577 0.382523 x

x Se 13 0.666677 0.655954 0.128173 x

x Se 14 0.736657 0.343822 0.631587 x

x Se 15 0.731352 0.331761 0.876085 x

x Se 16 0.668270 0.658697 0.370554 x

x Se 17 0.867496 0.658475 0.128201 x

x Se 18 0.932649 0.337054 0.623821 x

x Se 19 0.933081 0.339286 0.878286 x

x Se 20 0.868092 0.661224 0.372368 x

x Nb 1 0.002491 0.001524 0.248180 x

x Nb 2 -0.002976 -0.002598 0.751266 x

x Nb 3 -0.000252 -0.000535 0.000104 x

x Nb 4 0.000959 0.001840 0.499718 x

x Nb 5 0.195716 -0.011128 0.245850 x

x Nb 6 0.199162 0.003417 0.749979 x

x Nb 7 0.200290 0.006281 -0.001919 x

x Nb 8 0.201968 0.008309 0.498958 x

x Nb 9 0.402133 -0.001821 0.253208 x

x Nb 10 0.403048 0.015692 0.750686 x

x Nb 11 0.402593 0.001204 -0.000574 x

x Nb 12 0.382787 -0.041592 0.500128 x

x Nb 13 0.596971 -0.015728 0.249638 x

x Nb 14 0.597767 0.001387 0.746972 x

x Nb 15 0.597394 -0.001385 0.000893 x

x Nb 16 0.617083 0.041171 0.500132 x

x Nb 17 0.800759 -0.003319 0.250334 x

x Nb 18 0.804889 0.012580 0.754083 x

x Nb 19 0.799904 -0.005307 0.002070 x

x Nb 20 0.797279 -0.010143 0.501067 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599865E+004 60412.06 <-- SCF

1 -3.62601944E+004 5.19551504E-003 60439.25 <-- SCF

2 -3.62602070E+004 3.14947507E-004 60466.25 <-- SCF

3 -3.62602029E+004 -1.00821490E-004 60492.78 <-- SCF

4 -3.62600186E+004 -4.60827874E-003 60518.86 <-- SCF

5 -3.62600292E+004 2.64591167E-004 60545.38 <-- SCF

6 -3.62600258E+004 -8.42565946E-005 60570.08 <-- SCF

7 -3.62600245E+004 -3.35879550E-005 60592.03 <-- SCF

8 -3.62600243E+004 -4.12046640E-006 60611.95 <-- SCF

9 -3.62600243E+004 9.42855706E-007 60629.67 <-- SCF

10 -3.62600244E+004 4.88326282E-007 60646.47 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02436046 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00452 0.01271 0.01669 \*

\* Se 2 -0.00777 0.01611 -0.00774 \*

\* Se 3 -0.00852 -0.00270 -0.00112 \*

\* Se 4 -0.04507 0.00199 -0.03701 \*

\* Se 5 0.02881 0.02867 0.01333 \*

\* Se 6 0.01828 -0.01232 0.00959 \*

\* Se 7 -0.01024 -0.01175 0.03054 \*

\* Se 8 0.00658 0.02095 0.00952 \*

\* Se 9 -0.01332 0.01494 0.00160 \*

\* Se 10 0.02271 -0.02846 0.00579 \*

\* Se 11 0.00425 -0.00932 -0.02061 \*

\* Se 12 -0.02845 0.01398 -0.00194 \*

\* Se 13 -0.00168 -0.00385 0.04627 \*

\* Se 14 -0.00216 -0.01731 -0.00761 \*

\* Se 15 -0.01039 -0.02034 -0.00641 \*

\* Se 16 -0.01375 0.00292 -0.03216 \*

\* Se 17 -0.00089 -0.00603 0.01054 \*

\* Se 18 0.01280 0.00892 0.02675 \*

\* Se 19 -0.00161 -0.01576 -0.02403 \*

\* Se 20 0.01947 -0.01273 0.01145 \*

\* Nb 1 -0.00345 0.00105 -0.02475 \*

\* Nb 2 -0.00416 -0.00209 0.01751 \*

\* Nb 3 -0.00304 -0.00144 -0.00080 \*

\* Nb 4 0.02409 -0.00100 -0.01139 \*

\* Nb 5 0.03186 -0.00396 -0.02124 \*

\* Nb 6 0.00325 -0.00641 0.00413 \*

\* Nb 7 0.00169 -0.00613 0.00384 \*

\* Nb 8 -0.00941 0.00184 0.00833 \*

\* Nb 9 -0.01444 0.00641 -0.00222 \*

\* Nb 10 0.02386 0.02358 -0.00954 \*

\* Nb 11 0.01933 0.01132 -0.00988 \*

\* Nb 12 0.02534 0.02038 0.01458 \*

\* Nb 13 -0.00697 -0.01354 -0.00114 \*

\* Nb 14 0.00901 -0.00319 0.00240 \*

\* Nb 15 -0.01454 -0.01439 0.01404 \*

\* Nb 16 -0.02697 -0.00586 -0.01591 \*

\* Nb 17 -0.01590 0.00524 -0.00878 \*

\* Nb 18 -0.01042 0.00298 0.01078 \*

\* Nb 19 0.01194 0.00671 -0.00711 \*

\* Nb 20 -0.01464 -0.00210 -0.00628 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.009293 -0.038924 0.000330 \*

\* y -0.038924 -0.003827 -0.025852 \*

\* z 0.000330 -0.025852 -0.028942 \*

\* \*

\* Pressure: 0.0140 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.635E-006 | -36260.024842 | <-- min BFGS

| trial step | 1.000000 | 1.961E-006 | -36260.024894 | <-- min BFGS

| line step | -5.021955 | 4.738E-006 | -36260.024408 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 91 with quad minimization (lambda= 3.760315)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8566630 -8.2998643 0.0057697 0.4205338 -0.0042720 -0.0001628

0.0343276 3.3791472 0.0004649 1.0329156 1.8489067 -0.0005987

0.0054211 0.0014940 13.9664246 -0.0002081 -0.0000598 0.4498780

Lattice parameters(A) Cell Angles

a = 17.017879 alpha = 89.985763

b = 3.379322 beta = 89.964149

c = 13.966426 gamma = 118.608432

Current cell volume = 705.133444 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067034 0.661042 0.121719 x

x Se 2 0.131972 0.339423 0.627978 x

x Se 3 0.132243 0.340882 0.871982 x

x Se 4 0.067534 0.662272 0.373916 x

x Se 5 0.268807 0.669188 0.124284 x

x Se 6 0.331537 0.341067 0.629641 x

x Se 7 0.333391 0.344390 0.871728 x

x Se 8 0.263405 0.656516 0.368623 x

x Se 9 0.466859 0.653294 0.128855 x

x Se 10 0.531573 0.339439 0.617732 x

x Se 11 0.533173 0.346761 0.871283 x

x Se 12 0.468380 0.660569 0.382430 x

x Se 13 0.666626 0.655779 0.128220 x

x Se 14 0.736573 0.343385 0.631516 x

x Se 15 0.731414 0.331750 0.876027 x

x Se 16 0.668262 0.658530 0.370507 x

x Se 17 0.867486 0.658426 0.128246 x

x Se 18 0.932612 0.337012 0.623948 x

x Se 19 0.933051 0.339244 0.878250 x

x Se 20 0.868102 0.661206 0.372357 x

x Nb 1 0.002516 0.001837 0.248135 x

x Nb 2 -0.003021 -0.002970 0.751287 x

x Nb 3 -0.000249 -0.000547 0.000105 x

x Nb 4 0.000992 0.001916 0.499712 x

x Nb 5 0.195804 -0.010819 0.245895 x

x Nb 6 0.199197 0.003298 0.750013 x

x Nb 7 0.200274 0.006148 -0.001934 x

x Nb 8 0.201868 0.008370 0.499073 x

x Nb 9 0.402049 -0.001604 0.253194 x

x Nb 10 0.403118 0.015966 0.750605 x

x Nb 11 0.402604 0.001260 -0.000532 x

x Nb 12 0.383105 -0.040836 0.500208 x

x Nb 13 0.596928 -0.015866 0.249705 x

x Nb 14 0.597838 0.001105 0.746978 x

x Nb 15 0.597393 -0.001427 0.000866 x

x Nb 16 0.616764 0.040484 0.500058 x

x Nb 17 0.800706 -0.003275 0.250323 x

x Nb 18 0.804812 0.012283 0.754027 x

x Nb 19 0.799936 -0.005164 0.002092 x

x Nb 20 0.797333 -0.010335 0.500950 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599506E+004 60750.00 <-- SCF

1 -3.62601554E+004 5.11894620E-003 60776.97 <-- SCF

2 -3.62601650E+004 2.39243369E-004 60805.11 <-- SCF

3 -3.62601159E+004 -1.22800723E-003 60832.02 <-- SCF

4 -3.62600266E+004 -2.23070503E-003 60857.73 <-- SCF

5 -3.62600278E+004 2.99217438E-005 60884.39 <-- SCF

6 -3.62600253E+004 -6.24005356E-005 60909.00 <-- SCF

7 -3.62600249E+004 -1.01123032E-005 60929.52 <-- SCF

8 -3.62600249E+004 -9.35515113E-007 60950.12 <-- SCF

9 -3.62600249E+004 -2.94459587E-007 60967.59 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02487025 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00323 0.01054 0.00508 \*

\* Se 2 -0.00752 0.01595 -0.00147 \*

\* Se 3 -0.01004 0.00016 0.00614 \*

\* Se 4 -0.03762 0.00147 -0.00328 \*

\* Se 5 0.04683 0.01452 0.00144 \*

\* Se 6 0.02567 -0.01352 0.00052 \*

\* Se 7 -0.01693 -0.00389 0.02682 \*

\* Se 8 -0.00575 0.00089 0.01228 \*

\* Se 9 -0.01359 0.00089 -0.00489 \*

\* Se 10 -0.01506 -0.01195 -0.02460 \*

\* Se 11 0.00587 0.00347 -0.00794 \*

\* Se 12 0.00859 -0.00361 0.02316 \*

\* Se 13 0.00637 -0.00428 0.02548 \*

\* Se 14 0.00925 0.00063 -0.01213 \*

\* Se 15 -0.03227 -0.00831 0.00658 \*

\* Se 16 -0.02308 0.00460 -0.01170 \*

\* Se 17 -0.00202 -0.00681 0.00282 \*

\* Se 18 0.02085 0.01677 -0.00208 \*

\* Se 19 -0.00323 -0.01475 -0.01231 \*

\* Se 20 0.01797 -0.01591 0.00925 \*

\* Nb 1 -0.01775 -0.00158 -0.02528 \*

\* Nb 2 0.00887 0.00099 0.01861 \*

\* Nb 3 -0.00307 -0.00188 -0.00183 \*

\* Nb 4 0.02139 -0.00097 -0.01089 \*

\* Nb 5 0.03091 0.00612 -0.01822 \*

\* Nb 6 0.00152 -0.00466 -0.00100 \*

\* Nb 7 0.00005 -0.00506 0.01223 \*

\* Nb 8 0.00846 -0.00245 -0.00516 \*

\* Nb 9 -0.01135 0.00596 0.00023 \*

\* Nb 10 0.01624 0.01536 -0.00101 \*

\* Nb 11 0.01599 0.01360 -0.01491 \*

\* Nb 12 -0.00903 0.02411 0.00822 \*

\* Nb 13 -0.00741 -0.00978 -0.00512 \*

\* Nb 14 0.00693 -0.00200 0.00146 \*

\* Nb 15 -0.01072 -0.01799 0.01748 \*

\* Nb 16 0.00766 -0.01138 -0.01240 \*

\* Nb 17 -0.00956 0.00308 -0.00507 \*

\* Nb 18 -0.00839 -0.00698 0.01110 \*

\* Nb 19 0.01310 0.00592 -0.01476 \*

\* Nb 20 -0.03137 0.00272 0.00715 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.014945 0.016347 -0.000251 \*

\* y 0.016347 -0.002243 0.014685 \*

\* z -0.000251 0.014685 0.012062 \*

\* \*

\* Pressure: -0.0083 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.635E-006 | -36260.024842 | <-- min BFGS

| trial step | 1.000000 | 1.961E-006 | -36260.024894 | <-- min BFGS

| line step | -5.021955 | 4.738E-006 | -36260.024408 | <-- min BFGS

| quad step | 3.760315 | -8.537E-007 | -36260.024902 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 91 with enthalpy= -3.62600249E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.502297E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 4.905402E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.092298E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.634725E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 92 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 4.536E-006 | -36260.024902 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 92 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8567204 -8.3005045 0.0060009 0.4205410 -0.0042559 -0.0001629

0.0341979 3.3791823 0.0003750 1.0330022 1.8489263 -0.0005604

0.0054236 0.0012030 13.9663220 -0.0002084 -0.0000478 0.4498813

Lattice parameters(A) Cell Angles

a = 17.018242 alpha = 89.988482

b = 3.379355 beta = 89.962780

c = 13.966323 gamma = 118.612426

Current cell volume = 705.123509 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067030 0.661038 0.121722 x

x Se 2 0.131971 0.339437 0.627974 x

x Se 3 0.132244 0.340902 0.871986 x

x Se 4 0.067513 0.662207 0.373926 x

x Se 5 0.268829 0.669212 0.124283 x

x Se 6 0.331535 0.341020 0.629647 x

x Se 7 0.333378 0.344346 0.871739 x

x Se 8 0.263389 0.656472 0.368606 x

x Se 9 0.466858 0.653270 0.128854 x

x Se 10 0.531561 0.339424 0.617710 x

x Se 11 0.533172 0.346785 0.871281 x

x Se 12 0.468387 0.660541 0.382450 x

x Se 13 0.666635 0.655805 0.128225 x

x Se 14 0.736591 0.343437 0.631531 x

x Se 15 0.731393 0.331729 0.876029 x

x Se 16 0.668264 0.658581 0.370502 x

x Se 17 0.867482 0.658398 0.128243 x

x Se 18 0.932628 0.337078 0.623938 x

x Se 19 0.933055 0.339243 0.878245 x

x Se 20 0.868105 0.661202 0.372362 x

x Nb 1 0.002504 0.001778 0.248129 x

x Nb 2 -0.003009 -0.002908 0.751294 x

x Nb 3 -0.000251 -0.000547 0.000103 x

x Nb 4 0.000995 0.001920 0.499708 x

x Nb 5 0.195807 -0.010830 0.245875 x

x Nb 6 0.199183 0.003256 0.750012 x

x Nb 7 0.200282 0.006184 -0.001926 x

x Nb 8 0.201871 0.008339 0.499051 x

x Nb 9 0.402063 -0.001621 0.253195 x

x Nb 10 0.403114 0.015964 0.750618 x

x Nb 11 0.402604 0.001236 -0.000538 x

x Nb 12 0.383036 -0.040978 0.500200 x

x Nb 13 0.596932 -0.015872 0.249691 x

x Nb 14 0.597825 0.001134 0.746979 x

x Nb 15 0.597393 -0.001402 0.000870 x

x Nb 16 0.616831 0.040623 0.500063 x

x Nb 17 0.800722 -0.003227 0.250319 x

x Nb 18 0.804815 0.012311 0.754047 x

x Nb 19 0.799930 -0.005185 0.002082 x

x Nb 20 0.797331 -0.010298 0.500972 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600222E+004 61071.20 <-- SCF

1 -3.62600301E+004 1.97083420E-004 61097.80 <-- SCF

2 -3.62600305E+004 9.73357765E-006 61119.08 <-- SCF

3 -3.62600287E+004 -4.46163910E-005 61145.66 <-- SCF

4 -3.62600250E+004 -9.41595047E-005 61170.50 <-- SCF

5 -3.62600251E+004 4.12720823E-006 61191.94 <-- SCF

6 -3.62600250E+004 -3.26359819E-006 61210.25 <-- SCF

7 -3.62600250E+004 -9.11809502E-007 61226.45 <-- SCF

8 -3.62600250E+004 3.22184992E-007 61244.23 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02496800 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00493 0.01037 0.00185 \*

\* Se 2 -0.00634 0.01370 -0.00128 \*

\* Se 3 -0.00912 -0.00164 0.00778 \*

\* Se 4 -0.03080 0.00161 -0.00660 \*

\* Se 5 0.04233 0.01808 0.00190 \*

\* Se 6 0.02368 -0.01050 0.00053 \*

\* Se 7 -0.01149 -0.00282 0.02206 \*

\* Se 8 -0.00241 0.00123 0.01425 \*

\* Se 9 -0.01238 0.00216 -0.00476 \*

\* Se 10 -0.00842 -0.01382 -0.01640 \*

\* Se 11 0.00596 0.00152 -0.00618 \*

\* Se 12 0.00314 0.00018 0.01584 \*

\* Se 13 0.00241 -0.00440 0.02318 \*

\* Se 14 0.00491 -0.00020 -0.01427 \*

\* Se 15 -0.02787 -0.01166 0.00692 \*

\* Se 16 -0.02127 0.00135 -0.01266 \*

\* Se 17 -0.00267 -0.00486 0.00107 \*

\* Se 18 0.01433 0.01515 0.00236 \*

\* Se 19 -0.00454 -0.01427 -0.00816 \*

\* Se 20 0.01578 -0.01358 0.00879 \*

\* Nb 1 -0.01924 -0.00226 -0.02477 \*

\* Nb 2 0.01056 0.00199 0.01852 \*

\* Nb 3 -0.00374 -0.00174 -0.00144 \*

\* Nb 4 0.02234 -0.00120 -0.01161 \*

\* Nb 5 0.03288 0.00499 -0.01957 \*

\* Nb 6 0.00269 -0.00284 0.00014 \*

\* Nb 7 0.00260 -0.00411 0.01250 \*

\* Nb 8 0.00394 -0.00293 -0.00501 \*

\* Nb 9 -0.01046 0.00483 -0.00287 \*

\* Nb 10 0.01730 0.01435 0.00007 \*

\* Nb 11 0.01666 0.01299 -0.01389 \*

\* Nb 12 -0.00031 0.02282 0.00964 \*

\* Nb 13 -0.00761 -0.00909 -0.00531 \*

\* Nb 14 0.00499 -0.00112 0.00413 \*

\* Nb 15 -0.01251 -0.01692 0.01799 \*

\* Nb 16 -0.00053 -0.01048 -0.01416 \*

\* Nb 17 -0.01118 0.00088 -0.00542 \*

\* Nb 18 -0.01085 -0.00590 0.01253 \*

\* Nb 19 0.01044 0.00492 -0.01377 \*

\* Nb 20 -0.02813 0.00323 0.00612 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.001288 0.012071 0.000081 \*

\* y 0.012071 -0.006586 0.008140 \*

\* z 0.000081 0.008140 0.002753 \*

\* \*

\* Pressure: 0.0008 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 4.536E-006 | -36260.024902 | <-- min BFGS

| trial step | 1.000000 | 2.966E-006 | -36260.024995 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 92 with line minimization (lambda= 2.888537)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8568288 -8.3017135 0.0064377 0.4205546 -0.0042255 -0.0001633

0.0339528 3.3792484 0.0002051 1.0331658 1.8489634 -0.0004881

0.0054283 0.0006535 13.9661282 -0.0002090 -0.0000252 0.4498875

Lattice parameters(A) Cell Angles

a = 17.018926 alpha = 89.993617

b = 3.379419 beta = 89.960194

c = 13.966129 gamma = 118.619967

Current cell volume = 705.104739 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067024 0.661030 0.121727 x

x Se 2 0.131970 0.339463 0.627967 x

x Se 3 0.132246 0.340939 0.871995 x

x Se 4 0.067473 0.662084 0.373944 x

x Se 5 0.268871 0.669257 0.124281 x

x Se 6 0.331532 0.340929 0.629660 x

x Se 7 0.333354 0.344264 0.871761 x

x Se 8 0.263359 0.656389 0.368574 x

x Se 9 0.466854 0.653223 0.128853 x

x Se 10 0.531539 0.339395 0.617669 x

x Se 11 0.533169 0.346832 0.871277 x

x Se 12 0.468400 0.660489 0.382487 x

x Se 13 0.666653 0.655853 0.128235 x

x Se 14 0.736624 0.343537 0.631560 x

x Se 15 0.731352 0.331688 0.876034 x

x Se 16 0.668270 0.658677 0.370494 x

x Se 17 0.867475 0.658343 0.128238 x

x Se 18 0.932660 0.337201 0.623918 x

x Se 19 0.933061 0.339239 0.878236 x

x Se 20 0.868112 0.661193 0.372373 x

x Nb 1 0.002483 0.001666 0.248119 x

x Nb 2 -0.002988 -0.002791 0.751308 x

x Nb 3 -0.000253 -0.000546 0.000101 x

x Nb 4 0.001002 0.001928 0.499702 x

x Nb 5 0.195812 -0.010853 0.245836 x

x Nb 6 0.199155 0.003175 0.750010 x

x Nb 7 0.200297 0.006251 -0.001910 x

x Nb 8 0.201875 0.008279 0.499010 x

x Nb 9 0.402089 -0.001652 0.253196 x

x Nb 10 0.403107 0.015960 0.750641 x

x Nb 11 0.402604 0.001189 -0.000548 x

x Nb 12 0.382906 -0.041246 0.500184 x

x Nb 13 0.596942 -0.015882 0.249667 x

x Nb 14 0.597800 0.001188 0.746981 x

x Nb 15 0.597393 -0.001355 0.000878 x

x Nb 16 0.616960 0.040887 0.500074 x

x Nb 17 0.800751 -0.003134 0.250310 x

x Nb 18 0.804820 0.012365 0.754084 x

x Nb 19 0.799919 -0.005224 0.002061 x

x Nb 20 0.797327 -0.010230 0.501014 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600152E+004 61347.42 <-- SCF

1 -3.62600482E+004 8.25493053E-004 61374.58 <-- SCF

2 -3.62600497E+004 3.70132169E-005 61399.14 <-- SCF

3 -3.62600454E+004 -1.07573127E-004 61425.81 <-- SCF

4 -3.62600250E+004 -5.09789815E-004 61450.98 <-- SCF

5 -3.62600257E+004 1.84508584E-005 61475.72 <-- SCF

6 -3.62600252E+004 -1.34590950E-005 61496.77 <-- SCF

7 -3.62600251E+004 -2.89717011E-006 61515.03 <-- SCF

8 -3.62600250E+004 -4.50834611E-007 61533.78 <-- SCF

9 -3.62600250E+004 7.80792368E-008 61549.67 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02504600 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00368 0.01001 0.00020 \*

\* Se 2 -0.00476 0.00964 -0.00098 \*

\* Se 3 -0.00825 -0.00481 0.00799 \*

\* Se 4 -0.02233 0.00187 -0.01262 \*

\* Se 5 0.03324 0.02339 0.00532 \*

\* Se 6 0.01887 -0.00655 0.00037 \*

\* Se 7 -0.00725 -0.00170 0.01297 \*

\* Se 8 -0.00184 0.00106 0.01320 \*

\* Se 9 -0.00997 0.00318 -0.00635 \*

\* Se 10 -0.00014 -0.01573 -0.00930 \*

\* Se 11 0.00500 -0.00051 -0.00223 \*

\* Se 12 -0.00320 0.00505 0.00956 \*

\* Se 13 0.00073 -0.00327 0.01975 \*

\* Se 14 0.00307 -0.00010 -0.01285 \*

\* Se 15 -0.01809 -0.01645 0.00342 \*

\* Se 16 -0.01659 -0.00278 -0.01371 \*

\* Se 17 -0.00275 -0.00126 -0.00017 \*

\* Se 18 0.00702 0.01235 0.01018 \*

\* Se 19 -0.00305 -0.01295 -0.00559 \*

\* Se 20 0.01286 -0.00899 0.00731 \*

\* Nb 1 -0.01534 -0.00140 -0.02087 \*

\* Nb 2 0.00694 0.00084 0.01306 \*

\* Nb 3 -0.00368 -0.00210 -0.00093 \*

\* Nb 4 0.02197 -0.00084 -0.00894 \*

\* Nb 5 0.02742 0.00401 -0.01421 \*

\* Nb 6 0.00183 -0.00003 -0.00090 \*

\* Nb 7 -0.00078 -0.00461 0.00940 \*

\* Nb 8 -0.00486 -0.00080 0.00250 \*

\* Nb 9 -0.01219 0.00505 0.00073 \*

\* Nb 10 0.01678 0.01310 -0.00256 \*

\* Nb 11 0.01780 0.01304 -0.01248 \*

\* Nb 12 0.01345 0.02037 0.01269 \*

\* Nb 13 -0.00891 -0.00744 -0.00069 \*

\* Nb 14 0.00672 -0.00275 -0.00032 \*

\* Nb 15 -0.01296 -0.01738 0.01650 \*

\* Nb 16 -0.01531 -0.00864 -0.01523 \*

\* Nb 17 -0.01013 -0.00240 -0.00082 \*

\* Nb 18 -0.00799 -0.00479 0.00712 \*

\* Nb 19 0.01249 0.00476 -0.01010 \*

\* Nb 20 -0.01949 0.00057 -0.00040 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.010678 0.003087 -0.000904 \*

\* y 0.003087 -0.005567 -0.003421 \*

\* z -0.000904 -0.003421 -0.002744 \*

\* \*

\* Pressure: 0.0063 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 4.536E-006 | -36260.024902 | <-- min BFGS

| trial step | 1.000000 | 2.966E-006 | -36260.024995 | <-- min BFGS

| line step | 2.888537 | 9.930E-008 | -36260.025078 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 92 with enthalpy= -3.62600251E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 4.386104E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 4.099197E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.994097E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.067758E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 93 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.551E-006 | -36260.025078 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 93 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8563394 -8.3018004 0.0062571 0.4205679 -0.0042263 -0.0001594

0.0339590 3.3792916 0.0002104 1.0331962 1.8489375 -0.0004808

0.0053002 0.0006697 13.9663921 -0.0002040 -0.0000260 0.4498790

Lattice parameters(A) Cell Angles

a = 17.018541 alpha = 89.993467

b = 3.379462 beta = 89.961294

c = 13.966393 gamma = 118.620930

Current cell volume = 705.104695 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067027 0.661096 0.121726 x

x Se 2 0.131967 0.339480 0.627972 x

x Se 3 0.132242 0.340917 0.872012 x

x Se 4 0.067452 0.662042 0.373908 x

x Se 5 0.268900 0.669391 0.124292 x

x Se 6 0.331540 0.340961 0.629663 x

x Se 7 0.333349 0.344252 0.871779 x

x Se 8 0.263355 0.656383 0.368588 x

x Se 9 0.466851 0.653201 0.128849 x

x Se 10 0.531539 0.339360 0.617660 x

x Se 11 0.533171 0.346862 0.871273 x

x Se 12 0.468397 0.660475 0.382493 x

x Se 13 0.666653 0.655841 0.128256 x

x Se 14 0.736630 0.343551 0.631546 x

x Se 15 0.731335 0.331608 0.876034 x

x Se 16 0.668264 0.658624 0.370490 x

x Se 17 0.867469 0.658313 0.128231 x

x Se 18 0.932668 0.337248 0.623941 x

x Se 19 0.933058 0.339164 0.878230 x

x Se 20 0.868122 0.661187 0.372378 x

x Nb 1 0.002467 0.001647 0.248090 x

x Nb 2 -0.002982 -0.002795 0.751328 x

x Nb 3 -0.000255 -0.000556 0.000101 x

x Nb 4 0.001020 0.001965 0.499692 x

x Nb 5 0.195848 -0.010754 0.245829 x

x Nb 6 0.199146 0.003159 0.750007 x

x Nb 7 0.200296 0.006227 -0.001896 x

x Nb 8 0.201851 0.008249 0.499012 x

x Nb 9 0.402079 -0.001671 0.253194 x

x Nb 10 0.403122 0.016039 0.750630 x

x Nb 11 0.402610 0.001231 -0.000559 x

x Nb 12 0.382921 -0.041134 0.500212 x

x Nb 13 0.596933 -0.015926 0.249670 x

x Nb 14 0.597806 0.001206 0.746984 x

x Nb 15 0.597391 -0.001399 0.000893 x

x Nb 16 0.616942 0.040812 0.500041 x

x Nb 17 0.800754 -0.003138 0.250306 x

x Nb 18 0.804801 0.012303 0.754086 x

x Nb 19 0.799929 -0.005174 0.002047 x

x Nb 20 0.797331 -0.010249 0.501012 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600234E+004 61653.47 <-- SCF

1 -3.62600296E+004 1.56508478E-004 61680.47 <-- SCF

2 -3.62600299E+004 7.86237913E-006 61700.75 <-- SCF

3 -3.62600281E+004 -4.62376052E-005 61727.30 <-- SCF

4 -3.62600251E+004 -7.35431828E-005 61752.19 <-- SCF

5 -3.62600253E+004 4.20660935E-006 61772.06 <-- SCF

6 -3.62600252E+004 -1.74983504E-006 61789.42 <-- SCF

7 -3.62600252E+004 -9.95198553E-007 61805.03 <-- SCF

8 -3.62600252E+004 7.16238247E-007 61823.28 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02522608 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00352 0.00485 0.00054 \*

\* Se 2 -0.00444 0.00824 0.00067 \*

\* Se 3 -0.00769 -0.00515 0.00673 \*

\* Se 4 -0.01467 0.00158 -0.00817 \*

\* Se 5 0.02741 0.02171 0.00731 \*

\* Se 6 0.01656 -0.00621 -0.00014 \*

\* Se 7 -0.00560 -0.00053 0.00622 \*

\* Se 8 -0.00093 0.00081 0.00933 \*

\* Se 9 -0.00961 0.00424 -0.00525 \*

\* Se 10 -0.00047 -0.01297 -0.00688 \*

\* Se 11 0.00553 -0.00267 0.00035 \*

\* Se 12 -0.00350 0.00536 0.00875 \*

\* Se 13 0.00117 -0.00228 0.00963 \*

\* Se 14 0.00154 -0.00054 -0.01000 \*

\* Se 15 -0.01394 -0.01668 0.00261 \*

\* Se 16 -0.01501 -0.00141 -0.01309 \*

\* Se 17 -0.00213 -0.00002 -0.00050 \*

\* Se 18 0.00520 0.01231 0.00755 \*

\* Se 19 -0.00293 -0.00776 -0.00253 \*

\* Se 20 0.01041 -0.00681 0.00378 \*

\* Nb 1 -0.01755 -0.00005 -0.02265 \*

\* Nb 2 0.00798 -0.00040 0.01481 \*

\* Nb 3 -0.00460 -0.00229 -0.00054 \*

\* Nb 4 0.02406 -0.00082 -0.00906 \*

\* Nb 5 0.02806 0.00489 -0.01546 \*

\* Nb 6 -0.00051 -0.00025 0.00123 \*

\* Nb 7 -0.00140 -0.00459 0.01086 \*

\* Nb 8 -0.00525 -0.00066 0.00293 \*

\* Nb 9 -0.01353 0.00509 0.00022 \*

\* Nb 10 0.01732 0.01221 -0.00102 \*

\* Nb 11 0.01700 0.01324 -0.00953 \*

\* Nb 12 0.01187 0.02030 0.01091 \*

\* Nb 13 -0.01046 -0.00774 -0.00001 \*

\* Nb 14 0.00681 -0.00358 0.00005 \*

\* Nb 15 -0.01322 -0.01808 0.01671 \*

\* Nb 16 -0.01292 -0.00911 -0.01391 \*

\* Nb 17 -0.00784 -0.00342 -0.00063 \*

\* Nb 18 -0.00851 -0.00536 0.00940 \*

\* Nb 19 0.01413 0.00432 -0.00922 \*

\* Nb 20 -0.02184 0.00023 -0.00201 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.011532 0.003960 -0.003241 \*

\* y 0.003960 -0.002029 -0.003660 \*

\* z -0.003241 -0.003660 0.003822 \*

\* \*

\* Pressure: 0.0032 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.551E-006 | -36260.025078 | <-- min BFGS

| trial step | 1.000000 | 5.793E-006 | -36260.025255 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 93 with line minimization (lambda= 8.637321)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8526018 -8.3024643 0.0048773 0.4206700 -0.0042328 -0.0001299

0.0340056 3.3796219 0.0002507 1.0334285 1.8487402 -0.0004248

0.0043216 0.0007936 13.9684078 -0.0001654 -0.0000317 0.4498140

Lattice parameters(A) Cell Angles

a = 17.015602 alpha = 89.992317

b = 3.379793 beta = 89.969692

c = 13.968408 gamma = 118.628287

Current cell volume = 705.104318 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067051 0.661606 0.121714 x

x Se 2 0.131945 0.339614 0.628010 x

x Se 3 0.132213 0.340747 0.872142 x

x Se 4 0.067291 0.661723 0.373636 x

x Se 5 0.269123 0.670414 0.124376 x

x Se 6 0.331603 0.341202 0.629684 x

x Se 7 0.333314 0.344161 0.871917 x

x Se 8 0.263324 0.656341 0.368693 x

x Se 9 0.466825 0.653033 0.128819 x

x Se 10 0.531544 0.339089 0.617585 x

x Se 11 0.533183 0.347091 0.871246 x

x Se 12 0.468372 0.660371 0.382534 x

x Se 13 0.666650 0.655753 0.128418 x

x Se 14 0.736674 0.343653 0.631440 x

x Se 15 0.731204 0.330999 0.876038 x

x Se 16 0.668217 0.658226 0.370458 x

x Se 17 0.867421 0.658086 0.128180 x

x Se 18 0.932728 0.337606 0.624116 x

x Se 19 0.933034 0.338589 0.878183 x

x Se 20 0.868198 0.661137 0.372419 x

x Nb 1 0.002349 0.001502 0.247870 x

x Nb 2 -0.002935 -0.002828 0.751484 x

x Nb 3 -0.000268 -0.000633 0.000102 x

x Nb 4 0.001158 0.002247 0.499617 x

x Nb 5 0.196124 -0.010002 0.245771 x

x Nb 6 0.199078 0.003033 0.749986 x

x Nb 7 0.200289 0.006046 -0.001788 x

x Nb 8 0.201662 0.008020 0.499030 x

x Nb 9 0.402000 -0.001815 0.253181 x

x Nb 10 0.403235 0.016642 0.750546 x

x Nb 11 0.402656 0.001548 -0.000645 x

x Nb 12 0.383036 -0.040275 0.500428 x

x Nb 13 0.596868 -0.016258 0.249694 x

x Nb 14 0.597846 0.001344 0.747003 x

x Nb 15 0.597379 -0.001736 0.001013 x

x Nb 16 0.616811 0.040239 0.499793 x

x Nb 17 0.800773 -0.003165 0.250276 x

x Nb 18 0.804655 0.011832 0.754098 x

x Nb 19 0.800008 -0.004788 0.001937 x

x Nb 20 0.797361 -0.010393 0.500998 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599193E+004 61926.91 <-- SCF

1 -3.62602344E+004 7.87829748E-003 61953.97 <-- SCF

2 -3.62602528E+004 4.58588505E-004 61982.33 <-- SCF

3 -3.62601610E+004 -2.29498100E-003 62009.09 <-- SCF

4 -3.62600261E+004 -3.37183666E-003 62035.27 <-- SCF

5 -3.62600302E+004 1.02367632E-004 62062.02 <-- SCF

6 -3.62600264E+004 -9.41049837E-005 62087.23 <-- SCF

7 -3.62600255E+004 -2.40939640E-005 62110.22 <-- SCF

8 -3.62600255E+004 5.98587529E-007 62130.62 <-- SCF

9 -3.62600255E+004 2.81524417E-007 62148.36 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02548970 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00706 -0.02955 0.00424 \*

\* Se 2 0.00093 0.00072 0.00631 \*

\* Se 3 0.00329 -0.00778 -0.00224 \*

\* Se 4 0.03285 0.00286 0.00191 \*

\* Se 5 -0.01087 0.00494 0.02125 \*

\* Se 6 -0.00497 0.00088 0.00338 \*

\* Se 7 0.00945 0.00998 -0.05506 \*

\* Se 8 0.00808 0.00022 0.00701 \*

\* Se 9 -0.00495 0.01207 0.00846 \*

\* Se 10 0.01261 0.00571 0.01718 \*

\* Se 11 0.01064 -0.01795 0.01072 \*

\* Se 12 -0.01052 0.00945 -0.00451 \*

\* Se 13 0.00219 0.00351 -0.05261 \*

\* Se 14 -0.01713 -0.00495 -0.00425 \*

\* Se 15 0.00931 -0.02013 -0.00692 \*

\* Se 16 -0.00213 0.00585 -0.01300 \*

\* Se 17 -0.00832 0.00784 -0.00040 \*

\* Se 18 -0.01099 0.01332 -0.02184 \*

\* Se 19 -0.00544 0.02667 0.01294 \*

\* Se 20 -0.00832 0.00741 -0.01167 \*

\* Nb 1 -0.01878 0.00498 -0.00505 \*

\* Nb 2 0.01032 -0.00355 -0.00152 \*

\* Nb 3 -0.00695 -0.00252 -0.00293 \*

\* Nb 4 0.01631 0.00136 0.00504 \*

\* Nb 5 0.00503 0.01096 -0.00226 \*

\* Nb 6 0.00533 -0.00218 0.01284 \*

\* Nb 7 -0.00072 0.00294 0.00834 \*

\* Nb 8 0.00877 -0.00512 0.00461 \*

\* Nb 9 0.00239 0.00085 0.01793 \*

\* Nb 10 0.00472 0.00170 0.01722 \*

\* Nb 11 0.01844 0.00850 -0.00115 \*

\* Nb 12 -0.01216 0.01010 -0.01926 \*

\* Nb 13 -0.01344 -0.00804 0.00932 \*

\* Nb 14 -0.00237 -0.00413 -0.01535 \*

\* Nb 15 -0.01225 -0.01323 0.00825 \*

\* Nb 16 0.00594 -0.01319 0.01791 \*

\* Nb 17 0.00111 -0.00922 0.01687 \*

\* Nb 18 -0.00395 -0.00798 0.00808 \*

\* Nb 19 0.00602 -0.00555 0.00197 \*

\* Nb 20 -0.02652 0.00223 -0.00177 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.026450 0.009979 -0.001011 \*

\* y 0.009979 0.022891 0.000945 \*

\* z -0.001011 0.000945 0.043867 \*

\* \*

\* Pressure: -0.0134 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.551E-006 | -36260.025078 | <-- min BFGS

| trial step | 1.000000 | 5.793E-006 | -36260.025255 | <-- min BFGS

| line step | 8.637321 | -2.836E-006 | -36260.025518 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 93 with enthalpy= -3.62600255E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.102224E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 5.674473E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 5.106660E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.386663E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 94 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000016 | -36260.025518 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 94 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8578143 -8.3031176 0.0055556 0.4205474 -0.0041877 -0.0001455

0.0336504 3.3792984 0.0002494 1.0333076 1.8490271 -0.0004627

0.0048382 0.0007912 13.9656142 -0.0001857 -0.0000314 0.4499040

Lattice parameters(A) Cell Angles

a = 17.020471 alpha = 89.992328

b = 3.379466 beta = 89.965555

c = 13.965615 gamma = 118.627612

Current cell volume = 705.101289 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067043 0.661423 0.121699 x

x Se 2 0.131944 0.339491 0.627990 x

x Se 3 0.132199 0.340637 0.872102 x

x Se 4 0.067379 0.661899 0.373672 x

x Se 5 0.269052 0.670360 0.124370 x

x Se 6 0.331635 0.341200 0.629659 x

x Se 7 0.333347 0.344239 0.871874 x

x Se 8 0.263361 0.656428 0.368664 x

x Se 9 0.466811 0.653116 0.128838 x

x Se 10 0.531525 0.338948 0.617597 x

x Se 11 0.533202 0.346983 0.871243 x

x Se 12 0.468401 0.660649 0.382531 x

x Se 13 0.666629 0.655743 0.128383 x

x Se 14 0.736630 0.343536 0.631472 x

x Se 15 0.731260 0.330987 0.876023 x

x Se 16 0.668180 0.658234 0.370471 x

x Se 17 0.867454 0.658283 0.128204 x

x Se 18 0.932675 0.337459 0.624100 x

x Se 19 0.933039 0.338773 0.878210 x

x Se 20 0.868183 0.661228 0.372422 x

x Nb 1 0.002357 0.001394 0.247925 x

x Nb 2 -0.002925 -0.002698 0.751435 x

x Nb 3 -0.000266 -0.000638 0.000102 x

x Nb 4 0.001128 0.002207 0.499634 x

x Nb 5 0.196021 -0.010263 0.245793 x

x Nb 6 0.199131 0.003156 0.749994 x

x Nb 7 0.200272 0.005952 -0.001844 x

x Nb 8 0.201802 0.008253 0.499057 x

x Nb 9 0.402018 -0.001630 0.253229 x

x Nb 10 0.403235 0.016597 0.750557 x

x Nb 11 0.402681 0.001680 -0.000633 x

x Nb 12 0.383042 -0.040410 0.500327 x

x Nb 13 0.596857 -0.016217 0.249696 x

x Nb 14 0.597833 0.001141 0.746952 x

x Nb 15 0.597348 -0.001879 0.001004 x

x Nb 16 0.616813 0.040374 0.499905 x

x Nb 17 0.800724 -0.003282 0.250291 x

x Nb 18 0.804721 0.012005 0.754083 x

x Nb 19 0.800010 -0.004769 0.002001 x

x Nb 20 0.797246 -0.010587 0.500973 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600033E+004 62251.91 <-- SCF

1 -3.62600813E+004 1.94894513E-003 62279.28 <-- SCF

2 -3.62600853E+004 9.98821159E-005 62306.50 <-- SCF

3 -3.62600871E+004 4.52383952E-005 62333.27 <-- SCF

4 -3.62600242E+004 -1.57269332E-003 62359.03 <-- SCF

5 -3.62600270E+004 7.03684419E-005 62385.09 <-- SCF

6 -3.62600260E+004 -2.42020722E-005 62408.78 <-- SCF

7 -3.62600258E+004 -6.75254378E-006 62428.00 <-- SCF

8 -3.62600257E+004 -2.34244269E-006 62447.91 <-- SCF

9 -3.62600257E+004 4.30247170E-007 62464.92 <-- SCF

10 -3.62600257E+004 2.65231788E-007 62481.03 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02570502 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00819 -0.01638 0.00790 \*

\* Se 2 0.00560 0.00527 0.00300 \*

\* Se 3 0.00700 -0.00187 -0.00012 \*

\* Se 4 0.01162 0.00307 0.01044 \*

\* Se 5 0.00993 -0.00294 0.01336 \*

\* Se 6 -0.00695 0.00375 0.00683 \*

\* Se 7 0.00066 0.00918 -0.03772 \*

\* Se 8 0.00019 0.00154 0.01105 \*

\* Se 9 -0.00401 0.00918 0.00588 \*

\* Se 10 0.01323 0.01010 0.01260 \*

\* Se 11 0.00727 -0.01154 0.00489 \*

\* Se 12 -0.01260 -0.00150 -0.00282 \*

\* Se 13 0.00718 0.00012 -0.03983 \*

\* Se 14 -0.00671 -0.00484 -0.00718 \*

\* Se 15 -0.01135 -0.01100 -0.00073 \*

\* Se 16 0.00231 0.00312 -0.01143 \*

\* Se 17 -0.01160 -0.00068 -0.00056 \*

\* Se 18 0.00038 0.01423 -0.02341 \*

\* Se 19 -0.00697 0.01358 0.00428 \*

\* Se 20 -0.00833 0.00179 -0.00440 \*

\* Nb 1 -0.01819 0.00413 -0.00791 \*

\* Nb 2 0.00806 -0.00189 0.00272 \*

\* Nb 3 -0.00761 -0.00224 -0.00270 \*

\* Nb 4 0.02242 0.00054 0.00038 \*

\* Nb 5 0.01736 0.01104 -0.00698 \*

\* Nb 6 0.00220 -0.00407 0.00706 \*

\* Nb 7 0.00225 0.00365 0.01171 \*

\* Nb 8 -0.00641 -0.00322 0.00225 \*

\* Nb 9 -0.00539 0.00137 0.00569 \*

\* Nb 10 0.00753 0.00064 0.01221 \*

\* Nb 11 0.01587 0.00771 -0.00251 \*

\* Nb 12 -0.00054 0.01042 -0.00699 \*

\* Nb 13 -0.01032 -0.00772 0.00734 \*

\* Nb 14 -0.00153 -0.00329 -0.00539 \*

\* Nb 15 -0.01167 -0.01227 0.00800 \*

\* Nb 16 -0.00270 -0.01201 0.00446 \*

\* Nb 17 0.00088 -0.00493 0.01280 \*

\* Nb 18 -0.00764 -0.00872 0.01099 \*

\* Nb 19 0.00634 -0.00440 -0.00555 \*

\* Nb 20 -0.01593 0.00109 0.00040 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.004452 -0.002250 0.000627 \*

\* y -0.002250 0.000785 -0.000758 \*

\* z 0.000627 -0.000758 0.006521 \*

\* \*

\* Pressure: -0.0010 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000016 | -36260.025518 | <-- min BFGS

| trial step | 1.000000 | 1.146E-006 | -36260.025746 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 94 with enthalpy= -3.62600257E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 5.676528E-006 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 4.047030E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.151396E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 6.521301E-003 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 95 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.489E-006 | -36260.025746 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 95 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8585391 -8.3028186 0.0054699 0.4205231 -0.0041946 -0.0001457

0.0337074 3.3792785 0.0002869 1.0332168 1.8490214 -0.0004793

0.0048460 0.0009120 13.9648271 -0.0001859 -0.0000363 0.4499294

Lattice parameters(A) Cell Angles

a = 17.020958 alpha = 89.991196

b = 3.379447 beta = 89.966056

c = 13.964828 gamma = 118.624573

Current cell volume = 705.098096 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067048 0.661406 0.121703 x

x Se 2 0.131943 0.339503 0.627977 x

x Se 3 0.132203 0.340626 0.872107 x

x Se 4 0.067384 0.661912 0.373646 x

x Se 5 0.269057 0.670413 0.124384 x

x Se 6 0.331635 0.341224 0.629659 x

x Se 7 0.333341 0.344195 0.871871 x

x Se 8 0.263382 0.656482 0.368674 x

x Se 9 0.466809 0.653165 0.128845 x

x Se 10 0.531531 0.338878 0.617595 x

x Se 11 0.533205 0.346933 0.871234 x

x Se 12 0.468395 0.660733 0.382541 x

x Se 13 0.666635 0.655777 0.128386 x

x Se 14 0.736609 0.343477 0.631465 x

x Se 15 0.731261 0.330956 0.876010 x

x Se 16 0.668181 0.658195 0.370465 x

x Se 17 0.867448 0.658284 0.128202 x

x Se 18 0.932668 0.337452 0.624116 x

x Se 19 0.933035 0.338795 0.878208 x

x Se 20 0.868185 0.661230 0.372435 x

x Nb 1 0.002338 0.001336 0.247912 x

x Nb 2 -0.002909 -0.002656 0.751441 x

x Nb 3 -0.000268 -0.000651 0.000102 x

x Nb 4 0.001138 0.002232 0.499631 x

x Nb 5 0.196029 -0.010225 0.245787 x

x Nb 6 0.199131 0.003093 0.750005 x

x Nb 7 0.200270 0.005920 -0.001845 x

x Nb 8 0.201800 0.008250 0.499065 x

x Nb 9 0.402011 -0.001580 0.253234 x

x Nb 10 0.403250 0.016631 0.750554 x

x Nb 11 0.402689 0.001714 -0.000627 x

x Nb 12 0.383051 -0.040388 0.500321 x

x Nb 13 0.596845 -0.016223 0.249696 x

x Nb 14 0.597836 0.001073 0.746945 x

x Nb 15 0.597342 -0.001915 0.001004 x

x Nb 16 0.616803 0.040371 0.499911 x

x Nb 17 0.800721 -0.003239 0.250286 x

x Nb 18 0.804716 0.011973 0.754085 x

x Nb 19 0.800016 -0.004733 0.002005 x

x Nb 20 0.797235 -0.010619 0.500965 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600247E+004 62584.95 <-- SCF

1 -3.62600326E+004 1.96395687E-004 62612.09 <-- SCF

2 -3.62600330E+004 1.16441811E-005 62632.66 <-- SCF

3 -3.62600348E+004 4.38333672E-005 62659.17 <-- SCF

4 -3.62600254E+004 -2.34573221E-004 62684.39 <-- SCF

5 -3.62600258E+004 1.09463015E-005 62706.83 <-- SCF

6 -3.62600258E+004 -2.11694944E-006 62724.83 <-- SCF

7 -3.62600257E+004 -1.20608997E-006 62742.58 <-- SCF

8 -3.62600257E+004 -4.42596418E-008 62759.47 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02571399 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00720 -0.01480 0.00654 \*

\* Se 2 0.00745 0.00243 0.00602 \*

\* Se 3 0.00602 -0.00121 0.00107 \*

\* Se 4 0.01050 0.00330 0.01082 \*

\* Se 5 0.01159 -0.00573 0.01156 \*

\* Se 6 -0.00688 0.00237 0.00754 \*

\* Se 7 0.00441 0.01239 -0.03576 \*

\* Se 8 -0.00509 0.00143 0.00797 \*

\* Se 9 -0.00417 0.00669 0.00391 \*

\* Se 10 0.01051 0.01603 0.01340 \*

\* Se 11 0.00760 -0.00904 0.00798 \*

\* Se 12 -0.00928 -0.00863 -0.00666 \*

\* Se 13 0.00358 -0.00185 -0.04196 \*

\* Se 14 -0.00172 -0.00463 -0.00434 \*

\* Se 15 -0.01473 -0.00947 0.00093 \*

\* Se 16 0.00116 0.00606 -0.01023 \*

\* Se 17 -0.01134 -0.00166 -0.00069 \*

\* Se 18 0.00202 0.01469 -0.02654 \*

\* Se 19 -0.00646 0.01152 0.00529 \*

\* Se 20 -0.00898 0.00346 -0.00669 \*

\* Nb 1 -0.01842 0.00475 -0.00927 \*

\* Nb 2 0.00771 -0.00188 0.00407 \*

\* Nb 3 -0.00777 -0.00219 -0.00224 \*

\* Nb 4 0.02291 0.00066 0.00046 \*

\* Nb 5 0.02267 0.01148 -0.00553 \*

\* Nb 6 0.00436 -0.00363 0.00559 \*

\* Nb 7 0.00367 0.00376 0.01329 \*

\* Nb 8 -0.00250 -0.00304 0.00219 \*

\* Nb 9 -0.00332 0.00233 0.00590 \*

\* Nb 10 0.00854 -0.00028 0.01299 \*

\* Nb 11 0.01812 0.00786 -0.00343 \*

\* Nb 12 0.00059 0.01157 -0.00650 \*

\* Nb 13 -0.01190 -0.00758 0.00738 \*

\* Nb 14 -0.00304 -0.00397 -0.00545 \*

\* Nb 15 -0.01317 -0.01250 0.00902 \*

\* Nb 16 -0.00408 -0.01322 0.00381 \*

\* Nb 17 -0.00128 -0.00503 0.01387 \*

\* Nb 18 -0.01210 -0.00933 0.01029 \*

\* Nb 19 0.00525 -0.00406 -0.00674 \*

\* Nb 20 -0.01963 0.00096 0.00014 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.001519 -0.001853 0.000845 \*

\* y -0.001853 -0.000543 0.001204 \*

\* z 0.000845 0.001204 -0.002049 \*

\* \*

\* Pressure: 0.0014 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.489E-006 | -36260.025746 | <-- min BFGS

| trial step | 1.000000 | 8.527E-007 | -36260.025758 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 95 with line minimization (lambda= 2.340122)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8595105 -8.3024179 0.0053552 0.4204906 -0.0042038 -0.0001459

0.0337838 3.3792518 0.0003372 1.0330952 1.8490139 -0.0005015

0.0048564 0.0010739 13.9637724 -0.0001862 -0.0000430 0.4499634

Lattice parameters(A) Cell Angles

a = 17.021611 alpha = 89.989678

b = 3.379421 beta = 89.966728

c = 13.963773 gamma = 118.620501

Current cell volume = 705.093810 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067054 0.661384 0.121709 x

x Se 2 0.131942 0.339518 0.627959 x

x Se 3 0.132209 0.340612 0.872112 x

x Se 4 0.067392 0.661929 0.373610 x

x Se 5 0.269064 0.670484 0.124403 x

x Se 6 0.331635 0.341255 0.629659 x

x Se 7 0.333333 0.344136 0.871867 x

x Se 8 0.263410 0.656555 0.368689 x

x Se 9 0.466806 0.653231 0.128854 x

x Se 10 0.531538 0.338785 0.617593 x

x Se 11 0.533208 0.346865 0.871221 x

x Se 12 0.468387 0.660845 0.382554 x

x Se 13 0.666643 0.655824 0.128390 x

x Se 14 0.736581 0.343398 0.631456 x

x Se 15 0.731262 0.330914 0.875992 x

x Se 16 0.668183 0.658142 0.370458 x

x Se 17 0.867439 0.658285 0.128199 x

x Se 18 0.932657 0.337443 0.624138 x

x Se 19 0.933029 0.338823 0.878204 x

x Se 20 0.868186 0.661233 0.372454 x

x Nb 1 0.002312 0.001257 0.247894 x

x Nb 2 -0.002889 -0.002600 0.751449 x

x Nb 3 -0.000271 -0.000668 0.000103 x

x Nb 4 0.001151 0.002267 0.499626 x

x Nb 5 0.196039 -0.010173 0.245778 x

x Nb 6 0.199130 0.003009 0.750020 x

x Nb 7 0.200268 0.005877 -0.001845 x

x Nb 8 0.201799 0.008244 0.499076 x

x Nb 9 0.402002 -0.001513 0.253240 x

x Nb 10 0.403270 0.016677 0.750551 x

x Nb 11 0.402701 0.001760 -0.000619 x

x Nb 12 0.383064 -0.040358 0.500312 x

x Nb 13 0.596830 -0.016231 0.249697 x

x Nb 14 0.597840 0.000982 0.746937 x

x Nb 15 0.597333 -0.001962 0.001004 x

x Nb 16 0.616790 0.040367 0.499919 x

x Nb 17 0.800717 -0.003181 0.250281 x

x Nb 18 0.804711 0.011930 0.754088 x

x Nb 19 0.800023 -0.004685 0.002010 x

x Nb 20 0.797221 -0.010661 0.500955 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600242E+004 62862.73 <-- SCF

1 -3.62600285E+004 1.07151225E-004 62889.31 <-- SCF

2 -3.62600287E+004 5.68329847E-006 62908.81 <-- SCF

3 -3.62600279E+004 -2.10047896E-005 62935.11 <-- SCF

4 -3.62600257E+004 -5.38212596E-005 62959.23 <-- SCF

5 -3.62600258E+004 2.57927808E-006 62979.17 <-- SCF

6 -3.62600258E+004 -1.24777406E-006 62996.48 <-- SCF

7 -3.62600257E+004 -6.15082014E-007 63012.59 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02573862 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00296 -0.01257 0.00549 \*

\* Se 2 0.00567 -0.00080 0.01046 \*

\* Se 3 0.00216 -0.00024 -0.00038 \*

\* Se 4 0.00538 0.00306 0.01482 \*

\* Se 5 0.00904 -0.01014 0.00838 \*

\* Se 6 -0.00972 0.00042 0.00905 \*

\* Se 7 0.00574 0.01659 -0.03335 \*

\* Se 8 -0.01771 0.00175 0.00344 \*

\* Se 9 -0.00282 0.00237 -0.00180 \*

\* Se 10 0.00764 0.02556 0.01436 \*

\* Se 11 0.00674 -0.00452 0.01475 \*

\* Se 12 -0.00609 -0.02037 -0.01154 \*

\* Se 13 0.00181 -0.00431 -0.04513 \*

\* Se 14 0.01126 -0.00440 -0.00049 \*

\* Se 15 -0.01474 -0.00694 0.00342 \*

\* Se 16 0.00319 0.01026 -0.00835 \*

\* Se 17 -0.00787 -0.00287 0.00103 \*

\* Se 18 0.00853 0.01554 -0.03154 \*

\* Se 19 -0.00272 0.00875 0.00516 \*

\* Se 20 -0.00633 0.00511 -0.01064 \*

\* Nb 1 -0.01997 0.00521 -0.00900 \*

\* Nb 2 0.00862 -0.00172 0.00345 \*

\* Nb 3 -0.00884 -0.00210 -0.00189 \*

\* Nb 4 0.02604 0.00070 0.00089 \*

\* Nb 5 0.02366 0.01209 -0.00563 \*

\* Nb 6 -0.00502 -0.00254 0.00484 \*

\* Nb 7 -0.00121 0.00418 0.01406 \*

\* Nb 8 -0.00917 -0.00293 0.00373 \*

\* Nb 9 -0.00899 0.00347 0.00670 \*

\* Nb 10 0.00700 -0.00162 0.01272 \*

\* Nb 11 0.01897 0.00866 -0.00141 \*

\* Nb 12 -0.00035 0.01305 -0.00756 \*

\* Nb 13 -0.00868 -0.00634 0.00714 \*

\* Nb 14 0.00155 -0.00511 -0.00704 \*

\* Nb 15 -0.01398 -0.01389 0.00956 \*

\* Nb 16 -0.00214 -0.01424 0.00526 \*

\* Nb 17 0.00752 -0.00562 0.01430 \*

\* Nb 18 -0.01139 -0.00991 0.01053 \*

\* Nb 19 0.01160 -0.00439 -0.00697 \*

\* Nb 20 -0.01736 0.00084 -0.00084 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.009194 -0.002796 0.000801 \*

\* y -0.002796 -0.003298 0.005962 \*

\* z 0.000801 0.005962 -0.014319 \*

\* \*

\* Pressure: 0.0028 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.489E-006 | -36260.025746 | <-- min BFGS

| trial step | 1.000000 | 8.527E-007 | -36260.025758 | <-- min BFGS

| line step | 2.340122 | -4.548E-007 | -36260.025776 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 95 with enthalpy= -3.62600258E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.522371E-007 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 4.537370E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 8.801689E-004 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.431898E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 96 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.688E-006 | -36260.025776 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 96 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8590050 -8.3022130 0.0053522 0.4205019 -0.0042093 -0.0001441

0.0338269 3.3792419 0.0003068 1.0331005 1.8490061 -0.0004839

0.0047953 0.0009750 13.9641698 -0.0001839 -0.0000390 0.4499506

Lattice parameters(A) Cell Angles

a = 17.021069 alpha = 89.990602

b = 3.379411 beta = 89.966759

c = 13.964171 gamma = 118.619996

Current cell volume = 705.092865 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067056 0.661398 0.121708 x

x Se 2 0.131933 0.339498 0.627966 x

x Se 3 0.132202 0.340595 0.872120 x

x Se 4 0.067377 0.661889 0.373582 x

x Se 5 0.269077 0.670507 0.124410 x

x Se 6 0.331624 0.341231 0.629667 x

x Se 7 0.333337 0.344156 0.871871 x

x Se 8 0.263396 0.656538 0.368690 x

x Se 9 0.466806 0.653233 0.128853 x

x Se 10 0.531535 0.338811 0.617585 x

x Se 11 0.533209 0.346867 0.871223 x

x Se 12 0.468386 0.660785 0.382557 x

x Se 13 0.666638 0.655806 0.128390 x

x Se 14 0.736595 0.343415 0.631454 x

x Se 15 0.731253 0.330903 0.875991 x

x Se 16 0.668191 0.658179 0.370455 x

x Se 17 0.867439 0.658271 0.128198 x

x Se 18 0.932666 0.337489 0.624150 x

x Se 19 0.933028 0.338798 0.878202 x

x Se 20 0.868198 0.661258 0.372454 x

x Nb 1 0.002296 0.001233 0.247874 x

x Nb 2 -0.002879 -0.002586 0.751465 x

x Nb 3 -0.000272 -0.000669 0.000102 x

x Nb 4 0.001163 0.002288 0.499624 x

x Nb 5 0.196064 -0.010102 0.245769 x

x Nb 6 0.199114 0.002974 0.750021 x

x Nb 7 0.200273 0.005892 -0.001835 x

x Nb 8 0.201769 0.008208 0.499076 x

x Nb 9 0.402008 -0.001514 0.253247 x

x Nb 10 0.403282 0.016741 0.750548 x

x Nb 11 0.402703 0.001741 -0.000618 x

x Nb 12 0.383045 -0.040365 0.500324 x

x Nb 13 0.596823 -0.016292 0.249703 x

x Nb 14 0.597832 0.000986 0.746931 x

x Nb 15 0.597334 -0.001941 0.001004 x

x Nb 16 0.616808 0.040379 0.499906 x

x Nb 17 0.800732 -0.003150 0.250281 x

x Nb 18 0.804696 0.011883 0.754098 x

x Nb 19 0.800024 -0.004682 0.002001 x

x Nb 20 0.797238 -0.010651 0.500954 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600242E+004 63116.09 <-- SCF

1 -3.62600424E+004 4.55267668E-004 63143.56 <-- SCF

2 -3.62600438E+004 3.30881650E-005 63164.31 <-- SCF

3 -3.62600473E+004 8.93039888E-005 63191.28 <-- SCF

4 -3.62600245E+004 -5.70200869E-004 63217.62 <-- SCF

5 -3.62600260E+004 3.78628197E-005 63241.23 <-- SCF

6 -3.62600259E+004 -2.11924224E-006 63260.98 <-- SCF

7 -3.62600258E+004 -4.35957912E-006 63279.23 <-- SCF

8 -3.62600257E+004 -7.35711073E-007 63296.59 <-- SCF

9 -3.62600258E+004 1.34349178E-006 63315.08 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02579753 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00672 -0.01365 0.00432 \*

\* Se 2 0.01050 -0.00048 0.00984 \*

\* Se 3 0.00716 -0.00103 0.00158 \*

\* Se 4 0.01191 0.00325 0.01011 \*

\* Se 5 0.01240 -0.00840 0.00847 \*

\* Se 6 -0.00706 0.00181 0.00941 \*

\* Se 7 0.00807 0.01625 -0.03555 \*

\* Se 8 -0.01065 0.00014 0.00466 \*

\* Se 9 -0.00292 0.00279 0.00033 \*

\* Se 10 0.00897 0.02158 0.01694 \*

\* Se 11 0.00663 -0.00509 0.01314 \*

\* Se 12 -0.00646 -0.01411 -0.01110 \*

\* Se 13 0.00023 -0.00452 -0.04417 \*

\* Se 14 0.00334 -0.00324 -0.00082 \*

\* Se 15 -0.01798 -0.00894 0.00344 \*

\* Se 16 0.00008 0.00711 -0.01020 \*

\* Se 17 -0.01180 -0.00206 -0.00159 \*

\* Se 18 0.00261 0.01514 -0.03209 \*

\* Se 19 -0.00579 0.01052 0.00746 \*

\* Se 20 -0.01023 0.00556 -0.00895 \*

\* Nb 1 -0.01443 0.00574 -0.00256 \*

\* Nb 2 0.00379 -0.00173 -0.00168 \*

\* Nb 3 -0.00782 -0.00184 -0.00204 \*

\* Nb 4 0.02100 0.00110 0.00189 \*

\* Nb 5 0.02039 0.01129 -0.00070 \*

\* Nb 6 0.00252 -0.00024 0.00217 \*

\* Nb 7 0.00362 0.00503 0.01456 \*

\* Nb 8 -0.00532 -0.00335 0.00043 \*

\* Nb 9 -0.00376 0.00121 0.00445 \*

\* Nb 10 0.00091 -0.00319 0.01500 \*

\* Nb 11 0.01716 0.00820 -0.00440 \*

\* Nb 12 -0.00196 0.01271 -0.00358 \*

\* Nb 13 -0.00621 -0.00563 0.00673 \*

\* Nb 14 -0.00097 -0.00309 -0.00341 \*

\* Nb 15 -0.01293 -0.01291 0.00887 \*

\* Nb 16 -0.00235 -0.01560 0.00170 \*

\* Nb 17 0.00112 -0.00778 0.01718 \*

\* Nb 18 -0.00918 -0.00925 0.00660 \*

\* Nb 19 0.00494 -0.00521 -0.00893 \*

\* Nb 20 -0.01625 0.00189 0.00247 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.001384 0.001339 -0.000010 \*

\* y 0.001339 -0.003576 0.004059 \*

\* z -0.000010 0.004059 -0.005788 \*

\* \*

\* Pressure: 0.0027 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.688E-006 | -36260.025776 | <-- min BFGS

| trial step | 1.000000 | 8.635E-007 | -36260.025839 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 96 with line minimization (lambda= 2.047141)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8584757 -8.3019984 0.0053491 0.4205137 -0.0042150 -0.0001422

0.0338720 3.3792315 0.0002749 1.0331060 1.8489979 -0.0004654

0.0047314 0.0008714 13.9645860 -0.0001814 -0.0000348 0.4499372

Lattice parameters(A) Cell Angles

a = 17.020503 alpha = 89.991570

b = 3.379401 beta = 89.966791

c = 13.964587 gamma = 118.619468

Current cell volume = 705.091875 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067058 0.661414 0.121707 x

x Se 2 0.131923 0.339477 0.627973 x

x Se 3 0.132196 0.340577 0.872127 x

x Se 4 0.067361 0.661847 0.373552 x

x Se 5 0.269091 0.670532 0.124418 x

x Se 6 0.331613 0.341207 0.629674 x

x Se 7 0.333341 0.344176 0.871874 x

x Se 8 0.263381 0.656521 0.368692 x

x Se 9 0.466806 0.653235 0.128852 x

x Se 10 0.531531 0.338838 0.617576 x

x Se 11 0.533209 0.346868 0.871225 x

x Se 12 0.468386 0.660722 0.382559 x

x Se 13 0.666634 0.655788 0.128391 x

x Se 14 0.736609 0.343432 0.631452 x

x Se 15 0.731244 0.330891 0.875990 x

x Se 16 0.668200 0.658218 0.370452 x

x Se 17 0.867439 0.658257 0.128197 x

x Se 18 0.932675 0.337538 0.624162 x

x Se 19 0.933028 0.338772 0.878200 x

x Se 20 0.868211 0.661284 0.372453 x

x Nb 1 0.002279 0.001207 0.247854 x

x Nb 2 -0.002869 -0.002571 0.751481 x

x Nb 3 -0.000273 -0.000670 0.000102 x

x Nb 4 0.001176 0.002310 0.499622 x

x Nb 5 0.196090 -0.010027 0.245760 x

x Nb 6 0.199097 0.002937 0.750021 x

x Nb 7 0.200278 0.005907 -0.001825 x

x Nb 8 0.201739 0.008171 0.499076 x

x Nb 9 0.402015 -0.001515 0.253254 x

x Nb 10 0.403294 0.016808 0.750544 x

x Nb 11 0.402705 0.001720 -0.000617 x

x Nb 12 0.383026 -0.040372 0.500337 x

x Nb 13 0.596814 -0.016357 0.249708 x

x Nb 14 0.597824 0.000991 0.746926 x

x Nb 15 0.597334 -0.001920 0.001004 x

x Nb 16 0.616827 0.040391 0.499892 x

x Nb 17 0.800748 -0.003118 0.250280 x

x Nb 18 0.804679 0.011833 0.754110 x

x Nb 19 0.800025 -0.004678 0.001991 x

x Nb 20 0.797256 -0.010642 0.500953 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600238E+004 63418.78 <-- SCF

1 -3.62600556E+004 7.96689677E-004 63446.70 <-- SCF

2 -3.62600582E+004 6.49101053E-005 63468.41 <-- SCF

3 -3.62600673E+004 2.26050177E-004 63495.06 <-- SCF

4 -3.62600233E+004 -1.09919387E-003 63521.28 <-- SCF

5 -3.62600262E+004 7.22646507E-005 63546.42 <-- SCF

6 -3.62600261E+004 -2.20533338E-006 63566.75 <-- SCF

7 -3.62600258E+004 -7.68298837E-006 63585.84 <-- SCF

8 -3.62600257E+004 -1.59049343E-006 63604.20 <-- SCF

9 -3.62600258E+004 2.07128237E-007 63621.47 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02575237 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00787 -0.01422 0.00485 \*

\* Se 2 0.01266 -0.00000 0.01053 \*

\* Se 3 0.00995 -0.00148 0.00245 \*

\* Se 4 0.01519 0.00360 0.00565 \*

\* Se 5 0.01258 -0.00754 0.00889 \*

\* Se 6 -0.00597 0.00284 0.00833 \*

\* Se 7 0.00718 0.01572 -0.03642 \*

\* Se 8 -0.00673 -0.00137 0.00431 \*

\* Se 9 -0.00294 0.00216 -0.00025 \*

\* Se 10 0.01040 0.01943 0.01774 \*

\* Se 11 0.00649 -0.00442 0.01408 \*

\* Se 12 -0.00734 -0.01016 -0.00963 \*

\* Se 13 0.00159 -0.00428 -0.04426 \*

\* Se 14 -0.00088 -0.00186 -0.00056 \*

\* Se 15 -0.01815 -0.01015 0.00338 \*

\* Se 16 -0.00112 0.00482 -0.01073 \*

\* Se 17 -0.01340 -0.00151 -0.00327 \*

\* Se 18 -0.00023 0.01443 -0.03228 \*

\* Se 19 -0.00672 0.01199 0.00845 \*

\* Se 20 -0.01218 0.00555 -0.00938 \*

\* Nb 1 -0.01583 0.00630 -0.00297 \*

\* Nb 2 0.00517 -0.00216 -0.00188 \*

\* Nb 3 -0.00821 -0.00213 -0.00163 \*

\* Nb 4 0.02177 0.00134 0.00178 \*

\* Nb 5 0.02072 0.01137 -0.00102 \*

\* Nb 6 0.00321 -0.00026 0.00419 \*

\* Nb 7 0.00490 0.00457 0.01396 \*

\* Nb 8 -0.00434 -0.00395 0.00040 \*

\* Nb 9 -0.00269 0.00112 0.00386 \*

\* Nb 10 0.00232 -0.00369 0.01647 \*

\* Nb 11 0.01756 0.00832 -0.00364 \*

\* Nb 12 -0.00121 0.01147 -0.00456 \*

\* Nb 13 -0.00836 -0.00496 0.00564 \*

\* Nb 14 -0.00284 -0.00324 -0.00279 \*

\* Nb 15 -0.01364 -0.01336 0.00896 \*

\* Nb 16 -0.00350 -0.01463 0.00264 \*

\* Nb 17 0.00003 -0.00780 0.01641 \*

\* Nb 18 -0.00967 -0.00937 0.00699 \*

\* Nb 19 0.00386 -0.00485 -0.00756 \*

\* Nb 20 -0.01752 0.00236 0.00287 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.005987 0.006011 0.000098 \*

\* y 0.006011 0.002138 0.001838 \*

\* z 0.000098 0.001838 0.001414 \*

\* \*

\* Pressure: 0.0008 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.688E-006 | -36260.025776 | <-- min BFGS

| trial step | 1.000000 | 8.635E-007 | -36260.025839 | <-- min BFGS

| line step | 2.047141 | 5.891E-007 | -36260.025799 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 96 with enthalpy= -3.62600258E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 5.851260E-007 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 4.449498E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 9.325973E-004 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 6.010940E-003 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 97 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 4.226E-006 | -36260.025799 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 97 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8597695 -8.3026257 0.0054648 0.4204920 -0.0041881 -0.0001394

0.0336563 3.3791207 0.0001793 1.0331645 1.8491239 -0.0004173

0.0046346 0.0005620 13.9645152 -0.0001778 -0.0000221 0.4499394

Lattice parameters(A) Cell Angles

a = 17.021938 alpha = 89.994465

b = 3.379288 beta = 89.966130

c = 13.964516 gamma = 118.622826

Current cell volume = 705.101663 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067064 0.661509 0.121703 x

x Se 2 0.131915 0.339450 0.628004 x

x Se 3 0.132186 0.340541 0.872154 x

x Se 4 0.067338 0.661808 0.373485 x

x Se 5 0.269140 0.670694 0.124445 x

x Se 6 0.331604 0.341217 0.629693 x

x Se 7 0.333340 0.344223 0.871877 x

x Se 8 0.263346 0.656428 0.368695 x

x Se 9 0.466799 0.653151 0.128842 x

x Se 10 0.531530 0.338898 0.617570 x

x Se 11 0.533219 0.346967 0.871240 x

x Se 12 0.468382 0.660598 0.382554 x

x Se 13 0.666636 0.655774 0.128374 x

x Se 14 0.736642 0.343518 0.631448 x

x Se 15 0.731207 0.330751 0.875991 x

x Se 16 0.668205 0.658213 0.370445 x

x Se 17 0.867431 0.658203 0.128186 x

x Se 18 0.932691 0.337633 0.624186 x

x Se 19 0.933022 0.338654 0.878199 x

x Se 20 0.868228 0.661322 0.372441 x

x Nb 1 0.002240 0.001134 0.247806 x

x Nb 2 -0.002850 -0.002537 0.751514 x

x Nb 3 -0.000279 -0.000691 0.000101 x

x Nb 4 0.001213 0.002384 0.499613 x

x Nb 5 0.196160 -0.009855 0.245749 x

x Nb 6 0.199065 0.002929 0.750011 x

x Nb 7 0.200284 0.005920 -0.001796 x

x Nb 8 0.201677 0.008090 0.499078 x

x Nb 9 0.402018 -0.001587 0.253268 x

x Nb 10 0.403314 0.016975 0.750541 x

x Nb 11 0.402715 0.001750 -0.000627 x

x Nb 12 0.382990 -0.040320 0.500367 x

x Nb 13 0.596799 -0.016519 0.249717 x

x Nb 14 0.597812 0.001060 0.746914 x

x Nb 15 0.597332 -0.001957 0.001022 x

x Nb 16 0.616857 0.040370 0.499854 x

x Nb 17 0.800775 -0.003137 0.250292 x

x Nb 18 0.804639 0.011732 0.754121 x

x Nb 19 0.800035 -0.004641 0.001967 x

x Nb 20 0.797278 -0.010654 0.500952 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600194E+004 63724.91 <-- SCF

1 -3.62600398E+004 5.10567105E-004 63751.72 <-- SCF

2 -3.62600409E+004 2.76694005E-005 63776.84 <-- SCF

3 -3.62600375E+004 -8.68526364E-005 63803.66 <-- SCF

4 -3.62600257E+004 -2.93780450E-004 63829.38 <-- SCF

5 -3.62600263E+004 1.45887138E-005 63853.97 <-- SCF

6 -3.62600260E+004 -8.51108445E-006 63873.66 <-- SCF

7 -3.62600259E+004 -2.45136751E-006 63891.75 <-- SCF

8 -3.62600258E+004 -4.88091943E-007 63908.09 <-- SCF

9 -3.62600259E+004 1.46601457E-006 63926.58 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02589705 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00479 -0.02030 0.00814 \*

\* Se 2 0.00820 0.00283 0.00377 \*

\* Se 3 0.01096 -0.00243 0.00037 \*

\* Se 4 0.01519 0.00473 -0.00222 \*

\* Se 5 -0.00263 -0.00956 0.01168 \*

\* Se 6 -0.01272 0.00304 0.00347 \*

\* Se 7 0.00020 0.01196 -0.03834 \*

\* Se 8 -0.00309 -0.00019 0.00608 \*

\* Se 9 0.00051 0.00520 0.00489 \*

\* Se 10 0.01350 0.01492 0.01606 \*

\* Se 11 0.00430 -0.00762 0.00851 \*

\* Se 12 -0.00840 -0.00136 -0.00295 \*

\* Se 13 0.00802 -0.00373 -0.03590 \*

\* Se 14 -0.00451 -0.00269 -0.00154 \*

\* Se 15 -0.00432 -0.01065 -0.00213 \*

\* Se 16 0.00568 0.00360 -0.00991 \*

\* Se 17 -0.01250 0.00046 -0.00291 \*

\* Se 18 -0.00124 0.01212 -0.03460 \*

\* Se 19 -0.00381 0.01931 0.00657 \*

\* Se 20 -0.01049 0.00478 -0.00347 \*

\* Nb 1 -0.01022 0.00690 0.00036 \*

\* Nb 2 -0.00059 -0.00189 -0.00480 \*

\* Nb 3 -0.00870 -0.00227 -0.00140 \*

\* Nb 4 0.02229 0.00205 0.00247 \*

\* Nb 5 0.01172 0.01124 -0.00288 \*

\* Nb 6 0.00111 -0.00207 0.00837 \*

\* Nb 7 0.00246 0.00637 0.01207 \*

\* Nb 8 -0.00642 -0.00493 0.00361 \*

\* Nb 9 -0.00766 0.00034 0.00389 \*

\* Nb 10 0.00331 -0.00696 0.01863 \*

\* Nb 11 0.01640 0.00892 -0.00210 \*

\* Nb 12 -0.00076 0.00856 -0.00953 \*

\* Nb 13 -0.00666 -0.00088 0.00320 \*

\* Nb 14 0.00346 -0.00372 -0.00315 \*

\* Nb 15 -0.01289 -0.01328 0.00730 \*

\* Nb 16 -0.00412 -0.01298 0.00910 \*

\* Nb 17 0.00145 -0.00651 0.01474 \*

\* Nb 18 -0.00418 -0.00950 0.00912 \*

\* Nb 19 0.00643 -0.00708 -0.00491 \*

\* Nb 20 -0.01406 0.00327 0.00035 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.006763 -0.004507 0.001556 \*

\* y -0.004507 -0.007807 -0.005629 \*

\* z 0.001556 -0.005629 0.000181 \*

\* \*

\* Pressure: 0.0003 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 4.226E-006 | -36260.025799 | <-- min BFGS

| trial step | 1.000000 | 1.264E-006 | -36260.025946 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 97 with line minimization (lambda= 1.426673)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8603216 -8.3028933 0.0055141 0.4204827 -0.0041766 -0.0001382

0.0335643 3.3790734 0.0001385 1.0331894 1.8491776 -0.0003968

0.0045934 0.0004301 13.9644849 -0.0001763 -0.0000167 0.4499404

Lattice parameters(A) Cell Angles

a = 17.022551 alpha = 89.995700

b = 3.379240 beta = 89.965848

c = 13.964486 gamma = 118.624258

Current cell volume = 705.105836 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067067 0.661550 0.121702 x

x Se 2 0.131912 0.339439 0.628017 x

x Se 3 0.132181 0.340525 0.872166 x

x Se 4 0.067328 0.661792 0.373457 x

x Se 5 0.269162 0.670763 0.124456 x

x Se 6 0.331600 0.341222 0.629702 x

x Se 7 0.333340 0.344244 0.871879 x

x Se 8 0.263332 0.656389 0.368697 x

x Se 9 0.466796 0.653116 0.128838 x

x Se 10 0.531530 0.338923 0.617568 x

x Se 11 0.533224 0.347009 0.871247 x

x Se 12 0.468381 0.660545 0.382552 x

x Se 13 0.666636 0.655767 0.128367 x

x Se 14 0.736656 0.343554 0.631446 x

x Se 15 0.731191 0.330692 0.875992 x

x Se 16 0.668208 0.658210 0.370442 x

x Se 17 0.867428 0.658180 0.128182 x

x Se 18 0.932698 0.337673 0.624197 x

x Se 19 0.933019 0.338604 0.878199 x

x Se 20 0.868235 0.661337 0.372435 x

x Nb 1 0.002223 0.001102 0.247785 x

x Nb 2 -0.002842 -0.002522 0.751528 x

x Nb 3 -0.000281 -0.000700 0.000101 x

x Nb 4 0.001229 0.002416 0.499609 x

x Nb 5 0.196190 -0.009782 0.245745 x

x Nb 6 0.199052 0.002926 0.750007 x

x Nb 7 0.200286 0.005926 -0.001784 x

x Nb 8 0.201651 0.008055 0.499078 x

x Nb 9 0.402019 -0.001618 0.253274 x

x Nb 10 0.403322 0.017047 0.750540 x

x Nb 11 0.402719 0.001763 -0.000631 x

x Nb 12 0.382974 -0.040298 0.500380 x

x Nb 13 0.596793 -0.016588 0.249721 x

x Nb 14 0.597807 0.001090 0.746908 x

x Nb 15 0.597331 -0.001973 0.001029 x

x Nb 16 0.616870 0.040361 0.499838 x

x Nb 17 0.800786 -0.003144 0.250296 x

x Nb 18 0.804622 0.011690 0.754126 x

x Nb 19 0.800039 -0.004625 0.001957 x

x Nb 20 0.797287 -0.010659 0.500951 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600236E+004 64030.14 <-- SCF

1 -3.62600669E+004 1.08151268E-003 64058.17 <-- SCF

2 -3.62600700E+004 7.84872342E-005 64080.64 <-- SCF

3 -3.62600837E+004 3.42868211E-004 64107.66 <-- SCF

4 -3.62600232E+004 -1.51343847E-003 64133.73 <-- SCF

5 -3.62600266E+004 8.43366597E-005 64159.19 <-- SCF

6 -3.62600262E+004 -9.19898245E-006 64179.30 <-- SCF

7 -3.62600259E+004 -8.70874960E-006 64199.31 <-- SCF

8 -3.62600258E+004 -2.73758921E-007 64217.50 <-- SCF

9 -3.62600259E+004 3.70805648E-007 64234.12 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02586426 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00485 -0.02290 0.00969 \*

\* Se 2 0.00772 0.00426 0.00065 \*

\* Se 3 0.01362 -0.00290 -0.00051 \*

\* Se 4 0.01565 0.00512 -0.00645 \*

\* Se 5 -0.00670 -0.01058 0.01249 \*

\* Se 6 -0.01384 0.00349 0.00160 \*

\* Se 7 -0.00082 0.01058 -0.04030 \*

\* Se 8 -0.00058 0.00030 0.00883 \*

\* Se 9 0.00263 0.00627 0.00626 \*

\* Se 10 0.01483 0.01326 0.01569 \*

\* Se 11 0.00228 -0.00877 0.00615 \*

\* Se 12 -0.00986 0.00208 0.00026 \*

\* Se 13 0.00848 -0.00369 -0.03144 \*

\* Se 14 -0.00723 -0.00319 -0.00363 \*

\* Se 15 -0.00124 -0.01077 -0.00417 \*

\* Se 16 0.00703 0.00285 -0.00993 \*

\* Se 17 -0.01370 0.00117 -0.00249 \*

\* Se 18 -0.00290 0.01125 -0.03708 \*

\* Se 19 -0.00366 0.02234 0.00573 \*

\* Se 20 -0.01053 0.00426 0.00053 \*

\* Nb 1 -0.01055 0.00708 0.00202 \*

\* Nb 2 -0.00060 -0.00174 -0.00629 \*

\* Nb 3 -0.00917 -0.00228 -0.00093 \*

\* Nb 4 0.02330 0.00215 0.00277 \*

\* Nb 5 0.01098 0.01121 -0.00319 \*

\* Nb 6 0.00107 -0.00297 0.00903 \*

\* Nb 7 0.00293 0.00774 0.01105 \*

\* Nb 8 -0.00592 -0.00543 0.00508 \*

\* Nb 9 -0.00829 -0.00113 0.00380 \*

\* Nb 10 0.00433 -0.00666 0.02034 \*

\* Nb 11 0.01782 0.00918 -0.00148 \*

\* Nb 12 -0.00277 0.00841 -0.00933 \*

\* Nb 13 -0.00695 -0.00042 0.00155 \*

\* Nb 14 0.00342 -0.00287 -0.00243 \*

\* Nb 15 -0.01410 -0.01369 0.00802 \*

\* Nb 16 -0.00167 -0.01276 0.00984 \*

\* Nb 17 0.00157 -0.00584 0.01492 \*

\* Nb 18 -0.00357 -0.00935 0.00960 \*

\* Nb 19 0.00648 -0.00858 -0.00494 \*

\* Nb 20 -0.01433 0.00355 -0.00128 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.016734 -0.010875 0.002653 \*

\* y -0.010875 -0.013358 -0.007798 \*

\* z 0.002653 -0.007798 0.000157 \*

\* \*

\* Pressure: -0.0012 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 4.226E-006 | -36260.025799 | <-- min BFGS

| trial step | 1.000000 | 1.264E-006 | -36260.025946 | <-- min BFGS

| line step | 1.426673 | 4.556E-007 | -36260.025917 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 97 with enthalpy= -3.62600259E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.960240E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 4.167590E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.513354E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.673404E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 98 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.671E-006 | -36260.025917 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 98 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8593251 -8.3021606 0.0051256 0.4204941 -0.0042070 -0.0001290

0.0338085 3.3791923 0.0001327 1.0330900 1.8490389 -0.0003713

0.0042866 0.0004089 13.9644002 -0.0001642 -0.0000160 0.4499431

Lattice parameters(A) Cell Angles

a = 17.021323 alpha = 89.995897

b = 3.379361 beta = 89.968211

c = 13.964401 gamma = 118.619621

Current cell volume = 705.107177 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067079 0.661528 0.121718 x

x Se 2 0.131909 0.339440 0.628024 x

x Se 3 0.132197 0.340519 0.872213 x

x Se 4 0.067304 0.661730 0.373322 x

x Se 5 0.269217 0.670927 0.124530 x

x Se 6 0.331555 0.341197 0.629724 x

x Se 7 0.333339 0.344281 0.871831 x

x Se 8 0.263314 0.656373 0.368712 x

x Se 9 0.466795 0.653093 0.128843 x

x Se 10 0.531546 0.339023 0.617565 x

x Se 11 0.533231 0.347050 0.871253 x

x Se 12 0.468363 0.660448 0.382562 x

x Se 13 0.666644 0.655785 0.128340 x

x Se 14 0.736665 0.343536 0.631438 x

x Se 15 0.731150 0.330533 0.875954 x

x Se 16 0.668244 0.658233 0.370413 x

x Se 17 0.867392 0.658088 0.128152 x

x Se 18 0.932717 0.337823 0.624247 x

x Se 19 0.933012 0.338618 0.878195 x

x Se 20 0.868244 0.661383 0.372444 x

x Nb 1 0.002138 0.000963 0.247710 x

x Nb 2 -0.002791 -0.002452 0.751576 x

x Nb 3 -0.000293 -0.000748 0.000102 x

x Nb 4 0.001293 0.002548 0.499600 x

x Nb 5 0.196296 -0.009505 0.245719 x

x Nb 6 0.198977 0.002685 0.750026 x

x Nb 7 0.200298 0.005932 -0.001737 x

x Nb 8 0.201528 0.007842 0.499086 x

x Nb 9 0.402024 -0.001615 0.253299 x

x Nb 10 0.403361 0.017190 0.750549 x

x Nb 11 0.402735 0.001750 -0.000624 x

x Nb 12 0.382900 -0.040325 0.500412 x

x Nb 13 0.596764 -0.016720 0.249737 x

x Nb 14 0.597786 0.001045 0.746884 x

x Nb 15 0.597328 -0.001965 0.001042 x

x Nb 16 0.616934 0.040404 0.499803 x

x Nb 17 0.800854 -0.002967 0.250312 x

x Nb 18 0.804554 0.011503 0.754154 x

x Nb 19 0.800052 -0.004563 0.001925 x

x Nb 20 0.797345 -0.010610 0.500948 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62600082E+004 64337.66 <-- SCF

1 -3.62600577E+004 1.23650864E-003 64364.33 <-- SCF

2 -3.62600603E+004 6.63463725E-005 64391.25 <-- SCF

3 -3.62600469E+004 -3.34902745E-004 64418.06 <-- SCF

4 -3.62600265E+004 -5.10250685E-004 64443.80 <-- SCF

5 -3.62600269E+004 1.09154223E-005 64469.64 <-- SCF

6 -3.62600262E+004 -1.95862267E-005 64492.41 <-- SCF

7 -3.62600260E+004 -3.37411977E-006 64511.38 <-- SCF

8 -3.62600260E+004 -3.24206799E-007 64529.39 <-- SCF

9 -3.62600260E+004 2.41773353E-007 64545.53 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02602766 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00356 -0.01925 0.00453 \*

\* Se 2 0.00766 0.00458 0.00254 \*

\* Se 3 0.00986 -0.00234 -0.00157 \*

\* Se 4 0.01354 0.00620 -0.02706 \*

\* Se 5 -0.00952 -0.01300 0.00672 \*

\* Se 6 -0.00949 0.00102 -0.00082 \*

\* Se 7 -0.00067 0.00740 -0.02186 \*

\* Se 8 0.00163 -0.00234 0.00720 \*

\* Se 9 0.00348 0.00691 0.00552 \*

\* Se 10 0.01090 0.00936 0.01155 \*

\* Se 11 0.00182 -0.00873 0.00517 \*

\* Se 12 -0.00605 0.00521 0.00462 \*

\* Se 13 0.00563 -0.00578 -0.01676 \*

\* Se 14 -0.00779 0.00105 -0.00183 \*

\* Se 15 0.00053 -0.00978 -0.00571 \*

\* Se 16 0.00178 0.00373 -0.00415 \*

\* Se 17 -0.01073 0.00071 -0.00167 \*

\* Se 18 -0.00800 0.00868 -0.04290 \*

\* Se 19 -0.00173 0.02030 0.00836 \*

\* Se 20 -0.00847 0.00279 0.00326 \*

\* Nb 1 -0.01129 0.00662 0.00542 \*

\* Nb 2 0.00097 0.00069 -0.00779 \*

\* Nb 3 -0.00954 -0.00210 0.00033 \*

\* Nb 4 0.02525 0.00329 0.00194 \*

\* Nb 5 0.00916 0.01316 0.00004 \*

\* Nb 6 0.00136 -0.00291 0.00835 \*

\* Nb 7 0.00466 0.00820 0.01185 \*

\* Nb 8 -0.00331 -0.00588 0.00451 \*

\* Nb 9 -0.00756 -0.00158 0.00475 \*

\* Nb 10 0.00486 -0.00752 0.01640 \*

\* Nb 11 0.01761 0.00982 -0.00042 \*

\* Nb 12 0.00080 0.00687 -0.00866 \*

\* Nb 13 -0.00449 0.00175 -0.00096 \*

\* Nb 14 0.00405 -0.00273 -0.00103 \*

\* Nb 15 -0.01490 -0.01393 0.00652 \*

\* Nb 16 -0.00566 -0.01029 0.01022 \*

\* Nb 17 -0.00057 -0.00424 0.01091 \*

\* Nb 18 -0.00199 -0.01148 0.00864 \*

\* Nb 19 0.00712 -0.00893 -0.00544 \*

\* Nb 20 -0.01448 0.00445 -0.00071 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.016208 -0.003165 -0.000441 \*

\* y -0.003165 -0.006723 -0.008959 \*

\* z -0.000441 -0.008959 0.003293 \*

\* \*

\* Pressure: -0.0043 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.671E-006 | -36260.025917 | <-- min BFGS

| trial step | 1.000000 | 4.912E-006 | -36260.026074 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 98 with line minimization (lambda= 3.793249)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8565417 -8.3001137 0.0040402 0.4205261 -0.0042918 -0.0001032

0.0344906 3.3795243 0.0001164 1.0328124 1.8486516 -0.0003000

0.0034298 0.0003499 13.9641633 -0.0001303 -0.0000142 0.4499507

Lattice parameters(A) Cell Angles

a = 17.017895 alpha = 89.996447

b = 3.379700 beta = 89.974813

c = 13.964164 gamma = 118.606670

Current cell volume = 705.110873 A\*\*3

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Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067112 0.661464 0.121761 x

x Se 2 0.131900 0.339443 0.628044 x

x Se 3 0.132242 0.340501 0.872343 x

x Se 4 0.067236 0.661559 0.372944 x

x Se 5 0.269372 0.671384 0.124735 x

x Se 6 0.331428 0.341126 0.629789 x

x Se 7 0.333337 0.344385 0.871699 x

x Se 8 0.263267 0.656327 0.368755 x

x Se 9 0.466792 0.653028 0.128859 x

x Se 10 0.531591 0.339304 0.617557 x

x Se 11 0.533252 0.347164 0.871268 x

x Se 12 0.468312 0.660176 0.382589 x

x Se 13 0.666667 0.655836 0.128263 x

x Se 14 0.736690 0.343485 0.631416 x

x Se 15 0.731038 0.330088 0.875848 x

x Se 16 0.668344 0.658298 0.370331 x

x Se 17 0.867290 0.657832 0.128070 x

x Se 18 0.932771 0.338241 0.624386 x

x Se 19 0.932991 0.338659 0.878185 x

x Se 20 0.868269 0.661509 0.372470 x

x Nb 1 0.001898 0.000575 0.247498 x

x Nb 2 -0.002647 -0.002255 0.751709 x

x Nb 3 -0.000326 -0.000882 0.000104 x

x Nb 4 0.001473 0.002918 0.499574 x

x Nb 5 0.196590 -0.008731 0.245646 x

x Nb 6 0.198766 0.002014 0.750078 x

x Nb 7 0.200331 0.005949 -0.001605 x

x Nb 8 0.201186 0.007246 0.499106 x

x Nb 9 0.402037 -0.001608 0.253369 x

x Nb 10 0.403468 0.017592 0.750574 x

x Nb 11 0.402780 0.001715 -0.000604 x

x Nb 12 0.382694 -0.040398 0.500502 x

x Nb 13 0.596682 -0.017088 0.249782 x

x Nb 14 0.597729 0.000919 0.746815 x

x Nb 15 0.597320 -0.001943 0.001078 x

x Nb 16 0.617112 0.040522 0.499705 x

x Nb 17 0.801045 -0.002471 0.250355 x

x Nb 18 0.804366 0.010982 0.754232 x

x Nb 19 0.800089 -0.004389 0.001834 x

x Nb 20 0.797505 -0.010473 0.500937 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62598871E+004 64649.06 <-- SCF

1 -3.62602721E+004 9.62409848E-003 64675.81 <-- SCF

2 -3.62602927E+004 5.16538754E-004 64704.41 <-- SCF

3 -3.62601855E+004 -2.68105572E-003 64731.33 <-- SCF

4 -3.62600304E+004 -3.87838249E-003 64757.05 <-- SCF

5 -3.62600337E+004 8.43598514E-005 64783.70 <-- SCF

6 -3.62600272E+004 -1.63348716E-004 64809.59 <-- SCF

7 -3.62600262E+004 -2.41992883E-005 64831.78 <-- SCF

8 -3.62600261E+004 -3.32229355E-006 64853.17 <-- SCF

9 -3.62600261E+004 3.71837510E-007 64871.38 <-- SCF

10 -3.62600261E+004 -2.91684031E-008 64888.44 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02612395 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00406 -0.00921 -0.00568 \*

\* Se 2 0.00414 0.00579 0.00744 \*

\* Se 3 0.00440 -0.00212 -0.01142 \*

\* Se 4 -0.00229 0.00675 -0.07197 \*

\* Se 5 -0.02864 -0.02159 -0.01649 \*

\* Se 6 0.00017 -0.00568 -0.00853 \*

\* Se 7 -0.00134 -0.00119 0.03004 \*

\* Se 8 0.00606 -0.01009 0.00477 \*

\* Se 9 0.00735 0.00812 -0.00191 \*

\* Se 10 0.00055 -0.00075 -0.00403 \*

\* Se 11 -0.00219 -0.00797 0.00547 \*

\* Se 12 0.00525 0.01257 0.02201 \*

\* Se 13 -0.00016 -0.01066 0.02430 \*

\* Se 14 -0.00661 0.01324 0.00061 \*

\* Se 15 0.00863 -0.00422 -0.01298 \*

\* Se 16 -0.00996 0.00722 0.01653 \*

\* Se 17 -0.00304 -0.00037 0.00661 \*

\* Se 18 -0.02015 -0.00067 -0.05840 \*

\* Se 19 0.00248 0.01451 0.00797 \*

\* Se 20 0.00191 -0.00160 0.01191 \*

\* Nb 1 -0.01298 0.00471 0.02401 \*

\* Nb 2 0.00629 0.00800 -0.02133 \*

\* Nb 3 -0.00595 -0.00083 0.00243 \*

\* Nb 4 0.02720 0.00652 0.00173 \*

\* Nb 5 0.00335 0.01784 0.01092 \*

\* Nb 6 0.00621 -0.00078 0.00353 \*

\* Nb 7 0.01409 0.01195 0.00836 \*

\* Nb 8 0.01047 -0.00802 0.00532 \*

\* Nb 9 -0.00788 -0.00313 0.00794 \*

\* Nb 10 0.00741 -0.00859 0.00569 \*

\* Nb 11 0.01515 0.01251 0.00126 \*

\* Nb 12 0.01163 0.00195 -0.00623 \*

\* Nb 13 0.00181 0.00741 -0.00492 \*

\* Nb 14 0.00820 -0.00143 0.00079 \*

\* Nb 15 -0.01736 -0.01567 0.00224 \*

\* Nb 16 -0.01589 -0.00260 0.01091 \*

\* Nb 17 -0.00691 -0.00074 0.00422 \*

\* Nb 18 0.00530 -0.01655 0.00023 \*

\* Nb 19 0.00519 -0.01366 -0.00454 \*

\* Nb 20 -0.02595 0.00902 0.00119 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.016978 0.020105 -0.009158 \*

\* y 0.020105 0.007952 -0.013128 \*

\* z -0.009158 -0.013128 0.008006 \*

\* \*

\* Pressure: -0.0110 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.671E-006 | -36260.025917 | <-- min BFGS

| trial step | 1.000000 | 4.912E-006 | -36260.026074 | <-- min BFGS

| line step | 3.793249 | -3.524E-006 | -36260.026166 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 98 with enthalpy= -3.62600262E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 6.222545E-006 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 7.231764E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.286516E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.010546E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 99 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000011 | -36260.026166 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 99 with trial guess (lambda= 1.000000)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8569969 -8.3008236 0.0043249 0.4205321 -0.0042576 -0.0001204

0.0342138 3.3793402 0.0003029 1.0329717 1.8488354 -0.0004228

0.0040076 0.0009545 13.9642364 -0.0001527 -0.0000388 0.4499484

Lattice parameters(A) Cell Angles

a = 17.018638 alpha = 89.990782

b = 3.379513 beta = 89.972995

c = 13.964237 gamma = 118.612669

Current cell volume = 705.066079 A\*\*3

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Cell Contents

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xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067102 0.661367 0.121751 x

x Se 2 0.131893 0.339399 0.628017 x

x Se 3 0.132220 0.340378 0.872310 x

x Se 4 0.067279 0.661643 0.373021 x

x Se 5 0.269311 0.671330 0.124693 x

x Se 6 0.331491 0.341178 0.629752 x

x Se 7 0.333355 0.344376 0.871728 x

x Se 8 0.263320 0.656451 0.368761 x

x Se 9 0.466797 0.653269 0.128866 x

x Se 10 0.531562 0.339008 0.617555 x

x Se 11 0.533244 0.346899 0.871256 x

x Se 12 0.468343 0.660502 0.382594 x

x Se 13 0.666644 0.655809 0.128275 x

x Se 14 0.736640 0.343372 0.631410 x

x Se 15 0.731095 0.330154 0.875859 x

x Se 16 0.668289 0.658236 0.370364 x

x Se 17 0.867323 0.658005 0.128094 x

x Se 18 0.932734 0.338142 0.624359 x

x Se 19 0.932996 0.338750 0.878186 x

x Se 20 0.868272 0.661526 0.372490 x

x Nb 1 0.001918 0.000532 0.247545 x

x Nb 2 -0.002644 -0.002178 0.751673 x

x Nb 3 -0.000320 -0.000870 0.000102 x

x Nb 4 0.001438 0.002873 0.499578 x

x Nb 5 0.196503 -0.008816 0.245665 x

x Nb 6 0.198849 0.002116 0.750083 x

x Nb 7 0.200311 0.005838 -0.001644 x

x Nb 8 0.201332 0.007486 0.499117 x

x Nb 9 0.402016 -0.001404 0.253371 x

x Nb 10 0.403480 0.017477 0.750545 x

x Nb 11 0.402802 0.001899 -0.000610 x

x Nb 12 0.382844 -0.040161 0.500463 x

x Nb 13 0.596668 -0.016934 0.249793 x

x Nb 14 0.597757 0.000717 0.746812 x

x Nb 15 0.597291 -0.002135 0.001080 x

x Nb 16 0.616973 0.040319 0.499746 x

x Nb 17 0.800962 -0.002566 0.250339 x

x Nb 18 0.804426 0.011008 0.754209 x

x Nb 19 0.800098 -0.004336 0.001868 x

x Nb 20 0.797385 -0.010661 0.500926 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599999E+004 64991.84 <-- SCF

1 -3.62600889E+004 2.22578015E-003 65019.11 <-- SCF

2 -3.62600931E+004 1.03708011E-004 65046.00 <-- SCF

3 -3.62600883E+004 -1.20579916E-004 65072.55 <-- SCF

4 -3.62600258E+004 -1.56212776E-003 65098.05 <-- SCF

5 -3.62600280E+004 5.56413638E-005 65124.45 <-- SCF

6 -3.62600267E+004 -3.24793641E-005 65148.16 <-- SCF

7 -3.62600264E+004 -8.27381844E-006 65167.95 <-- SCF

8 -3.62600263E+004 -1.34295876E-006 65187.97 <-- SCF

9 -3.62600263E+004 1.91437618E-007 65204.91 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02631931 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00335 -0.00357 -0.00600 \*

\* Se 2 0.01350 0.00219 0.01188 \*

\* Se 3 0.00951 0.00060 -0.00452 \*

\* Se 4 -0.00562 0.00698 -0.06501 \*

\* Se 5 -0.01195 -0.02488 -0.01266 \*

\* Se 6 -0.00207 -0.00241 -0.00263 \*

\* Se 7 -0.00198 0.00278 0.01849 \*

\* Se 8 -0.00086 -0.00624 0.00260 \*

\* Se 9 0.00380 0.00017 -0.00038 \*

\* Se 10 0.00808 0.01220 0.00401 \*

\* Se 11 0.00178 0.00021 0.00418 \*

\* Se 12 -0.00109 -0.00068 0.00986 \*

\* Se 13 0.00209 -0.01141 0.01578 \*

\* Se 14 -0.00000 0.00843 0.00357 \*

\* Se 15 -0.00586 -0.00151 -0.00573 \*

\* Se 16 -0.00765 0.00662 0.00919 \*

\* Se 17 -0.00990 -0.00485 0.00236 \*

\* Se 18 -0.01156 -0.00049 -0.05559 \*

\* Se 19 0.00190 0.00816 0.01062 \*

\* Se 20 -0.00648 0.00258 0.00540 \*

\* Nb 1 -0.01447 0.00456 0.02019 \*

\* Nb 2 0.00534 0.00771 -0.01763 \*

\* Nb 3 -0.00737 -0.00087 0.00146 \*

\* Nb 4 0.02812 0.00569 0.00241 \*

\* Nb 5 0.01149 0.01323 0.01039 \*

\* Nb 6 -0.00005 0.00185 0.00130 \*

\* Nb 7 0.01016 0.01124 0.01048 \*

\* Nb 8 0.00291 -0.00575 0.00305 \*

\* Nb 9 -0.00746 -0.00243 0.00489 \*

\* Nb 10 0.00407 -0.00705 0.00803 \*

\* Nb 11 0.01126 0.01180 0.00099 \*

\* Nb 12 0.00156 0.00424 -0.00576 \*

\* Nb 13 0.00283 0.00338 -0.00342 \*

\* Nb 14 0.00446 -0.00125 0.00220 \*

\* Nb 15 -0.01259 -0.01436 0.00292 \*

\* Nb 16 -0.00532 -0.00572 0.00926 \*

\* Nb 17 0.00058 -0.00368 0.00800 \*

\* Nb 18 0.00009 -0.01266 0.00082 \*

\* Nb 19 0.00678 -0.01194 -0.00821 \*

\* Nb 20 -0.02139 0.00712 0.00322 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.002024 0.004587 -0.002540 \*

\* y 0.004587 -0.002696 -0.001108 \*

\* z -0.002540 -0.001108 -0.000336 \*

\* \*

\* Pressure: 0.0003 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000011 | -36260.026166 | <-- min BFGS

| trial step | 1.000000 | 1.329E-006 | -36260.026362 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 99 with enthalpy= -3.62600264E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 4.886339E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 6.562450E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.346391E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.586699E-003 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 100 ...

================================================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.870E-006 | -36260.026362 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 100 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8565504 -8.3006702 0.0041088 0.4205440 -0.0042590 -0.0001245

0.0342236 3.3792956 0.0004603 1.0329956 1.8488565 -0.0005002

0.0041482 0.0014601 13.9640319 -0.0001578 -0.0000597 0.4499550

Lattice parameters(A) Cell Angles

a = 17.018174 alpha = 89.986032

b = 3.379469 beta = 89.974231

c = 13.964033 gamma = 118.612777

Current cell volume = 705.026480 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067112 0.661252 0.121764 x

x Se 2 0.131869 0.339309 0.628007 x

x Se 3 0.132214 0.340164 0.872382 x

x Se 4 0.067269 0.661578 0.372803 x

x Se 5 0.269377 0.671754 0.124791 x

x Se 6 0.331495 0.341180 0.629752 x

x Se 7 0.333372 0.344440 0.871698 x

x Se 8 0.263343 0.656534 0.368799 x

x Se 9 0.466795 0.653477 0.128879 x

x Se 10 0.531549 0.338763 0.617531 x

x Se 11 0.533254 0.346708 0.871257 x

x Se 12 0.468353 0.660733 0.382627 x

x Se 13 0.666630 0.655801 0.128249 x

x Se 14 0.736606 0.343242 0.631385 x

x Se 15 0.731063 0.329800 0.875801 x

x Se 16 0.668279 0.658199 0.370355 x

x Se 17 0.867292 0.658032 0.128054 x

x Se 18 0.932733 0.338374 0.624450 x

x Se 19 0.932989 0.338827 0.878176 x

x Se 20 0.868308 0.661675 0.372539 x

x Nb 1 0.001741 0.000107 0.247432 x

x Nb 2 -0.002516 -0.001865 0.751736 x

x Nb 3 -0.000338 -0.000962 0.000102 x

x Nb 4 0.001540 0.003117 0.499554 x

x Nb 5 0.196628 -0.008307 0.245634 x

x Nb 6 0.198789 0.001751 0.750116 x

x Nb 7 0.200310 0.005676 -0.001582 x

x Nb 8 0.201267 0.007344 0.499135 x

x Nb 9 0.401999 -0.001130 0.253434 x

x Nb 10 0.403580 0.017660 0.750512 x

x Nb 11 0.402870 0.002160 -0.000620 x

x Nb 12 0.382874 -0.039855 0.500495 x

x Nb 13 0.596586 -0.017015 0.249842 x

x Nb 14 0.597746 0.000367 0.746751 x

x Nb 15 0.597244 -0.002424 0.001131 x

x Nb 16 0.616935 0.040133 0.499704 x

x Nb 17 0.801002 -0.002329 0.250347 x

x Nb 18 0.804360 0.010641 0.754234 x

x Nb 19 0.800144 -0.004084 0.001830 x

x Nb 20 0.797333 -0.010828 0.500916 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -3.62599874E+004 65309.03 <-- SCF

1 -3.62601440E+004 3.91480978E-003 65336.22 <-- SCF

2 -3.62601526E+004 2.16951767E-004 65363.98 <-- SCF

3 -3.62601443E+004 -2.08339763E-004 65390.77 <-- SCF

4 -3.62600242E+004 -3.00215374E-003 65416.42 <-- SCF

5 -3.62600290E+004 1.20365777E-004 65443.02 <-- SCF

6 -3.62600270E+004 -4.98226146E-005 65468.03 <-- SCF

7 -3.62600264E+004 -1.48200391E-005 65488.30 <-- SCF

8 -3.62600263E+004 -3.08618639E-006 65508.64 <-- SCF

9 -3.62600263E+004 6.09506925E-007 65526.20 <-- SCF

10 -3.62600264E+004 3.51135916E-007 65542.77 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -36260.02635927 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00349 0.00653 -0.00760 \*

\* Se 2 0.02481 0.00000 0.01654 \*

\* Se 3 0.01511 0.00298 -0.01087 \*

\* Se 4 -0.02004 0.00785 -0.07447 \*

\* Se 5 -0.02117 -0.03934 -0.02525 \*

\* Se 6 -0.00698 0.00044 0.00211 \*

\* Se 7 -0.00395 0.00061 0.02989 \*

\* Se 8 -0.00577 -0.00483 -0.00140 \*

\* Se 9 0.00316 -0.00509 -0.00036 \*

\* Se 10 0.01457 0.02422 0.01070 \*

\* Se 11 0.00331 0.00679 0.00282 \*

\* Se 12 -0.00391 -0.01065 0.00033 \*

\* Se 13 0.00352 -0.01331 0.03010 \*

\* Se 14 0.00675 0.00888 0.00768 \*

\* Se 15 -0.01002 0.00977 -0.00330 \*

\* Se 16 -0.00508 0.00711 0.00852 \*

\* Se 17 -0.01301 -0.00978 0.00569 \*

\* Se 18 -0.01162 -0.01112 -0.06513 \*

\* Se 19 0.00467 0.00064 0.01118 \*

\* Se 20 -0.01214 0.00506 0.00545 \*

\* Nb 1 -0.00745 0.00547 0.03032 \*

\* Nb 2 -0.00139 0.01049 -0.02492 \*

\* Nb 3 -0.00777 -0.00026 0.00154 \*

\* Nb 4 0.02655 0.00742 0.00313 \*

\* Nb 5 0.01095 0.01115 0.01667 \*

\* Nb 6 -0.00175 0.00505 -0.00231 \*

\* Nb 7 0.01444 0.01446 0.01110 \*

\* Nb 8 0.00329 -0.00595 0.00103 \*

\* Nb 9 -0.00195 -0.00698 0.00131 \*

\* Nb 10 -0.00199 -0.00574 0.01042 \*

\* Nb 11 0.00756 0.01096 0.00336 \*

\* Nb 12 0.00276 0.00239 -0.00811 \*

\* Nb 13 0.01121 0.00075 -0.00778 \*

\* Nb 14 0.00188 0.00334 0.00803 \*

\* Nb 15 -0.00964 -0.01273 -0.00127 \*

\* Nb 16 -0.00708 -0.00457 0.01251 \*

\* Nb 17 0.00360 -0.00495 0.00901 \*

\* Nb 18 0.00095 -0.01025 -0.00327 \*

\* Nb 19 0.00583 -0.01462 -0.00937 \*

\* Nb 20 -0.01570 0.00780 0.00598 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.006951 -0.002284 0.001161 \*

\* y -0.002284 0.004784 0.007521 \*

\* z 0.001161 0.007521 0.005227 \*

\* \*

\* Pressure: -0.0010 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.870E-006 | -36260.026362 | <-- min BFGS

| trial step | 1.000000 | -2.434E-006 | -36260.026399 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 100 with enthalpy= -3.62600264E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 9.308823E-007 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 7.751634E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.075266E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 7.520606E-003 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

BFGS: WARNING - Geometry optimization failed to converge after 100 steps

================================================================================

BFGS: Final Configuration:

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8565504 -8.3006702 0.0041088 0.4205440 -0.0042590 -0.0001245

0.0342236 3.3792956 0.0004603 1.0329956 1.8488565 -0.0005002

0.0041482 0.0014601 13.9640319 -0.0001578 -0.0000597 0.4499550

Lattice parameters(A) Cell Angles

a = 17.018174 alpha = 89.986032

b = 3.379469 beta = 89.974231

c = 13.964033 gamma = 118.612777

Current cell volume = 705.026480 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.067112 0.661252 0.121764 x

x Se 2 0.131869 0.339309 0.628007 x

x Se 3 0.132214 0.340164 0.872382 x

x Se 4 0.067269 0.661578 0.372803 x

x Se 5 0.269377 0.671754 0.124791 x

x Se 6 0.331495 0.341180 0.629752 x

x Se 7 0.333372 0.344440 0.871698 x

x Se 8 0.263343 0.656534 0.368799 x

x Se 9 0.466795 0.653477 0.128879 x

x Se 10 0.531549 0.338763 0.617531 x

x Se 11 0.533254 0.346708 0.871257 x

x Se 12 0.468353 0.660733 0.382627 x

x Se 13 0.666630 0.655801 0.128249 x

x Se 14 0.736606 0.343242 0.631385 x

x Se 15 0.731063 0.329800 0.875801 x

x Se 16 0.668279 0.658199 0.370355 x

x Se 17 0.867292 0.658032 0.128054 x

x Se 18 0.932733 0.338374 0.624450 x

x Se 19 0.932989 0.338827 0.878176 x

x Se 20 0.868308 0.661675 0.372539 x

x Nb 1 0.001741 0.000107 0.247432 x

x Nb 2 -0.002516 -0.001865 0.751736 x

x Nb 3 -0.000338 -0.000962 0.000102 x

x Nb 4 0.001540 0.003117 0.499554 x

x Nb 5 0.196628 -0.008307 0.245634 x

x Nb 6 0.198789 0.001751 0.750116 x

x Nb 7 0.200310 0.005676 -0.001582 x

x Nb 8 0.201267 0.007344 0.499135 x

x Nb 9 0.401999 -0.001130 0.253434 x

x Nb 10 0.403580 0.017660 0.750512 x

x Nb 11 0.402870 0.002160 -0.000620 x

x Nb 12 0.382874 -0.039855 0.500495 x

x Nb 13 0.596586 -0.017015 0.249842 x

x Nb 14 0.597746 0.000367 0.746751 x

x Nb 15 0.597244 -0.002424 0.001131 x

x Nb 16 0.616935 0.040133 0.499704 x

x Nb 17 0.801002 -0.002329 0.250347 x

x Nb 18 0.804360 0.010641 0.754234 x

x Nb 19 0.800144 -0.004084 0.001830 x

x Nb 20 0.797333 -0.010828 0.500916 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

BFGS: Final Enthalpy = -3.62600264E+004 eV

BFGS: Final <frequency> = 1436.58331 cm-1

BFGS: Final bulk modulus = 276.80115 GPa

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\* There were at least 1 warnings during this run \*\*\*

\*\*\* => please check the whole of this file carefully! \*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00349 0.00653 -0.00760 \*

\* Se 2 0.02481 0.00000 0.01654 \*

\* Se 3 0.01511 0.00298 -0.01087 \*

\* Se 4 -0.02004 0.00785 -0.07447 \*

\* Se 5 -0.02117 -0.03934 -0.02525 \*

\* Se 6 -0.00698 0.00044 0.00211 \*

\* Se 7 -0.00395 0.00061 0.02989 \*

\* Se 8 -0.00577 -0.00483 -0.00140 \*

\* Se 9 0.00316 -0.00509 -0.00036 \*

\* Se 10 0.01457 0.02422 0.01070 \*

\* Se 11 0.00331 0.00679 0.00282 \*

\* Se 12 -0.00391 -0.01065 0.00033 \*

\* Se 13 0.00352 -0.01331 0.03010 \*

\* Se 14 0.00675 0.00888 0.00768 \*

\* Se 15 -0.01002 0.00977 -0.00330 \*

\* Se 16 -0.00508 0.00711 0.00852 \*

\* Se 17 -0.01301 -0.00978 0.00569 \*

\* Se 18 -0.01162 -0.01112 -0.06513 \*

\* Se 19 0.00467 0.00064 0.01118 \*

\* Se 20 -0.01214 0.00506 0.00545 \*

\* Nb 1 -0.00745 0.00547 0.03032 \*

\* Nb 2 -0.00139 0.01049 -0.02492 \*

\* Nb 3 -0.00777 -0.00026 0.00154 \*

\* Nb 4 0.02655 0.00742 0.00313 \*

\* Nb 5 0.01095 0.01115 0.01667 \*

\* Nb 6 -0.00175 0.00505 -0.00231 \*

\* Nb 7 0.01444 0.01446 0.01110 \*

\* Nb 8 0.00329 -0.00595 0.00103 \*

\* Nb 9 -0.00195 -0.00698 0.00131 \*

\* Nb 10 -0.00199 -0.00574 0.01042 \*

\* Nb 11 0.00756 0.01096 0.00336 \*

\* Nb 12 0.00276 0.00239 -0.00811 \*

\* Nb 13 0.01121 0.00075 -0.00778 \*

\* Nb 14 0.00188 0.00334 0.00803 \*

\* Nb 15 -0.00964 -0.01273 -0.00127 \*

\* Nb 16 -0.00708 -0.00457 0.01251 \*

\* Nb 17 0.00360 -0.00495 0.00901 \*

\* Nb 18 0.00095 -0.01025 -0.00327 \*

\* Nb 19 0.00583 -0.01462 -0.00937 \*

\* Nb 20 -0.01570 0.00780 0.00598 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.006951 -0.002284 0.001161 \*

\* y -0.002284 0.004784 0.007521 \*

\* z 0.001161 0.007521 0.005227 \*

\* \*

\* Pressure: -0.0010 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Pseudo atomic calculation performed for Se 4s2 4p4

Converged in 17 iterations to a total energy of -256.4822 eV

Pseudo atomic calculation performed for Nb 4s2 4p6 4d4 5s1

Converged in 18 iterations to a total energy of -1541.3312 eV

Charge spilling parameter for spin component 1 = 0.27%

Atomic Populations (Mulliken)

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Species Ion s p d f Total Charge (e)

==============================================================

Se 1 1.38 4.22 0.00 0.00 5.60 0.40

Se 2 1.37 4.22 0.00 0.00 5.59 0.41

Se 3 1.38 4.22 0.00 0.00 5.60 0.40

Se 4 1.38 4.22 0.00 0.00 5.60 0.40

Se 5 1.38 4.22 0.00 0.00 5.60 0.40

Se 6 1.36 4.22 0.00 0.00 5.58 0.42

Se 7 1.38 4.22 0.00 0.00 5.60 0.40

Se 8 1.33 4.21 0.00 0.00 5.55 0.45

Se 9 1.38 4.21 0.00 0.00 5.59 0.41

Se 10 1.42 4.25 0.00 0.00 5.67 0.33

Se 11 1.39 4.21 0.00 0.00 5.60 0.40

Se 12 1.42 4.25 0.00 0.00 5.68 0.32

Se 13 1.38 4.22 0.00 0.00 5.60 0.40

Se 14 1.33 4.21 0.00 0.00 5.55 0.45

Se 15 1.38 4.22 0.00 0.00 5.61 0.39

Se 16 1.36 4.22 0.00 0.00 5.58 0.42

Se 17 1.37 4.22 0.00 0.00 5.59 0.41

Se 18 1.38 4.22 0.00 0.00 5.60 0.40

Se 19 1.38 4.21 0.00 0.00 5.59 0.41

Se 20 1.38 4.23 0.00 0.00 5.60 0.40

Nb 1 2.59 6.67 4.14 0.00 13.39 -0.39

Nb 2 2.59 6.67 4.14 0.00 13.39 -0.39

Nb 3 2.55 6.60 4.26 0.00 13.41 -0.41

Nb 4 2.56 6.63 4.22 0.00 13.41 -0.41

Nb 5 2.59 6.67 4.14 0.00 13.41 -0.41

Nb 6 2.59 6.66 4.15 0.00 13.40 -0.40

Nb 7 2.55 6.61 4.23 0.00 13.40 -0.40

Nb 8 2.58 6.65 4.21 0.00 13.43 -0.43

Nb 9 2.59 6.67 4.13 0.00 13.38 -0.38

Nb 10 2.59 6.68 4.14 0.00 13.41 -0.41

Nb 11 2.56 6.63 4.22 0.00 13.41 -0.41

Nb 12 2.57 6.59 4.21 0.00 13.37 -0.37

Nb 13 2.59 6.68 4.14 0.00 13.41 -0.41

Nb 14 2.59 6.67 4.12 0.00 13.38 -0.38

Nb 15 2.56 6.63 4.22 0.00 13.41 -0.41

Nb 16 2.57 6.59 4.22 0.00 13.38 -0.38

Nb 17 2.59 6.66 4.15 0.00 13.40 -0.40

Nb 18 2.59 6.68 4.14 0.00 13.41 -0.41

Nb 19 2.55 6.61 4.23 0.00 13.40 -0.40

Nb 20 2.58 6.64 4.21 0.00 13.42 -0.42

==============================================================

Bond Population Length (A)

============================================================

Se 8 -- Nb 12 -1.35 2.56474

Se 14 -- Nb 16 -1.37 2.56600

Se 11 -- Nb 10 -1.37 2.56970

Se 9 -- Nb 13 -1.39 2.57304

Se 16 -- Nb 16 -0.77 2.57634

Se 6 -- Nb 12 -0.75 2.57738

Se 19 -- Nb 18 -1.54 2.58774

Se 16 -- Nb 17 -1.32 2.59614

Se 19 -- Nb 3 -0.84 2.59677

Se 1 -- Nb 5 -1.57 2.59695

Se 17 -- Nb 17 -1.86 2.59727

Se 3 -- Nb 6 -1.84 2.59747

Se 2 -- Nb 6 -1.87 2.59825

Se 1 -- Nb 3 -0.84 2.59911

Se 6 -- Nb 6 -1.32 2.59915

Se 20 -- Nb 17 -1.82 2.59987

Se 8 -- Nb 5 -2.00 2.60047

Se 7 -- Nb 10 -1.69 2.60264

Se 14 -- Nb 18 -2.03 2.60343

Se 11 -- Nb 14 -1.81 2.60411

Se 13 -- Nb 13 -1.72 2.60536

Se 9 -- Nb 9 -1.82 2.60672

Se 16 -- Nb 13 -2.00 2.60938

Se 17 -- Nb 1 -1.45 2.61181

Se 6 -- Nb 10 -1.99 2.61333

Se 5 -- Nb 5 -1.92 2.61352

Se 4 -- Nb 1 -1.94 2.61535

Se 1 -- Nb 1 -1.93 2.61683

Se 19 -- Nb 2 -1.95 2.61865

Se 8 -- Nb 9 -1.26 2.62349

Se 4 -- Nb 5 -1.69 2.62444

Se 15 -- Nb 18 -1.91 2.62463

Se 14 -- Nb 14 -1.24 2.62591

Se 3 -- Nb 2 -1.48 2.62632

Se 18 -- Nb 2 -1.91 2.62868

Se 19 -- Nb 19 -1.23 2.63094

Se 1 -- Nb 7 -1.20 2.63215

Se 7 -- Nb 6 -1.67 2.63313

Se 18 -- Nb 4 -0.85 2.63369

Se 13 -- Nb 17 -1.70 2.63535

Se 4 -- Nb 4 -0.84 2.63590

Se 18 -- Nb 18 -1.72 2.63854

Se 17 -- Nb 19 -0.88 2.63952

Se 3 -- Nb 7 -0.90 2.64079

Se 13 -- Nb 15 -0.93 2.64225

Se 9 -- Nb 15 -1.19 2.64306

Se 14 -- Nb 20 -0.95 2.64349

Se 11 -- Nb 11 -1.18 2.64596

Se 7 -- Nb 11 -0.90 2.64656

Se 9 -- Nb 11 -0.78 2.64739

Se 2 -- Nb 2 -1.60 2.64854

Se 15 -- Nb 19 -0.80 2.64874

Se 8 -- Nb 8 -0.98 2.64920

Se 2 -- Nb 4 -1.18 2.64928

Se 11 -- Nb 15 -0.77 2.65003

Se 20 -- Nb 1 -1.63 2.65040

Se 5 -- Nb 7 -0.83 2.65184

Se 5 -- Nb 11 -1.15 2.65342

Se 16 -- Nb 20 -1.50 2.65525

Se 15 -- Nb 15 -1.12 2.65637

Se 10 -- Nb 14 -1.45 2.65852

Se 12 -- Nb 9 -1.47 2.65939

Se 18 -- Nb 20 -1.22 2.66047

Se 7 -- Nb 7 -1.10 2.66123

Se 13 -- Nb 19 -1.12 2.66349

Se 10 -- Nb 10 -1.60 2.66468

Se 3 -- Nb 3 -1.22 2.66516

Se 17 -- Nb 3 -1.21 2.66534

Se 12 -- Nb 13 -1.61 2.66566

Se 20 -- Nb 4 -1.10 2.66776

Se 6 -- Nb 8 -1.47 2.66855

Se 12 -- Nb 12 -0.72 2.66982

Se 4 -- Nb 8 -1.27 2.67024

Se 10 -- Nb 16 -0.71 2.67094

Se 5 -- Nb 9 -1.63 2.67543

Se 2 -- Nb 8 -1.00 2.67581

Se 20 -- Nb 20 -0.97 2.67897

Se 15 -- Nb 14 -1.63 2.68697

Se 12 -- Nb 16 -0.90 2.75864

Se 10 -- Nb 12 -0.89 2.75933

============================================================

Hirshfeld Analysis

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Species Ion Hirshfeld Charge (e) Spin (hbar/2)

===================================================

Se 1 -0.16 0.00

Se 2 -0.16 0.00

Se 3 -0.16 0.00

Se 4 -0.16 0.00

Se 5 -0.16 0.00

Se 6 -0.16 0.00

Se 7 -0.16 0.00

Se 8 -0.16 0.00

Se 9 -0.16 0.00

Se 10 -0.15 0.00

Se 11 -0.16 0.00

Se 12 -0.15 0.00

Se 13 -0.16 0.00

Se 14 -0.16 0.00

Se 15 -0.16 0.00

Se 16 -0.16 0.00

Se 17 -0.16 0.00

Se 18 -0.16 0.00

Se 19 -0.16 0.00

Se 20 -0.16 0.00

Nb 1 0.17 0.00

Nb 2 0.17 0.00

Nb 3 0.15 0.00

Nb 4 0.16 0.00

Nb 5 0.17 0.00

Nb 6 0.17 0.00

Nb 7 0.15 0.00

Nb 8 0.14 0.00

Nb 9 0.17 0.00

Nb 10 0.17 0.00

Nb 11 0.15 0.00

Nb 12 0.15 0.00

Nb 13 0.17 0.00

Nb 14 0.17 0.00

Nb 15 0.15 0.00

Nb 16 0.15 0.00

Nb 17 0.17 0.00

Nb 18 0.17 0.00

Nb 19 0.15 0.00

Nb 20 0.15 0.00

===================================================

Writing analysis data to 2H-Nb1.1Se2-7-UF.castep\_bin

Writing model to 2H-Nb1.1Se2-7-UF.check

A BibTeX formatted list of references used in this run has been written to

2H-Nb1.1Se2-7-UF.bib

Initialisation time = 1.62 s

Calculation time = 65643.91 s

Finalisation time = 5.44 s

Total time = 65650.97 s

Overall parallel efficiency rating: Very good (84%)

Data was distributed by:-

G-vector (2-way); efficiency rating: Very good (88%)

k-point (7-way); efficiency rating: Excellent (95%)