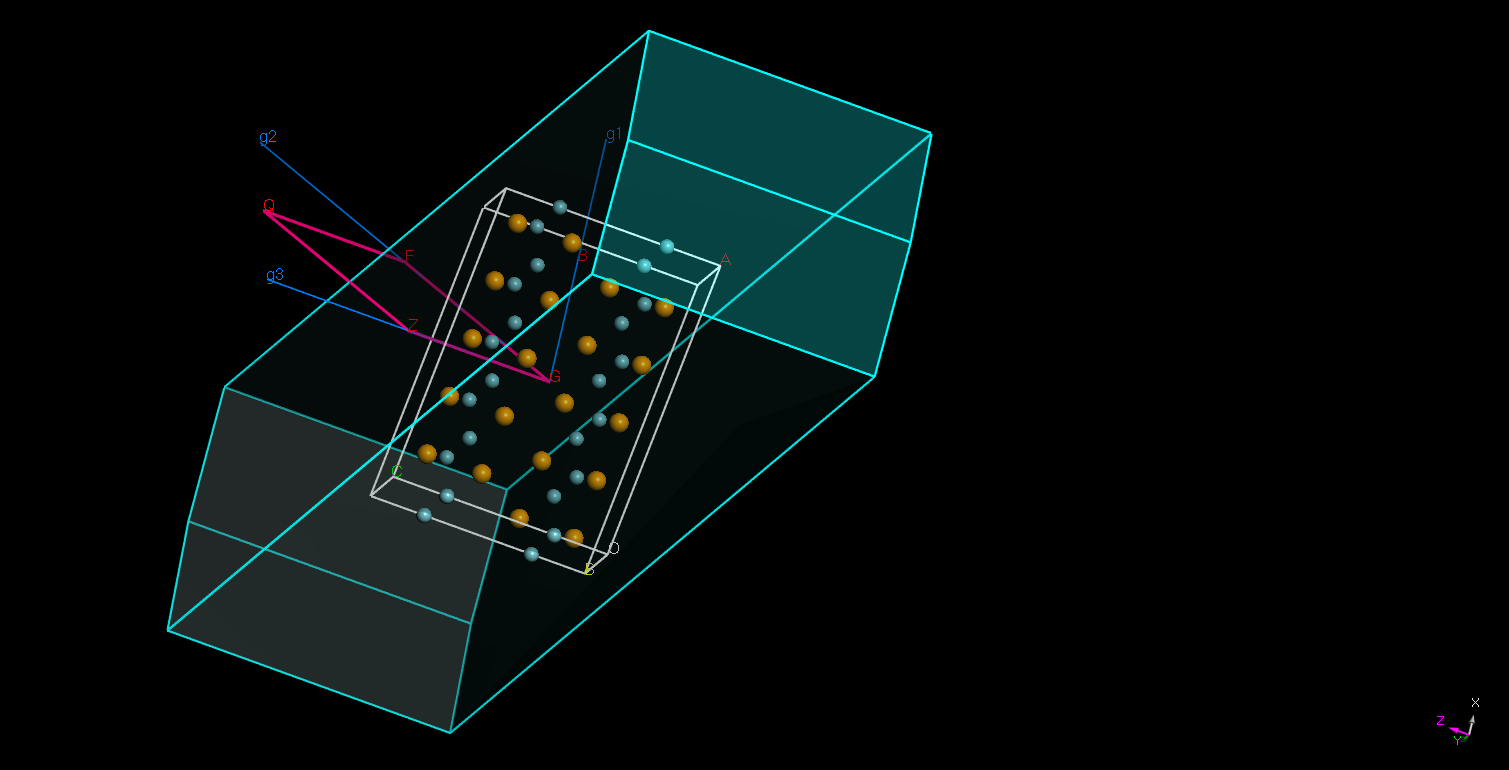
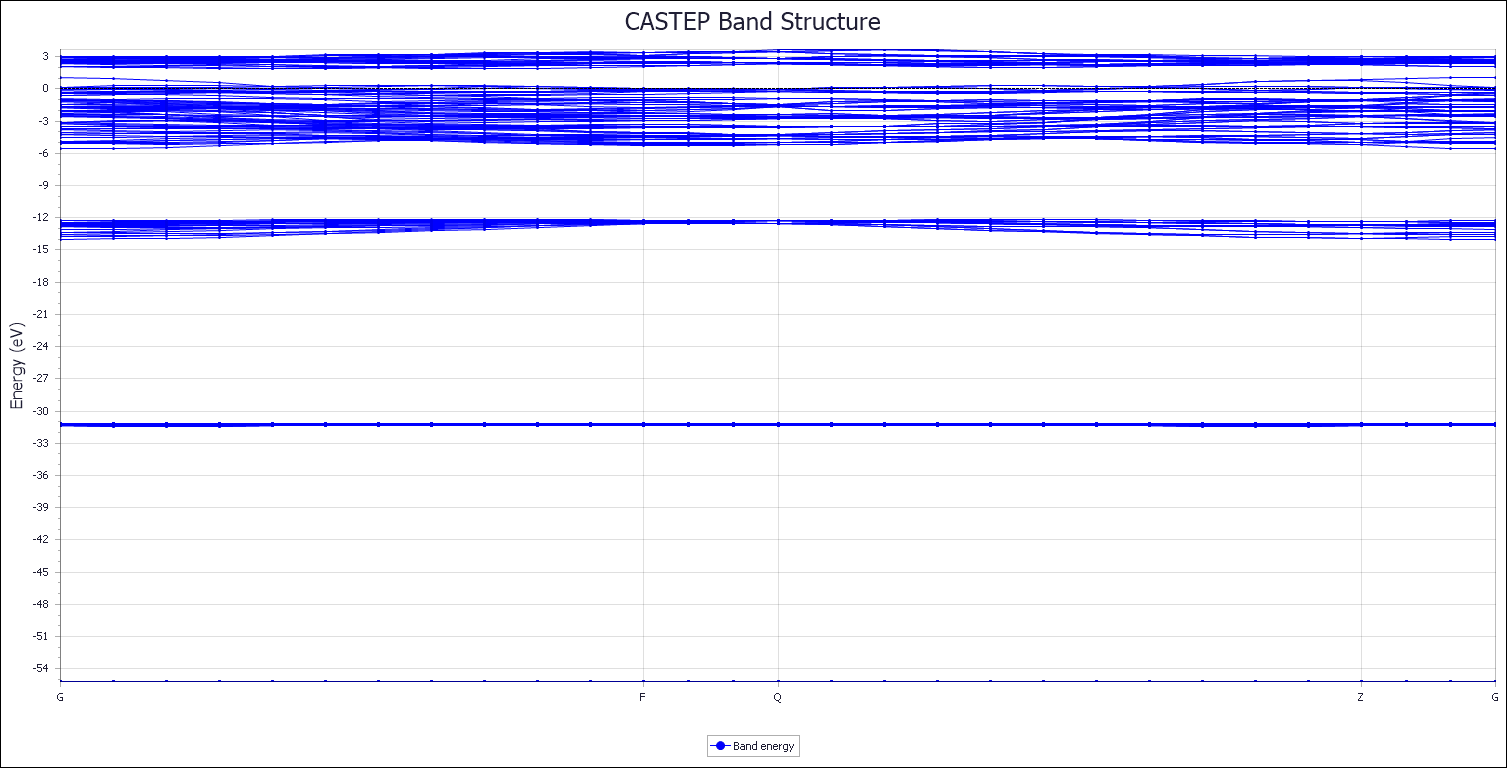
2H-Nb1Se2-7 CASTEP GeomOpt

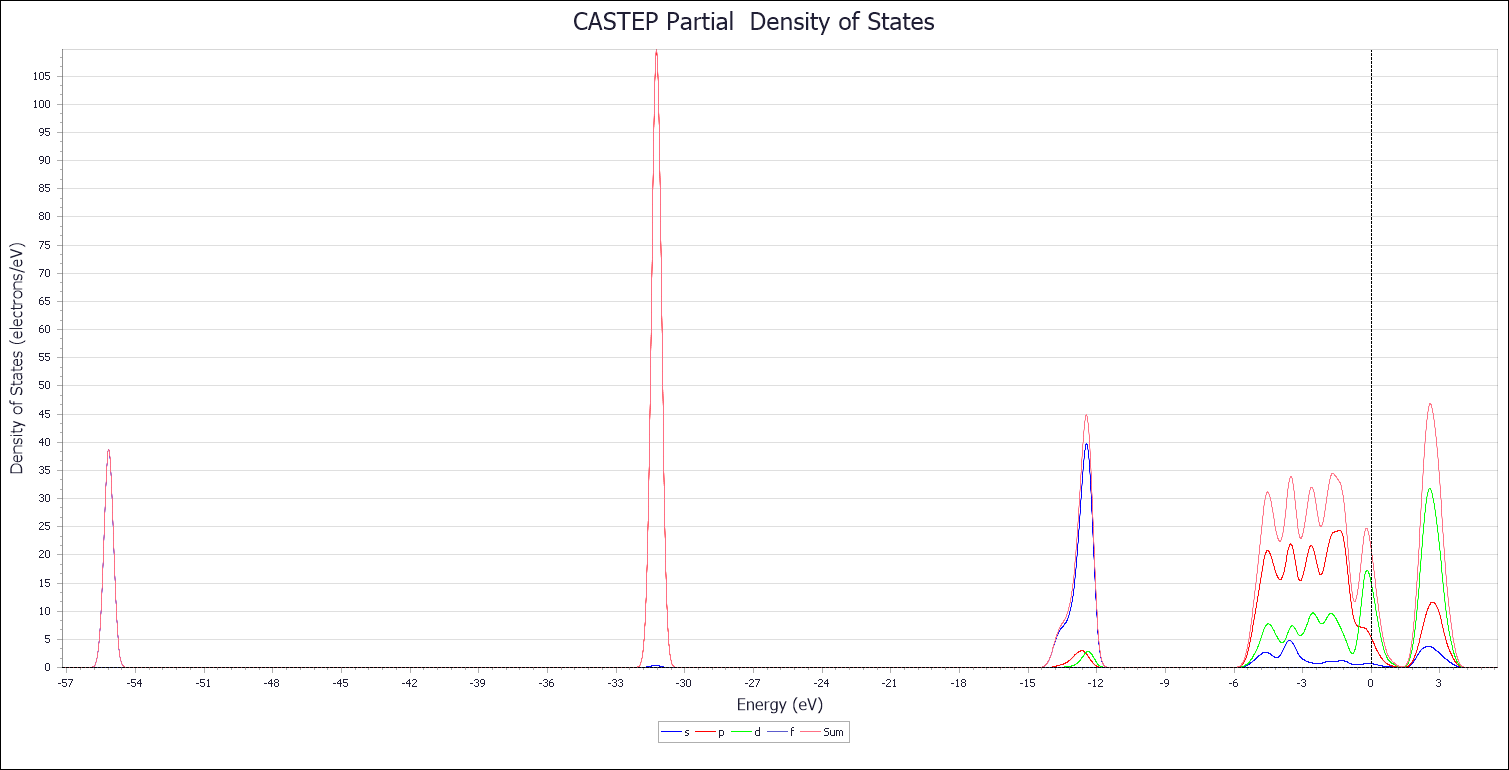
2H-Nb1Se2-7-US



2H-Nb1Se2-7 Band Structure



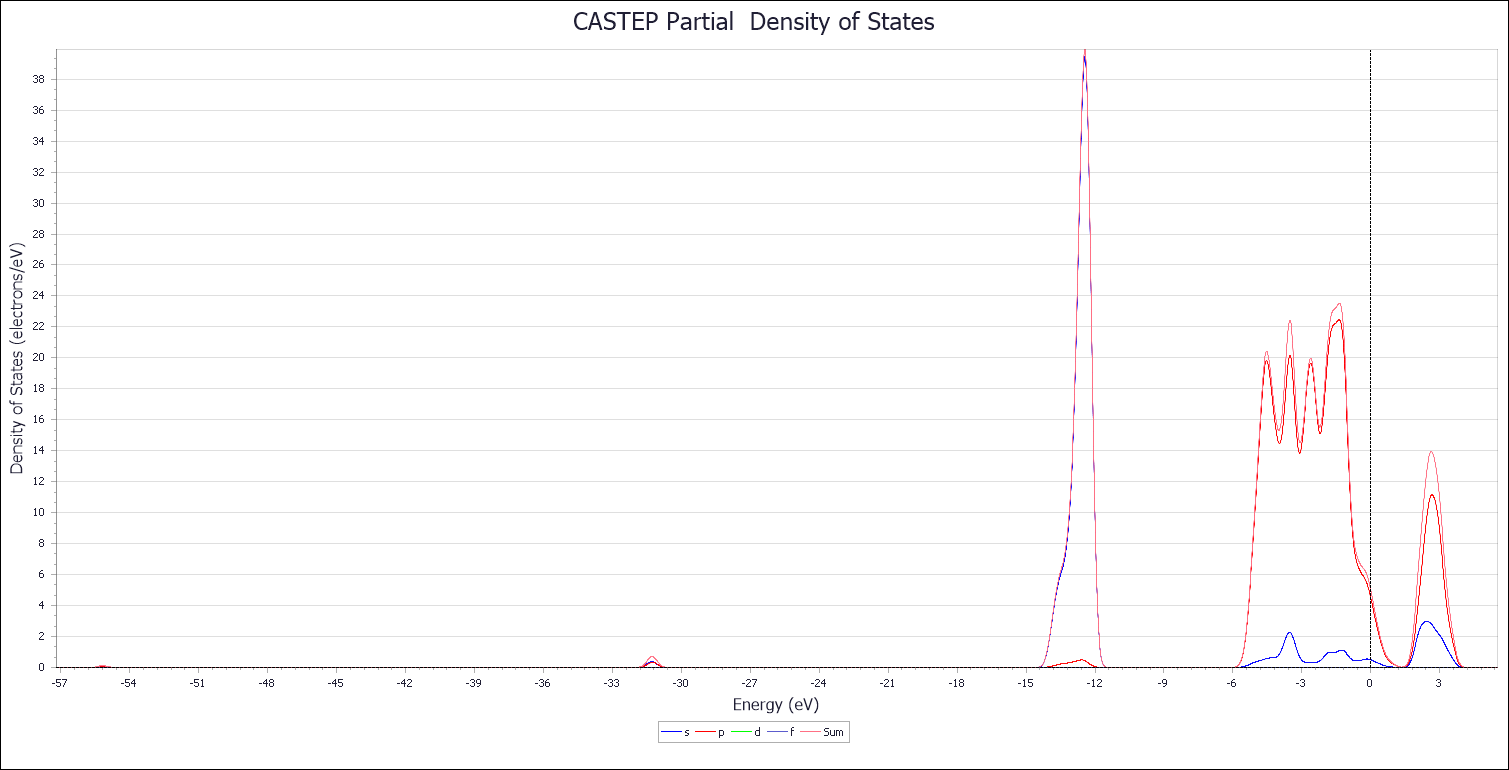
2H-Nb1Se2-7-US- PDOS-Total



2H-Nb1Se2-7 -US-PDOS-Nb



2H-Nb1Se2-7-US- PDOS-Se



Job started on host DESKTOP-UVBHK2J

at Thu Mar 5 08:50:08 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 |

| |

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| |

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| |

| 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 19 iterations to a total energy of -256.4822 eV

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

Converged in 19 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-Nb1Se2-7.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 (85009576)

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 : 2.0000

size of fine grid : 3.0000

size of fine gmax : 34.3673 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 : 250.0

net charge of system : 0.000

net spin of system : 0.000

number of up spins : 125.0

number of down spins : 125.0

treating system as non-spin-polarized

number of bands : 125

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* 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. : 0.5000E-06 eV

eigen-energy convergence tolerance : 0.1200E-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 = 30

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 0.200000 -0.000000 0.250000 x

x Nb 4 0.200000 -0.000000 0.750000 x

x Nb 5 0.400000 -0.000000 0.250000 x

x Nb 6 0.400000 -0.000000 0.750000 x

x Nb 7 0.600000 -0.000000 0.250000 x

x Nb 8 0.600000 -0.000000 0.750000 x

x Nb 9 0.800000 -0.000000 0.250000 x

x Nb 10 0.800000 -0.000000 0.750000 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 171.1 MB 880.0 MB |

| Electronic energy minimisation requirements 81.1 MB 0.0 MB |

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

| Approx. total storage required per process 252.1 MB 880.0 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 -1.31409114E+004 13.62 <-- SCF

1 -1.99975233E+004 2.28553729E+002 34.36 <-- SCF

2 -2.07286881E+004 2.43721597E+001 49.23 <-- SCF

3 -2.07571550E+004 9.48896478E-001 64.64 <-- SCF

4 -2.07471205E+004 -3.34484578E-001 92.25 <-- SCF

5 -2.07458474E+004 -4.24360834E-002 121.39 <-- SCF

6 -2.07457769E+004 -2.34807162E-003 148.33 <-- SCF

7 -2.07458188E+004 1.39677814E-003 178.28 <-- SCF

8 -2.07458317E+004 4.29435719E-004 206.47 <-- SCF

9 -2.07458366E+004 1.64203756E-004 234.86 <-- SCF

10 -2.07458384E+004 5.88820378E-005 260.89 <-- SCF

11 -2.07458393E+004 2.90355934E-005 285.56 <-- SCF

12 -2.07458397E+004 1.51078539E-005 309.67 <-- SCF

13 -2.07458399E+004 5.99854761E-006 330.55 <-- SCF

14 -2.07458400E+004 2.78011465E-006 351.03 <-- SCF

15 -2.07458400E+004 1.35017251E-006 371.83 <-- SCF

16 -2.07458401E+004 7.88921771E-007 392.55 <-- SCF

17 -2.07458401E+004 4.92666569E-007 412.89 <-- SCF

18 -2.07458401E+004 3.55314874E-007 433.28 <-- SCF

19 -2.07458401E+004 3.12884103E-007 453.72 <-- SCF

20 -2.07458401E+004 2.35738353E-007 474.20 <-- SCF

21 -2.07458401E+004 1.98392184E-007 494.59 <-- SCF

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

Final energy = -20745.84011441 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 -2.07458401E+004 519.95 <-- SCF

1 -2.07458448E+004 1.56804941E-004 536.00 <-- SCF

2 -2.07458448E+004 5.48883347E-007 557.00 <-- SCF

3 -2.07458448E+004 3.20392831E-007 578.55 <-- SCF

4 -2.07458448E+004 -5.04085578E-007 598.81 <-- SCF

5 -2.07458448E+004 2.32337894E-007 619.56 <-- SCF

6 -2.07458448E+004 2.73247038E-007 639.69 <-- SCF

7 -2.07458448E+004 3.76635699E-008 659.77 <-- SCF

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

Final energy = -20745.84484505 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 -2.07458448E+004 685.17 <-- SCF

1 -2.07458512E+004 2.12687479E-004 701.06 <-- SCF

2 -2.07458513E+004 4.60071628E-006 724.02 <-- SCF

3 -2.07458635E+004 4.04961972E-004 751.66 <-- SCF

4 -2.07458449E+004 -6.19852005E-004 778.42 <-- SCF

5 -2.07458473E+004 8.10929703E-005 802.84 <-- SCF

6 -2.07458484E+004 3.61898599E-005 823.23 <-- SCF

7 -2.07458490E+004 1.88534231E-005 843.28 <-- SCF

8 -2.07458494E+004 1.42017994E-005 863.55 <-- SCF

9 -2.07458495E+004 5.34751767E-006 883.70 <-- SCF

10 -2.07458496E+004 1.98144357E-006 903.69 <-- SCF

11 -2.07458496E+004 -5.26050589E-007 923.73 <-- SCF

12 -2.07458496E+004 -2.92875367E-007 943.69 <-- SCF

13 -2.07458496E+004 3.61135128E-007 963.56 <-- SCF

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

Final energy = -20745.84959423 eV

(energy not corrected for finite basis set)

For future reference: finite basis dEtot/dlog(Ecut) = -0.468686eV

Total energy corrected for finite basis set = -20745.849632 eV

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

| Memory Disk |

| Model and support data 171.1 MB 880.0 MB |

| Electronic energy minimisation requirements 81.1 MB 0.0 MB |

| Geometry minimisation requirements 101.5 MB 0.0 MB |

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

| Approx. total storage required per process 353.7 MB 880.0 MB |

| |

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

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

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.05559 -0.01833 0.17413 \*

\* Se 2 0.00406 0.02971 0.13206 \*

\* Se 3 -0.03458 0.02985 -0.13572 \*

\* Se 4 0.01727 -0.01816 -0.17011 \*

\* Se 5 0.01139 -0.01411 0.13631 \*

\* Se 6 -0.00892 0.02747 0.17046 \*

\* Se 7 -0.04798 0.02764 -0.17435 \*

\* Se 8 -0.02649 -0.01394 -0.13262 \*

\* Se 9 0.07473 -0.01923 0.17575 \*

\* Se 10 -0.04041 0.01896 0.16704 \*

\* Se 11 -0.07909 0.01902 -0.17087 \*

\* Se 12 0.03664 -0.01914 -0.17176 \*

\* Se 13 0.03992 -0.02760 0.17905 \*

\* Se 14 0.02720 0.01359 0.12235 \*

\* Se 15 -0.01180 0.01375 -0.12601 \*

\* Se 16 0.00180 -0.02738 -0.17514 \*

\* Se 17 0.03618 -0.03044 0.14679 \*

\* Se 18 -0.02757 0.01857 0.16898 \*

\* Se 19 -0.06642 0.01868 -0.17289 \*

\* Se 20 -0.00154 -0.03031 -0.14301 \*

\* Nb 1 -0.06238 0.03521 -0.00117 \*

\* Nb 2 0.06368 -0.03507 0.00113 \*

\* Nb 3 -0.06197 0.03211 -0.00110 \*

\* Nb 4 0.07374 -0.03494 0.00126 \*

\* Nb 5 -0.05796 0.03659 -0.00135 \*

\* Nb 6 0.06641 -0.03266 0.00097 \*

\* Nb 7 -0.06350 0.03231 -0.00114 \*

\* Nb 8 0.06757 -0.03584 0.00134 \*

\* Nb 9 -0.05844 0.03570 -0.00130 \*

\* Nb 10 0.07288 -0.03200 0.00089 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.330567 -0.379724 0.139042 \*

\* y -0.379724 -0.139999 -0.000829 \*

\* z 0.139042 -0.000829 -0.104877 \*

\* \*

\* Pressure: -0.0286 \*

\* \*

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

BFGS: finished iteration 0 with enthalpy= -2.07458496E+004 eV

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

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

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

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

| |F|max | 1.919436E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

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

| Smax | 3.797239E-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 | 0.000072 | -20745.849632 | <-- min BFGS

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

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

BFGS: starting iteration 1 with trial guess (lambda= 1.000000)

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

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

| Memory Disk |

| Model and support data 171.1 MB 880.0 MB |

| Electronic energy minimisation requirements 81.1 MB 0.0 MB |

| Geometry minimisation requirements 101.6 MB 0.0 MB |

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

| Approx. total storage required per process 353.8 MB 880.0 MB |

| |

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

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

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Unit Cell

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

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

14.9226412 -8.6157754 -0.0013885 0.4209890 -0.0001066 0.0000390

0.0008727 3.4478218 0.0000019 1.0520110 1.8220974 0.0000965

-0.0011652 0.0000069 12.5710789 0.0000463 -0.0000003 0.4998127

Lattice parameters(A) Cell Angles

a = 17.231274 alpha = 89.999938

b = 3.447822 beta = 90.009232

c = 12.571079 gamma = 119.986028

Current cell volume = 646.884162 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 0.066671 0.666671 0.117316 x

x Se 2 0.133334 0.333344 0.617312 x

x Se 3 0.133331 0.333337 0.882687 x

x Se 4 0.066668 0.666664 0.382684 x

x Se 5 0.266668 0.666664 0.117313 x

x Se 6 0.333333 0.333341 0.617316 x

x Se 7 0.333330 0.333333 0.882684 x

x Se 8 0.266665 0.666657 0.382688 x

x Se 9 0.466673 0.666675 0.117316 x

x Se 10 0.533330 0.333332 0.617316 x

x Se 11 0.533327 0.333324 0.882684 x

x Se 12 0.466670 0.666667 0.382684 x

x Se 13 0.666670 0.666665 0.117317 x

x Se 14 0.733335 0.333343 0.617311 x

x Se 15 0.733332 0.333336 0.882688 x

x Se 16 0.666667 0.666658 0.382684 x

x Se 17 0.866670 0.666663 0.117314 x

x Se 18 0.933331 0.333334 0.617316 x

x Se 19 0.933328 0.333327 0.882684 x

x Se 20 0.866667 0.666656 0.382687 x

x Nb 1 -0.000005 -0.000000 0.250000 x

x Nb 2 0.000005 0.000001 0.750000 x

x Nb 3 0.199995 -0.000001 0.250000 x

x Nb 4 0.200006 0.000003 0.750000 x

x Nb 5 0.399995 0.000001 0.250000 x

x Nb 6 0.400005 0.000002 0.750000 x

x Nb 7 0.599995 -0.000001 0.250000 x

x Nb 8 0.600005 0.000001 0.750000 x

x Nb 9 0.799995 0.000001 0.250000 x

x Nb 10 0.800006 0.000003 0.750000 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07458374E+004 1344.64 <-- SCF

1 -2.07462209E+004 1.27822594E-002 1363.66 <-- SCF

2 -2.07462283E+004 2.48307641E-004 1390.69 <-- SCF

3 -2.07460518E+004 -5.88427775E-003 1417.81 <-- SCF

4 -2.07457919E+004 -8.66290638E-003 1444.94 <-- SCF

5 -2.07458765E+004 2.81949168E-003 1474.17 <-- SCF

6 -2.07458685E+004 -2.66207182E-004 1501.16 <-- SCF

7 -2.07458496E+004 -6.28110588E-004 1527.41 <-- SCF

8 -2.07458486E+004 -3.54539103E-005 1553.72 <-- SCF

9 -2.07458519E+004 1.11270313E-004 1579.14 <-- SCF

10 -2.07458532E+004 4.41352301E-005 1601.95 <-- SCF

11 -2.07458530E+004 -6.87994318E-006 1624.94 <-- SCF

12 -2.07458520E+004 -3.47385541E-005 1649.00 <-- SCF

13 -2.07458519E+004 -2.13179994E-006 1671.22 <-- SCF

14 -2.07458520E+004 5.11149966E-007 1692.42 <-- SCF

15 -2.07458513E+004 -2.08128038E-005 1715.22 <-- SCF

16 -2.07458514E+004 2.21808721E-006 1735.45 <-- SCF

17 -2.07458513E+004 -3.58024971E-006 1758.19 <-- SCF

18 -2.07458513E+004 1.75844323E-006 1778.28 <-- SCF

19 -2.07458513E+004 2.90623553E-007 1798.31 <-- SCF

20 -2.07458513E+004 5.10774199E-008 1818.91 <-- SCF

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

Final energy = -20745.85134784 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.05112 -0.02029 0.17278 \*

\* Se 2 0.00320 0.02985 0.13043 \*

\* Se 3 -0.03291 0.03022 -0.13462 \*

\* Se 4 0.01555 -0.01999 -0.16845 \*

\* Se 5 0.00332 -0.01451 0.13637 \*

\* Se 6 -0.01336 0.02652 0.16979 \*

\* Se 7 -0.04979 0.02703 -0.17405 \*

\* Se 8 -0.03097 -0.01426 -0.13231 \*

\* Se 9 0.06980 -0.02139 0.17370 \*

\* Se 10 -0.04333 0.01976 0.16437 \*

\* Se 11 -0.07912 0.01994 -0.16841 \*

\* Se 12 0.03413 -0.02112 -0.16932 \*

\* Se 13 0.03267 -0.02879 0.17924 \*

\* Se 14 0.02510 0.01270 0.12294 \*

\* Se 15 -0.01138 0.01297 -0.12640 \*

\* Se 16 -0.00265 -0.02839 -0.17494 \*

\* Se 17 0.03089 -0.03143 0.14367 \*

\* Se 18 -0.03314 0.01830 0.16453 \*

\* Se 19 -0.06909 0.01862 -0.16928 \*

\* Se 20 -0.00462 -0.03097 -0.13987 \*

\* Nb 1 -0.06476 0.04003 -0.00189 \*

\* Nb 2 0.07490 -0.03631 0.00087 \*

\* Nb 3 -0.03905 0.03443 -0.00030 \*

\* Nb 4 0.07089 -0.03525 0.00101 \*

\* Nb 5 -0.05751 0.03983 -0.00030 \*

\* Nb 6 0.07205 -0.03172 0.00026 \*

\* Nb 7 -0.05070 0.03633 -0.00049 \*

\* Nb 8 0.07452 -0.03845 0.00149 \*

\* Nb 9 -0.04473 0.03680 -0.00031 \*

\* Nb 10 0.06897 -0.03045 -0.00051 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.299691 -0.349257 0.135621 \*

\* y -0.349257 -0.136015 -0.001882 \*

\* z 0.135621 -0.001882 -0.106641 \*

\* \*

\* Pressure: -0.0190 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000072 | -20745.849632 | <-- min BFGS

| trial step | 1.000000 | 0.000068 | -20745.851343 | <-- min BFGS

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

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

BFGS: improving iteration 1 with line minimization (lambda= 19.378742)

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Unit Cell

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

14.8220790 -8.5611054 -0.0269078 0.4227129 -0.0020700 0.0007583

0.0169124 3.4537354 0.0000369 1.0478191 1.8141124 0.0018602

-0.0225799 0.0001347 12.5872316 0.0009006 -0.0000097 0.4991730

Lattice parameters(A) Cell Angles

a = 17.116871 alpha = 89.999278

b = 3.453777 beta = 90.179378

c = 12.587252 gamma = 119.729754

Current cell volume = 646.180156 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 0.066751 0.666757 0.117614 x

x Se 2 0.133339 0.333544 0.617538 x

x Se 3 0.133281 0.333398 0.882455 x

x Se 4 0.066693 0.666613 0.382393 x

x Se 5 0.266684 0.666617 0.117546 x

x Se 6 0.333320 0.333480 0.617607 x

x Se 7 0.333260 0.333333 0.882386 x

x Se 8 0.266626 0.666475 0.382461 x

x Se 9 0.466780 0.666824 0.117617 x

x Se 10 0.533272 0.333305 0.617601 x

x Se 11 0.533213 0.333158 0.882392 x

x Se 12 0.466722 0.666680 0.382390 x

x Se 13 0.666727 0.666637 0.117623 x

x Se 14 0.733375 0.333526 0.617521 x

x Se 15 0.733315 0.333379 0.882473 x

x Se 16 0.666669 0.666493 0.382384 x

x Se 17 0.866722 0.666604 0.117565 x

x Se 18 0.933291 0.333351 0.617605 x

x Se 19 0.933233 0.333204 0.882388 x

x Se 20 0.866664 0.666462 0.382442 x

x Nb 1 -0.000095 -0.000005 0.249998 x

x Nb 2 0.000097 0.000011 0.750002 x

x Nb 3 0.199906 -0.000024 0.249998 x

x Nb 4 0.200112 0.000050 0.750002 x

x Nb 5 0.399912 0.000021 0.249998 x

x Nb 6 0.400101 0.000037 0.750002 x

x Nb 7 0.599904 -0.000029 0.249998 x

x Nb 8 0.600103 0.000021 0.750002 x

x Nb 9 0.799911 0.000013 0.249998 x

x Nb 10 0.800111 0.000066 0.750002 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07453645E+004 2200.36 <-- SCF

1 -2.07460841E+004 2.39848231E-002 2216.75 <-- SCF

2 -2.07461358E+004 1.72467890E-003 2249.31 <-- SCF

3 -2.07459237E+004 -7.07067474E-003 2277.47 <-- SCF

4 -2.07458762E+004 -1.58214529E-003 2305.00 <-- SCF

5 -2.07458663E+004 -3.30641147E-004 2332.47 <-- SCF

6 -2.07458648E+004 -5.11294700E-005 2362.12 <-- SCF

7 -2.07458647E+004 -2.12983872E-006 2390.33 <-- SCF

8 -2.07458648E+004 2.99384056E-006 2415.75 <-- SCF

9 -2.07458648E+004 8.63829835E-007 2436.47 <-- SCF

10 -2.07458648E+004 7.54073150E-007 2457.83 <-- SCF

11 -2.07458648E+004 3.42848071E-007 2477.88 <-- SCF

12 -2.07458648E+004 1.29473491E-007 2498.94 <-- SCF

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

Final energy = -20745.86484186 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00196 -0.03149 0.13304 \*

\* Se 2 -0.00402 0.04071 0.11418 \*

\* Se 3 0.01240 0.04525 -0.12242 \*

\* Se 4 0.02049 -0.02792 -0.12619 \*

\* Se 5 -0.03736 -0.02456 0.11415 \*

\* Se 6 -0.00956 0.03604 0.13504 \*

\* Se 7 0.01048 0.04023 -0.13906 \*

\* Se 8 -0.02032 -0.02256 -0.11401 \*

\* Se 9 0.00844 -0.03533 0.13536 \*

\* Se 10 -0.02466 0.03321 0.12827 \*

\* Se 11 -0.00768 0.03552 -0.13835 \*

\* Se 12 0.02589 -0.03303 -0.12552 \*

\* Se 13 -0.00838 -0.04007 0.13709 \*

\* Se 14 0.02125 0.02254 0.11439 \*

\* Se 15 0.03846 0.02489 -0.11447 \*

\* Se 16 0.01134 -0.03598 -0.13287 \*

\* Se 17 -0.01072 -0.04520 0.12078 \*

\* Se 18 -0.01930 0.02827 0.12825 \*

\* Se 19 -0.00077 0.03178 -0.13523 \*

\* Se 20 0.00611 -0.04092 -0.11245 \*

\* Nb 1 -0.00498 0.07527 -0.00074 \*

\* Nb 2 0.00408 -0.07521 0.00149 \*

\* Nb 3 0.00358 0.07396 -0.00131 \*

\* Nb 4 -0.00390 -0.07401 0.00100 \*

\* Nb 5 -0.01098 0.07666 -0.00161 \*

\* Nb 6 -0.00543 -0.07311 0.00096 \*

\* Nb 7 0.00206 0.07268 -0.00054 \*

\* Nb 8 0.00872 -0.07710 0.00157 \*

\* Nb 9 0.00084 0.07371 -0.00173 \*

\* Nb 10 -0.00805 -0.07426 0.00093 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.439481 0.261503 -0.121558 \*

\* y 0.261503 -0.046397 -0.017845 \*

\* z -0.121558 -0.017845 -0.376180 \*

\* \*

\* Pressure: 0.2874 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000072 | -20745.849632 | <-- min BFGS

| trial step | 1.000000 | 0.000068 | -20745.851343 | <-- min BFGS

| line step | 19.378742 | -0.000014 | -20745.864916 | <-- min BFGS

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

BFGS: finished iteration 1 with enthalpy= -2.07458649E+004 eV

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

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

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

| dE/ion | 5.094616E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.451417E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.344199E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.394807E-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 | 0.000089 | -20745.864916 | <-- min BFGS

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

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BFGS: starting iteration 2 with trial guess (lambda= 1.000000)

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Unit Cell

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

14.8398794 -8.5705071 -0.0227088 0.4223854 -0.0017562 0.0006372

0.0143572 3.4530715 0.0000656 1.0483585 1.8152343 0.0015467

-0.0189873 0.0002400 12.5878039 0.0007565 -0.0000126 0.4991498

Lattice parameters(A) Cell Angles

a = 17.136981 alpha = 89.998179

b = 3.453101 beta = 90.151311

c = 12.587818 gamma = 119.769564

Current cell volume = 646.586330 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 0.066741 0.666737 0.117586 x

x Se 2 0.133338 0.333529 0.617518 x

x Se 3 0.133288 0.333405 0.882475 x

x Se 4 0.066691 0.666615 0.382421 x

x Se 5 0.266679 0.666610 0.117525 x

x Se 6 0.333321 0.333471 0.617581 x

x Se 7 0.333270 0.333346 0.882413 x

x Se 8 0.266630 0.666488 0.382481 x

x Se 9 0.466767 0.666796 0.117589 x

x Se 10 0.533278 0.333313 0.617575 x

x Se 11 0.533227 0.333188 0.882419 x

x Se 12 0.466717 0.666673 0.382418 x

x Se 13 0.666719 0.666628 0.117594 x

x Se 14 0.733371 0.333512 0.617503 x

x Se 15 0.733320 0.333387 0.882491 x

x Se 16 0.666670 0.666506 0.382412 x

x Se 17 0.866714 0.666597 0.117542 x

x Se 18 0.933295 0.333354 0.617578 x

x Se 19 0.933245 0.333229 0.882416 x

x Se 20 0.866665 0.666476 0.382465 x

x Nb 1 -0.000084 0.000016 0.249998 x

x Nb 2 0.000085 -0.000011 0.750002 x

x Nb 3 0.199918 0.000001 0.249998 x

x Nb 4 0.200098 0.000022 0.750002 x

x Nb 5 0.399922 0.000038 0.249998 x

x Nb 6 0.400088 0.000011 0.750002 x

x Nb 7 0.599915 -0.000004 0.249998 x

x Nb 8 0.600091 -0.000002 0.750002 x

x Nb 9 0.799922 0.000033 0.249998 x

x Nb 10 0.800097 0.000036 0.750001 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07458539E+004 2878.41 <-- SCF

1 -2.07458696E+004 5.22107995E-004 2894.52 <-- SCF

2 -2.07458703E+004 2.18068348E-005 2925.45 <-- SCF

3 -2.07458675E+004 -9.18823807E-005 2953.02 <-- SCF

4 -2.07458668E+004 -2.24497448E-005 2980.58 <-- SCF

5 -2.07458667E+004 -5.36420947E-006 3007.73 <-- SCF

6 -2.07458666E+004 -2.32794939E-006 3030.98 <-- SCF

7 -2.07458666E+004 6.69142621E-008 3051.69 <-- SCF

8 -2.07458666E+004 2.00475295E-007 3071.88 <-- SCF

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

Final energy = -20745.86661130 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.01098 -0.02759 0.14396 \*

\* Se 2 -0.00289 0.03792 0.12104 \*

\* Se 3 0.00426 0.04159 -0.12865 \*

\* Se 4 0.01978 -0.02481 -0.13717 \*

\* Se 5 -0.02844 -0.02196 0.12293 \*

\* Se 6 -0.00874 0.03327 0.14403 \*

\* Se 7 0.00112 0.03660 -0.14859 \*

\* Se 8 -0.02078 -0.02018 -0.12181 \*

\* Se 9 0.01768 -0.03179 0.14521 \*

\* Se 10 -0.02460 0.02994 0.13807 \*

\* Se 11 -0.01708 0.03167 -0.14726 \*

\* Se 12 0.02548 -0.02994 -0.13614 \*

\* Se 13 0.00121 -0.03679 0.14720 \*

\* Se 14 0.02227 0.02034 0.12276 \*

\* Se 15 0.03009 0.02206 -0.12382 \*

\* Se 16 0.01084 -0.03331 -0.14258 \*

\* Se 17 -0.00297 -0.04178 0.12820 \*

\* Se 18 -0.01958 0.02528 0.13819 \*

\* Se 19 -0.01083 0.02803 -0.14511 \*

\* Se 20 0.00432 -0.03813 -0.12042 \*

\* Nb 1 -0.01296 0.06694 -0.00141 \*

\* Nb 2 0.01046 -0.06718 0.00166 \*

\* Nb 3 -0.00590 0.06614 -0.00153 \*

\* Nb 4 0.00574 -0.06624 0.00147 \*

\* Nb 5 -0.02025 0.06901 -0.00175 \*

\* Nb 6 0.00670 -0.06502 0.00133 \*

\* Nb 7 -0.00832 0.06529 -0.00107 \*

\* Nb 8 0.01946 -0.06917 0.00173 \*

\* Nb 9 -0.00788 0.06645 -0.00184 \*

\* Nb 10 0.00084 -0.06665 0.00137 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.282850 0.160281 -0.077285 \*

\* y 0.160281 -0.026998 -0.014650 \*

\* z -0.077285 -0.014650 -0.293522 \*

\* \*

\* Pressure: 0.2011 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000089 | -20745.864916 | <-- min BFGS

| trial step | 1.000000 | 0.000042 | -20745.866724 | <-- min BFGS

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

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BFGS: improving iteration 2 with line minimization (lambda= 1.898007)

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Unit Cell

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

14.8558644 -8.5789498 -0.0189382 0.4220921 -0.0014748 0.0005285

0.0120626 3.4524752 0.0000913 1.0488437 1.8162428 0.0012649

-0.0157612 0.0003346 12.5883178 0.0006274 -0.0000154 0.4991291

Lattice parameters(A) Cell Angles

a = 17.155041 alpha = 89.997213

b = 3.452496 beta = 90.126135

c = 12.588328 gamma = 119.805330

Current cell volume = 646.950247 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 0.066732 0.666720 0.117561 x

x Se 2 0.133338 0.333516 0.617500 x

x Se 3 0.133295 0.333412 0.882493 x

x Se 4 0.066689 0.666617 0.382445 x

x Se 5 0.266675 0.666604 0.117506 x

x Se 6 0.333322 0.333463 0.617557 x

x Se 7 0.333279 0.333358 0.882437 x

x Se 8 0.266633 0.666500 0.382499 x

x Se 9 0.466755 0.666771 0.117564 x

x Se 10 0.533283 0.333321 0.617551 x

x Se 11 0.533240 0.333215 0.882442 x

x Se 12 0.466713 0.666667 0.382443 x

x Se 13 0.666712 0.666619 0.117569 x

x Se 14 0.733368 0.333500 0.617487 x

x Se 15 0.733324 0.333394 0.882508 x

x Se 16 0.666670 0.666517 0.382437 x

x Se 17 0.866708 0.666590 0.117522 x

x Se 18 0.933299 0.333356 0.617554 x

x Se 19 0.933256 0.333251 0.882440 x

x Se 20 0.866666 0.666489 0.382485 x

x Nb 1 -0.000073 0.000035 0.249998 x

x Nb 2 0.000075 -0.000031 0.750002 x

x Nb 3 0.199928 0.000023 0.249998 x

x Nb 4 0.200086 -0.000003 0.750002 x

x Nb 5 0.399931 0.000054 0.249998 x

x Nb 6 0.400077 -0.000013 0.750001 x

x Nb 7 0.599926 0.000018 0.249998 x

x Nb 8 0.600080 -0.000023 0.750002 x

x Nb 9 0.799932 0.000050 0.249998 x

x Nb 10 0.800084 0.000008 0.750001 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07458569E+004 3444.44 <-- SCF

1 -2.07458711E+004 4.71844256E-004 3460.64 <-- SCF

2 -2.07458721E+004 3.51722805E-005 3491.27 <-- SCF

3 -2.07458733E+004 4.04173788E-005 3518.62 <-- SCF

4 -2.07458652E+004 -2.72179541E-004 3547.11 <-- SCF

5 -2.07458672E+004 6.66518829E-005 3574.28 <-- SCF

6 -2.07458682E+004 3.51132879E-005 3601.28 <-- SCF

7 -2.07458678E+004 -1.43895816E-005 3625.83 <-- SCF

8 -2.07458673E+004 -1.59020836E-005 3648.39 <-- SCF

9 -2.07458671E+004 -6.10151771E-006 3670.56 <-- SCF

10 -2.07458671E+004 -7.17929351E-007 3693.77 <-- SCF

11 -2.07458672E+004 2.02000016E-006 3715.39 <-- SCF

12 -2.07458672E+004 1.25118230E-006 3736.53 <-- SCF

13 -2.07458672E+004 2.75866781E-007 3756.62 <-- SCF

14 -2.07458672E+004 -2.53886096E-007 3776.97 <-- SCF

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

Final energy = -20745.86721709 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.01920 -0.02411 0.15315 \*

\* Se 2 -0.00083 0.03551 0.12857 \*

\* Se 3 -0.00219 0.03839 -0.13553 \*

\* Se 4 0.01922 -0.02216 -0.14678 \*

\* Se 5 -0.02093 -0.01957 0.13037 \*

\* Se 6 -0.00810 0.03104 0.15314 \*

\* Se 7 -0.00753 0.03365 -0.15769 \*

\* Se 8 -0.02165 -0.01833 -0.12868 \*

\* Se 9 0.02636 -0.02812 0.15388 \*

\* Se 10 -0.02566 0.02690 0.14592 \*

\* Se 11 -0.02665 0.02815 -0.15407 \*

\* Se 12 0.02566 -0.02690 -0.14581 \*

\* Se 13 0.00873 -0.03339 0.15776 \*

\* Se 14 0.02164 0.01832 0.12827 \*

\* Se 15 0.02080 0.01954 -0.13007 \*

\* Se 16 0.00932 -0.03073 -0.15319 \*

\* Se 17 0.00233 -0.03831 0.13502 \*

\* Se 18 -0.01861 0.02243 0.14614 \*

\* Se 19 -0.01872 0.02445 -0.15267 \*

\* Se 20 0.00120 -0.03548 -0.12799 \*

\* Nb 1 -0.02069 0.05880 -0.00137 \*

\* Nb 2 0.02181 -0.05904 0.00151 \*

\* Nb 3 -0.01235 0.05913 -0.00172 \*

\* Nb 4 0.01685 -0.05950 0.00158 \*

\* Nb 5 -0.02691 0.06112 -0.00156 \*

\* Nb 6 0.01272 -0.05817 0.00142 \*

\* Nb 7 -0.01418 0.05748 -0.00125 \*

\* Nb 8 0.02645 -0.06126 0.00165 \*

\* Nb 9 -0.01898 0.05899 -0.00168 \*

\* Nb 10 0.01169 -0.05883 0.00170 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.147895 0.070277 -0.037598 \*

\* y 0.070277 -0.013791 -0.011120 \*

\* z -0.037598 -0.011120 -0.219678 \*

\* \*

\* Pressure: 0.1271 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000089 | -20745.864916 | <-- min BFGS

| trial step | 1.000000 | 0.000042 | -20745.866724 | <-- min BFGS

| line step | 1.898007 | 7.875E-007 | -20745.867266 | <-- min BFGS

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

BFGS: finished iteration 2 with enthalpy= -2.07458673E+004 eV

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

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

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

| dE/ion | 7.834291E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.614910E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.623207E-004 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.196780E-001 | 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 | 0.000081 | -20745.867266 | <-- min BFGS

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

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

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

| Memory Disk |

| Model and support data 171.1 MB 880.0 MB |

| Electronic energy minimisation requirements 81.1 MB 0.0 MB |

| Geometry minimisation requirements 101.6 MB 0.0 MB |

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

| Approx. total storage required per process 353.9 MB 880.0 MB |

| |

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

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

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Unit Cell

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

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

14.8561020 -8.5785312 -0.0193933 0.4220564 -0.0015250 0.0005367

0.0124765 3.4530269 0.0001556 1.0485363 1.8158280 0.0012510

-0.0160145 0.0005706 12.5942162 0.0006370 -0.0000248 0.4988953

Lattice parameters(A) Cell Angles

a = 17.155038 alpha = 89.995086

b = 3.453049 beta = 90.129162

c = 12.594226 gamma = 119.796886

Current cell volume = 647.411557 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.066739 0.666712 0.117608 x

x Se 2 0.133338 0.333554 0.617538 x

x Se 3 0.133292 0.333445 0.882454 x

x Se 4 0.066694 0.666604 0.382400 x

x Se 5 0.266672 0.666575 0.117545 x

x Se 6 0.333319 0.333491 0.617603 x

x Se 7 0.333274 0.333383 0.882390 x

x Se 8 0.266627 0.666466 0.382461 x

x Se 9 0.466765 0.666768 0.117611 x

x Se 10 0.533275 0.333330 0.617596 x

x Se 11 0.533229 0.333218 0.882395 x

x Se 12 0.466720 0.666658 0.382398 x

x Se 13 0.666716 0.666593 0.117617 x

x Se 14 0.733374 0.333535 0.617523 x

x Se 15 0.733328 0.333423 0.882471 x

x Se 16 0.666672 0.666488 0.382390 x

x Se 17 0.866711 0.666557 0.117562 x

x Se 18 0.933293 0.333366 0.617599 x

x Se 19 0.933247 0.333257 0.882393 x

x Se 20 0.866666 0.666451 0.382446 x

x Nb 1 -0.000082 0.000074 0.249998 x

x Nb 2 0.000083 -0.000069 0.750002 x

x Nb 3 0.199921 0.000063 0.249998 x

x Nb 4 0.200094 -0.000040 0.750002 x

x Nb 5 0.399922 0.000093 0.249997 x

x Nb 6 0.400084 -0.000051 0.750002 x

x Nb 7 0.599919 0.000056 0.249998 x

x Nb 8 0.600090 -0.000060 0.750003 x

x Nb 9 0.799925 0.000091 0.249997 x

x Nb 10 0.800092 -0.000030 0.750002 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07458645E+004 4152.86 <-- SCF

1 -2.07458933E+004 9.61497221E-004 4170.48 <-- SCF

2 -2.07458955E+004 7.40347307E-005 4199.22 <-- SCF

3 -2.07459536E+004 1.93451437E-003 4226.12 <-- SCF

4 -2.07458462E+004 -3.57954949E-003 4252.92 <-- SCF

5 -2.07458572E+004 3.66622302E-004 4279.88 <-- SCF

6 -2.07458669E+004 3.23332372E-004 4307.02 <-- SCF

7 -2.07458702E+004 1.10234170E-004 4331.92 <-- SCF

8 -2.07458721E+004 6.43633180E-005 4355.73 <-- SCF

9 -2.07458716E+004 -1.88191093E-005 4378.61 <-- SCF

10 -2.07458709E+004 -2.06673399E-005 4398.98 <-- SCF

11 -2.07458697E+004 -4.10442538E-005 4422.66 <-- SCF

12 -2.07458691E+004 -1.99630161E-005 4445.41 <-- SCF

13 -2.07458692E+004 4.42090639E-006 4467.75 <-- SCF

14 -2.07458694E+004 4.92207441E-006 4487.48 <-- SCF

15 -2.07458694E+004 -7.84154776E-007 4507.83 <-- SCF

16 -2.07458693E+004 -1.39734904E-006 4528.98 <-- SCF

17 -2.07458693E+004 1.88683201E-007 4548.92 <-- SCF

18 -2.07458693E+004 5.98818413E-008 4568.12 <-- SCF

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

Final energy = -20745.86933653 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.01812 -0.02155 0.15758 \*

\* Se 2 -0.00009 0.03431 0.13719 \*

\* Se 3 -0.00067 0.03660 -0.14432 \*

\* Se 4 0.01874 -0.02002 -0.15133 \*

\* Se 5 -0.02128 -0.01758 0.13845 \*

\* Se 6 -0.00734 0.02852 0.15722 \*

\* Se 7 -0.00574 0.03053 -0.16146 \*

\* Se 8 -0.02140 -0.01692 -0.13709 \*

\* Se 9 0.02418 -0.02646 0.15840 \*

\* Se 10 -0.02307 0.02569 0.15168 \*

\* Se 11 -0.02332 0.02637 -0.15980 \*

\* Se 12 0.02398 -0.02576 -0.15032 \*

\* Se 13 0.00796 -0.03032 0.16125 \*

\* Se 14 0.02134 0.01702 0.13783 \*

\* Se 15 0.02131 0.01761 -0.13928 \*

\* Se 16 0.00943 -0.02828 -0.15695 \*

\* Se 17 0.00123 -0.03666 0.14322 \*

\* Se 18 -0.01670 0.02027 0.15089 \*

\* Se 19 -0.01604 0.02184 -0.15716 \*

\* Se 20 0.00060 -0.03438 -0.13607 \*

\* Nb 1 -0.01946 0.05612 -0.00111 \*

\* Nb 2 0.01971 -0.05644 0.00117 \*

\* Nb 3 -0.01122 0.05611 -0.00165 \*

\* Nb 4 0.01297 -0.05581 0.00145 \*

\* Nb 5 -0.02653 0.05855 -0.00135 \*

\* Nb 6 0.01007 -0.05481 0.00118 \*

\* Nb 7 -0.01152 0.05422 -0.00115 \*

\* Nb 8 0.02431 -0.05857 0.00136 \*

\* Nb 9 -0.01614 0.05577 -0.00146 \*

\* Nb 10 0.00656 -0.05598 0.00163 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.117190 0.083406 -0.041168 \*

\* y 0.083406 0.032914 -0.008695 \*

\* z -0.041168 -0.008695 -0.165377 \*

\* \*

\* Pressure: 0.0832 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000081 | -20745.867266 | <-- min BFGS

| trial step | 1.000000 | 0.000077 | -20745.869399 | <-- min BFGS

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

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

BFGS: improving iteration 3 with line minimization (lambda= 20.714681)

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

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

| Memory Disk |

| Model and support data 172.0 MB 880.0 MB |

| Electronic energy minimisation requirements 81.8 MB 0.0 MB |

| Geometry minimisation requirements 102.5 MB 0.0 MB |

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

| Approx. total storage required per process 356.3 MB 880.0 MB |

| |

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

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

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Unit Cell

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

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

14.8607874 -8.5702783 -0.0283657 0.4213564 -0.0025107 0.0006975

0.0206374 3.4639025 0.0014237 1.0425055 1.8076921 0.0009801

-0.0210085 0.0052240 12.7105012 0.0008236 -0.0002081 0.4943317

Lattice parameters(A) Cell Angles

a = 17.154984 alpha = 89.953468

b = 3.463964 beta = 90.188539

c = 12.710520 gamma = 119.630871

Current cell volume = 656.535972 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 0.066882 0.666554 0.118532 x

x Se 2 0.133339 0.334307 0.618284 x

x Se 3 0.133238 0.334109 0.881672 x

x Se 4 0.066788 0.666360 0.381509 x

x Se 5 0.266609 0.666008 0.118305 x

x Se 6 0.333275 0.334051 0.618522 x

x Se 7 0.333182 0.333869 0.881446 x

x Se 8 0.266512 0.665792 0.381714 x

x Se 9 0.466967 0.666698 0.118545 x

x Se 10 0.533119 0.333489 0.618482 x

x Se 11 0.533019 0.333267 0.881468 x

x Se 12 0.466871 0.666483 0.381505 x

x Se 13 0.666797 0.666082 0.118568 x

x Se 14 0.733492 0.334212 0.618246 x

x Se 15 0.733392 0.333989 0.881735 x

x Se 16 0.666706 0.665907 0.381464 x

x Se 17 0.866771 0.665904 0.118367 x

x Se 18 0.933181 0.333573 0.618490 x

x Se 19 0.933085 0.333374 0.881469 x

x Se 20 0.866673 0.665714 0.381677 x

x Nb 1 -0.000245 0.000832 0.249991 x

x Nb 2 0.000250 -0.000820 0.750010 x

x Nb 3 0.199783 0.000854 0.249990 x

x Nb 4 0.200262 -0.000783 0.750010 x

x Nb 5 0.399749 0.000864 0.249989 x

x Nb 6 0.400229 -0.000818 0.750008 x

x Nb 7 0.599773 0.000809 0.249992 x

x Nb 8 0.600278 -0.000790 0.750011 x

x Nb 9 0.799780 0.000892 0.249988 x

x Nb 10 0.800244 -0.000784 0.750009 x

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07442099E+004 4963.73 <-- SCF

1 -2.07489110E+004 1.56703244E-001 4981.45 <-- SCF

2 -2.07492937E+004 1.27558437E-002 5016.14 <-- SCF

3 -2.07467956E+004 -8.32702073E-002 5044.70 <-- SCF

4 -2.07459620E+004 -2.77842489E-002 5073.53 <-- SCF

5 -2.07459025E+004 -1.98436658E-003 5101.88 <-- SCF

6 -2.07458960E+004 -2.15435173E-004 5130.28 <-- SCF

7 -2.07458933E+004 -9.18984312E-005 5159.20 <-- SCF

8 -2.07458934E+004 4.97844185E-006 5189.42 <-- SCF

9 -2.07458933E+004 -3.94320128E-006 5218.05 <-- SCF

10 -2.07458936E+004 1.05179262E-005 5244.56 <-- SCF

11 -2.07458937E+004 2.73597932E-006 5270.33 <-- SCF

12 -2.07458938E+004 1.45617298E-006 5292.77 <-- SCF

13 -2.07458938E+004 1.47850674E-007 5314.28 <-- SCF

14 -2.07458938E+004 2.23818185E-008 5334.86 <-- SCF

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

Final energy = -20745.89376781 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.02929 -0.00325 0.27852 \*

\* Se 2 0.01659 0.01514 0.30143 \*

\* Se 3 0.03200 0.00442 -0.30416 \*

\* Se 4 -0.01091 -0.00826 -0.27857 \*

\* Se 5 -0.03143 0.00738 0.30347 \*

\* Se 6 0.01006 0.01210 0.26919 \*

\* Se 7 0.03397 0.00299 -0.27076 \*

\* Se 8 -0.01552 -0.00177 -0.30381 \*

\* Se 9 -0.03139 0.00664 0.27509 \*

\* Se 10 0.01568 0.00274 0.27566 \*

\* Se 11 0.03282 -0.00675 -0.27735 \*

\* Se 12 -0.01432 -0.00274 -0.27357 \*

\* Se 13 -0.02986 -0.00339 0.27057 \*

\* Se 14 0.01580 0.00194 0.30747 \*

\* Se 15 0.03171 -0.00735 -0.30685 \*

\* Se 16 -0.00608 -0.01248 -0.26909 \*

\* Se 17 -0.03302 -0.00336 0.29816 \*

\* Se 18 0.01597 0.00884 0.27795 \*

\* Se 19 0.03424 0.00387 -0.27766 \*

\* Se 20 -0.01772 -0.01437 -0.29621 \*

\* Nb 1 0.02571 0.00086 0.00384 \*

\* Nb 2 -0.02411 -0.00199 -0.00389 \*

\* Nb 3 0.04819 0.00370 0.00125 \*

\* Nb 4 -0.05218 0.00486 -0.00252 \*

\* Nb 5 0.01252 0.00386 0.00296 \*

\* Nb 6 -0.04113 0.00109 -0.00349 \*

\* Nb 7 0.03861 -0.00145 0.00354 \*

\* Nb 8 -0.01422 -0.00432 -0.00282 \*

\* Nb 9 0.04197 -0.00519 0.00281 \*

\* Nb 10 -0.05468 -0.00377 -0.00115 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.471673 0.302316 -0.106612 \*

\* y 0.302316 0.915100 0.035745 \*

\* z -0.106612 0.035745 0.789064 \*

\* \*

\* Pressure: -0.7253 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000081 | -20745.867266 | <-- min BFGS

| trial step | 1.000000 | 0.000077 | -20745.869399 | <-- min BFGS

| line step | 20.714681 | 0.000018 | -20745.893713 | <-- min BFGS

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

BFGS: finished iteration 3 with enthalpy= -2.07458937E+004 eV

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

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

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

| dE/ion | 8.815684E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 3.085692E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.302013E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 9.150999E-001 | 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 | 0.000544 | -20745.893713 | <-- min BFGS

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

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BFGS: starting iteration 4 with trial guess (lambda= 1.000000)

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

| Memory Disk |

| Model and support data 171.9 MB 880.0 MB |

| Electronic energy minimisation requirements 82.1 MB 0.0 MB |

| Geometry minimisation requirements 103.0 MB 0.0 MB |

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

| Approx. total storage required per process 357.0 MB 880.0 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)

14.8553740 -8.5604358 -0.0328105 0.4212094 -0.0030358 0.0007787

0.0249878 3.4675285 0.0020275 1.0398557 1.8045129 0.0008655

-0.0235504 0.0074469 12.7678356 0.0009173 -0.0002943 0.4921123

Lattice parameters(A) Cell Angles

a = 17.145386 alpha = 89.933845

b = 3.467619 beta = 90.217897

c = 12.767860 gamma = 119.539902

Current cell volume = 660.418135 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 0.066963 0.666459 0.119096 x

x Se 2 0.133341 0.334747 0.618748 x

x Se 3 0.133208 0.334493 0.881187 x

x Se 4 0.066841 0.666214 0.380964 x

x Se 5 0.266571 0.665684 0.118777 x

x Se 6 0.333251 0.334378 0.619081 x

x Se 7 0.333131 0.334151 0.880873 x

x Se 8 0.266444 0.665403 0.381249 x

x Se 9 0.467082 0.666660 0.119113 x

x Se 10 0.533030 0.333583 0.619023 x

x Se 11 0.532900 0.333293 0.880903 x

x Se 12 0.466956 0.666381 0.380960 x

x Se 13 0.666842 0.665785 0.119147 x

x Se 14 0.733561 0.334604 0.618697 x

x Se 15 0.733430 0.334314 0.881277 x

x Se 16 0.666725 0.665567 0.380900 x

x Se 17 0.866803 0.665526 0.118864 x

x Se 18 0.933118 0.333698 0.619034 x

x Se 19 0.932993 0.333445 0.880906 x

x Se 20 0.866676 0.665282 0.381201 x

x Nb 1 -0.000338 0.001264 0.249988 x

x Nb 2 0.000345 -0.001247 0.750014 x

x Nb 3 0.199707 0.001309 0.249985 x

x Nb 4 0.200355 -0.001208 0.750014 x

x Nb 5 0.399650 0.001302 0.249984 x

x Nb 6 0.400310 -0.001256 0.750012 x

x Nb 7 0.599691 0.001239 0.249989 x

x Nb 8 0.600386 -0.001204 0.750016 x

x Nb 9 0.799699 0.001351 0.249984 x

x Nb 10 0.800328 -0.001218 0.750012 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07454201E+004 5714.41 <-- SCF

1 -2.07468502E+004 4.76719777E-002 5733.44 <-- SCF

2 -2.07469619E+004 3.72219318E-003 5763.88 <-- SCF

3 -2.07461453E+004 -2.72198065E-002 5793.09 <-- SCF

4 -2.07459294E+004 -7.19695233E-003 5819.78 <-- SCF

5 -2.07459077E+004 -7.21408593E-004 5845.48 <-- SCF

6 -2.07459077E+004 -5.83892732E-007 5874.02 <-- SCF

7 -2.07459065E+004 -4.16997423E-005 5902.14 <-- SCF

8 -2.07459074E+004 3.12409554E-005 5930.00 <-- SCF

9 -2.07459069E+004 -1.54923560E-005 5955.06 <-- SCF

10 -2.07459069E+004 -2.60026165E-006 5981.39 <-- SCF

11 -2.07459069E+004 1.47445560E-006 6004.61 <-- SCF

12 -2.07459069E+004 -1.27460129E-006 6025.17 <-- SCF

13 -2.07459069E+004 6.68187221E-007 6045.31 <-- SCF

14 -2.07459069E+004 -2.09745196E-007 6064.70 <-- SCF

15 -2.07459069E+004 3.15818257E-007 6085.59 <-- SCF

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

Final energy = -20745.90689006 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.06065 0.00354 0.31554 \*

\* Se 2 0.02332 -0.01174 0.34767 \*

\* Se 3 0.04755 -0.03105 -0.34371 \*

\* Se 4 -0.02983 -0.00796 -0.32428 \*

\* Se 5 -0.03795 0.02489 0.35482 \*

\* Se 6 0.01934 -0.00518 0.30092 \*

\* Se 7 0.04831 -0.01920 -0.30382 \*

\* Se 8 -0.01066 0.01205 -0.35121 \*

\* Se 9 -0.05243 0.01990 0.30618 \*

\* Se 10 0.02621 -0.00936 0.31652 \*

\* Se 11 0.05561 -0.01995 -0.31032 \*

\* Se 12 -0.02331 0.00936 -0.31261 \*

\* Se 13 -0.04260 0.01809 0.30243 \*

\* Se 14 0.01238 -0.01186 0.35572 \*

\* Se 15 0.03978 -0.02480 -0.35890 \*

\* Se 16 -0.01404 0.00421 -0.29993 \*

\* Se 17 -0.04749 0.03286 0.33695 \*

\* Se 18 0.03664 0.00811 0.32431 \*

\* Se 19 0.06711 -0.00344 -0.31518 \*

\* Se 20 -0.02367 0.01340 -0.34158 \*

\* Nb 1 0.04695 -0.02904 0.00713 \*

\* Nb 2 -0.04668 0.02921 -0.00706 \*

\* Nb 3 0.07646 -0.02538 0.00348 \*

\* Nb 4 -0.08706 0.03944 -0.00545 \*

\* Nb 5 0.03131 -0.02668 0.00554 \*

\* Nb 6 -0.07108 0.03399 -0.00676 \*

\* Nb 7 0.06748 -0.03351 0.00700 \*

\* Nb 8 -0.03495 0.02571 -0.00550 \*

\* Nb 9 0.07418 -0.04065 0.00555 \*

\* Nb 10 -0.09023 0.02507 -0.00345 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.580243 0.418120 -0.141996 \*

\* y 0.418120 1.180188 0.055679 \*

\* z -0.141996 0.055679 1.007194 \*

\* \*

\* Pressure: -0.9225 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000544 | -20745.893713 | <-- min BFGS

| trial step | 1.000000 | 0.000437 | -20745.906844 | <-- min BFGS

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

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BFGS: improving iteration 4 with line minimization (lambda= 4.606845)

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

| Memory Disk |

| Model and support data 173.0 MB 880.0 MB |

| Electronic energy minimisation requirements 82.9 MB 0.0 MB |

| Geometry minimisation requirements 104.1 MB 0.0 MB |

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

| Approx. total storage required per process 360.0 MB 880.0 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)

14.8358488 -8.5249351 -0.0488422 0.4206912 -0.0049181 0.0010667

0.0406791 3.4806070 0.0042053 1.0303795 1.7931552 0.0004611

-0.0327184 0.0154645 12.9746321 0.0012497 -0.0005997 0.4842708

Lattice parameters(A) Cell Angles

a = 17.110795 alpha = 89.864182

b = 3.480847 beta = 90.322848

c = 12.974683 gamma = 119.212887

Current cell volume = 674.474979 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 0.067253 0.666120 0.121130 x

x Se 2 0.133350 0.336336 0.620422 x

x Se 3 0.133103 0.335879 0.879440 x

x Se 4 0.067030 0.665690 0.378997 x

x Se 5 0.266433 0.664514 0.120480 x

x Se 6 0.333163 0.335559 0.621099 x

x Se 7 0.332947 0.335170 0.878804 x

x Se 8 0.266200 0.663997 0.379572 x

x Se 9 0.467494 0.666524 0.121164 x

x Se 10 0.532711 0.333920 0.620977 x

x Se 11 0.532471 0.333386 0.878865 x

x Se 12 0.467263 0.666013 0.378994 x

x Se 13 0.667002 0.664715 0.121233 x

x Se 14 0.733811 0.336018 0.620323 x

x Se 15 0.733568 0.335483 0.879626 x

x Se 16 0.666793 0.664342 0.378866 x

x Se 17 0.866920 0.664162 0.120658 x

x Se 18 0.932892 0.334147 0.620999 x

x Se 19 0.932663 0.333701 0.878873 x

x Se 20 0.866685 0.663725 0.379482 x

x Nb 1 -0.000673 0.002820 0.249976 x

x Nb 2 0.000687 -0.002788 0.750029 x

x Nb 3 0.199433 0.002953 0.249970 x

x Nb 4 0.200692 -0.002742 0.750028 x

x Nb 5 0.399293 0.002882 0.249967 x

x Nb 6 0.400601 -0.002836 0.750024 x

x Nb 7 0.599397 0.002790 0.249979 x

x Nb 8 0.600776 -0.002696 0.750033 x

x Nb 9 0.799410 0.003003 0.249966 x

x Nb 10 0.800632 -0.002787 0.750026 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07395775E+004 6462.30 <-- SCF

1 -2.07580929E+004 6.17180246E-001 6479.95 <-- SCF

2 -2.07601581E+004 6.88401352E-002 6513.41 <-- SCF

3 -2.07503336E+004 -3.27481600E-001 6541.64 <-- SCF

4 -2.07463267E+004 -1.33564039E-001 6570.50 <-- SCF

5 -2.07459924E+004 -1.11414608E-002 6598.30 <-- SCF

6 -2.07458987E+004 -3.12472854E-003 6626.33 <-- SCF

7 -2.07459038E+004 1.69965588E-004 6655.97 <-- SCF

8 -2.07459043E+004 1.72468951E-005 6684.09 <-- SCF

9 -2.07459053E+004 3.31310937E-005 6713.53 <-- SCF

10 -2.07459058E+004 1.70021070E-005 6738.81 <-- SCF

11 -2.07459060E+004 6.25893692E-006 6763.59 <-- SCF

12 -2.07459061E+004 1.38579257E-006 6784.50 <-- SCF

13 -2.07459061E+004 7.08884662E-007 6804.84 <-- SCF

14 -2.07459061E+004 5.14173112E-007 6825.19 <-- SCF

15 -2.07459061E+004 3.52839085E-007 6845.67 <-- SCF

16 -2.07459061E+004 2.52296204E-007 6866.22 <-- SCF

17 -2.07459061E+004 1.95048028E-007 6886.72 <-- SCF

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

Final energy = -20745.90611705 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.13700 0.05896 0.29747 \*

\* Se 2 0.05302 -0.08652 0.42237 \*

\* Se 3 0.09326 -0.11348 -0.40117 \*

\* Se 4 -0.06561 0.03493 -0.32126 \*

\* Se 5 -0.05470 0.08519 0.42006 \*

\* Se 6 0.05191 -0.04668 0.28234 \*

\* Se 7 0.11432 -0.07782 -0.26379 \*

\* Se 8 0.00885 0.05645 -0.42789 \*

\* Se 9 -0.13798 0.08044 0.28426 \*

\* Se 10 0.09087 -0.05998 0.32180 \*

\* Se 11 0.14199 -0.07883 -0.29379 \*

\* Se 12 -0.08754 0.06130 -0.31215 \*

\* Se 13 -0.10431 0.07603 0.25964 \*

\* Se 14 -0.00859 -0.05690 0.44847 \*

\* Se 15 0.05593 -0.08485 -0.44003 \*

\* Se 16 -0.04223 0.04466 -0.27808 \*

\* Se 17 -0.09427 0.11412 0.37689 \*

\* Se 18 0.08226 -0.03426 0.32223 \*

\* Se 19 0.15159 -0.05828 -0.29752 \*

\* Se 20 -0.05313 0.08737 -0.40075 \*

\* Nb 1 0.12201 -0.13955 0.01821 \*

\* Nb 2 -0.12278 0.14006 -0.01794 \*

\* Nb 3 0.18756 -0.13294 0.01151 \*

\* Nb 4 -0.21334 0.16475 -0.01553 \*

\* Nb 5 0.09838 -0.13967 0.01454 \*

\* Nb 6 -0.17195 0.15406 -0.01799 \*

\* Nb 7 0.16487 -0.15367 0.01835 \*

\* Nb 8 -0.10602 0.13909 -0.01416 \*

\* Nb 9 0.19239 -0.16563 0.01556 \*

\* Nb 10 -0.20974 0.13166 -0.01164 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.961294 0.823673 -0.254900 \*

\* y 0.823673 2.104098 0.113352 \*

\* z -0.254900 0.113352 1.778994 \*

\* \*

\* Pressure: -1.6148 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000544 | -20745.893713 | <-- min BFGS

| trial step | 1.000000 | 0.000437 | -20745.906844 | <-- min BFGS

| line step | 4.606845 | -0.000563 | -20745.906098 | <-- min BFGS

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

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

BFGS: improving iteration 4 with quad minimization (lambda= 2.576591)

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Unit Cell

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

14.8468393 -8.5449181 -0.0398181 0.4209806 -0.0038608 0.0009055

0.0318466 3.4732453 0.0029794 1.0356979 1.7995273 0.0006870

-0.0275578 0.0109515 12.8582286 0.0010637 -0.0004289 0.4886536

Lattice parameters(A) Cell Angles

a = 17.130261 alpha = 89.903181

b = 3.473393 beta = 90.263951

c = 12.858263 gamma = 119.396750

Current cell volume = 666.552067 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 0.666311 0.119985 x

x Se 2 0.133345 0.335442 0.619480 x

x Se 3 0.133163 0.335099 0.880423 x

x Se 4 0.066923 0.665985 0.380104 x

x Se 5 0.266511 0.665173 0.119521 x

x Se 6 0.333212 0.334894 0.619963 x

x Se 7 0.333050 0.334596 0.879968 x

x Se 8 0.266338 0.664788 0.380516 x

x Se 9 0.467262 0.666601 0.120010 x

x Se 10 0.532891 0.333730 0.619877 x

x Se 11 0.532712 0.333333 0.880012 x

x Se 12 0.467090 0.666220 0.380101 x

x Se 13 0.666912 0.665317 0.120059 x

x Se 14 0.733670 0.335222 0.619408 x

x Se 15 0.733490 0.334825 0.880555 x

x Se 16 0.666755 0.665031 0.380011 x

x Se 17 0.866854 0.664930 0.119649 x

x Se 18 0.933019 0.333894 0.619893 x

x Se 19 0.932849 0.333557 0.880017 x

x Se 20 0.866680 0.664602 0.380449 x

x Nb 1 -0.000485 0.001944 0.249983 x

x Nb 2 0.000494 -0.001921 0.750021 x

x Nb 3 0.199587 0.002028 0.249979 x

x Nb 4 0.200502 -0.001879 0.750020 x

x Nb 5 0.399494 0.001993 0.249977 x

x Nb 6 0.400437 -0.001947 0.750017 x

x Nb 7 0.599563 0.001917 0.249985 x

x Nb 8 0.600556 -0.001856 0.750023 x

x Nb 9 0.799573 0.002073 0.249976 x

x Nb 10 0.800461 -0.001904 0.750018 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07439169E+004 7269.61 <-- SCF

1 -2.07498689E+004 1.98399215E-001 7286.91 <-- SCF

2 -2.07502187E+004 1.16598947E-002 7320.06 <-- SCF

3 -2.07465783E+004 -1.21346608E-001 7349.09 <-- SCF

4 -2.07460099E+004 -1.89459925E-002 7377.70 <-- SCF

5 -2.07459098E+004 -3.33628917E-003 7405.66 <-- SCF

6 -2.07459170E+004 2.38969019E-004 7435.77 <-- SCF

7 -2.07459170E+004 -2.90636752E-007 7465.47 <-- SCF

8 -2.07459179E+004 3.06337128E-005 7492.55 <-- SCF

9 -2.07459180E+004 2.32290624E-006 7518.27 <-- SCF

10 -2.07459181E+004 5.03520629E-006 7542.16 <-- SCF

11 -2.07459182E+004 3.45871887E-006 7563.44 <-- SCF

12 -2.07459183E+004 1.50671841E-006 7584.14 <-- SCF

13 -2.07459183E+004 3.77379395E-007 7604.00 <-- SCF

14 -2.07459183E+004 2.83465017E-007 7624.28 <-- SCF

15 -2.07459183E+004 2.43323802E-007 7644.31 <-- SCF

16 -2.07459183E+004 2.90050519E-007 7664.78 <-- SCF

17 -2.07459183E+004 2.22476707E-007 7685.23 <-- SCF

18 -2.07459183E+004 3.01736504E-007 7705.95 <-- SCF

19 -2.07459183E+004 2.11365302E-007 7726.17 <-- SCF

20 -2.07459183E+004 1.44022374E-007 7746.62 <-- SCF

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

Final energy = -20745.91833095 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.09791 0.02645 0.32100 \*

\* Se 2 0.03716 -0.04818 0.40605 \*

\* Se 3 0.06758 -0.07367 -0.39551 \*

\* Se 4 -0.05152 0.01019 -0.33112 \*

\* Se 5 -0.04002 0.05268 0.41585 \*

\* Se 6 0.02358 -0.01745 0.32632 \*

\* Se 7 0.06578 -0.04066 -0.31841 \*

\* Se 8 0.00609 0.03466 -0.41571 \*

\* Se 9 -0.10598 0.03707 0.30425 \*

\* Se 10 0.06683 -0.02444 0.33115 \*

\* Se 11 0.10950 -0.03572 -0.30965 \*

\* Se 12 -0.06388 0.02540 -0.32604 \*

\* Se 13 -0.05980 0.03888 0.31662 \*

\* Se 14 -0.00523 -0.03464 0.42484 \*

\* Se 15 0.04094 -0.05262 -0.42638 \*

\* Se 16 -0.01816 0.01602 -0.32456 \*

\* Se 17 -0.06730 0.07379 0.38333 \*

\* Se 18 0.06258 -0.00990 0.33142 \*

\* Se 19 0.10809 -0.02609 -0.32090 \*

\* Se 20 -0.03742 0.04931 -0.39347 \*

\* Nb 1 0.08020 -0.07846 0.01252 \*

\* Nb 2 -0.08001 0.07869 -0.01231 \*

\* Nb 3 0.12830 -0.07343 0.00664 \*

\* Nb 4 -0.14267 0.09494 -0.01000 \*

\* Nb 5 0.05859 -0.07746 0.01075 \*

\* Nb 6 -0.11896 0.08856 -0.01155 \*

\* Nb 7 0.11479 -0.08734 0.01140 \*

\* Nb 8 -0.06193 0.07649 -0.01034 \*

\* Nb 9 0.12702 -0.09611 0.01045 \*

\* Nb 10 -0.14624 0.07303 -0.00662 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.762058 0.601291 -0.190468 \*

\* y 0.601291 1.603451 0.084215 \*

\* z -0.190468 0.084215 1.364933 \*

\* \*

\* Pressure: -1.2435 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000544 | -20745.893713 | <-- min BFGS

| trial step | 1.000000 | 0.000437 | -20745.906844 | <-- min BFGS

| line step | 4.606845 | -0.000563 | -20745.906098 | <-- min BFGS

| quad step | 2.576591 | 0.000086 | -20745.918407 | <-- min BFGS

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

BFGS: finished iteration 4 with enthalpy= -2.07459184E+004 eV

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

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

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

| dE/ion | 8.231078E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 4.315593E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.956297E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.603451E+000 | 2.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 5 ...

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

Writing analysis data to 2H-Nb1Se2-7.castep\_bin

Writing model to 2H-Nb1Se2-7.check

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

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

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

| previous | 0.000000 | 0.001266 | -20745.918407 | <-- 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)

14.8509319 -8.5344366 -0.0386502 0.4207306 -0.0040982 0.0008261

0.0338175 3.4725282 0.0036751 1.0340263 1.7993278 0.0001353

-0.0252595 0.0135437 12.9310352 0.0009637 -0.0005236 0.4859021

Lattice parameters(A) Cell Angles

a = 17.128581 alpha = 89.880447

b = 3.472695 beta = 90.256226

c = 12.931067 gamma = 119.326935

Current cell volume = 670.585825 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 0.067195 0.666127 0.120887 x

x Se 2 0.133352 0.336108 0.620245 x

x Se 3 0.133132 0.335698 0.879627 x

x Se 4 0.066999 0.665750 0.379230 x

x Se 5 0.266441 0.664668 0.120299 x

x Se 6 0.333178 0.335398 0.620860 x

x Se 7 0.332989 0.335055 0.879051 x

x Se 8 0.266236 0.664207 0.379748 x

x Se 9 0.467415 0.666499 0.120917 x

x Se 10 0.532766 0.333894 0.620747 x

x Se 11 0.532553 0.333420 0.879108 x

x Se 12 0.467211 0.666046 0.379227 x

x Se 13 0.666966 0.664842 0.120982 x

x Se 14 0.733775 0.335807 0.620158 x

x Se 15 0.733561 0.335331 0.879795 x

x Se 16 0.666783 0.664514 0.379108 x

x Se 17 0.866889 0.664341 0.120460 x

x Se 18 0.932932 0.334105 0.620768 x

x Se 19 0.932731 0.333714 0.879115 x

x Se 20 0.866680 0.663949 0.379669 x

x Nb 1 -0.000609 0.002632 0.249980 x

x Nb 2 0.000622 -0.002602 0.750025 x

x Nb 3 0.199495 0.002775 0.249973 x

x Nb 4 0.200618 -0.002574 0.750025 x

x Nb 5 0.399356 0.002680 0.249971 x

x Nb 6 0.400537 -0.002657 0.750021 x

x Nb 7 0.599460 0.002612 0.249981 x

x Nb 8 0.600706 -0.002514 0.750029 x

x Nb 9 0.799472 0.002804 0.249970 x

x Nb 10 0.800562 -0.002630 0.750023 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07449446E+004 8131.73 <-- SCF

1 -2.07480744E+004 1.04329139E-001 8149.38 <-- SCF

2 -2.07483440E+004 8.98704121E-003 8181.45 <-- SCF

3 -2.07464951E+004 -6.16311410E-002 8212.73 <-- SCF

4 -2.07460121E+004 -1.61001440E-002 8244.12 <-- SCF

5 -2.07459478E+004 -2.14272259E-003 8270.70 <-- SCF

6 -2.07459469E+004 -3.07290469E-005 8299.83 <-- SCF

7 -2.07459455E+004 -4.68049526E-005 8328.64 <-- SCF

8 -2.07459468E+004 4.24647665E-005 8358.34 <-- SCF

9 -2.07459463E+004 -1.59430813E-005 8384.88 <-- SCF

10 -2.07459470E+004 2.32597789E-005 8413.55 <-- SCF

11 -2.07459466E+004 -1.36881673E-005 8438.06 <-- SCF

12 -2.07459465E+004 -2.85300178E-006 8460.14 <-- SCF

13 -2.07459464E+004 -1.54703957E-006 8482.94 <-- SCF

14 -2.07459465E+004 3.00240450E-006 8504.56 <-- SCF

15 -2.07459466E+004 1.43277657E-006 8526.20 <-- SCF

16 -2.07459466E+004 2.95925221E-007 8548.03 <-- SCF

17 -2.07459466E+004 -1.92184201E-007 8569.25 <-- SCF

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

Final energy = -20745.94657916 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.11116 0.05141 0.25994 \*

\* Se 2 0.05013 -0.07809 0.37587 \*

\* Se 3 0.07556 -0.10362 -0.35851 \*

\* Se 4 -0.06115 0.02987 -0.27916 \*

\* Se 5 -0.04081 0.08137 0.36757 \*

\* Se 6 0.04818 -0.04468 0.24817 \*

\* Se 7 0.09171 -0.07359 -0.23133 \*

\* Se 8 0.00568 0.05562 -0.37482 \*

\* Se 9 -0.11718 0.07469 0.24517 \*

\* Se 10 0.08872 -0.05261 0.28065 \*

\* Se 11 0.12070 -0.07273 -0.25571 \*

\* Se 12 -0.08562 0.05407 -0.26996 \*

\* Se 13 -0.08248 0.07211 0.22593 \*

\* Se 14 -0.00539 -0.05549 0.39474 \*

\* Se 15 0.04211 -0.08073 -0.38713 \*

\* Se 16 -0.03941 0.04321 -0.24274 \*

\* Se 17 -0.07661 0.10495 0.33587 \*

\* Se 18 0.07550 -0.02922 0.28274 \*

\* Se 19 0.12417 -0.05054 -0.26252 \*

\* Se 20 -0.05048 0.07986 -0.35547 \*

\* Nb 1 0.09784 -0.13254 0.01705 \*

\* Nb 2 -0.10051 0.13360 -0.01678 \*

\* Nb 3 0.15688 -0.12839 0.01053 \*

\* Nb 4 -0.17807 0.15686 -0.01421 \*

\* Nb 5 0.08033 -0.13456 0.01400 \*

\* Nb 6 -0.14258 0.14900 -0.01665 \*

\* Nb 7 0.13452 -0.14869 0.01693 \*

\* Nb 8 -0.08580 0.13288 -0.01398 \*

\* Nb 9 0.16212 -0.16001 0.01421 \*

\* Nb 10 -0.17691 0.12601 -0.01039 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.750738 0.596133 -0.178869 \*

\* y 0.596133 1.575769 0.107623 \*

\* z -0.178869 0.107623 1.262942 \*

\* \*

\* Pressure: -1.1965 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.001266 | -20745.918407 | <-- min BFGS

| trial step | 1.000000 | 0.000787 | -20745.946512 | <-- min BFGS

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

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BFGS: improving iteration 5 with line minimization (lambda= 2.641235)

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

| Memory Disk |

| Model and support data 172.8 MB 880.0 MB |

| Electronic energy minimisation requirements 83.2 MB 0.0 MB |

| Geometry minimisation requirements 104.4 MB 0.0 MB |

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

| Approx. total storage required per process 360.4 MB 880.0 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)

14.8576488 -8.5172340 -0.0367334 0.4203216 -0.0044873 0.0006982

0.0370521 3.4713514 0.0048169 1.0312881 1.7990047 -0.0007555

-0.0214873 0.0177981 13.0505280 0.0008024 -0.0006766 0.4814529

Lattice parameters(A) Cell Angles

a = 17.125839 alpha = 89.843373

b = 3.471553 beta = 90.243598

c = 13.050558 gamma = 119.212300

Current cell volume = 677.210949 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 0.067366 0.665826 0.122368 x

x Se 2 0.133363 0.337202 0.621501 x

x Se 3 0.133083 0.336681 0.878320 x

x Se 4 0.067122 0.665364 0.377794 x

x Se 5 0.266327 0.663840 0.121577 x

x Se 6 0.333121 0.336224 0.622332 x

x Se 7 0.332887 0.335808 0.877545 x

x Se 8 0.266068 0.663254 0.378487 x

x Se 9 0.467667 0.666332 0.122407 x

x Se 10 0.532561 0.334163 0.622174 x

x Se 11 0.532292 0.333563 0.877625 x

x Se 12 0.467409 0.665761 0.377794 x

x Se 13 0.667055 0.664061 0.122498 x

x Se 14 0.733946 0.336766 0.621388 x

x Se 15 0.733676 0.336161 0.878547 x

x Se 16 0.666829 0.663665 0.377627 x

x Se 17 0.866946 0.663374 0.121792 x

x Se 18 0.932788 0.334452 0.622202 x

x Se 19 0.932537 0.333971 0.877634 x

x Se 20 0.866680 0.662877 0.378388 x

x Nb 1 -0.000813 0.003761 0.249974 x

x Nb 2 0.000831 -0.003721 0.750033 x

x Nb 3 0.199344 0.004000 0.249963 x

x Nb 4 0.200807 -0.003715 0.750033 x

x Nb 5 0.399129 0.003809 0.249962 x

x Nb 6 0.400701 -0.003823 0.750026 x

x Nb 7 0.599292 0.003753 0.249977 x

x Nb 8 0.600952 -0.003594 0.750039 x

x Nb 9 0.799307 0.004005 0.249960 x

x Nb 10 0.800726 -0.003821 0.750031 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07432448E+004 8951.72 <-- SCF

1 -2.07516755E+004 2.81025436E-001 8969.59 <-- SCF

2 -2.07525166E+004 2.80350532E-002 9002.88 <-- SCF

3 -2.07476151E+004 -1.63381718E-001 9031.44 <-- SCF

4 -2.07461501E+004 -4.88346150E-002 9060.84 <-- SCF

5 -2.07459683E+004 -6.06124200E-003 9087.88 <-- SCF

6 -2.07459612E+004 -2.34831168E-004 9117.11 <-- SCF

7 -2.07459524E+004 -2.93134944E-004 9146.61 <-- SCF

8 -2.07459552E+004 9.32825218E-005 9176.30 <-- SCF

9 -2.07459544E+004 -2.83986524E-005 9205.03 <-- SCF

10 -2.07459550E+004 2.14834330E-005 9233.38 <-- SCF

11 -2.07459555E+004 1.59446875E-005 9260.55 <-- SCF

12 -2.07459555E+004 -4.50839664E-007 9283.64 <-- SCF

13 -2.07459555E+004 1.27143347E-006 9306.91 <-- SCF

14 -2.07459555E+004 1.51532649E-007 9328.05 <-- SCF

15 -2.07459555E+004 8.97296349E-007 9349.56 <-- SCF

16 -2.07459555E+004 4.84669571E-008 9370.64 <-- SCF

17 -2.07459555E+004 -4.48422137E-007 9391.69 <-- SCF

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

Final energy = -20745.95553329 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.14933 0.10238 0.12206 \*

\* Se 2 0.05273 -0.13873 0.28785 \*

\* Se 3 0.08007 -0.16237 -0.25317 \*

\* Se 4 -0.10500 0.06819 -0.15283 \*

\* Se 5 -0.02924 0.13994 0.25052 \*

\* Se 6 0.07274 -0.10914 0.08365 \*

\* Se 7 0.11589 -0.15038 -0.05945 \*

\* Se 8 0.00952 0.10436 -0.26602 \*

\* Se 9 -0.15662 0.11495 0.12696 \*

\* Se 10 0.11417 -0.08841 0.17884 \*

\* Se 11 0.16246 -0.11411 -0.13775 \*

\* Se 12 -0.11043 0.08906 -0.16776 \*

\* Se 13 -0.10717 0.15081 0.05252 \*

\* Se 14 -0.00978 -0.10350 0.29263 \*

\* Se 15 0.03078 -0.13891 -0.27815 \*

\* Se 16 -0.06303 0.10886 -0.07592 \*

\* Se 17 -0.08115 0.16264 0.22830 \*

\* Se 18 0.12009 -0.06595 0.15509 \*

\* Se 19 0.16176 -0.10007 -0.12367 \*

\* Se 20 -0.05205 0.13713 -0.26548 \*

\* Nb 1 0.12859 -0.23114 0.02503 \*

\* Nb 2 -0.13322 0.23051 -0.02434 \*

\* Nb 3 0.21003 -0.22462 0.01593 \*

\* Nb 4 -0.24300 0.26200 -0.02103 \*

\* Nb 5 0.11096 -0.23173 0.02051 \*

\* Nb 6 -0.18596 0.25100 -0.02387 \*

\* Nb 7 0.17851 -0.25237 0.02427 \*

\* Nb 8 -0.11558 0.23128 -0.02012 \*

\* Nb 9 0.22423 -0.26293 0.02133 \*

\* Nb 10 -0.23099 0.22125 -0.01590 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.741899 0.587194 -0.158077 \*

\* y 0.587194 1.548953 0.145929 \*

\* z -0.158077 0.145929 1.142044 \*

\* \*

\* Pressure: -1.1443 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.001266 | -20745.918407 | <-- min BFGS

| trial step | 1.000000 | 0.000787 | -20745.946512 | <-- min BFGS

| line step | 2.641235 | -0.000351 | -20745.955489 | <-- min BFGS

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

BFGS: finished iteration 5 with enthalpy= -2.07459555E+004 eV

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

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

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

| dE/ion | 1.236077E-003 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 3.579572E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.236398E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.548953E+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 | 0.002949 | -20745.955489 | <-- 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)

14.8805897 -8.5336134 -0.0179237 0.4205564 -0.0029370 0.0002695

0.0241299 3.4555270 0.0036020 1.0385859 1.8110490 -0.0012156

-0.0082082 0.0134044 12.9570565 0.0002930 -0.0005075 0.4849245

Lattice parameters(A) Cell Angles

a = 17.153858 alpha = 89.881259

b = 3.455613 beta = 90.120841

c = 12.957066 gamma = 119.433045

Current cell volume = 668.922552 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 0.067242 0.665876 0.121802 x

x Se 2 0.133367 0.336683 0.621080 x

x Se 3 0.133142 0.336255 0.878767 x

x Se 4 0.067051 0.665512 0.378337 x

x Se 5 0.266351 0.664211 0.121143 x

x Se 6 0.333157 0.335848 0.621767 x

x Se 7 0.332976 0.335520 0.878128 x

x Se 8 0.266146 0.663731 0.378911 x

x Se 9 0.467498 0.666316 0.121833 x

x Se 10 0.532681 0.334085 0.621637 x

x Se 11 0.532468 0.333599 0.878191 x

x Se 12 0.467295 0.665855 0.378338 x

x Se 13 0.666978 0.664377 0.121907 x

x Se 14 0.733866 0.336287 0.620988 x

x Se 15 0.733652 0.335791 0.878958 x

x Se 16 0.666804 0.664065 0.378200 x

x Se 17 0.866883 0.663792 0.121323 x

x Se 18 0.932877 0.334343 0.621660 x

x Se 19 0.932680 0.333962 0.878200 x

x Se 20 0.866670 0.663385 0.378832 x

x Nb 1 -0.000676 0.003292 0.249981 x

x Nb 2 0.000691 -0.003260 0.750025 x

x Nb 3 0.199476 0.003548 0.249969 x

x Nb 4 0.200649 -0.003289 0.750026 x

x Nb 5 0.399266 0.003317 0.249970 x

x Nb 6 0.400565 -0.003370 0.750020 x

x Nb 7 0.599426 0.003302 0.249983 x

x Nb 8 0.600801 -0.003141 0.750031 x

x Nb 9 0.799441 0.003516 0.249968 x

x Nb 10 0.800578 -0.003411 0.750026 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07448978E+004 9777.95 <-- SCF

1 -2.07475084E+004 8.70196475E-002 9795.16 <-- SCF

2 -2.07476671E+004 5.29057624E-003 9827.16 <-- SCF

3 -2.07462840E+004 -4.61060742E-002 9855.30 <-- SCF

4 -2.07460335E+004 -8.34779616E-003 9882.17 <-- SCF

5 -2.07460072E+004 -8.76342887E-004 9908.38 <-- SCF

6 -2.07460088E+004 5.28927194E-005 9937.67 <-- SCF

7 -2.07460065E+004 -7.64042527E-005 9965.67 <-- SCF

8 -2.07460084E+004 6.27971752E-005 9991.83 <-- SCF

9 -2.07460062E+004 -7.50027961E-005 10018.28 <-- SCF

10 -2.07460065E+004 1.07123717E-005 10043.86 <-- SCF

11 -2.07460068E+004 9.82981886E-006 10068.30 <-- SCF

12 -2.07460067E+004 -3.48469553E-006 10091.25 <-- SCF

13 -2.07460067E+004 1.66187559E-006 10111.77 <-- SCF

14 -2.07460068E+004 7.06876827E-007 10132.20 <-- SCF

15 -2.07460068E+004 3.59273930E-007 10152.22 <-- SCF

16 -2.07460068E+004 2.58964718E-007 10172.55 <-- SCF

17 -2.07460068E+004 1.37481316E-007 10192.97 <-- SCF

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

Final energy = -20746.00677392 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.09075 0.08762 0.04921 \*

\* Se 2 0.05309 -0.13777 0.18408 \*

\* Se 3 0.05136 -0.15293 -0.15358 \*

\* Se 4 -0.08120 0.06063 -0.07801 \*

\* Se 5 0.00422 0.12701 0.16326 \*

\* Se 6 0.05918 -0.09349 0.02766 \*

\* Se 7 0.06590 -0.12796 -0.00470 \*

\* Se 8 0.00725 0.09761 -0.17351 \*

\* Se 9 -0.09718 0.11106 0.05311 \*

\* Se 10 0.10277 -0.09041 0.08974 \*

\* Se 11 0.09982 -0.10996 -0.06097 \*

\* Se 12 -0.10120 0.09132 -0.08168 \*

\* Se 13 -0.05886 0.12740 -0.00038 \*

\* Se 14 -0.00520 -0.09713 0.19244 \*

\* Se 15 -0.00097 -0.12635 -0.18296 \*

\* Se 16 -0.05186 0.09263 -0.02253 \*

\* Se 17 -0.05116 0.15195 0.13523 \*

\* Se 18 0.09313 -0.05995 0.07984 \*

\* Se 19 0.10110 -0.08586 -0.05088 \*

\* Se 20 -0.05265 0.13648 -0.16656 \*

\* Nb 1 0.08432 -0.21814 0.02109 \*

\* Nb 2 -0.08720 0.21858 -0.02113 \*

\* Nb 3 0.14422 -0.21415 0.01208 \*

\* Nb 4 -0.17382 0.24612 -0.01679 \*

\* Nb 5 0.06702 -0.21940 0.01836 \*

\* Nb 6 -0.12878 0.23767 -0.01922 \*

\* Nb 7 0.12174 -0.23728 0.01928 \*

\* Nb 8 -0.07259 0.21916 -0.01812 \*

\* Nb 9 0.16023 -0.24707 0.01747 \*

\* Nb 10 -0.16195 0.21260 -0.01183 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.269831 0.160763 -0.011873 \*

\* y 0.160763 0.477245 0.123528 \*

\* z -0.011873 0.123528 0.126539 \*

\* \*

\* Pressure: -0.2912 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.002949 | -20745.955489 | <-- min BFGS

| trial step | 1.000000 | 0.000773 | -20746.006813 | <-- min BFGS

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

BFGS: finished iteration 6 with enthalpy= -2.07460068E+004 eV

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

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

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

| dE/ion | 1.710807E-003 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 3.017815E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.964184E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.772454E-001 | 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 | 0.000393 | -20746.006813 | <-- 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)

14.8887050 -8.5356622 -0.0098567 0.4206377 -0.0023941 0.0000887

0.0196273 3.4485691 0.0030310 1.0411334 1.8160445 -0.0013831

-0.0026635 0.0113848 12.9437098 0.0000765 -0.0004271 0.4854242

Lattice parameters(A) Cell Angles

a = 17.161910 alpha = 89.899315

b = 3.448626 beta = 90.068200

c = 12.943715 gamma = 119.499478

Current cell volume = 666.759207 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 0.067218 0.665855 0.121859 x

x Se 2 0.133375 0.336645 0.621166 x

x Se 3 0.133159 0.336225 0.878684 x

x Se 4 0.067039 0.665504 0.378276 x

x Se 5 0.266340 0.664251 0.121226 x

x Se 6 0.333165 0.335833 0.621821 x

x Se 7 0.332997 0.335512 0.878077 x

x Se 8 0.266146 0.663777 0.378826 x

x Se 9 0.467472 0.666304 0.121890 x

x Se 10 0.532698 0.334091 0.621701 x

x Se 11 0.532495 0.333615 0.878131 x

x Se 12 0.467279 0.665852 0.378277 x

x Se 13 0.666961 0.664391 0.121957 x

x Se 14 0.733867 0.336243 0.621078 x

x Se 15 0.733664 0.335753 0.878869 x

x Se 16 0.666798 0.664086 0.378147 x

x Se 17 0.866866 0.663822 0.121399 x

x Se 18 0.932892 0.334362 0.621722 x

x Se 19 0.932706 0.333994 0.878142 x

x Se 20 0.866662 0.663424 0.378752 x

x Nb 1 -0.000654 0.003254 0.249985 x

x Nb 2 0.000669 -0.003222 0.750021 x

x Nb 3 0.199510 0.003547 0.249971 x

x Nb 4 0.200609 -0.003276 0.750023 x

x Nb 5 0.399281 0.003266 0.249973 x

x Nb 6 0.400534 -0.003346 0.750016 x

x Nb 7 0.599456 0.003273 0.249987 x

x Nb 8 0.600783 -0.003096 0.750028 x

x Nb 9 0.799475 0.003487 0.249971 x

x Nb 10 0.800539 -0.003424 0.750024 x

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07459458E+004 10577.69 <-- SCF

1 -2.07460375E+004 3.05503398E-003 10593.55 <-- SCF

2 -2.07460422E+004 1.57081775E-004 10624.12 <-- SCF

3 -2.07460224E+004 -6.59907290E-004 10651.77 <-- SCF

4 -2.07460134E+004 -2.98961521E-004 10679.27 <-- SCF

5 -2.07460148E+004 4.48754921E-005 10706.41 <-- SCF

6 -2.07460132E+004 -5.42066698E-005 10733.88 <-- SCF

7 -2.07460125E+004 -2.06422479E-005 10758.84 <-- SCF

8 -2.07460126E+004 3.66826236E-006 10781.45 <-- SCF

9 -2.07460128E+004 6.47982301E-006 10802.12 <-- SCF

10 -2.07460130E+004 3.91954553E-006 10822.61 <-- SCF

11 -2.07460129E+004 -2.68122735E-007 10843.00 <-- SCF

12 -2.07460129E+004 -1.77783428E-006 10863.41 <-- SCF

13 -2.07460129E+004 -8.78934015E-007 10885.09 <-- SCF

14 -2.07460129E+004 3.88632588E-008 10906.14 <-- SCF

15 -2.07460129E+004 9.20729778E-008 10926.22 <-- SCF

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

Final energy = -20746.01287404 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.07474 0.08929 -0.00679 \*

\* Se 2 0.05172 -0.14346 0.12309 \*

\* Se 3 0.03921 -0.15395 -0.09280 \*

\* Se 4 -0.07979 0.06401 -0.02088 \*

\* Se 5 0.01750 0.12876 0.09723 \*

\* Se 6 0.05583 -0.09925 -0.02992 \*

\* Se 7 0.04842 -0.12972 0.05118 \*

\* Se 8 0.00757 0.10365 -0.10858 \*

\* Se 9 -0.08451 0.11035 0.00118 \*

\* Se 10 0.10354 -0.09195 0.03578 \*

\* Se 11 0.08638 -0.10957 -0.00805 \*

\* Se 12 -0.10269 0.09249 -0.02851 \*

\* Se 13 -0.04333 0.13005 -0.05629 \*

\* Se 14 -0.00774 -0.10308 0.12630 \*

\* Se 15 -0.01679 -0.12806 -0.11594 \*

\* Se 16 -0.05051 0.09931 0.03486 \*

\* Se 17 -0.03965 0.15224 0.07484 \*

\* Se 18 0.09010 -0.06299 0.02252 \*

\* Se 19 0.08381 -0.08717 0.00563 \*

\* Se 20 -0.05245 0.14112 -0.10583 \*

\* Nb 1 0.07072 -0.22893 0.02050 \*

\* Nb 2 -0.07312 0.22886 -0.02084 \*

\* Nb 3 0.12513 -0.22391 0.01154 \*

\* Nb 4 -0.15058 0.25526 -0.01606 \*

\* Nb 5 0.05415 -0.22880 0.01821 \*

\* Nb 6 -0.10764 0.24566 -0.01844 \*

\* Nb 7 0.10372 -0.24734 0.01837 \*

\* Nb 8 -0.05874 0.23013 -0.01805 \*

\* Nb 9 0.14045 -0.25499 0.01691 \*

\* Nb 10 -0.13600 0.22197 -0.01116 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.038464 -0.008185 0.044160 \*

\* y -0.008185 -0.008156 0.110444 \*

\* z 0.044160 0.110444 -0.327090 \*

\* \*

\* Pressure: 0.0989 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000393 | -20746.006813 | <-- min BFGS

| trial step | 1.000000 | 0.000048 | -20746.012899 | <-- min BFGS

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

BFGS: finished iteration 7 with enthalpy= -2.07460129E+004 eV

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

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

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

| dE/ion | 2.028621E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.968020E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.182862E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.270899E-001 | 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 | 0.000079 | -20746.012899 | <-- 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)

14.8893303 -8.5358430 -0.0082426 0.4206717 -0.0023039 0.0000718

0.0188799 3.4473494 0.0026278 1.0416081 1.8169098 -0.0012241

-0.0021562 0.0099573 12.9442660 0.0000564 -0.0003703 0.4854033

Lattice parameters(A) Cell Angles

a = 17.162542 alpha = 89.912304

b = 3.447402 beta = 90.057718

c = 12.944270 gamma = 119.511264

Current cell volume = 666.498307 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 0.067208 0.665870 0.121868 x

x Se 2 0.133381 0.336593 0.621193 x

x Se 3 0.133166 0.336168 0.878661 x

x Se 4 0.067030 0.665510 0.378264 x

x Se 5 0.266340 0.664314 0.121251 x

x Se 6 0.333172 0.335804 0.621826 x

x Se 7 0.333005 0.335470 0.878075 x

x Se 8 0.266147 0.663828 0.378800 x

x Se 9 0.467460 0.666326 0.121899 x

x Se 10 0.532710 0.334079 0.621715 x

x Se 11 0.532508 0.333595 0.878121 x

x Se 12 0.467267 0.665864 0.378265 x

x Se 13 0.666954 0.664435 0.121958 x

x Se 14 0.733866 0.336192 0.621107 x

x Se 15 0.733664 0.335691 0.878842 x

x Se 16 0.666792 0.664118 0.378143 x

x Se 17 0.866859 0.663880 0.121420 x

x Se 18 0.932903 0.334360 0.621734 x

x Se 19 0.932719 0.333983 0.878133 x

x Se 20 0.866656 0.663475 0.378727 x

x Nb 1 -0.000644 0.003172 0.249988 x

x Nb 2 0.000659 -0.003141 0.750018 x

x Nb 3 0.199527 0.003486 0.249973 x

x Nb 4 0.200589 -0.003207 0.750021 x

x Nb 5 0.399289 0.003178 0.249976 x

x Nb 6 0.400518 -0.003268 0.750013 x

x Nb 7 0.599470 0.003193 0.249989 x

x Nb 8 0.600774 -0.003011 0.750025 x

x Nb 9 0.799493 0.003413 0.249973 x

x Nb 10 0.800519 -0.003369 0.750022 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460113E+004 11311.41 <-- SCF

1 -2.07460246E+004 4.43142195E-004 11328.64 <-- SCF

2 -2.07460258E+004 4.11671529E-005 11357.09 <-- SCF

3 -2.07460776E+004 1.72371268E-003 11384.89 <-- SCF

4 -2.07459948E+004 -2.76022741E-003 11412.58 <-- SCF

5 -2.07460002E+004 1.83182127E-004 11438.55 <-- SCF

6 -2.07460092E+004 2.98527183E-004 11465.36 <-- SCF

7 -2.07460150E+004 1.93856839E-004 11491.61 <-- SCF

8 -2.07460174E+004 8.08817141E-005 11515.56 <-- SCF

9 -2.07460185E+004 3.48421018E-005 11536.09 <-- SCF

10 -2.07460187E+004 8.59082226E-006 11556.56 <-- SCF

11 -2.07460187E+004 -9.13852757E-008 11576.84 <-- SCF

12 -2.07460185E+004 -7.96085607E-006 11597.55 <-- SCF

13 -2.07460182E+004 -1.01777252E-005 11617.98 <-- SCF

14 -2.07460185E+004 1.07723182E-005 11638.77 <-- SCF

15 -2.07460200E+004 5.00523995E-005 11659.72 <-- SCF

16 -2.07460191E+004 -3.05127404E-005 11680.17 <-- SCF

17 -2.07460177E+004 -4.67673702E-005 11701.16 <-- SCF

18 -2.07460163E+004 -4.71372980E-005 11724.16 <-- SCF

19 -2.07460154E+004 -3.00310517E-005 11745.28 <-- SCF

20 -2.07460143E+004 -3.54811874E-005 11770.25 <-- SCF

21 -2.07460147E+004 1.24712066E-005 11790.66 <-- SCF

22 -2.07460149E+004 5.68501973E-006 11811.38 <-- SCF

23 -2.07460149E+004 2.42881060E-006 11831.89 <-- SCF

24 -2.07460150E+004 1.50791222E-007 11852.05 <-- SCF

25 -2.07460149E+004 -4.73470516E-007 11872.05 <-- SCF

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

Final energy = -20746.01493606 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.07110 0.08541 -0.00843 \*

\* Se 2 0.04966 -0.14306 0.11010 \*

\* Se 3 0.03779 -0.14975 -0.08078 \*

\* Se 4 -0.07516 0.06340 -0.01844 \*

\* Se 5 0.01862 0.12250 0.09121 \*

\* Se 6 0.05328 -0.09682 -0.03872 \*

\* Se 7 0.04627 -0.12341 0.05914 \*

\* Se 8 0.00962 0.10151 -0.10241 \*

\* Se 9 -0.08218 0.10647 0.00265 \*

\* Se 10 0.10056 -0.09147 0.03030 \*

\* Se 11 0.08362 -0.10579 -0.00328 \*

\* Se 12 -0.09949 0.09193 -0.02950 \*

\* Se 13 -0.04193 0.12420 -0.05553 \*

\* Se 14 -0.00755 -0.10166 0.11220 \*

\* Se 15 -0.01594 -0.12265 -0.10197 \*

\* Se 16 -0.04836 0.09735 0.03525 \*

\* Se 17 -0.03853 0.14711 0.07182 \*

\* Se 18 0.08383 -0.06228 0.01534 \*

\* Se 19 0.07812 -0.08327 0.01187 \*

\* Se 20 -0.05047 0.13987 -0.10202 \*

\* Nb 1 0.06607 -0.22485 0.01993 \*

\* Nb 2 -0.08038 0.22345 -0.02029 \*

\* Nb 3 0.11588 -0.21549 0.01135 \*

\* Nb 4 -0.13565 0.25348 -0.01558 \*

\* Nb 5 0.05146 -0.22468 0.01745 \*

\* Nb 6 -0.09876 0.23541 -0.01771 \*

\* Nb 7 0.10172 -0.24320 0.01788 \*

\* Nb 8 -0.06657 0.23096 -0.01764 \*

\* Nb 9 0.13266 -0.24900 0.01633 \*

\* Nb 10 -0.11710 0.21434 -0.01050 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.006587 -0.031112 0.043213 \*

\* y -0.031112 -0.087955 0.094738 \*

\* z 0.043213 0.094738 -0.364784 \*

\* \*

\* Pressure: 0.1487 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000079 | -20746.012899 | <-- min BFGS

| trial step | 1.000000 | 0.000070 | -20746.014965 | <-- min BFGS

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

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BFGS: improving iteration 8 with line minimization (lambda= 8.299527)

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Unit Cell

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

14.8938950 -8.5371635 0.0035396 0.4209211 -0.0016434 -0.0000503

0.0134249 3.4384462 -0.0003153 1.0450862 1.8232524 -0.0000597

0.0015468 -0.0004625 12.9483260 -0.0000896 0.0000449 0.4852508

Lattice parameters(A) Cell Angles

a = 17.167157 alpha = 90.007274

b = 3.438472 beta = 89.981231

c = 12.948326 gamma = 119.597584

Current cell volume = 664.591816 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 0.067128 0.665978 0.121927 x

x Se 2 0.133424 0.336212 0.621394 x

x Se 3 0.133213 0.335745 0.878489 x

x Se 4 0.066962 0.665553 0.378178 x

x Se 5 0.266339 0.664770 0.121427 x

x Se 6 0.333219 0.335587 0.621862 x

x Se 7 0.333062 0.335163 0.878060 x

x Se 8 0.266153 0.664202 0.378612 x

x Se 9 0.467371 0.666488 0.121963 x

x Se 10 0.532801 0.333994 0.621815 x

x Se 11 0.532600 0.333443 0.878048 x

x Se 12 0.467178 0.665957 0.378173 x

x Se 13 0.666903 0.664760 0.121966 x

x Se 14 0.733860 0.335820 0.621315 x

x Se 15 0.733665 0.335240 0.878644 x

x Se 16 0.666752 0.664351 0.378114 x

x Se 17 0.866811 0.664296 0.121569 x

x Se 18 0.932982 0.334351 0.621823 x

x Se 19 0.932809 0.333910 0.878073 x

x Se 20 0.866612 0.663847 0.378548 x

x Nb 1 -0.000570 0.002575 0.250010 x

x Nb 2 0.000582 -0.002550 0.749997 x

x Nb 3 0.199653 0.003040 0.249985 x

x Nb 4 0.200440 -0.002700 0.750004 x

x Nb 5 0.399345 0.002537 0.249994 x

x Nb 6 0.400407 -0.002703 0.749994 x

x Nb 7 0.599576 0.002610 0.250009 x

x Nb 8 0.600712 -0.002383 0.750007 x

x Nb 9 0.799628 0.002870 0.249991 x

x Nb 10 0.800380 -0.002965 0.750011 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07458380E+004 12260.59 <-- SCF

1 -2.07461214E+004 9.44784545E-003 12276.06 <-- SCF

2 -2.07461427E+004 7.09157862E-004 12306.84 <-- SCF

3 -2.07460684E+004 -2.47745387E-003 12334.89 <-- SCF

4 -2.07460255E+004 -1.42901793E-003 12362.03 <-- SCF

5 -2.07460252E+004 -1.08127823E-005 12389.89 <-- SCF

6 -2.07460229E+004 -7.50399710E-005 12417.58 <-- SCF

7 -2.07460219E+004 -3.27317915E-005 12444.66 <-- SCF

8 -2.07460219E+004 -2.73811409E-007 12469.92 <-- SCF

9 -2.07460220E+004 3.09328903E-006 12494.52 <-- SCF

10 -2.07460220E+004 7.56611635E-007 12516.14 <-- SCF

11 -2.07460220E+004 -2.19221130E-007 12537.34 <-- SCF

12 -2.07460220E+004 -1.87285111E-008 12558.17 <-- SCF

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

Final energy = -20746.02203413 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.04108 0.05556 -0.04156 \*

\* Se 2 0.04464 -0.13228 0.04551 \*

\* Se 3 0.02756 -0.11226 -0.02448 \*

\* Se 4 -0.05412 0.05729 0.02250 \*

\* Se 5 0.03488 0.08385 0.02385 \*

\* Se 6 0.03417 -0.08486 -0.06311 \*

\* Se 7 0.01869 -0.08291 0.07535 \*

\* Se 8 0.01928 0.09210 -0.03259 \*

\* Se 9 -0.06035 0.07459 -0.03081 \*

\* Se 10 0.08966 -0.08244 -0.00351 \*

\* Se 11 0.06244 -0.07307 0.02442 \*

\* Se 12 -0.08816 0.08374 0.01038 \*

\* Se 13 -0.01123 0.08092 -0.07948 \*

\* Se 14 -0.01777 -0.09093 0.04443 \*

\* Se 15 -0.03260 -0.08292 -0.03638 \*

\* Se 16 -0.02706 0.08286 0.06696 \*

\* Se 17 -0.02568 0.11114 0.01255 \*

\* Se 18 0.06187 -0.05873 -0.02044 \*

\* Se 19 0.04864 -0.05624 0.04010 \*

\* Se 20 -0.04419 0.13050 -0.03343 \*

\* Nb 1 0.03869 -0.19188 0.01344 \*

\* Nb 2 -0.04208 0.19484 -0.01413 \*

\* Nb 3 0.05658 -0.18366 0.00760 \*

\* Nb 4 -0.08021 0.20776 -0.00997 \*

\* Nb 5 0.03068 -0.19255 0.01241 \*

\* Nb 6 -0.06413 0.20464 -0.01259 \*

\* Nb 7 0.05789 -0.19993 0.01211 \*

\* Nb 8 -0.03159 0.19064 -0.01257 \*

\* Nb 9 0.06840 -0.20883 0.01081 \*

\* Nb 10 -0.07380 0.18305 -0.00734 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.236517 -0.182756 0.073197 \*

\* y -0.182756 -0.675928 -0.010569 \*

\* z 0.073197 -0.010569 -0.650737 \*

\* \*

\* Pressure: 0.5211 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000079 | -20746.012899 | <-- min BFGS

| trial step | 1.000000 | 0.000070 | -20746.014965 | <-- min BFGS

| line step | 8.299527 | 1.461E-006 | -20746.022125 | <-- min BFGS

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

BFGS: finished iteration 8 with enthalpy= -2.07460221E+004 eV

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

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

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

| dE/ion | 3.075241E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.229342E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.261417E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 6.759278E-001 | 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 | 0.000430 | -20746.022125 | <-- 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)

14.8888451 -8.5349468 0.0042316 0.4210047 -0.0017471 0.0000384

0.0142716 3.4390256 -0.0019052 1.0448462 1.8226894 0.0009501

-0.0012091 -0.0060719 12.9781863 0.0000161 0.0002681 0.4841344

Lattice parameters(A) Cell Angles

a = 17.161674 alpha = 90.058569

b = 3.439056 beta = 89.977172

c = 12.978188 gamma = 119.585481

Current cell volume = 666.104281 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 0.067103 0.666063 0.122057 x

x Se 2 0.133455 0.336028 0.621592 x

x Se 3 0.133229 0.335513 0.878308 x

x Se 4 0.066929 0.665565 0.378032 x

x Se 5 0.266341 0.665035 0.121609 x

x Se 6 0.333245 0.335495 0.621975 x

x Se 7 0.333079 0.334984 0.877958 x

x Se 8 0.266143 0.664386 0.378424 x

x Se 9 0.467347 0.666623 0.122100 x

x Se 10 0.532841 0.333936 0.621971 x

x Se 11 0.532624 0.333311 0.877906 x

x Se 12 0.467138 0.666017 0.378022 x

x Se 13 0.666888 0.664944 0.122065 x

x Se 14 0.733870 0.335640 0.621513 x

x Se 15 0.733665 0.334979 0.878451 x

x Se 16 0.666728 0.664448 0.378003 x

x Se 17 0.866795 0.664526 0.121742 x

x Se 18 0.933019 0.334351 0.621969 x

x Se 19 0.932837 0.333838 0.877942 x

x Se 20 0.866582 0.664027 0.378359 x

x Nb 1 -0.000551 0.002208 0.250023 x

x Nb 2 0.000562 -0.002185 0.749983 x

x Nb 3 0.199706 0.002769 0.249992 x

x Nb 4 0.200375 -0.002382 0.749994 x

x Nb 5 0.399354 0.002148 0.250006 x

x Nb 6 0.400364 -0.002350 0.749982 x

x Nb 7 0.599617 0.002247 0.250021 x

x Nb 8 0.600703 -0.001993 0.749995 x

x Nb 9 0.799689 0.002542 0.250001 x

x Nb 10 0.800321 -0.002713 0.750004 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07459422E+004 12944.91 <-- SCF

1 -2.07461635E+004 7.37911505E-003 12962.17 <-- SCF

2 -2.07461923E+004 9.59242210E-004 12992.67 <-- SCF

3 -2.07460985E+004 -3.12660910E-003 13020.47 <-- SCF

4 -2.07460334E+004 -2.17179014E-003 13048.20 <-- SCF

5 -2.07460340E+004 2.20611509E-005 13076.50 <-- SCF

6 -2.07460327E+004 -4.43768301E-005 13103.70 <-- SCF

7 -2.07460319E+004 -2.50667830E-005 13130.73 <-- SCF

8 -2.07460320E+004 1.78005877E-006 13156.59 <-- SCF

9 -2.07460321E+004 2.50530288E-006 13179.16 <-- SCF

10 -2.07460321E+004 1.43727834E-006 13200.45 <-- SCF

11 -2.07460321E+004 1.15392315E-006 13222.17 <-- SCF

12 -2.07460322E+004 2.02103960E-007 13243.44 <-- SCF

13 -2.07460322E+004 2.41435895E-007 13264.20 <-- SCF

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

Final energy = -20746.03216080 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.04039 0.03507 -0.01782 \*

\* Se 2 0.03949 -0.12161 0.04793 \*

\* Se 3 0.03093 -0.08548 -0.03381 \*

\* Se 4 -0.04341 0.05238 0.00224 \*

\* Se 5 0.02974 0.05457 0.03077 \*

\* Se 6 0.02159 -0.07194 -0.03914 \*

\* Se 7 0.01561 -0.05291 0.04699 \*

\* Se 8 0.02453 0.07944 -0.03757 \*

\* Se 9 -0.06059 0.05062 -0.00682 \*

\* Se 10 0.07985 -0.07420 0.01700 \*

\* Se 11 0.06225 -0.04937 0.00002 \*

\* Se 12 -0.07865 0.07527 -0.00972 \*

\* Se 13 -0.00951 0.05042 -0.05134 \*

\* Se 14 -0.02355 -0.07833 0.04834 \*

\* Se 15 -0.02789 -0.05347 -0.04175 \*

\* Se 16 -0.01607 0.06949 0.04323 \*

\* Se 17 -0.02949 0.08495 0.02333 \*

\* Se 18 0.05070 -0.05390 0.00039 \*

\* Se 19 0.04761 -0.03604 0.01548 \*

\* Se 20 -0.03968 0.12000 -0.03714 \*

\* Nb 1 0.03653 -0.16060 0.00936 \*

\* Nb 2 -0.03798 0.16401 -0.00993 \*

\* Nb 3 0.04063 -0.14922 0.00576 \*

\* Nb 4 -0.06085 0.17028 -0.00661 \*

\* Nb 5 0.02552 -0.15941 0.00848 \*

\* Nb 6 -0.05441 0.16971 -0.00949 \*

\* Nb 7 0.05026 -0.16430 0.00922 \*

\* Nb 8 -0.02723 0.15796 -0.00886 \*

\* Nb 9 0.04981 -0.17244 0.00708 \*

\* Nb 10 -0.05537 0.14909 -0.00560 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.177165 -0.117418 0.033292 \*

\* y -0.117418 -0.601203 -0.073404 \*

\* z 0.033292 -0.073404 -0.391498 \*

\* \*

\* Pressure: 0.3900 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000430 | -20746.022125 | <-- min BFGS

| trial step | 1.000000 | 0.000311 | -20746.032169 | <-- min BFGS

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

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BFGS: improving iteration 9 with line minimization (lambda= 3.619665)

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Unit Cell

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

14.8756159 -8.5291399 0.0060444 0.4212242 -0.0020184 0.0002687

0.0164899 3.4405432 -0.0060700 1.0442205 1.8212205 0.0035708

-0.0084284 -0.0207666 13.0564101 0.0002905 0.0008476 0.4812353

Lattice parameters(A) Cell Angles

a = 17.147309 alpha = 90.192390

b = 3.440588 beta = 89.966561

c = 13.056429 gamma = 119.553782

Current cell volume = 670.063853 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 0.067037 0.666284 0.122399 x

x Se 2 0.133534 0.335545 0.622111 x

x Se 3 0.133273 0.334905 0.877831 x

x Se 4 0.066842 0.665596 0.377652 x

x Se 5 0.266345 0.665729 0.122087 x

x Se 6 0.333312 0.335253 0.622271 x

x Se 7 0.333122 0.334514 0.877692 x

x Se 8 0.266118 0.664867 0.377930 x

x Se 9 0.467285 0.666977 0.122459 x

x Se 10 0.532944 0.333784 0.622378 x

x Se 11 0.532686 0.332964 0.877536 x

x Se 12 0.467035 0.666172 0.377627 x

x Se 13 0.666850 0.665427 0.122325 x

x Se 14 0.733897 0.335166 0.622031 x

x Se 15 0.733663 0.334295 0.877948 x

x Se 16 0.666667 0.664703 0.377714 x

x Se 17 0.866753 0.665128 0.122193 x

x Se 18 0.933116 0.334352 0.622353 x

x Se 19 0.932910 0.333650 0.877598 x

x Se 20 0.866505 0.664500 0.377864 x

x Nb 1 -0.000501 0.001248 0.250058 x

x Nb 2 0.000509 -0.001229 0.749948 x

x Nb 3 0.199845 0.002058 0.250010 x

x Nb 4 0.200207 -0.001548 0.749968 x

x Nb 5 0.399376 0.001129 0.250036 x

x Nb 6 0.400249 -0.001426 0.749951 x

x Nb 7 0.599724 0.001296 0.250052 x

x Nb 8 0.600680 -0.000972 0.749966 x

x Nb 9 0.799849 0.001684 0.250029 x

x Nb 10 0.800167 -0.002051 0.749986 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07454324E+004 13651.77 <-- SCF

1 -2.07469131E+004 4.93571016E-002 13669.19 <-- SCF

2 -2.07470287E+004 3.85060305E-003 13700.62 <-- SCF

3 -2.07462650E+004 -2.54564547E-002 13728.84 <-- SCF

4 -2.07460668E+004 -6.60673699E-003 13756.62 <-- SCF

5 -2.07460454E+004 -7.12991641E-004 13783.73 <-- SCF

6 -2.07460441E+004 -4.10417817E-005 13812.80 <-- SCF

7 -2.07460431E+004 -3.54483732E-005 13841.11 <-- SCF

8 -2.07460433E+004 8.75344280E-006 13869.69 <-- SCF

9 -2.07460434E+004 2.39137801E-006 13894.95 <-- SCF

10 -2.07460436E+004 7.70287779E-006 13920.17 <-- SCF

11 -2.07460435E+004 -3.86120459E-006 13943.14 <-- SCF

12 -2.07460435E+004 3.41729640E-007 13964.42 <-- SCF

13 -2.07460436E+004 1.58547292E-006 13985.05 <-- SCF

14 -2.07460436E+004 3.28120276E-007 14005.78 <-- SCF

15 -2.07460436E+004 1.45042017E-007 14026.64 <-- SCF

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

Final energy = -20746.04360418 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.03760 -0.01494 0.05150 \*

\* Se 2 0.02482 -0.08422 0.05571 \*

\* Se 3 0.03221 -0.01554 -0.05729 \*

\* Se 4 -0.02071 0.04226 -0.05515 \*

\* Se 5 0.02146 -0.02398 0.05149 \*

\* Se 6 -0.00719 -0.03918 0.02181 \*

\* Se 7 0.00590 0.02324 -0.02610 \*

\* Se 8 0.03922 0.04191 -0.04977 \*

\* Se 9 -0.06011 -0.01320 0.05813 \*

\* Se 10 0.05360 -0.04885 0.06442 \*

\* Se 11 0.06162 0.01397 -0.06061 \*

\* Se 12 -0.05234 0.04949 -0.06141 \*

\* Se 13 -0.00157 -0.02495 0.02566 \*

\* Se 14 -0.03947 -0.04191 0.05391 \*

\* Se 15 -0.02087 0.02366 -0.05535 \*

\* Se 16 0.01072 0.03762 -0.02175 \*

\* Se 17 -0.03172 0.01505 0.05330 \*

\* Se 18 0.02739 -0.04360 0.05493 \*

\* Se 19 0.04446 0.01390 -0.05117 \*

\* Se 20 -0.02563 0.08287 -0.05163 \*

\* Nb 1 0.02546 -0.08174 -0.00015 \*

\* Nb 2 -0.02652 0.08441 -0.00023 \*

\* Nb 3 0.00059 -0.06202 0.00142 \*

\* Nb 4 -0.01024 0.07933 0.00178 \*

\* Nb 5 0.01192 -0.07830 -0.00014 \*

\* Nb 6 -0.03614 0.08320 -0.00226 \*

\* Nb 7 0.03313 -0.07997 0.00220 \*

\* Nb 8 -0.01722 0.07847 -0.00016 \*

\* Nb 9 0.00268 -0.08042 -0.00155 \*

\* Nb 10 -0.00783 0.06346 -0.00154 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.039021 0.052939 -0.054845 \*

\* y 0.052939 -0.417393 -0.232919 \*

\* z -0.054845 -0.232919 0.257665 \*

\* \*

\* Pressure: 0.0662 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000430 | -20746.022125 | <-- min BFGS

| trial step | 1.000000 | 0.000311 | -20746.032169 | <-- min BFGS

| line step | 3.619665 | 0.000016 | -20746.043533 | <-- min BFGS

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

BFGS: finished iteration 9 with enthalpy= -2.07460435E+004 eV

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

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

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

| dE/ion | 7.135977E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.039861E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.004151E-002 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.173926E-001 | 2.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 10 ...

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

Writing analysis data to 2H-Nb1Se2-7.castep\_bin

Writing model to 2H-Nb1Se2-7.check

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

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

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

| previous | 0.000000 | 0.000050 | -20746.043533 | <-- 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)

14.8758414 -8.5320235 0.0052146 0.4212117 -0.0020283 0.0002698

0.0165778 3.4418420 -0.0057498 1.0441484 1.8205064 0.0034136

-0.0084603 -0.0196373 13.0605896 0.0002915 0.0008023 0.4810812

Lattice parameters(A) Cell Angles

a = 17.148939 alpha = 90.182039

b = 3.441887 beta = 89.971913

c = 13.060607 gamma = 119.560403

Current cell volume = 670.551423 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 0.067031 0.666284 0.122434 x

x Se 2 0.133541 0.335497 0.622156 x

x Se 3 0.133278 0.334873 0.877788 x

x Se 4 0.066835 0.665607 0.377614 x

x Se 5 0.266346 0.665765 0.122129 x

x Se 6 0.333316 0.335228 0.622300 x

x Se 7 0.333124 0.334498 0.877664 x

x Se 8 0.266119 0.664914 0.377887 x

x Se 9 0.467278 0.666982 0.122496 x

x Se 10 0.532954 0.333770 0.622418 x

x Se 11 0.532693 0.332960 0.877499 x

x Se 12 0.467025 0.666187 0.377588 x

x Se 13 0.666848 0.665444 0.122352 x

x Se 14 0.733897 0.335119 0.622076 x

x Se 15 0.733662 0.334260 0.877904 x

x Se 16 0.666664 0.664730 0.377685 x

x Se 17 0.866749 0.665159 0.122234 x

x Se 18 0.933124 0.334344 0.622390 x

x Se 19 0.932917 0.333653 0.877563 x

x Se 20 0.866499 0.664547 0.377821 x

x Nb 1 -0.000497 0.001170 0.250060 x

x Nb 2 0.000505 -0.001151 0.749946 x

x Nb 3 0.199853 0.001998 0.250011 x

x Nb 4 0.200197 -0.001476 0.749966 x

x Nb 5 0.399377 0.001046 0.250038 x

x Nb 6 0.400240 -0.001352 0.749949 x

x Nb 7 0.599732 0.001221 0.250054 x

x Nb 8 0.600678 -0.000889 0.749964 x

x Nb 9 0.799858 0.001609 0.250030 x

x Nb 10 0.800158 -0.001995 0.749985 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460402E+004 14419.47 <-- SCF

1 -2.07460596E+004 6.46915961E-004 14437.73 <-- SCF

2 -2.07460619E+004 7.44223962E-005 14467.25 <-- SCF

3 -2.07461029E+004 1.36935516E-003 14495.59 <-- SCF

4 -2.07460237E+004 -2.64084187E-003 14523.91 <-- SCF

5 -2.07460296E+004 1.95095717E-004 14551.09 <-- SCF

6 -2.07460404E+004 3.61394443E-004 14578.94 <-- SCF

7 -2.07460480E+004 2.52059220E-004 14606.02 <-- SCF

8 -2.07460494E+004 4.91351857E-005 14631.25 <-- SCF

9 -2.07460479E+004 -5.06203414E-005 14654.77 <-- SCF

10 -2.07460460E+004 -6.23025789E-005 14678.50 <-- SCF

11 -2.07460445E+004 -5.30369307E-005 14704.41 <-- SCF

12 -2.07460449E+004 1.31170334E-005 14726.00 <-- SCF

13 -2.07460449E+004 1.47754454E-006 14746.83 <-- SCF

14 -2.07460449E+004 -2.43067138E-007 14768.98 <-- SCF

15 -2.07460449E+004 3.66183639E-007 14789.78 <-- SCF

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

Final energy = -20746.04490036 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.03790 -0.01451 0.05442 \*

\* Se 2 0.02549 -0.07731 0.05532 \*

\* Se 3 0.03134 -0.01350 -0.05802 \*

\* Se 4 -0.02193 0.03975 -0.05647 \*

\* Se 5 0.02170 -0.02635 0.04997 \*

\* Se 6 -0.00635 -0.03402 0.02655 \*

\* Se 7 0.00574 0.02506 -0.03159 \*

\* Se 8 0.03856 0.03605 -0.04766 \*

\* Se 9 -0.05870 -0.01377 0.05964 \*

\* Se 10 0.05365 -0.04534 0.06637 \*

\* Se 11 0.06156 0.01491 -0.06415 \*

\* Se 12 -0.05135 0.04639 -0.06113 \*

\* Se 13 -0.00019 -0.02586 0.02920 \*

\* Se 14 -0.03951 -0.03592 0.05417 \*

\* Se 15 -0.02165 0.02588 -0.05614 \*

\* Se 16 0.01103 0.03353 -0.02451 \*

\* Se 17 -0.03048 0.01292 0.05322 \*

\* Se 18 0.02895 -0.03989 0.05694 \*

\* Se 19 0.04526 0.01458 -0.05471 \*

\* Se 20 -0.02602 0.07624 -0.05018 \*

\* Nb 1 0.02497 -0.07811 -0.00103 \*

\* Nb 2 -0.02851 0.07875 0.00041 \*

\* Nb 3 -0.00089 -0.05677 0.00104 \*

\* Nb 4 -0.00788 0.07300 0.00230 \*

\* Nb 5 0.00939 -0.07373 -0.00074 \*

\* Nb 6 -0.03835 0.07815 -0.00183 \*

\* Nb 7 0.03526 -0.07656 0.00135 \*

\* Nb 8 -0.01796 0.07334 0.00046 \*

\* Nb 9 0.00231 -0.07405 -0.00208 \*

\* Nb 10 -0.00755 0.05713 -0.00113 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.007293 0.062649 -0.051276 \*

\* y 0.062649 -0.344069 -0.219743 \*

\* z -0.051276 -0.219743 0.294692 \*

\* \*

\* Pressure: 0.0189 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000050 | -20746.043533 | <-- min BFGS

| trial step | 1.000000 | 0.000043 | -20746.044799 | <-- min BFGS

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

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BFGS: improving iteration 10 with line minimization (lambda= 7.028712)

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Unit Cell

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

14.8772012 -8.5494081 0.0002122 0.4211365 -0.0020882 0.0002764

0.0171079 3.4496717 -0.0038193 1.0437142 1.8162131 0.0024706

-0.0086526 -0.0128285 13.0857865 0.0002978 0.0005301 0.4801541

Lattice parameters(A) Cell Angles

a = 17.158773 alpha = 90.119791

b = 3.449716 beta = 90.004153

c = 13.085796 gamma = 119.600316

Current cell volume = 673.494612 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 0.066995 0.666282 0.122645 x

x Se 2 0.133583 0.335203 0.622428 x

x Se 3 0.133308 0.334682 0.877529 x

x Se 4 0.066797 0.665670 0.377387 x

x Se 5 0.266355 0.665977 0.122384 x

x Se 6 0.333336 0.335073 0.622475 x

x Se 7 0.333139 0.334400 0.877497 x

x Se 8 0.266122 0.665200 0.377629 x

x Se 9 0.467236 0.667013 0.122718 x

x Se 10 0.533011 0.333682 0.622660 x

x Se 11 0.532736 0.332934 0.877271 x

x Se 12 0.466968 0.666278 0.377352 x

x Se 13 0.666837 0.665547 0.122518 x

x Se 14 0.733894 0.334836 0.622345 x

x Se 15 0.733655 0.334052 0.877638 x

x Se 16 0.666648 0.664890 0.377512 x

x Se 17 0.866720 0.665348 0.122482 x

x Se 18 0.933168 0.334297 0.622618 x

x Se 19 0.932958 0.333671 0.877351 x

x Se 20 0.866457 0.664833 0.377559 x

x Nb 1 -0.000474 0.000699 0.250073 x

x Nb 2 0.000481 -0.000678 0.749933 x

x Nb 3 0.199899 0.001637 0.250018 x

x Nb 4 0.200136 -0.001040 0.749958 x

x Nb 5 0.399382 0.000544 0.250049 x

x Nb 6 0.400187 -0.000906 0.749935 x

x Nb 7 0.599781 0.000767 0.250068 x

x Nb 8 0.600672 -0.000391 0.749953 x

x Nb 9 0.799912 0.001156 0.250039 x

x Nb 10 0.800103 -0.001657 0.749977 x

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07458913E+004 15177.66 <-- SCF

1 -2.07462943E+004 1.34359758E-002 15195.56 <-- SCF

2 -2.07463309E+004 1.21828778E-003 15226.56 <-- SCF

3 -2.07461098E+004 -7.36793244E-003 15255.09 <-- SCF

4 -2.07460529E+004 -1.89842186E-003 15282.30 <-- SCF

5 -2.07460499E+004 -9.94474786E-005 15309.94 <-- SCF

6 -2.07460493E+004 -1.92928856E-005 15338.55 <-- SCF

7 -2.07460493E+004 -2.15891205E-007 15367.36 <-- SCF

8 -2.07460479E+004 -4.59556306E-005 15396.16 <-- SCF

9 -2.07460487E+004 2.43787207E-005 15422.25 <-- SCF

10 -2.07460484E+004 -8.17999326E-006 15446.95 <-- SCF

11 -2.07460485E+004 1.48714710E-006 15470.66 <-- SCF

12 -2.07460486E+004 3.74884033E-006 15490.94 <-- SCF

13 -2.07460485E+004 -2.35364721E-006 15512.30 <-- SCF

14 -2.07460485E+004 -1.38569646E-006 15533.03 <-- SCF

15 -2.07460485E+004 1.08642482E-007 15553.45 <-- SCF

16 -2.07460485E+004 9.12319375E-008 15573.61 <-- SCF

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

Final energy = -20746.04847852 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.03757 -0.01593 0.07697 \*

\* Se 2 0.02592 -0.03647 0.04786 \*

\* Se 3 0.02777 -0.00074 -0.06034 \*

\* Se 4 -0.02222 0.02035 -0.07014 \*

\* Se 5 0.01743 -0.03355 0.05092 \*

\* Se 6 -0.00707 -0.00884 0.04778 \*

\* Se 7 0.00284 0.03060 -0.05759 \*

\* Se 8 0.03480 0.00736 -0.04495 \*

\* Se 9 -0.05541 -0.01896 0.08053 \*

\* Se 10 0.04569 -0.02545 0.07645 \*

\* Se 11 0.05766 0.01957 -0.08306 \*

\* Se 12 -0.04401 0.02584 -0.07331 \*

\* Se 13 -0.00011 -0.03205 0.05702 \*

\* Se 14 -0.03590 -0.00694 0.04657 \*

\* Se 15 -0.01773 0.03357 -0.05227 \*

\* Se 16 0.00905 0.00757 -0.04738 \*

\* Se 17 -0.02762 0.00086 0.05924 \*

\* Se 18 0.02721 -0.02191 0.07188 \*

\* Se 19 0.04299 0.01440 -0.07868 \*

\* Se 20 -0.02677 0.03644 -0.04676 \*

\* Nb 1 0.02715 -0.04325 -0.00660 \*

\* Nb 2 -0.02811 0.04535 0.00627 \*

\* Nb 3 -0.00382 -0.02111 -0.00338 \*

\* Nb 4 0.00239 0.03254 0.00739 \*

\* Nb 5 0.01597 -0.03879 -0.00631 \*

\* Nb 6 -0.03924 0.04248 0.00365 \*

\* Nb 7 0.03738 -0.03942 -0.00380 \*

\* Nb 8 -0.02051 0.03843 0.00606 \*

\* Nb 9 -0.00756 -0.03365 -0.00732 \*

\* Nb 10 -0.00057 0.02172 0.00329 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.170579 0.118671 -0.046538 \*

\* y 0.118671 0.074917 -0.143100 \*

\* z -0.046538 -0.143100 0.481769 \*

\* \*

\* Pressure: -0.2424 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000050 | -20746.043533 | <-- min BFGS

| trial step | 1.000000 | 0.000043 | -20746.044799 | <-- min BFGS

| line step | 7.028712 | 3.215E-006 | -20746.048422 | <-- min BFGS

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

BFGS: finished iteration 10 with enthalpy= -2.07460484E+004 eV

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

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

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

| dE/ion | 1.629816E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.029842E-001 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.514608E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.817687E-001 | 2.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 11 ...

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

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

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

| previous | 0.000000 | 0.000161 | -20746.048422 | <-- 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)

14.8788613 -8.5610691 -0.0003909 0.4212223 -0.0018546 0.0001910

0.0151953 3.4509998 -0.0022808 1.0449478 1.8160854 0.0015068

-0.0059622 -0.0074203 13.0778282 0.0001948 0.0003167 0.4804459

Lattice parameters(A) Cell Angles

a = 17.166025 alpha = 90.070491

b = 3.451034 beta = 90.007732

c = 13.077832 gamma = 119.663175

Current cell volume = 673.207448 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 0.066962 0.666254 0.122708 x

x Se 2 0.133606 0.335011 0.622528 x

x Se 3 0.133332 0.334578 0.877435 x

x Se 4 0.066771 0.665718 0.377316 x

x Se 5 0.266361 0.666080 0.122476 x

x Se 6 0.333346 0.334961 0.622518 x

x Se 7 0.333155 0.334361 0.877457 x

x Se 8 0.266135 0.665388 0.377535 x

x Se 9 0.467193 0.666984 0.122786 x

x Se 10 0.533054 0.333638 0.622740 x

x Se 11 0.532780 0.332968 0.877199 x

x Se 12 0.466926 0.666327 0.377276 x

x Se 13 0.666824 0.665592 0.122556 x

x Se 14 0.733881 0.334648 0.622446 x

x Se 15 0.733648 0.333950 0.877539 x

x Se 16 0.666640 0.665006 0.377471 x

x Se 17 0.866697 0.665450 0.122569 x

x Se 18 0.933199 0.334261 0.622690 x

x Se 19 0.932997 0.333712 0.877287 x

x Se 20 0.866434 0.665021 0.377466 x

x Nb 1 -0.000447 0.000440 0.250079 x

x Nb 2 0.000453 -0.000416 0.749927 x

x Nb 3 0.199932 0.001430 0.250022 x

x Nb 4 0.200094 -0.000796 0.749954 x

x Nb 5 0.399399 0.000266 0.250053 x

x Nb 6 0.400144 -0.000664 0.749929 x

x Nb 7 0.599821 0.000523 0.250074 x

x Nb 8 0.600651 -0.000120 0.749948 x

x Nb 9 0.799948 0.000894 0.250043 x

x Nb 10 0.800064 -0.001467 0.749974 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460267E+004 15966.11 <-- SCF

1 -2.07460675E+004 1.35815742E-003 15983.02 <-- SCF

2 -2.07460707E+004 1.06998175E-004 16015.03 <-- SCF

3 -2.07460580E+004 -4.23131120E-004 16043.81 <-- SCF

4 -2.07460512E+004 -2.26415496E-004 16071.83 <-- SCF

5 -2.07460534E+004 7.39402229E-005 16100.05 <-- SCF

6 -2.07460527E+004 -2.55372020E-005 16128.12 <-- SCF

7 -2.07460517E+004 -3.08440205E-005 16154.12 <-- SCF

8 -2.07460516E+004 -4.12552357E-006 16178.56 <-- SCF

9 -2.07460518E+004 5.23516661E-006 16200.72 <-- SCF

10 -2.07460518E+004 2.38109445E-006 16222.11 <-- SCF

11 -2.07460518E+004 2.02722469E-007 16242.72 <-- SCF

12 -2.07460518E+004 -7.34839561E-007 16263.52 <-- SCF

13 -2.07460518E+004 -3.04249622E-007 16284.73 <-- SCF

14 -2.07460518E+004 1.51392201E-007 16305.50 <-- SCF

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

Final energy = -20746.05181327 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.02899 -0.01378 0.05048 \*

\* Se 2 0.02522 -0.01470 0.00699 \*

\* Se 3 0.01842 0.00304 -0.02439 \*

\* Se 4 -0.02163 0.00808 -0.03930 \*

\* Se 5 0.01904 -0.03328 0.01561 \*

\* Se 6 -0.00664 0.00671 0.02222 \*

\* Se 7 -0.00558 0.03123 -0.03472 \*

\* Se 8 0.03000 -0.00805 -0.00723 \*

\* Se 9 -0.04655 -0.01719 0.05399 \*

\* Se 10 0.04314 -0.01319 0.04302 \*

\* Se 11 0.04839 0.01783 -0.05515 \*

\* Se 12 -0.04192 0.01347 -0.04125 \*

\* Se 13 0.00636 -0.03137 0.03500 \*

\* Se 14 -0.03273 0.00830 0.00682 \*

\* Se 15 -0.02098 0.03308 -0.01490 \*

\* Se 16 0.00684 -0.00681 -0.02256 \*

\* Se 17 -0.01886 -0.00298 0.02501 \*

\* Se 18 0.02565 -0.00895 0.03961 \*

\* Se 19 0.03337 0.01290 -0.05086 \*

\* Se 20 -0.02650 0.01486 -0.00764 \*

\* Nb 1 0.02182 -0.03047 -0.00971 \*

\* Nb 2 -0.02280 0.03159 0.00928 \*

\* Nb 3 -0.00975 -0.00761 -0.00584 \*

\* Nb 4 0.01542 0.01572 0.01000 \*

\* Nb 5 0.01296 -0.02492 -0.00924 \*

\* Nb 6 -0.03268 0.02726 0.00663 \*

\* Nb 7 0.03345 -0.02722 -0.00680 \*

\* Nb 8 -0.01744 0.02540 0.00896 \*

\* Nb 9 -0.01816 -0.01666 -0.00988 \*

\* Nb 10 0.01111 0.00774 0.00584 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.098883 0.068225 -0.013117 \*

\* y 0.068225 0.057577 -0.083468 \*

\* z -0.013117 -0.083468 0.256919 \*

\* \*

\* Pressure: -0.1378 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000161 | -20746.048422 | <-- min BFGS

| trial step | 1.000000 | 0.000084 | -20746.051754 | <-- min BFGS

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

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BFGS: improving iteration 11 with line minimization (lambda= 2.097078)

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Unit Cell

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

14.8806827 -8.5738622 -0.0010526 0.4213168 -0.0015983 0.0000969

0.0130971 3.4524568 -0.0005930 1.0463020 1.8159480 0.0004476

-0.0030105 -0.0014870 13.0690974 0.0000814 0.0000823 0.4807666

Lattice parameters(A) Cell Angles

a = 17.173987 alpha = 90.016410

b = 3.452482 beta = 90.011693

c = 13.069098 gamma = 119.732072

Current cell volume = 672.891279 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 0.066925 0.666224 0.122778 x

x Se 2 0.133630 0.334800 0.622638 x

x Se 3 0.133358 0.334464 0.877332 x

x Se 4 0.066743 0.665771 0.377238 x

x Se 5 0.266369 0.666194 0.122576 x

x Se 6 0.333358 0.334839 0.622565 x

x Se 7 0.333173 0.334318 0.877413 x

x Se 8 0.266150 0.665595 0.377432 x

x Se 9 0.467145 0.666953 0.122861 x

x Se 10 0.533100 0.333588 0.622828 x

x Se 11 0.532829 0.333005 0.877120 x

x Se 12 0.466880 0.666381 0.377193 x

x Se 13 0.666810 0.665640 0.122597 x

x Se 14 0.733866 0.334442 0.622557 x

x Se 15 0.733641 0.333838 0.877430 x

x Se 16 0.666632 0.665134 0.377425 x

x Se 17 0.866671 0.665563 0.122664 x

x Se 18 0.933233 0.334221 0.622769 x

x Se 19 0.933039 0.333757 0.877217 x

x Se 20 0.866410 0.665227 0.377364 x

x Nb 1 -0.000418 0.000155 0.250085 x

x Nb 2 0.000422 -0.000130 0.749920 x

x Nb 3 0.199968 0.001204 0.250026 x

x Nb 4 0.200048 -0.000528 0.749950 x

x Nb 5 0.399417 -0.000038 0.250059 x

x Nb 6 0.400098 -0.000399 0.749923 x

x Nb 7 0.599865 0.000255 0.250080 x

x Nb 8 0.600629 0.000177 0.749943 x

x Nb 9 0.799988 0.000607 0.250047 x

x Nb 10 0.800021 -0.001257 0.749970 x

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460229E+004 16697.92 <-- SCF

1 -2.07460709E+004 1.60062274E-003 16714.19 <-- SCF

2 -2.07460741E+004 1.04861219E-004 16746.27 <-- SCF

3 -2.07460584E+004 -5.23500609E-004 16775.41 <-- SCF

4 -2.07460539E+004 -1.49137279E-004 16803.61 <-- SCF

5 -2.07460532E+004 -2.36581231E-005 16831.48 <-- SCF

6 -2.07460530E+004 -4.87030960E-006 16858.17 <-- SCF

7 -2.07460530E+004 -8.92833144E-007 16880.25 <-- SCF

8 -2.07460530E+004 3.78064828E-007 16901.14 <-- SCF

9 -2.07460530E+004 8.08607229E-008 16921.67 <-- SCF

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

Final energy = -20746.05302322 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.01840 -0.01246 0.02115 \*

\* Se 2 0.02300 0.00876 -0.03607 \*

\* Se 3 0.00739 0.00779 0.01389 \*

\* Se 4 -0.01959 -0.00634 -0.00530 \*

\* Se 5 0.02134 -0.03235 -0.02189 \*

\* Se 6 -0.00512 0.02284 -0.00556 \*

\* Se 7 -0.01337 0.03103 -0.00998 \*

\* Se 8 0.02542 -0.02454 0.03309 \*

\* Se 9 -0.03523 -0.01552 0.02480 \*

\* Se 10 0.03906 0.00138 0.00702 \*

\* Se 11 0.03731 0.01643 -0.02489 \*

\* Se 12 -0.03781 -0.00079 -0.00634 \*

\* Se 13 0.01379 -0.03109 0.01156 \*

\* Se 14 -0.02819 0.02487 -0.03542 \*

\* Se 15 -0.02331 0.03207 0.02443 \*

\* Se 16 0.00513 -0.02277 0.00402 \*

\* Se 17 -0.00901 -0.00737 -0.01135 \*

\* Se 18 0.02267 0.00548 0.00595 \*

\* Se 19 0.02207 0.01136 -0.02183 \*

\* Se 20 -0.02530 -0.00794 0.03336 \*

\* Nb 1 0.01730 -0.01805 -0.01282 \*

\* Nb 2 -0.01912 0.01875 0.01236 \*

\* Nb 3 -0.01871 0.00452 -0.00835 \*

\* Nb 4 0.02778 0.00019 0.01283 \*

\* Nb 5 0.01029 -0.01210 -0.01227 \*

\* Nb 6 -0.02603 0.01515 0.00950 \*

\* Nb 7 0.02824 -0.01578 -0.00974 \*

\* Nb 8 -0.01445 0.01190 0.01206 \*

\* Nb 9 -0.02768 -0.00163 -0.01260 \*

\* Nb 10 0.02056 -0.00380 0.00840 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.021205 0.012140 0.022496 \*

\* y 0.012140 0.036710 -0.017879 \*

\* z 0.022496 -0.017879 0.012242 \*

\* \*

\* Pressure: -0.0234 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000161 | -20746.048422 | <-- min BFGS

| trial step | 1.000000 | 0.000084 | -20746.051754 | <-- min BFGS

| line step | 2.097078 | 1.968E-006 | -20746.053011 | <-- min BFGS

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

BFGS: finished iteration 11 with enthalpy= -2.07460530E+004 eV

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

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

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

| dE/ion | 1.529522E-004 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 5.165484E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.349139E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.670997E-002 | 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 | 8.915E-006 | -20746.053011 | <-- 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)

14.8803721 -8.5739518 -0.0016143 0.4213387 -0.0015755 0.0001005

0.0129088 3.4521631 -0.0004301 1.0464564 1.8161590 0.0003785

-0.0031191 -0.0009243 13.0585091 0.0000866 0.0000596 0.4811564

Lattice parameters(A) Cell Angles

a = 17.173763 alpha = 90.011245

b = 3.452187 beta = 90.015219

c = 13.058510 gamma = 119.735955

Current cell volume = 672.253986 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 0.066922 0.666217 0.122688 x

x Se 2 0.133625 0.334798 0.622539 x

x Se 3 0.133357 0.334466 0.877428 x

x Se 4 0.066743 0.665778 0.377330 x

x Se 5 0.266375 0.666176 0.122481 x

x Se 6 0.333355 0.334829 0.622477 x

x Se 7 0.333173 0.334323 0.877499 x

x Se 8 0.266161 0.665595 0.377528 x

x Se 9 0.467137 0.666928 0.122769 x

x Se 10 0.533104 0.333596 0.622733 x

x Se 11 0.532838 0.333031 0.877213 x

x Se 12 0.466877 0.666374 0.377286 x

x Se 13 0.666810 0.665636 0.122511 x

x Se 14 0.733855 0.334441 0.622459 x

x Se 15 0.733634 0.333855 0.877526 x

x Se 16 0.666634 0.665143 0.377514 x

x Se 17 0.866671 0.665560 0.122569 x

x Se 18 0.933234 0.334214 0.622677 x

x Se 19 0.933043 0.333763 0.877307 x

x Se 20 0.866414 0.665229 0.377462 x

x Nb 1 -0.000411 0.000174 0.250081 x

x Nb 2 0.000416 -0.000149 0.749924 x

x Nb 3 0.199963 0.001200 0.250024 x

x Nb 4 0.200054 -0.000535 0.749953 x

x Nb 5 0.399426 -0.000014 0.250056 x

x Nb 6 0.400098 -0.000415 0.749926 x

x Nb 7 0.599866 0.000275 0.250077 x

x Nb 8 0.600619 0.000149 0.749946 x

x Nb 9 0.799981 0.000613 0.250045 x

x Nb 10 0.800027 -0.001251 0.749972 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460397E+004 17309.42 <-- SCF

1 -2.07460830E+004 1.44190576E-003 17327.28 <-- SCF

2 -2.07460869E+004 1.31036003E-004 17358.19 <-- SCF

3 -2.07460598E+004 -9.04688509E-004 17386.58 <-- SCF

4 -2.07460540E+004 -1.92621152E-004 17413.81 <-- SCF

5 -2.07460532E+004 -2.58438751E-005 17440.08 <-- SCF

6 -2.07460531E+004 -2.93002915E-006 17466.25 <-- SCF

7 -2.07460531E+004 -4.52012748E-007 17487.83 <-- SCF

8 -2.07460531E+004 4.69522906E-007 17508.56 <-- SCF

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

Final energy = -20746.05312270 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.01817 -0.01158 0.01753 \*

\* Se 2 0.02636 0.00676 -0.03316 \*

\* Se 3 0.01099 0.00601 0.01335 \*

\* Se 4 -0.02015 -0.00781 -0.00382 \*

\* Se 5 0.02145 -0.03239 -0.02040 \*

\* Se 6 -0.00400 0.02475 -0.00713 \*

\* Se 7 -0.01201 0.03100 -0.00746 \*

\* Se 8 0.02400 -0.02614 0.03081 \*

\* Se 9 -0.03587 -0.01391 0.02004 \*

\* Se 10 0.04278 0.00146 0.00426 \*

\* Se 11 0.03837 0.01453 -0.02137 \*

\* Se 12 -0.04111 -0.00129 -0.00257 \*

\* Se 13 0.01454 -0.03158 0.00731 \*

\* Se 14 -0.02569 0.02615 -0.03179 \*

\* Se 15 -0.02216 0.03197 0.02174 \*

\* Se 16 0.00585 -0.02529 0.00716 \*

\* Se 17 -0.01066 -0.00555 -0.01274 \*

\* Se 18 0.02373 0.00649 0.00531 \*

\* Se 19 0.02254 0.01010 -0.01901 \*

\* Se 20 -0.02707 -0.00599 0.03252 \*

\* Nb 1 0.01557 -0.01568 -0.01217 \*

\* Nb 2 -0.01707 0.01688 0.01183 \*

\* Nb 3 -0.02065 0.00647 -0.00815 \*

\* Nb 4 0.02662 -0.00220 0.01217 \*

\* Nb 5 0.00824 -0.01068 -0.01159 \*

\* Nb 6 -0.02629 0.01354 0.00924 \*

\* Nb 7 0.02406 -0.01212 -0.00943 \*

\* Nb 8 -0.01381 0.01071 0.01150 \*

\* Nb 9 -0.02997 0.00082 -0.01213 \*

\* Nb 10 0.01959 -0.00543 0.00816 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.002319 0.005709 0.024118 \*

\* y 0.005709 0.014264 -0.011250 \*

\* z 0.024118 -0.011250 -0.024991 \*

\* \*

\* Pressure: 0.0028 \*

\* \*

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

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

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

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

| previous | 0.000000 | 8.915E-006 | -20746.053011 | <-- min BFGS

| trial step | 1.000000 | 4.504E-006 | -20746.053172 | <-- min BFGS

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

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BFGS: improving iteration 12 with line minimization (lambda= 2.021293)

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Unit Cell

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

14.8800550 -8.5740434 -0.0021880 0.4213611 -0.0015523 0.0001043

0.0127165 3.4518632 -0.0002637 1.0466140 1.8163745 0.0003078

-0.0032300 -0.0003496 13.0476955 0.0000918 0.0000365 0.4815552

Lattice parameters(A) Cell Angles

a = 17.173534 alpha = 90.005965

b = 3.451887 beta = 90.018823

c = 13.047696 gamma = 119.739922

Current cell volume = 671.603275 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.066918 0.666211 0.122595 x

x Se 2 0.133620 0.334796 0.622438 x

x Se 3 0.133355 0.334468 0.877526 x

x Se 4 0.066742 0.665785 0.377425 x

x Se 5 0.266382 0.666158 0.122384 x

x Se 6 0.333352 0.334819 0.622386 x

x Se 7 0.333173 0.334328 0.877588 x

x Se 8 0.266172 0.665595 0.377627 x

x Se 9 0.467129 0.666902 0.122675 x

x Se 10 0.533108 0.333604 0.622637 x

x Se 11 0.532847 0.333058 0.877307 x

x Se 12 0.466873 0.666366 0.377382 x

x Se 13 0.666810 0.665631 0.122423 x

x Se 14 0.733843 0.334440 0.622360 x

x Se 15 0.733628 0.333871 0.877625 x

x Se 16 0.666637 0.665153 0.377604 x

x Se 17 0.866672 0.665557 0.122472 x

x Se 18 0.933235 0.334206 0.622582 x

x Se 19 0.933047 0.333769 0.877400 x

x Se 20 0.866418 0.665230 0.377562 x

x Nb 1 -0.000405 0.000194 0.250078 x

x Nb 2 0.000410 -0.000169 0.749927 x

x Nb 3 0.199957 0.001196 0.250022 x

x Nb 4 0.200061 -0.000542 0.749956 x

x Nb 5 0.399435 0.000011 0.250053 x

x Nb 6 0.400098 -0.000433 0.749929 x

x Nb 7 0.599867 0.000295 0.250074 x

x Nb 8 0.600609 0.000121 0.749948 x

x Nb 9 0.799974 0.000619 0.250042 x

x Nb 10 0.800033 -0.001244 0.749974 x

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460393E+004 17904.25 <-- SCF

1 -2.07460839E+004 1.48749815E-003 17922.22 <-- SCF

2 -2.07460870E+004 1.03107397E-004 17953.84 <-- SCF

3 -2.07460594E+004 -9.18797933E-004 17982.72 <-- SCF

4 -2.07460540E+004 -1.80991264E-004 18010.69 <-- SCF

5 -2.07460531E+004 -2.98418960E-005 18036.88 <-- SCF

6 -2.07460531E+004 1.21637379E-006 18063.12 <-- SCF

7 -2.07460531E+004 1.47704451E-007 18084.17 <-- SCF

8 -2.07460532E+004 2.46625267E-007 18104.73 <-- SCF

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

Final energy = -20746.05315484 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.01597 -0.01105 0.01846 \*

\* Se 2 0.02732 0.00502 -0.02837 \*

\* Se 3 0.01233 0.00476 0.01049 \*

\* Se 4 -0.01848 -0.00909 -0.00663 \*

\* Se 5 0.01997 -0.03207 -0.01403 \*

\* Se 6 -0.00456 0.02650 -0.00580 \*

\* Se 7 -0.01239 0.03118 -0.00799 \*

\* Se 8 0.02121 -0.02696 0.02363 \*

\* Se 9 -0.03734 -0.01274 0.01821 \*

\* Se 10 0.04593 0.00238 0.00257 \*

\* Se 11 0.03885 0.01343 -0.01902 \*

\* Se 12 -0.04496 -0.00222 -0.00146 \*

\* Se 13 0.01433 -0.03180 0.00867 \*

\* Se 14 -0.02272 0.02709 -0.02540 \*

\* Se 15 -0.02063 0.03183 0.01603 \*

\* Se 16 0.00585 -0.02708 0.00509 \*

\* Se 17 -0.01291 -0.00449 -0.00906 \*

\* Se 18 0.02268 0.00788 0.00668 \*

\* Se 19 0.02084 0.00973 -0.01846 \*

\* Se 20 -0.02899 -0.00442 0.02720 \*

\* Nb 1 0.01371 -0.01682 -0.01080 \*

\* Nb 2 -0.01464 0.01790 0.01040 \*

\* Nb 3 -0.01898 0.00390 -0.00725 \*

\* Nb 4 0.02409 0.00031 0.01096 \*

\* Nb 5 0.00599 -0.01201 -0.01038 \*

\* Nb 6 -0.02534 0.01537 0.00808 \*

\* Nb 7 0.02401 -0.01376 -0.00836 \*

\* Nb 8 -0.01037 0.01188 0.01010 \*

\* Nb 9 -0.02690 -0.00151 -0.01079 \*

\* Nb 10 0.01810 -0.00315 0.00723 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.025822 -0.002458 0.026015 \*

\* y -0.002458 -0.019690 -0.005019 \*

\* z 0.026015 -0.005019 -0.074909 \*

\* \*

\* Pressure: 0.0401 \*

\* \*

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

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

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

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

| previous | 0.000000 | 8.915E-006 | -20746.053011 | <-- min BFGS

| trial step | 1.000000 | 4.504E-006 | -20746.053172 | <-- min BFGS

| line step | 2.021293 | -4.870E-006 | -20746.053179 | <-- min BFGS

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

BFGS: reverting to earlier configuration

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Unit Cell

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

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

14.8803721 -8.5739518 -0.0016143 0.4213387 -0.0015755 0.0001005

0.0129088 3.4521631 -0.0004301 1.0464564 1.8161590 0.0003785

-0.0031191 -0.0009243 13.0585091 0.0000866 0.0000596 0.4811564

Lattice parameters(A) Cell Angles

a = 17.173763 alpha = 90.011245

b = 3.452187 beta = 90.015219

c = 13.058510 gamma = 119.735955

Current cell volume = 672.253986 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 0.066922 0.666217 0.122688 x

x Se 2 0.133625 0.334798 0.622539 x

x Se 3 0.133357 0.334466 0.877428 x

x Se 4 0.066743 0.665778 0.377330 x

x Se 5 0.266375 0.666176 0.122481 x

x Se 6 0.333355 0.334829 0.622477 x

x Se 7 0.333173 0.334323 0.877499 x

x Se 8 0.266161 0.665595 0.377528 x

x Se 9 0.467137 0.666928 0.122769 x

x Se 10 0.533104 0.333596 0.622733 x

x Se 11 0.532838 0.333031 0.877213 x

x Se 12 0.466877 0.666374 0.377286 x

x Se 13 0.666810 0.665636 0.122511 x

x Se 14 0.733855 0.334441 0.622459 x

x Se 15 0.733634 0.333855 0.877526 x

x Se 16 0.666634 0.665143 0.377514 x

x Se 17 0.866671 0.665560 0.122569 x

x Se 18 0.933234 0.334214 0.622677 x

x Se 19 0.933043 0.333763 0.877307 x

x Se 20 0.866414 0.665229 0.377462 x

x Nb 1 -0.000411 0.000174 0.250081 x

x Nb 2 0.000416 -0.000149 0.749924 x

x Nb 3 0.199963 0.001200 0.250024 x

x Nb 4 0.200054 -0.000535 0.749953 x

x Nb 5 0.399426 -0.000014 0.250056 x

x Nb 6 0.400098 -0.000415 0.749926 x

x Nb 7 0.599866 0.000275 0.250077 x

x Nb 8 0.600619 0.000149 0.749946 x

x Nb 9 0.799981 0.000613 0.250045 x

x Nb 10 0.800027 -0.001251 0.749972 x

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BFGS: finished iteration 12 with enthalpy= -2.07460532E+004 eV

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

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

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

| dE/ion | 5.388113E-006 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 4.852336E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.293945E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.499144E-002 | 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 | 8.155E-006 | -20746.053172 | <-- 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)

14.8803703 -8.5734973 -0.0027772 0.4213415 -0.0015709 0.0001195

0.0128696 3.4519105 -0.0002610 1.0464844 1.8163036 0.0003445

-0.0037026 -0.0003415 13.0463315 0.0001106 0.0000360 0.4816056

Lattice parameters(A) Cell Angles

a = 17.173534 alpha = 90.005892

b = 3.451935 beta = 90.022606

c = 13.046332 gamma = 119.735279

Current cell volume = 671.573486 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 0.666201 0.122568 x

x Se 2 0.133619 0.334824 0.622399 x

x Se 3 0.133354 0.334489 0.877562 x

x Se 4 0.066743 0.665775 0.377455 x

x Se 5 0.266385 0.666131 0.122348 x

x Se 6 0.333350 0.334838 0.622359 x

x Se 7 0.333170 0.334347 0.877612 x

x Se 8 0.266175 0.665570 0.377665 x

x Se 9 0.467128 0.666882 0.122648 x

x Se 10 0.533109 0.333622 0.622605 x

x Se 11 0.532848 0.333079 0.877335 x

x Se 12 0.466873 0.666349 0.377413 x

x Se 13 0.666813 0.665612 0.122398 x

x Se 14 0.733839 0.334464 0.622321 x

x Se 15 0.733624 0.333898 0.877662 x

x Se 16 0.666640 0.665135 0.377631 x

x Se 17 0.866673 0.665538 0.122437 x

x Se 18 0.933233 0.334215 0.622552 x

x Se 19 0.933046 0.333778 0.877427 x

x Se 20 0.866418 0.665203 0.377600 x

x Nb 1 -0.000406 0.000226 0.250075 x

x Nb 2 0.000410 -0.000201 0.749930 x

x Nb 3 0.199950 0.001217 0.250020 x

x Nb 4 0.200070 -0.000566 0.749958 x

x Nb 5 0.399436 0.000046 0.250050 x

x Nb 6 0.400100 -0.000466 0.749931 x

x Nb 7 0.599864 0.000329 0.250071 x

x Nb 8 0.600608 0.000085 0.749951 x

x Nb 9 0.799965 0.000643 0.250039 x

x Nb 10 0.800041 -0.001262 0.749975 x

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460313E+004 18518.88 <-- SCF

1 -2.07461034E+004 2.40168116E-003 18536.78 <-- SCF

2 -2.07461084E+004 1.68938500E-004 18568.41 <-- SCF

3 -2.07460632E+004 -1.50892891E-003 18597.31 <-- SCF

4 -2.07460546E+004 -2.86119847E-004 18625.20 <-- SCF

5 -2.07460531E+004 -4.85884320E-005 18652.36 <-- SCF

6 -2.07460532E+004 1.83000157E-006 18679.98 <-- SCF

7 -2.07460532E+004 4.71769358E-008 18701.94 <-- SCF

8 -2.07460532E+004 4.99205874E-007 18722.89 <-- SCF

9 -2.07460532E+004 1.49920380E-007 18743.34 <-- SCF

10 -2.07460532E+004 4.33294549E-008 18763.86 <-- SCF

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

Final energy = -20746.05321195 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.01657 -0.01037 0.02143 \*

\* Se 2 0.02748 0.00255 -0.02065 \*

\* Se 3 0.01413 0.00319 0.00429 \*

\* Se 4 -0.01791 -0.00841 -0.01095 \*

\* Se 5 0.01879 -0.03075 -0.00737 \*

\* Se 6 -0.00440 0.02528 -0.00116 \*

\* Se 7 -0.01077 0.02986 -0.01141 \*

\* Se 8 0.02062 -0.02545 0.01597 \*

\* Se 9 -0.03813 -0.01144 0.02091 \*

\* Se 10 0.04627 0.00123 0.00682 \*

\* Se 11 0.03967 0.01213 -0.02192 \*

\* Se 12 -0.04520 -0.00106 -0.00559 \*

\* Se 13 0.01286 -0.03049 0.01174 \*

\* Se 14 -0.02197 0.02551 -0.01692 \*

\* Se 15 -0.01929 0.03046 0.00860 \*

\* Se 16 0.00585 -0.02588 0.00084 \*

\* Se 17 -0.01458 -0.00298 -0.00335 \*

\* Se 18 0.02215 0.00723 0.01127 \*

\* Se 19 0.02144 0.00911 -0.02169 \*

\* Se 20 -0.02911 -0.00201 0.01989 \*

\* Nb 1 0.01344 -0.01863 -0.01017 \*

\* Nb 2 -0.01447 0.01963 0.00974 \*

\* Nb 3 -0.01828 0.00185 -0.00686 \*

\* Nb 4 0.02288 0.00263 0.01040 \*

\* Nb 5 0.00711 -0.01424 -0.00988 \*

\* Nb 6 -0.02618 0.01738 0.00771 \*

\* Nb 7 0.02528 -0.01572 -0.00792 \*

\* Nb 8 -0.01182 0.01409 0.00970 \*

\* Nb 9 -0.02581 -0.00377 -0.01033 \*

\* Nb 10 0.01651 -0.00091 0.00687 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.000461 0.000372 0.021108 \*

\* y 0.000372 0.003516 -0.005214 \*

\* z 0.021108 -0.005214 -0.035136 \*

\* \*

\* Pressure: 0.0107 \*

\* \*

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

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

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

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

| previous | 0.000000 | 8.155E-006 | -20746.053172 | <-- min BFGS

| trial step | 1.000000 | -3.444E-006 | -20746.053223 | <-- min BFGS

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

BFGS: finished iteration 13 with enthalpy= -2.07460532E+004 eV

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

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

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

| dE/ion | 1.673076E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 4.692149E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.835056E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.513620E-002 | 2.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 14 ...

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

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

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

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

| previous | 0.000000 | 3.601E-006 | -20746.053223 | <-- 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)

14.8802871 -8.5738705 -0.0030099 0.4213441 -0.0015704 0.0001235

0.0128665 3.4520547 -0.0002270 1.0464926 1.8162287 0.0003375

-0.0038270 -0.0002197 13.0502338 0.0001154 0.0000312 0.4814615

Lattice parameters(A) Cell Angles

a = 17.173649 alpha = 90.004795

b = 3.452079 beta = 90.024119

c = 13.050234 gamma = 119.736556

Current cell volume = 671.798328 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.066917 0.666194 0.122608 x

x Se 2 0.133625 0.334823 0.622438 x

x Se 3 0.133357 0.334486 0.877522 x

x Se 4 0.066740 0.665767 0.377416 x

x Se 5 0.266385 0.666136 0.122387 x

x Se 6 0.333351 0.334844 0.622394 x

x Se 7 0.333170 0.334351 0.877577 x

x Se 8 0.266174 0.665576 0.377627 x

x Se 9 0.467125 0.666877 0.122688 x

x Se 10 0.533114 0.333627 0.622646 x

x Se 11 0.532850 0.333085 0.877294 x

x Se 12 0.466868 0.666344 0.377373 x

x Se 13 0.666814 0.665608 0.122434 x

x Se 14 0.733841 0.334459 0.622360 x

x Se 15 0.733625 0.333893 0.877622 x

x Se 16 0.666639 0.665129 0.377596 x

x Se 17 0.866671 0.665541 0.122477 x

x Se 18 0.933237 0.334224 0.622591 x

x Se 19 0.933049 0.333786 0.877387 x

x Se 20 0.866413 0.665205 0.377562 x

x Nb 1 -0.000405 0.000198 0.250075 x

x Nb 2 0.000409 -0.000173 0.749930 x

x Nb 3 0.199952 0.001202 0.250020 x

x Nb 4 0.200068 -0.000542 0.749958 x

x Nb 5 0.399434 0.000017 0.250050 x

x Nb 6 0.400095 -0.000444 0.749931 x

x Nb 7 0.599869 0.000307 0.250072 x

x Nb 8 0.600609 0.000114 0.749951 x

x Nb 9 0.799967 0.000617 0.250039 x

x Nb 10 0.800038 -0.001249 0.749976 x

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460510E+004 19167.41 <-- SCF

1 -2.07460581E+004 2.36265172E-004 19185.58 <-- SCF

2 -2.07460586E+004 1.69898661E-005 19213.94 <-- SCF

3 -2.07460543E+004 -1.44889922E-004 19242.89 <-- SCF

4 -2.07460534E+004 -2.95375041E-005 19270.88 <-- SCF

5 -2.07460533E+004 -4.83921586E-006 19296.28 <-- SCF

6 -2.07460533E+004 1.52618494E-008 19317.83 <-- SCF

7 -2.07460533E+004 6.31349430E-008 19338.45 <-- SCF

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

Final energy = -20746.05326503 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.01670 -0.01047 0.02038 \*

\* Se 2 0.02679 0.00446 -0.02321 \*

\* Se 3 0.01371 0.00415 0.00642 \*

\* Se 4 -0.01760 -0.00868 -0.00930 \*

\* Se 5 0.01850 -0.03069 -0.01054 \*

\* Se 6 -0.00410 0.02537 -0.00301 \*

\* Se 7 -0.01010 0.02960 -0.00975 \*

\* Se 8 0.02116 -0.02584 0.01937 \*

\* Se 9 -0.03622 -0.01177 0.02130 \*

\* Se 10 0.04309 0.00158 0.00650 \*

\* Se 11 0.03786 0.01240 -0.02201 \*

\* Se 12 -0.04200 -0.00146 -0.00548 \*

\* Se 13 0.01218 -0.03029 0.01054 \*

\* Se 14 -0.02269 0.02590 -0.02046 \*

\* Se 15 -0.01918 0.03036 0.01191 \*

\* Se 16 0.00558 -0.02601 0.00227 \*

\* Se 17 -0.01418 -0.00391 -0.00519 \*

\* Se 18 0.02176 0.00740 0.00939 \*

\* Se 19 0.02153 0.00907 -0.02038 \*

\* Se 20 -0.02838 -0.00391 0.02210 \*

\* Nb 1 0.01255 -0.01755 -0.01015 \*

\* Nb 2 -0.01357 0.01865 0.00969 \*

\* Nb 3 -0.01755 0.00284 -0.00697 \*

\* Nb 4 0.02330 0.00108 0.01047 \*

\* Nb 5 0.00677 -0.01298 -0.01001 \*

\* Nb 6 -0.02487 0.01654 0.00767 \*

\* Nb 7 0.02387 -0.01473 -0.00794 \*

\* Nb 8 -0.01111 0.01291 0.00978 \*

\* Nb 9 -0.02671 -0.00216 -0.01038 \*

\* Nb 10 0.01631 -0.00184 0.00698 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.002284 0.001725 0.018816 \*

\* y 0.001725 0.006640 -0.004347 \*

\* z 0.018816 -0.004347 -0.026566 \*

\* \*

\* Pressure: 0.0074 \*

\* \*

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

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

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

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

| previous | 0.000000 | 3.601E-006 | -20746.053223 | <-- min BFGS

| trial step | 1.000000 | 2.457E-006 | -20746.053304 | <-- min BFGS

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

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BFGS: improving iteration 14 with line minimization (lambda= 3.147562)

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Unit Cell

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

14.8801085 -8.5746720 -0.0035095 0.4213496 -0.0015695 0.0001321

0.0128600 3.4523643 -0.0001540 1.0465102 1.8160677 0.0003223

-0.0040942 0.0000420 13.0586142 0.0001256 0.0000210 0.4811526

Lattice parameters(A) Cell Angles

a = 17.173894 alpha = 90.002439

b = 3.452388 beta = 90.027365

c = 13.058615 gamma = 119.739298

Current cell volume = 672.281238 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 0.066913 0.666179 0.122693 x

x Se 2 0.133637 0.334819 0.622522 x

x Se 3 0.133363 0.334479 0.877436 x

x Se 4 0.066733 0.665750 0.377331 x

x Se 5 0.266385 0.666148 0.122470 x

x Se 6 0.333354 0.334858 0.622469 x

x Se 7 0.333169 0.334361 0.877501 x

x Se 8 0.266172 0.665588 0.377544 x

x Se 9 0.467119 0.666865 0.122775 x

x Se 10 0.533125 0.333639 0.622732 x

x Se 11 0.532857 0.333098 0.877206 x

x Se 12 0.466857 0.666333 0.377288 x

x Se 13 0.666815 0.665599 0.122510 x

x Se 14 0.733843 0.334447 0.622443 x

x Se 15 0.733625 0.333882 0.877537 x

x Se 16 0.666636 0.665115 0.377522 x

x Se 17 0.866665 0.665547 0.122561 x

x Se 18 0.933245 0.334244 0.622676 x

x Se 19 0.933054 0.333805 0.877301 x

x Se 20 0.866401 0.665208 0.377479 x

x Nb 1 -0.000404 0.000140 0.250076 x

x Nb 2 0.000408 -0.000114 0.749929 x

x Nb 3 0.199956 0.001170 0.250020 x

x Nb 4 0.200063 -0.000490 0.749959 x

x Nb 5 0.399431 -0.000047 0.250050 x

x Nb 6 0.400085 -0.000397 0.749930 x

x Nb 7 0.599878 0.000257 0.250073 x

x Nb 8 0.600612 0.000177 0.749951 x

x Nb 9 0.799971 0.000561 0.250039 x

x Nb 10 0.800033 -0.001220 0.749976 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460432E+004 19741.53 <-- SCF

1 -2.07460756E+004 1.08120200E-003 19759.64 <-- SCF

2 -2.07460780E+004 7.95500224E-005 19791.09 <-- SCF

3 -2.07460580E+004 -6.65995637E-004 19820.14 <-- SCF

4 -2.07460539E+004 -1.35895933E-004 19848.25 <-- SCF

5 -2.07460534E+004 -1.69027012E-005 19874.97 <-- SCF

6 -2.07460535E+004 9.85299006E-007 19899.38 <-- SCF

7 -2.07460534E+004 -1.89961889E-006 19920.77 <-- SCF

8 -2.07460535E+004 2.89597145E-006 19946.44 <-- SCF

9 -2.07460534E+004 -1.73281439E-006 19969.84 <-- SCF

10 -2.07460533E+004 -4.61653033E-006 19992.94 <-- SCF

11 -2.07460534E+004 3.53119177E-006 20015.98 <-- SCF

12 -2.07460534E+004 -1.08457661E-006 20037.47 <-- SCF

13 -2.07460533E+004 -8.45222282E-007 20059.27 <-- SCF

14 -2.07460533E+004 -9.79584036E-008 20080.41 <-- SCF

15 -2.07460533E+004 -1.67101691E-007 20101.53 <-- SCF

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

Final energy = -20746.05334110 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.01707 -0.01092 0.01885 \*

\* Se 2 0.02329 0.00832 -0.02676 \*

\* Se 3 0.01057 0.00582 0.00922 \*

\* Se 4 -0.01709 -0.00950 -0.00680 \*

\* Se 5 0.01727 -0.02994 -0.01537 \*

\* Se 6 -0.00467 0.02580 -0.00469 \*

\* Se 7 -0.01001 0.02915 -0.00802 \*

\* Se 8 0.02148 -0.02622 0.02411 \*

\* Se 9 -0.03440 -0.01216 0.02146 \*

\* Se 10 0.03789 0.00257 0.00593 \*

\* Se 11 0.03537 0.01297 -0.02165 \*

\* Se 12 -0.03776 -0.00220 -0.00542 \*

\* Se 13 0.01142 -0.02959 0.00930 \*

\* Se 14 -0.02367 0.02669 -0.02554 \*

\* Se 15 -0.01863 0.03001 0.01703 \*

\* Se 16 0.00542 -0.02618 0.00341 \*

\* Se 17 -0.01289 -0.00515 -0.00804 \*

\* Se 18 0.02039 0.00831 0.00741 \*

\* Se 19 0.02113 0.00955 -0.01950 \*

\* Se 20 -0.02666 -0.00737 0.02564 \*

\* Nb 1 0.01234 -0.01436 -0.01035 \*

\* Nb 2 -0.01174 0.01549 0.00991 \*

\* Nb 3 -0.01749 0.00541 -0.00699 \*

\* Nb 4 0.02571 -0.00278 0.01053 \*

\* Nb 5 0.00798 -0.01029 -0.01018 \*

\* Nb 6 -0.02256 0.01302 0.00777 \*

\* Nb 7 0.02409 -0.01176 -0.00800 \*

\* Nb 8 -0.01012 0.00929 0.01008 \*

\* Nb 9 -0.02863 0.00109 -0.01037 \*

\* Nb 10 0.01902 -0.00507 0.00702 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.002819 0.004392 0.014620 \*

\* y 0.004392 0.021271 -0.001782 \*

\* z 0.014620 -0.001782 -0.020163 \*

\* \*

\* Pressure: -0.0013 \*

\* \*

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

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

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

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

| previous | 0.000000 | 3.601E-006 | -20746.053223 | <-- min BFGS

| trial step | 1.000000 | 2.457E-006 | -20746.053304 | <-- min BFGS

| line step | 3.147562 | 9.889E-007 | -20746.053385 | <-- min BFGS

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

BFGS: finished iteration 14 with enthalpy= -2.07460534E+004 eV

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

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

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

| dE/ion | 5.418713E-006 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 4.387064E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.694695E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.127090E-002 | 2.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 15 ...

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

Writing analysis data to 2H-Nb1Se2-7.castep\_bin

Writing model to 2H-Nb1Se2-7.check

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

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

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

| previous | 0.000000 | 7.811E-006 | -20746.053385 | <-- 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)

14.8801840 -8.5748910 -0.0049595 0.4213514 -0.0015627 0.0001587

0.0128038 3.4523560 0.0000208 1.0465439 1.8160889 0.0003024

-0.0049171 0.0006584 13.0638499 0.0001583 -0.0000035 0.4809598

Lattice parameters(A) Cell Angles

a = 17.174069 alpha = 89.996847

b = 3.452380 beta = 90.036673

c = 13.063851 gamma = 119.740737

Current cell volume = 672.546306 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 0.066905 0.666133 0.122752 x

x Se 2 0.133652 0.334860 0.622556 x

x Se 3 0.133369 0.334506 0.877392 x

x Se 4 0.066725 0.665709 0.377279 x

x Se 5 0.266391 0.666111 0.122510 x

x Se 6 0.333352 0.334908 0.622512 x

x Se 7 0.333164 0.334413 0.877450 x

x Se 8 0.266178 0.665564 0.377509 x

x Se 9 0.467105 0.666801 0.122836 x

x Se 10 0.533144 0.333689 0.622785 x

x Se 11 0.532871 0.333165 0.877145 x

x Se 12 0.466838 0.666284 0.377237 x

x Se 13 0.666821 0.665549 0.122561 x

x Se 14 0.733836 0.334469 0.622478 x

x Se 15 0.733618 0.333918 0.877498 x

x Se 16 0.666638 0.665066 0.377478 x

x Se 17 0.866659 0.665520 0.122605 x

x Se 18 0.933255 0.334287 0.622729 x

x Se 19 0.933063 0.333853 0.877242 x

x Se 20 0.866386 0.665165 0.377445 x

x Nb 1 -0.000399 0.000112 0.250071 x

x Nb 2 0.000403 -0.000085 0.749934 x

x Nb 3 0.199949 0.001157 0.250017 x

x Nb 4 0.200072 -0.000454 0.749964 x

x Nb 5 0.399431 -0.000076 0.250045 x

x Nb 6 0.400073 -0.000387 0.749933 x

x Nb 7 0.599890 0.000248 0.250069 x

x Nb 8 0.600611 0.000201 0.749956 x

x Nb 9 0.799961 0.000520 0.250033 x

x Nb 10 0.800039 -0.001207 0.749979 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460492E+004 20503.56 <-- SCF

1 -2.07460873E+004 1.27047741E-003 20522.12 <-- SCF

2 -2.07460904E+004 1.02356553E-004 20552.33 <-- SCF

3 -2.07462035E+004 3.76877710E-003 20581.14 <-- SCF

4 -2.07460202E+004 -6.10966914E-003 20609.39 <-- SCF

5 -2.07460252E+004 1.67102379E-004 20637.56 <-- SCF

6 -2.07460429E+004 5.89024973E-004 20666.59 <-- SCF

7 -2.07460547E+004 3.93106117E-004 20694.61 <-- SCF

8 -2.07460587E+004 1.34822822E-004 20720.95 <-- SCF

9 -2.07460592E+004 1.59693012E-005 20746.28 <-- SCF

10 -2.07460583E+004 -2.83760957E-005 20768.83 <-- SCF

11 -2.07460574E+004 -3.05618847E-005 20790.39 <-- SCF

12 -2.07460572E+004 -6.54053940E-006 20811.39 <-- SCF

13 -2.07460572E+004 -5.43024733E-007 20832.50 <-- SCF

14 -2.07460570E+004 -5.24629090E-006 20853.38 <-- SCF

15 -2.07460586E+004 5.04362009E-005 20876.23 <-- SCF

16 -2.07460597E+004 3.87827588E-005 20897.55 <-- SCF

17 -2.07460560E+004 -1.23324572E-004 20921.39 <-- SCF

18 -2.07460532E+004 -9.26852072E-005 20949.25 <-- SCF

19 -2.07460533E+004 4.40801834E-007 20975.69 <-- SCF

20 -2.07460535E+004 7.40094464E-006 20999.23 <-- SCF

21 -2.07460536E+004 2.77005826E-006 21020.58 <-- SCF

22 -2.07460535E+004 -1.51349200E-006 21041.91 <-- SCF

23 -2.07460536E+004 3.65050709E-006 21063.38 <-- SCF

24 -2.07460536E+004 6.56921757E-007 21084.52 <-- SCF

25 -2.07460536E+004 -1.50203999E-006 21105.38 <-- SCF

26 -2.07460536E+004 -1.66812751E-006 21126.44 <-- SCF

27 -2.07460535E+004 -4.98462075E-007 21147.17 <-- SCF

28 -2.07460535E+004 -1.79841244E-007 21168.14 <-- SCF

29 -2.07460535E+004 -1.36637595E-007 21189.38 <-- SCF

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

Final energy = -20746.05352842 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.01673 -0.01018 0.01478 \*

\* Se 2 0.02200 0.00901 -0.02671 \*

\* Se 3 0.01130 0.00453 0.01113 \*

\* Se 4 -0.01499 -0.00999 -0.00411 \*

\* Se 5 0.01584 -0.02681 -0.01605 \*

\* Se 6 -0.00425 0.02433 -0.00583 \*

\* Se 7 -0.00763 0.02556 -0.00498 \*

\* Se 8 0.02184 -0.02489 0.02295 \*

\* Se 9 -0.03083 -0.01033 0.01805 \*

\* Se 10 0.03336 0.00184 0.00469 \*

\* Se 11 0.03321 0.01039 -0.01835 \*

\* Se 12 -0.03156 -0.00215 -0.00393 \*

\* Se 13 0.01029 -0.02643 0.00617 \*

\* Se 14 -0.02272 0.02529 -0.02526 \*

\* Se 15 -0.01608 0.02685 0.01839 \*

\* Se 16 0.00642 -0.02502 0.00447 \*

\* Se 17 -0.01131 -0.00434 -0.00885 \*

\* Se 18 0.01886 0.00805 0.00395 \*

\* Se 19 0.02114 0.00801 -0.01472 \*

\* Se 20 -0.02292 -0.00845 0.02446 \*

\* Nb 1 0.00921 -0.01369 -0.00825 \*

\* Nb 2 -0.00828 0.01607 0.00799 \*

\* Nb 3 -0.01961 0.00400 -0.00554 \*

\* Nb 4 0.02155 -0.00159 0.00873 \*

\* Nb 5 0.00432 -0.01043 -0.00853 \*

\* Nb 6 -0.02167 0.01467 0.00627 \*

\* Nb 7 0.01898 -0.01232 -0.00630 \*

\* Nb 8 -0.00849 0.01041 0.00836 \*

\* Nb 9 -0.02708 0.00073 -0.00871 \*

\* Nb 10 0.01585 -0.00314 0.00572 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.005839 0.002074 0.006608 \*

\* y 0.002074 0.022732 0.004123 \*

\* z 0.006608 0.004123 -0.008668 \*

\* \*

\* Pressure: -0.0066 \*

\* \*

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

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

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

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

| previous | 0.000000 | 7.811E-006 | -20746.053385 | <-- min BFGS

| trial step | 1.000000 | 5.416E-006 | -20746.053546 | <-- min BFGS

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

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BFGS: improving iteration 15 with line minimization (lambda= 3.260857)

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Unit Cell

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

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

14.8803549 -8.5753863 -0.0082380 0.4213555 -0.0015472 0.0002186

0.0126769 3.4523374 0.0004161 1.0466200 1.8161369 0.0002575

-0.0067776 0.0020519 13.0756870 0.0002322 -0.0000588 0.4805244

Lattice parameters(A) Cell Angles

a = 17.174466 alpha = 89.984212

b = 3.452361 beta = 90.057703

c = 13.075689 gamma = 119.743990

Current cell volume = 673.145539 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 0.066889 0.666031 0.122884 x

x Se 2 0.133685 0.334955 0.622632 x

x Se 3 0.133384 0.334566 0.877294 x

x Se 4 0.066705 0.665617 0.377161 x

x Se 5 0.266405 0.666027 0.122600 x

x Se 6 0.333350 0.335019 0.622608 x

x Se 7 0.333151 0.334529 0.877337 x

x Se 8 0.266192 0.665510 0.377431 x

x Se 9 0.467073 0.666657 0.122972 x

x Se 10 0.533186 0.333802 0.622903 x

x Se 11 0.532905 0.333317 0.877006 x

x Se 12 0.466796 0.666175 0.377120 x

x Se 13 0.666835 0.665435 0.122675 x

x Se 14 0.733821 0.334520 0.622555 x

x Se 15 0.733603 0.333998 0.877409 x

x Se 16 0.666642 0.664956 0.377381 x

x Se 17 0.866643 0.665459 0.122704 x

x Se 18 0.933279 0.334386 0.622848 x

x Se 19 0.933084 0.333962 0.877109 x

x Se 20 0.866351 0.665069 0.377368 x

x Nb 1 -0.000390 0.000048 0.250059 x

x Nb 2 0.000393 -0.000018 0.749945 x

x Nb 3 0.199934 0.001128 0.250009 x

x Nb 4 0.200093 -0.000374 0.749977 x

x Nb 5 0.399430 -0.000140 0.250034 x

x Nb 6 0.400044 -0.000365 0.749942 x

x Nb 7 0.599917 0.000228 0.250061 x

x Nb 8 0.600608 0.000255 0.749967 x

x Nb 9 0.799937 0.000428 0.250021 x

x Nb 10 0.800053 -0.001178 0.749987 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460341E+004 21583.69 <-- SCF

1 -2.07461019E+004 2.25919382E-003 21601.69 <-- SCF

2 -2.07461096E+004 2.57685379E-004 21632.62 <-- SCF

3 -2.07461017E+004 -2.65440265E-004 21661.25 <-- SCF

4 -2.07460346E+004 -2.23687494E-003 21690.06 <-- SCF

5 -2.07460494E+004 4.95532696E-004 21719.03 <-- SCF

6 -2.07460588E+004 3.12600902E-004 21747.72 <-- SCF

7 -2.07460587E+004 -3.71748838E-006 21776.03 <-- SCF

8 -2.07460539E+004 -1.60347108E-004 21803.30 <-- SCF

9 -2.07460533E+004 -1.87414754E-005 21829.83 <-- SCF

10 -2.07460538E+004 1.40427246E-005 21855.39 <-- SCF

11 -2.07460537E+004 -3.06129506E-006 21878.83 <-- SCF

12 -2.07460537E+004 2.20601504E-006 21899.92 <-- SCF

13 -2.07460537E+004 -2.49476100E-007 21920.59 <-- SCF

14 -2.07460537E+004 -4.85131545E-007 21941.72 <-- SCF

15 -2.07460537E+004 1.89106815E-007 21962.55 <-- SCF

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

Final energy = -20746.05371429 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.01635 -0.00676 0.00664 \*

\* Se 2 0.01465 0.01162 -0.02223 \*

\* Se 3 0.00869 0.00280 0.01073 \*

\* Se 4 -0.01090 -0.00930 0.00077 \*

\* Se 5 0.00960 -0.02010 -0.01708 \*

\* Se 6 -0.00438 0.02133 -0.00735 \*

\* Se 7 -0.00291 0.01775 0.00097 \*

\* Se 8 0.01975 -0.02215 0.02003 \*

\* Se 9 -0.02493 -0.00477 0.01424 \*

\* Se 10 0.02007 0.00111 0.00508 \*

\* Se 11 0.02599 0.00529 -0.01402 \*

\* Se 12 -0.01999 -0.00087 -0.00494 \*

\* Se 13 0.00443 -0.01839 0.00015 \*

\* Se 14 -0.02185 0.02274 -0.02139 \*

\* Se 15 -0.01110 0.02034 0.01840 \*

\* Se 16 0.00557 -0.02199 0.00627 \*

\* Se 17 -0.01023 -0.00209 -0.00938 \*

\* Se 18 0.01299 0.00788 -0.00122 \*

\* Se 19 0.01911 0.00534 -0.00652 \*

\* Se 20 -0.01720 -0.01065 0.02072 \*

\* Nb 1 0.00135 -0.01487 -0.00315 \*

\* Nb 2 0.00089 0.01585 0.00296 \*

\* Nb 3 -0.01451 0.00211 -0.00227 \*

\* Nb 4 0.02037 -0.00240 0.00426 \*

\* Nb 5 -0.00022 -0.01172 -0.00428 \*

\* Nb 6 -0.01639 0.01561 0.00230 \*

\* Nb 7 0.01715 -0.01369 -0.00240 \*

\* Nb 8 -0.00081 0.01077 0.00420 \*

\* Nb 9 -0.02252 0.00065 -0.00384 \*

\* Nb 10 0.01367 -0.00146 0.00235 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.007325 -0.004223 -0.013530 \*

\* y -0.004223 0.020783 0.017253 \*

\* z -0.013530 0.017253 0.016288 \*

\* \*

\* Pressure: -0.0148 \*

\* \*

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

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

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

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

| previous | 0.000000 | 7.811E-006 | -20746.053385 | <-- min BFGS

| trial step | 1.000000 | 5.416E-006 | -20746.053546 | <-- min BFGS

| line step | 3.260857 | 9.788E-007 | -20746.053720 | <-- min BFGS

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

BFGS: finished iteration 15 with enthalpy= -2.07460537E+004 eV

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

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

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

| dE/ion | 1.117978E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 3.810772E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.727882E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.078291E-002 | 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 | 0.000013 | -20746.053720 | <-- min BFGS

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

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

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)

14.8797387 -8.5753938 -0.0112008 0.4213858 -0.0015250 0.0002756

0.0124926 3.4520190 0.0007279 1.0467927 1.8163596 0.0002480

-0.0085377 0.0031355 13.0718016 0.0003028 -0.0001024 0.4806673

Lattice parameters(A) Cell Angles

a = 17.173937 alpha = 89.974311

b = 3.452042 beta = 90.076653

c = 13.071805 gamma = 119.748079

Current cell volume = 672.834992 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 0.665947 0.122857 x

x Se 2 0.133706 0.335020 0.622552 x

x Se 3 0.133395 0.334603 0.877353 x

x Se 4 0.066687 0.665551 0.377202 x

x Se 5 0.266426 0.665951 0.122535 x

x Se 6 0.333345 0.335092 0.622555 x

x Se 7 0.333143 0.334615 0.877375 x

x Se 8 0.266218 0.665474 0.377506 x

x Se 9 0.467034 0.666517 0.122946 x

x Se 10 0.533228 0.333901 0.622860 x

x Se 11 0.532945 0.333464 0.877032 x

x Se 12 0.466756 0.666080 0.377164 x

x Se 13 0.666846 0.665350 0.122637 x

x Se 14 0.733792 0.334553 0.622479 x

x Se 15 0.733581 0.334071 0.877476 x

x Se 16 0.666648 0.664884 0.377433 x

x Se 17 0.866632 0.665422 0.122646 x

x Se 18 0.933301 0.334454 0.622807 x

x Se 19 0.933107 0.334050 0.877136 x

x Se 20 0.866328 0.665002 0.377447 x

x Nb 1 -0.000374 0.000003 0.250047 x

x Nb 2 0.000376 0.000029 0.749957 x

x Nb 3 0.199917 0.001083 0.250000 x

x Nb 4 0.200116 -0.000305 0.749989 x

x Nb 5 0.399442 -0.000179 0.250021 x

x Nb 6 0.400020 -0.000351 0.749951 x

x Nb 7 0.599942 0.000221 0.250051 x

x Nb 8 0.600592 0.000281 0.749979 x

x Nb 9 0.799912 0.000346 0.250009 x

x Nb 10 0.800070 -0.001131 0.749996 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460483E+004 22357.05 <-- SCF

1 -2.07460643E+004 5.33204456E-004 22374.34 <-- SCF

2 -2.07460655E+004 4.24162716E-005 22404.34 <-- SCF

3 -2.07460563E+004 -3.07594284E-004 22433.03 <-- SCF

4 -2.07460543E+004 -6.53831982E-005 22460.98 <-- SCF

5 -2.07460540E+004 -9.93879462E-006 22487.06 <-- SCF

6 -2.07460540E+004 -5.89303603E-007 22509.61 <-- SCF

7 -2.07460540E+004 1.51379414E-007 22531.42 <-- SCF

8 -2.07460540E+004 1.84089446E-007 22552.20 <-- SCF

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

Final energy = -20746.05403203 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.01458 -0.00611 0.00065 \*

\* Se 2 0.01255 0.01093 -0.01256 \*

\* Se 3 0.01191 0.00170 0.00814 \*

\* Se 4 -0.00608 -0.01153 0.00148 \*

\* Se 5 0.00511 -0.01722 -0.01201 \*

\* Se 6 -0.00545 0.02218 -0.00695 \*

\* Se 7 0.00091 0.01493 0.00540 \*

\* Se 8 0.01720 -0.02184 0.01052 \*

\* Se 9 -0.02131 -0.00228 0.00784 \*

\* Se 10 0.01475 0.00208 0.00262 \*

\* Se 11 0.02231 0.00252 -0.00767 \*

\* Se 12 -0.01462 -0.00205 -0.00261 \*

\* Se 13 0.00068 -0.01534 -0.00477 \*

\* Se 14 -0.01828 0.02212 -0.00998 \*

\* Se 15 -0.00573 0.01733 0.01167 \*

\* Se 16 0.00656 -0.02257 0.00640 \*

\* Se 17 -0.01279 -0.00137 -0.00713 \*

\* Se 18 0.00768 0.01044 -0.00163 \*

\* Se 19 0.01695 0.00486 -0.00080 \*

\* Se 20 -0.01459 -0.01038 0.01172 \*

\* Nb 1 -0.00922 -0.01353 0.00214 \*

\* Nb 2 0.00983 0.01415 -0.00238 \*

\* Nb 3 -0.00988 -0.00184 0.00143 \*

\* Nb 4 0.01549 -0.00037 -0.00041 \*

\* Nb 5 -0.00530 -0.01166 0.00018 \*

\* Nb 6 -0.01118 0.01654 -0.00172 \*

\* Nb 7 0.01117 -0.01507 0.00157 \*

\* Nb 8 0.00440 0.01132 -0.00024 \*

\* Nb 9 -0.01781 -0.00023 0.00055 \*

\* Nb 10 0.00931 0.00231 -0.00142 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.007198 -0.010429 -0.028933 \*

\* y -0.010429 -0.002271 0.027964 \*

\* z -0.028933 0.027964 0.012617 \*

\* \*

\* Pressure: -0.0010 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000013 | -20746.053720 | <-- min BFGS

| trial step | 1.000000 | 8.293E-006 | -20746.054035 | <-- min BFGS

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

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

BFGS: improving iteration 16 with line minimization (lambda= 2.663327)

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Unit Cell

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

14.8787136 -8.5754062 -0.0161289 0.4214363 -0.0014881 0.0003704

0.0121861 3.4514895 0.0012464 1.0470800 1.8167302 0.0002322

-0.0114653 0.0049380 13.0653388 0.0004204 -0.0001751 0.4809053

Lattice parameters(A) Cell Angles

a = 17.173059 alpha = 89.957833

b = 3.451511 beta = 90.108187

c = 13.065345 gamma = 119.754884

Current cell volume = 672.318527 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 0.665809 0.122810 x

x Se 2 0.133741 0.335128 0.622420 x

x Se 3 0.133413 0.334664 0.877452 x

x Se 4 0.066657 0.665443 0.377271 x

x Se 5 0.266461 0.665824 0.122427 x

x Se 6 0.333338 0.335212 0.622467 x

x Se 7 0.333129 0.334760 0.877438 x

x Se 8 0.266262 0.665413 0.377631 x

x Se 9 0.466970 0.666285 0.122903 x

x Se 10 0.533296 0.334064 0.622789 x

x Se 11 0.533013 0.333708 0.877074 x

x Se 12 0.466689 0.665923 0.377237 x

x Se 13 0.666863 0.665210 0.122575 x

x Se 14 0.733745 0.334606 0.622351 x

x Se 15 0.733545 0.334192 0.877587 x

x Se 16 0.666658 0.664766 0.377520 x

x Se 17 0.866612 0.665360 0.122550 x

x Se 18 0.933336 0.334569 0.622739 x

x Se 19 0.933147 0.334197 0.877181 x

x Se 20 0.866290 0.664891 0.377577 x

x Nb 1 -0.000346 -0.000072 0.250025 x

x Nb 2 0.000347 0.000108 0.749978 x

x Nb 3 0.199888 0.001008 0.249986 x

x Nb 4 0.200154 -0.000189 0.750011 x

x Nb 5 0.399462 -0.000243 0.250001 x

x Nb 6 0.399979 -0.000328 0.749968 x

x Nb 7 0.599983 0.000208 0.250034 x

x Nb 8 0.600564 0.000325 0.750000 x

x Nb 9 0.799869 0.000210 0.249987 x

x Nb 10 0.800098 -0.001051 0.750010 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460382E+004 22943.27 <-- SCF

1 -2.07460832E+004 1.50106700E-003 22960.73 <-- SCF

2 -2.07460875E+004 1.44167394E-004 22991.66 <-- SCF

3 -2.07460627E+004 -8.27584937E-004 23020.66 <-- SCF

4 -2.07460550E+004 -2.55291795E-004 23048.59 <-- SCF

5 -2.07460544E+004 -2.17877071E-005 23075.73 <-- SCF

6 -2.07460542E+004 -4.47534869E-006 23102.64 <-- SCF

7 -2.07460542E+004 -1.23401182E-006 23126.73 <-- SCF

8 -2.07460542E+004 4.99104714E-007 23148.42 <-- SCF

9 -2.07460542E+004 1.72676418E-007 23169.67 <-- SCF

10 -2.07460542E+004 9.26666351E-008 23191.08 <-- SCF

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

Final energy = -20746.05422653 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.01207 -0.00482 -0.00504 \*

\* Se 2 0.00621 0.00912 0.00846 \*

\* Se 3 0.01619 -0.00034 -0.00094 \*

\* Se 4 0.00169 -0.01517 -0.00108 \*

\* Se 5 -0.00377 -0.01192 0.00104 \*

\* Se 6 -0.00715 0.02273 -0.00229 \*

\* Se 7 0.00769 0.00975 0.00899 \*

\* Se 8 0.01138 -0.02058 -0.01021 \*

\* Se 9 -0.01392 0.00258 -0.00053 \*

\* Se 10 0.00374 0.00365 0.00122 \*

\* Se 11 0.01428 -0.00264 0.00043 \*

\* Se 12 -0.00395 -0.00386 -0.00120 \*

\* Se 13 -0.00654 -0.00976 -0.00966 \*

\* Se 14 -0.01235 0.02079 0.01171 \*

\* Se 15 0.00300 0.01213 -0.00241 \*

\* Se 16 0.00782 -0.02278 0.00307 \*

\* Se 17 -0.01670 0.00045 0.00063 \*

\* Se 18 -0.00065 0.01442 0.00056 \*

\* Se 19 0.01373 0.00390 0.00510 \*

\* Se 20 -0.00817 -0.00880 -0.00776 \*

\* Nb 1 -0.01995 -0.01203 0.00991 \*

\* Nb 2 0.02172 0.01220 -0.00999 \*

\* Nb 3 -0.00562 -0.00665 0.00648 \*

\* Nb 4 0.01003 0.00141 -0.00814 \*

\* Nb 5 -0.01636 -0.01192 0.00693 \*

\* Nb 6 -0.00209 0.01797 -0.00772 \*

\* Nb 7 0.00341 -0.01712 0.00765 \*

\* Nb 8 0.01547 0.01201 -0.00692 \*

\* Nb 9 -0.01115 -0.00165 0.00811 \*

\* Nb 10 0.00406 0.00691 -0.00641 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.013564 -0.021500 -0.057005 \*

\* y -0.021500 -0.021575 0.045203 \*

\* z -0.057005 0.045203 0.031491 \*

\* \*

\* Pressure: 0.0012 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000013 | -20746.053720 | <-- min BFGS

| trial step | 1.000000 | 8.293E-006 | -20746.054035 | <-- min BFGS

| line step | 2.663327 | -4.247E-007 | -20746.054241 | <-- min BFGS

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

BFGS: finished iteration 16 with enthalpy= -2.07460542E+004 eV

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

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

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

| dE/ion | 1.734091E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.686444E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.036748E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 5.700538E-002 | 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 | 3.304E-006 | -20746.054241 | <-- min BFGS

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

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

BFGS: starting iteration 17 with trial guess (lambda= 1.000000)

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Unit Cell

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

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

14.8786959 -8.5755856 -0.0147359 0.4214361 -0.0014891 0.0003439

0.0121952 3.4515744 0.0010936 1.0470758 1.8166828 0.0002414

-0.0106426 0.0043984 13.0597416 0.0003878 -0.0001538 0.4811114

Lattice parameters(A) Cell Angles

a = 17.173132 alpha = 89.962715

b = 3.451596 beta = 90.099253

c = 13.059747 gamma = 119.755284

Current cell volume = 672.047353 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 0.066838 0.665829 0.122753 x

x Se 2 0.133733 0.335099 0.622377 x

x Se 3 0.133411 0.334644 0.877500 x

x Se 4 0.066660 0.665464 0.377325 x

x Se 5 0.266460 0.665843 0.122381 x

x Se 6 0.333338 0.335184 0.622418 x

x Se 7 0.333133 0.334733 0.877492 x

x Se 8 0.266263 0.665431 0.377674 x

x Se 9 0.466972 0.666312 0.122845 x

x Se 10 0.533290 0.334040 0.622735 x

x Se 11 0.533011 0.333681 0.877133 x

x Se 12 0.466695 0.665947 0.377291 x

x Se 13 0.666858 0.665237 0.122521 x

x Se 14 0.733744 0.334589 0.622309 x

x Se 15 0.733546 0.334173 0.877632 x

x Se 16 0.666657 0.664794 0.377570 x

x Se 17 0.866613 0.665380 0.122501 x

x Se 18 0.933333 0.334547 0.622685 x

x Se 19 0.933146 0.334176 0.877239 x

x Se 20 0.866297 0.664920 0.377620 x

x Nb 1 -0.000347 -0.000075 0.250028 x

x Nb 2 0.000348 0.000111 0.749975 x

x Nb 3 0.199891 0.000997 0.249989 x

x Nb 4 0.200150 -0.000192 0.750008 x

x Nb 5 0.399465 -0.000245 0.250004 x

x Nb 6 0.399983 -0.000318 0.749966 x

x Nb 7 0.599979 0.000198 0.250036 x

x Nb 8 0.600562 0.000328 0.749997 x

x Nb 9 0.799874 0.000215 0.249991 x

x Nb 10 0.800095 -0.001041 0.750007 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460504E+004 23584.41 <-- SCF

1 -2.07460628E+004 4.15140729E-004 23602.14 <-- SCF

2 -2.07460639E+004 3.49475205E-005 23632.31 <-- SCF

3 -2.07460563E+004 -2.53899648E-004 23661.12 <-- SCF

4 -2.07460545E+004 -5.76317112E-005 23689.28 <-- SCF

5 -2.07460543E+004 -7.60833191E-006 23715.28 <-- SCF

6 -2.07460543E+004 -9.26024743E-007 23737.73 <-- SCF

7 -2.07460543E+004 -9.15309832E-008 23758.70 <-- SCF

8 -2.07460543E+004 7.06183660E-007 23780.27 <-- SCF

9 -2.07460543E+004 -2.55845671E-007 23801.22 <-- SCF

10 -2.07460543E+004 -7.96769143E-008 23821.36 <-- SCF

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

Final energy = -20746.05429194 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.01075 -0.00639 -0.00115 \*

\* Se 2 0.00863 0.00808 0.00773 \*

\* Se 3 0.01694 0.00080 -0.00157 \*

\* Se 4 0.00104 -0.01569 -0.00366 \*

\* Se 5 -0.00111 -0.01431 0.00481 \*

\* Se 6 -0.00663 0.02391 -0.00065 \*

\* Se 7 0.00603 0.01286 0.00621 \*

\* Se 8 0.01135 -0.02143 -0.01280 \*

\* Se 9 -0.01498 0.00022 0.00168 \*

\* Se 10 0.00805 0.00447 -0.00035 \*

\* Se 11 0.01578 -0.00065 0.00061 \*

\* Se 12 -0.00766 -0.00511 -0.00229 \*

\* Se 13 -0.00446 -0.01319 -0.00451 \*

\* Se 14 -0.01075 0.02129 0.01173 \*

\* Se 15 0.00200 0.01416 -0.00367 \*

\* Se 16 0.00768 -0.02429 -0.00102 \*

\* Se 17 -0.01648 -0.00080 0.00366 \*

\* Se 18 0.00159 0.01517 0.00107 \*

\* Se 19 0.01393 0.00567 0.00341 \*

\* Se 20 -0.00963 -0.00785 -0.00938 \*

\* Nb 1 -0.01956 -0.01147 0.00812 \*

\* Nb 2 0.01956 0.01134 -0.00822 \*

\* Nb 3 -0.00745 -0.00507 0.00524 \*

\* Nb 4 0.01294 0.00062 -0.00652 \*

\* Nb 5 -0.01517 -0.01000 0.00571 \*

\* Nb 6 -0.00585 0.01647 -0.00638 \*

\* Nb 7 0.00366 -0.01513 0.00649 \*

\* Nb 8 0.01187 0.01122 -0.00573 \*

\* Nb 9 -0.01505 -0.00083 0.00662 \*

\* Nb 10 0.00448 0.00593 -0.00520 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.027234 -0.020045 -0.048157 \*

\* y -0.020045 -0.032859 0.040239 \*

\* z -0.048157 0.040239 0.006650 \*

\* \*

\* Pressure: 0.0178 \*

\* \*

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

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

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

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

| previous | 0.000000 | 3.304E-006 | -20746.054241 | <-- min BFGS

| trial step | 1.000000 | 3.748E-007 | -20746.054308 | <-- min BFGS

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

BFGS: finished iteration 17 with enthalpy= -2.07460543E+004 eV

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

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

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

| dE/ion | 2.251668E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 2.741690E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.702507E-004 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.815698E-002 | 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 | 3.487E-006 | -20746.054308 | <-- 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)

14.8795047 -8.5762639 -0.0124427 0.4214089 -0.0014964 0.0002988

0.0122570 3.4519515 0.0008654 1.0469767 1.8164659 0.0002405

-0.0092479 0.0036016 13.0594497 0.0003321 -0.0001218 0.4811220

Lattice parameters(A) Cell Angles

a = 17.174170 alpha = 89.969979

b = 3.451973 beta = 90.084554

c = 13.059453 gamma = 119.754892

Current cell volume = 672.149231 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 0.066839 0.665839 0.122748 x

x Se 2 0.133730 0.335081 0.622388 x

x Se 3 0.133412 0.334634 0.877496 x

x Se 4 0.066663 0.665472 0.377325 x

x Se 5 0.266456 0.665857 0.122387 x

x Se 6 0.333338 0.335172 0.622418 x

x Se 7 0.333137 0.334719 0.877496 x

x Se 8 0.266261 0.665441 0.377664 x

x Se 9 0.466975 0.666337 0.122840 x

x Se 10 0.533285 0.334020 0.622735 x

x Se 11 0.533007 0.333654 0.877137 x

x Se 12 0.466701 0.665966 0.377290 x

x Se 13 0.666854 0.665251 0.122517 x

x Se 14 0.733747 0.334580 0.622320 x

x Se 15 0.733550 0.334160 0.877625 x

x Se 16 0.666657 0.664806 0.377569 x

x Se 17 0.866612 0.665390 0.122505 x

x Se 18 0.933330 0.334539 0.622684 x

x Se 19 0.933145 0.334165 0.877244 x

x Se 20 0.866300 0.664938 0.377610 x

x Nb 1 -0.000351 -0.000096 0.250033 x

x Nb 2 0.000353 0.000132 0.749970 x

x Nb 3 0.199896 0.000987 0.249992 x

x Nb 4 0.200144 -0.000188 0.750003 x

x Nb 5 0.399462 -0.000265 0.250008 x

x Nb 6 0.399986 -0.000296 0.749962 x

x Nb 7 0.599976 0.000176 0.250040 x

x Nb 8 0.600566 0.000350 0.749993 x

x Nb 9 0.799879 0.000211 0.249995 x

x Nb 10 0.800090 -0.001032 0.750004 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460533E+004 24219.00 <-- SCF

1 -2.07460860E+004 1.09045783E-003 24238.56 <-- SCF

2 -2.07460870E+004 3.14982173E-005 24265.12 <-- SCF

3 -2.07462296E+004 4.75460967E-003 24293.97 <-- SCF

4 -2.07460208E+004 -6.96233843E-003 24322.75 <-- SCF

5 -2.07460207E+004 -1.16937773E-006 24350.95 <-- SCF

6 -2.07460375E+004 5.58762081E-004 24377.81 <-- SCF

7 -2.07460462E+004 2.89153818E-004 24400.19 <-- SCF

8 -2.07460516E+004 1.80177405E-004 24422.11 <-- SCF

9 -2.07460558E+004 1.40327059E-004 24444.91 <-- SCF

10 -2.07460579E+004 7.16813199E-005 24467.27 <-- SCF

11 -2.07460582E+004 9.06442302E-006 24490.08 <-- SCF

12 -2.07460576E+004 -1.97520338E-005 24512.02 <-- SCF

13 -2.07460569E+004 -2.29285278E-005 24534.16 <-- SCF

14 -2.07460564E+004 -1.88218797E-005 24555.75 <-- SCF

15 -2.07460558E+004 -1.79552062E-005 24577.16 <-- SCF

16 -2.07460545E+004 -4.35837082E-005 24602.02 <-- SCF

17 -2.07460544E+004 -3.51862319E-006 24623.08 <-- SCF

18 -2.07460542E+004 -7.10452723E-006 24646.64 <-- SCF

19 -2.07460543E+004 3.68741088E-006 24667.89 <-- SCF

20 -2.07460547E+004 1.34565382E-005 24690.97 <-- SCF

21 -2.07460547E+004 1.34770415E-007 24711.69 <-- SCF

22 -2.07460543E+004 -1.51061321E-005 24734.23 <-- SCF

23 -2.07460542E+004 -8.59123680E-007 24755.42 <-- SCF

24 -2.07460543E+004 7.00274414E-007 24776.92 <-- SCF

25 -2.07460543E+004 1.90420419E-006 24797.81 <-- SCF

26 -2.07460543E+004 1.22504179E-006 24818.84 <-- SCF

27 -2.07460544E+004 6.34601398E-007 24839.73 <-- SCF

28 -2.07460543E+004 -6.57644519E-007 24860.55 <-- SCF

29 -2.07460543E+004 -2.95083768E-007 24881.80 <-- SCF

30 -2.07460543E+004 6.13464434E-008 24902.83 <-- SCF

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

Final energy = -20746.05433786 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00938 -0.00778 0.00108 \*

\* Se 2 0.01068 0.00882 0.00705 \*

\* Se 3 0.01501 0.00295 -0.00292 \*

\* Se 4 -0.00094 -0.01511 -0.00448 \*

\* Se 5 0.00024 -0.01590 0.00392 \*

\* Se 6 -0.00507 0.02419 0.00144 \*

\* Se 7 0.00364 0.01546 0.00284 \*

\* Se 8 0.00960 -0.02113 -0.01049 \*

\* Se 9 -0.01444 -0.00104 0.00357 \*

\* Se 10 0.01018 0.00476 0.00189 \*

\* Se 11 0.01471 0.00151 -0.00290 \*

\* Se 12 -0.01052 -0.00450 -0.00291 \*

\* Se 13 -0.00218 -0.01533 -0.00264 \*

\* Se 14 -0.01072 0.02152 0.01052 \*

\* Se 15 -0.00121 0.01615 -0.00400 \*

\* Se 16 0.00620 -0.02406 -0.00132 \*

\* Se 17 -0.01582 -0.00248 0.00285 \*

\* Se 18 0.00325 0.01468 0.00314 \*

\* Se 19 0.01237 0.00710 0.00000 \*

\* Se 20 -0.01300 -0.00804 -0.00695 \*

\* Nb 1 -0.01725 -0.01065 0.00687 \*

\* Nb 2 0.01910 0.01019 -0.00682 \*

\* Nb 3 -0.00704 -0.00353 0.00399 \*

\* Nb 4 0.01316 -0.00174 -0.00507 \*

\* Nb 5 -0.01310 -0.00954 0.00466 \*

\* Nb 6 -0.00351 0.01451 -0.00535 \*

\* Nb 7 0.00401 -0.01380 0.00522 \*

\* Nb 8 0.00956 0.00844 -0.00434 \*

\* Nb 9 -0.01519 0.00027 0.00522 \*

\* Nb 10 0.00767 0.00408 -0.00409 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.001084 -0.016128 -0.032794 \*

\* y -0.016128 0.004182 0.032496 \*

\* z -0.032794 0.032496 0.026360 \*

\* \*

\* Pressure: -0.0105 \*

\* \*

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

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

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

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

| previous | 0.000000 | 3.487E-006 | -20746.054308 | <-- min BFGS

| trial step | 1.000000 | 1.708E-006 | -20746.054373 | <-- min BFGS

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

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

BFGS: improving iteration 18 with line minimization (lambda= 1.959932)

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Unit Cell

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

14.8802810 -8.5769150 -0.0102413 0.4213828 -0.0015034 0.0002555

0.0123164 3.4523135 0.0006464 1.0468815 1.8162578 0.0002395

-0.0079091 0.0028368 13.0591695 0.0002786 -0.0000911 0.4811323

Lattice parameters(A) Cell Angles

a = 17.175166 alpha = 89.976951

b = 3.452336 beta = 90.070444

c = 13.059172 gamma = 119.754516

Current cell volume = 672.247009 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 0.066839 0.665850 0.122743 x

x Se 2 0.133727 0.335063 0.622398 x

x Se 3 0.133414 0.334624 0.877491 x

x Se 4 0.066666 0.665481 0.377326 x

x Se 5 0.266452 0.665871 0.122393 x

x Se 6 0.333339 0.335161 0.622418 x

x Se 7 0.333141 0.334705 0.877501 x

x Se 8 0.266259 0.665450 0.377654 x

x Se 9 0.466978 0.666362 0.122836 x

x Se 10 0.533279 0.334001 0.622735 x

x Se 11 0.533004 0.333628 0.877142 x

x Se 12 0.466706 0.665984 0.377290 x

x Se 13 0.666850 0.665265 0.122512 x

x Se 14 0.733749 0.334571 0.622331 x

x Se 15 0.733554 0.334147 0.877619 x

x Se 16 0.666657 0.664817 0.377569 x

x Se 17 0.866611 0.665400 0.122509 x

x Se 18 0.933327 0.334530 0.622684 x

x Se 19 0.933145 0.334155 0.877249 x

x Se 20 0.866303 0.664955 0.377600 x

x Nb 1 -0.000356 -0.000116 0.250037 x

x Nb 2 0.000357 0.000152 0.749966 x

x Nb 3 0.199900 0.000976 0.249995 x

x Nb 4 0.200139 -0.000184 0.749999 x

x Nb 5 0.399459 -0.000285 0.250012 x

x Nb 6 0.399988 -0.000276 0.749958 x

x Nb 7 0.599974 0.000155 0.250044 x

x Nb 8 0.600569 0.000371 0.749989 x

x Nb 9 0.799884 0.000208 0.249999 x

x Nb 10 0.800085 -0.001023 0.750001 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460539E+004 25298.33 <-- SCF

1 -2.07460546E+004 2.40812571E-005 25314.80 <-- SCF

2 -2.07460547E+004 2.12064224E-006 25338.41 <-- SCF

3 -2.07460545E+004 -6.11483896E-006 25366.45 <-- SCF

4 -2.07460544E+004 -3.71181322E-006 25392.03 <-- SCF

5 -2.07460544E+004 -3.67288974E-008 25413.69 <-- SCF

6 -2.07460544E+004 -1.01690288E-007 25434.73 <-- SCF

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

Final energy = -20746.05436962 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00924 -0.00912 0.00336 \*

\* Se 2 0.01214 0.00919 0.00404 \*

\* Se 3 0.01298 0.00437 -0.00236 \*

\* Se 4 -0.00337 -0.01485 -0.00454 \*

\* Se 5 0.00207 -0.01790 0.00310 \*

\* Se 6 -0.00373 0.02441 0.00099 \*

\* Se 7 0.00212 0.01768 0.00108 \*

\* Se 8 0.00913 -0.02158 -0.00775 \*

\* Se 9 -0.01417 -0.00309 0.00581 \*

\* Se 10 0.01199 0.00475 0.00206 \*

\* Se 11 0.01399 0.00309 -0.00484 \*

\* Se 12 -0.01255 -0.00491 -0.00320 \*

\* Se 13 -0.00100 -0.01761 -0.00035 \*

\* Se 14 -0.01072 0.02184 0.00743 \*

\* Se 15 -0.00342 0.01811 -0.00292 \*

\* Se 16 0.00439 -0.02433 -0.00167 \*

\* Se 17 -0.01440 -0.00418 0.00326 \*

\* Se 18 0.00476 0.01437 0.00258 \*

\* Se 19 0.01130 0.00835 -0.00181 \*

\* Se 20 -0.01474 -0.00872 -0.00468 \*

\* Nb 1 -0.02121 -0.01038 0.00902 \*

\* Nb 2 0.02299 0.01010 -0.00900 \*

\* Nb 3 -0.00337 -0.00500 0.00594 \*

\* Nb 4 0.01203 -0.00044 -0.00739 \*

\* Nb 5 -0.01456 -0.00907 0.00658 \*

\* Nb 6 -0.00238 0.01522 -0.00742 \*

\* Nb 7 0.00295 -0.01456 0.00707 \*

\* Nb 8 0.01287 0.00924 -0.00626 \*

\* Nb 9 -0.01082 -0.00004 0.00753 \*

\* Nb 10 0.00395 0.00507 -0.00565 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.012297 -0.012488 -0.016779 \*

\* y -0.012488 0.020495 0.023792 \*

\* z -0.016779 0.023792 0.021101 \*

\* \*

\* Pressure: -0.0180 \*

\* \*

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

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

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

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

| previous | 0.000000 | 3.487E-006 | -20746.054308 | <-- min BFGS

| trial step | 1.000000 | 1.708E-006 | -20746.054373 | <-- min BFGS

| line step | 1.959932 | 5.090E-007 | -20746.054395 | <-- min BFGS

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

BFGS: finished iteration 18 with enthalpy= -2.07460544E+004 eV

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

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

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

| dE/ion | 2.893091E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 2.667881E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.127287E-004 | 5.000000E-004 | A | Yes | <-- BFGS

| Smax | 2.379164E-002 | 2.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 19 ...

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

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

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

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

| previous | 0.000000 | 5.433E-006 | -20746.054395 | <-- min BFGS

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

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

BFGS: starting iteration 19 with trial guess (lambda= 1.000000)

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Unit Cell

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

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

14.8798255 -8.5765580 -0.0082863 0.4213869 -0.0015186 0.0002251

0.0124415 3.4523868 0.0003313 1.0468260 1.8161815 0.0003178

-0.0069697 0.0017321 13.0588071 0.0002408 -0.0000470 0.4811456

Lattice parameters(A) Cell Angles

a = 17.174592 alpha = 89.987012

b = 3.452409 beta = 90.057933

c = 13.058809 gamma = 119.752169

Current cell volume = 672.236105 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 0.066824 0.665789 0.122752 x

x Se 2 0.133743 0.335109 0.622389 x

x Se 3 0.133426 0.334650 0.877493 x

x Se 4 0.066655 0.665423 0.377320 x

x Se 5 0.266461 0.665821 0.122389 x

x Se 6 0.333336 0.335227 0.622414 x

x Se 7 0.333140 0.334769 0.877501 x

x Se 8 0.266274 0.665417 0.377659 x

x Se 9 0.466953 0.666286 0.122848 x

x Se 10 0.533304 0.334060 0.622739 x

x Se 11 0.533030 0.333708 0.877130 x

x Se 12 0.466682 0.665926 0.377286 x

x Se 13 0.666853 0.665204 0.122512 x

x Se 14 0.733733 0.334602 0.622325 x

x Se 15 0.733545 0.334196 0.877624 x

x Se 16 0.666661 0.664753 0.377574 x

x Se 17 0.866598 0.665373 0.122508 x

x Se 18 0.933340 0.334591 0.622688 x

x Se 19 0.933163 0.334220 0.877240 x

x Se 20 0.866286 0.664907 0.377608 x

x Nb 1 -0.000355 -0.000197 0.250036 x

x Nb 2 0.000357 0.000235 0.749967 x

x Nb 3 0.199893 0.000927 0.249994 x

x Nb 4 0.200151 -0.000121 0.750001 x

x Nb 5 0.399458 -0.000358 0.250009 x

x Nb 6 0.399973 -0.000225 0.749959 x

x Nb 7 0.599989 0.000109 0.250043 x

x Nb 8 0.600567 0.000438 0.749991 x

x Nb 9 0.799870 0.000137 0.249997 x

x Nb 10 0.800091 -0.000975 0.750002 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460533E+004 25832.58 <-- SCF

1 -2.07460596E+004 2.08982734E-004 25850.73 <-- SCF

2 -2.07460605E+004 2.90435812E-005 25879.02 <-- SCF

3 -2.07460844E+004 7.96950751E-004 25908.27 <-- SCF

4 -2.07460425E+004 -1.39578787E-003 25937.31 <-- SCF

5 -2.07460473E+004 1.60072782E-004 25964.14 <-- SCF

6 -2.07460524E+004 1.71429939E-004 25991.62 <-- SCF

7 -2.07460544E+004 6.68182084E-005 26017.44 <-- SCF

8 -2.07460551E+004 2.07704174E-005 26040.16 <-- SCF

9 -2.07460554E+004 1.16799276E-005 26061.98 <-- SCF

10 -2.07460554E+004 3.85621404E-007 26083.42 <-- SCF

11 -2.07460554E+004 -9.49279878E-007 26105.11 <-- SCF

12 -2.07460554E+004 -4.41641121E-007 26126.17 <-- SCF

13 -2.07460555E+004 3.91083917E-006 26147.47 <-- SCF

14 -2.07460555E+004 -1.42042392E-006 26168.69 <-- SCF

15 -2.07460554E+004 -1.45433746E-006 26189.83 <-- SCF

16 -2.07460556E+004 4.47862468E-006 26211.03 <-- SCF

17 -2.07460556E+004 1.80993292E-006 26232.44 <-- SCF

18 -2.07460561E+004 1.68999387E-005 26254.30 <-- SCF

19 -2.07460550E+004 -3.77246797E-005 26276.81 <-- SCF

20 -2.07460544E+004 -1.80149709E-005 26299.92 <-- SCF

21 -2.07460545E+004 2.36006690E-006 26321.55 <-- SCF

22 -2.07460545E+004 -9.36002351E-007 26343.08 <-- SCF

23 -2.07460543E+004 -5.26451495E-006 26365.19 <-- SCF

24 -2.07460544E+004 1.16848513E-006 26386.81 <-- SCF

25 -2.07460544E+004 2.74845788E-006 26408.36 <-- SCF

26 -2.07460545E+004 1.38023383E-006 26429.31 <-- SCF

27 -2.07460545E+004 2.01819866E-006 26450.58 <-- SCF

28 -2.07460546E+004 7.64479528E-007 26471.53 <-- SCF

29 -2.07460546E+004 3.31034734E-007 26492.52 <-- SCF

30 -2.07460545E+004 -2.08616577E-006 26513.62 <-- SCF

31 -2.07460545E+004 -8.06584545E-007 26534.86 <-- SCF

32 -2.07460545E+004 4.51629248E-007 26555.86 <-- SCF

33 -2.07460545E+004 1.42361742E-007 26577.44 <-- SCF

34 -2.07460545E+004 -1.07906314E-007 26598.34 <-- SCF

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

Final energy = -20746.05450420 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00625 -0.01162 0.00089 \*

\* Se 2 0.01241 0.00782 0.00624 \*

\* Se 3 0.01175 0.00652 -0.00089 \*

\* Se 4 -0.00336 -0.01442 -0.00420 \*

\* Se 5 0.00092 -0.01811 0.00364 \*

\* Se 6 -0.00110 0.02183 0.00087 \*

\* Se 7 0.00186 0.01794 0.00354 \*

\* Se 8 0.00432 -0.01900 -0.01006 \*

\* Se 9 -0.00761 -0.00394 0.00258 \*

\* Se 10 0.00821 0.00409 0.00038 \*

\* Se 11 0.00702 0.00374 -0.00082 \*

\* Se 12 -0.00916 -0.00449 -0.00245 \*

\* Se 13 -0.00093 -0.01803 -0.00204 \*

\* Se 14 -0.00423 0.01879 0.00958 \*

\* Se 15 -0.00074 0.01795 -0.00310 \*

\* Se 16 0.00174 -0.02195 -0.00227 \*

\* Se 17 -0.01202 -0.00681 0.00329 \*

\* Se 18 0.00257 0.01342 0.00214 \*

\* Se 19 0.00619 0.01033 0.00088 \*

\* Se 20 -0.01404 -0.00780 -0.00828 \*

\* Nb 1 -0.01877 -0.00624 0.00690 \*

\* Nb 2 0.02176 0.00687 -0.00700 \*

\* Nb 3 -0.00716 -0.00047 0.00393 \*

\* Nb 4 0.01273 -0.00397 -0.00528 \*

\* Nb 5 -0.01372 -0.00521 0.00489 \*

\* Nb 6 -0.00056 0.01028 -0.00546 \*

\* Nb 7 0.00334 -0.00989 0.00541 \*

\* Nb 8 0.01365 0.00605 -0.00467 \*

\* Nb 9 -0.01513 0.00435 0.00531 \*

\* Nb 10 0.00628 0.00198 -0.00395 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.017546 -0.007474 -0.009285 \*

\* y -0.007474 0.025686 0.014523 \*

\* z -0.009285 0.014523 0.021893 \*

\* \*

\* Pressure: -0.0217 \*

\* \*

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

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

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

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

| previous | 0.000000 | 5.433E-006 | -20746.054395 | <-- min BFGS

| trial step | 1.000000 | 3.963E-006 | -20746.054535 | <-- min BFGS

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

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

BFGS: improving iteration 19 with line minimization (lambda= 3.696754)

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Unit Cell

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

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

14.8785972 -8.5755953 -0.0030143 0.4213980 -0.0015597 0.0001430

0.0127789 3.4525847 -0.0005182 1.0466763 1.8159758 0.0005290

-0.0044364 -0.0012469 13.0578297 0.0001388 0.0000717 0.4811815

Lattice parameters(A) Cell Angles

a = 17.173046 alpha = 90.014143

b = 3.452608 beta = 90.024190

c = 13.057830 gamma = 119.745843

Current cell volume = 672.206600 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 0.066785 0.665626 0.122776 x

x Se 2 0.133787 0.335233 0.622366 x

x Se 3 0.133461 0.334721 0.877500 x

x Se 4 0.066627 0.665268 0.377306 x

x Se 5 0.266485 0.665685 0.122376 x

x Se 6 0.333327 0.335405 0.622400 x

x Se 7 0.333136 0.334941 0.877503 x

x Se 8 0.266316 0.665328 0.377675 x

x Se 9 0.466885 0.666081 0.122881 x

x Se 10 0.533371 0.334219 0.622751 x

x Se 11 0.533100 0.333923 0.877097 x

x Se 12 0.466616 0.665770 0.377275 x

x Se 13 0.666860 0.665038 0.122512 x

x Se 14 0.733689 0.334686 0.622309 x

x Se 15 0.733519 0.334327 0.877637 x

x Se 16 0.666672 0.664578 0.377586 x

x Se 17 0.866562 0.665300 0.122503 x

x Se 18 0.933375 0.334755 0.622701 x

x Se 19 0.933211 0.334394 0.877217 x

x Se 20 0.866238 0.664776 0.377631 x

x Nb 1 -0.000353 -0.000415 0.250033 x

x Nb 2 0.000355 0.000459 0.749969 x

x Nb 3 0.199872 0.000795 0.249992 x

x Nb 4 0.200183 0.000050 0.750007 x

x Nb 5 0.399456 -0.000557 0.250003 x

x Nb 6 0.399930 -0.000090 0.749960 x

x Nb 7 0.600032 -0.000016 0.250041 x

x Nb 8 0.600562 0.000619 0.749997 x

x Nb 9 0.799833 -0.000056 0.249992 x

x Nb 10 0.800109 -0.000845 0.750005 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460465E+004 26995.64 <-- SCF

1 -2.07460829E+004 1.21166612E-003 27013.50 <-- SCF

2 -2.07460865E+004 1.20826075E-004 27044.41 <-- SCF

3 -2.07461787E+004 3.07406812E-003 27073.75 <-- SCF

4 -2.07460239E+004 -5.16180044E-003 27102.64 <-- SCF

5 -2.07460325E+004 2.86648957E-004 27131.94 <-- SCF

6 -2.07460445E+004 3.99628869E-004 27161.22 <-- SCF

7 -2.07460546E+004 3.38197713E-004 27189.78 <-- SCF

8 -2.07460628E+004 2.74068382E-004 27215.86 <-- SCF

9 -2.07460632E+004 1.25598021E-005 27239.50 <-- SCF

10 -2.07460614E+004 -6.13819768E-005 27262.80 <-- SCF

11 -2.07460596E+004 -5.70594010E-005 27285.47 <-- SCF

12 -2.07460573E+004 -7.90134551E-005 27309.59 <-- SCF

13 -2.07460553E+004 -6.42064259E-005 27333.80 <-- SCF

14 -2.07460541E+004 -4.24047582E-005 27357.88 <-- SCF

15 -2.07460536E+004 -1.58169990E-005 27384.25 <-- SCF

16 -2.07460546E+004 3.49655961E-005 27407.02 <-- SCF

17 -2.07460551E+004 1.39363826E-005 27428.36 <-- SCF

18 -2.07460551E+004 -5.10704078E-008 27450.11 <-- SCF

19 -2.07460548E+004 -9.55378884E-006 27472.73 <-- SCF

20 -2.07460548E+004 -6.94701130E-007 27493.91 <-- SCF

21 -2.07460547E+004 -2.73020072E-007 27515.00 <-- SCF

22 -2.07460547E+004 3.36796623E-008 27536.28 <-- SCF

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

Final energy = -20746.05474961 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00291 -0.01874 -0.00449 \*

\* Se 2 0.01077 0.00468 0.00988 \*

\* Se 3 0.00671 0.01228 0.00184 \*

\* Se 4 -0.00067 -0.01409 -0.00161 \*

\* Se 5 -0.00172 -0.01971 0.00614 \*

\* Se 6 0.00611 0.01531 -0.00387 \*

\* Se 7 0.00311 0.01868 0.01230 \*

\* Se 8 -0.00615 -0.01362 -0.01537 \*

\* Se 9 0.00654 -0.00761 -0.00184 \*

\* Se 10 0.00091 0.00303 -0.00632 \*

\* Se 11 -0.00761 0.00632 0.01005 \*

\* Se 12 -0.00196 -0.00434 -0.00241 \*

\* Se 13 -0.00226 -0.02075 -0.00566 \*

\* Se 14 0.00659 0.01220 0.01037 \*

\* Se 15 0.00195 0.01836 -0.00112 \*

\* Se 16 -0.00523 -0.01743 -0.00268 \*

\* Se 17 -0.00829 -0.01314 0.00381 \*

\* Se 18 -0.00031 0.01178 -0.00573 \*

\* Se 19 -0.00347 0.01617 0.01169 \*

\* Se 20 -0.01334 -0.00523 -0.01513 \*

\* Nb 1 -0.02566 0.00172 0.01101 \*

\* Nb 2 0.02923 0.00251 -0.01103 \*

\* Nb 3 -0.00856 0.00136 0.00668 \*

\* Nb 4 0.01412 -0.00759 -0.00894 \*

\* Nb 5 -0.01404 -0.00038 0.00881 \*

\* Nb 6 0.00661 0.00981 -0.00919 \*

\* Nb 7 -0.00614 -0.00304 0.00892 \*

\* Nb 8 0.01547 0.00167 -0.00852 \*

\* Nb 9 -0.01301 0.00775 0.00909 \*

\* Nb 10 0.00740 0.00203 -0.00666 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.015794 0.010483 0.016321 \*

\* y 0.010483 0.024770 -0.014119 \*

\* z 0.016321 -0.014119 0.007515 \*

\* \*

\* Pressure: -0.0160 \*

\* \*

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

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

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

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

| previous | 0.000000 | 5.433E-006 | -20746.054395 | <-- min BFGS

| trial step | 1.000000 | 3.963E-006 | -20746.054535 | <-- min BFGS

| line step | 3.696754 | 3.197E-007 | -20746.054801 | <-- min BFGS

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

BFGS: finished iteration 19 with enthalpy= -2.07460548E+004 eV

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

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

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

| dE/ion | 1.352384E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 3.134052E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.565484E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.477013E-002 | 2.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 20 ...

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

Writing analysis data to 2H-Nb1Se2-7.castep\_bin

Writing model to 2H-Nb1Se2-7.check

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

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

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

| previous | 0.000000 | 3.039E-006 | -20746.054801 | <-- min BFGS

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

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

BFGS: starting iteration 20 with trial guess (lambda= 1.000000)

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

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Unit Cell

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

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

14.8783259 -8.5743064 -0.0034738 0.4213973 -0.0015745 0.0001513

0.0128990 3.4522805 -0.0004611 1.0466095 1.8160996 0.0005211

-0.0046926 -0.0010422 13.0574497 0.0001491 0.0000637 0.4811955

Lattice parameters(A) Cell Angles

a = 17.172167 alpha = 90.012303

b = 3.452305 beta = 90.027148

c = 13.057451 gamma = 119.740557

Current cell volume = 672.128936 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.066780 0.665553 0.122793 x

x Se 2 0.133799 0.335332 0.622345 x

x Se 3 0.133466 0.334799 0.877508 x

x Se 4 0.066623 0.665202 0.377298 x

x Se 5 0.266492 0.665583 0.122365 x

x Se 6 0.333321 0.335500 0.622405 x

x Se 7 0.333128 0.335040 0.877490 x

x Se 8 0.266326 0.665246 0.377690 x

x Se 9 0.466873 0.665986 0.122899 x

x Se 10 0.533386 0.334294 0.622756 x

x Se 11 0.533114 0.334020 0.877079 x

x Se 12 0.466602 0.665696 0.377269 x

x Se 13 0.666869 0.664939 0.122526 x

x Se 14 0.733677 0.334765 0.622291 x

x Se 15 0.733511 0.334427 0.877651 x

x Se 16 0.666679 0.664483 0.377580 x

x Se 17 0.866556 0.665222 0.122497 x

x Se 18 0.933380 0.334820 0.622709 x

x Se 19 0.933217 0.334466 0.877200 x

x Se 20 0.866225 0.664676 0.377648 x

x Nb 1 -0.000358 -0.000399 0.250028 x

x Nb 2 0.000360 0.000447 0.749974 x

x Nb 3 0.199852 0.000820 0.249988 x

x Nb 4 0.200210 0.000035 0.750013 x

x Nb 5 0.399451 -0.000531 0.249998 x

x Nb 6 0.399925 -0.000129 0.749964 x

x Nb 7 0.600037 0.000029 0.250037 x

x Nb 8 0.600564 0.000588 0.750003 x

x Nb 9 0.799806 -0.000045 0.249986 x

x Nb 10 0.800129 -0.000865 0.750008 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460444E+004 27934.44 <-- SCF

1 -2.07463709E+004 1.08833772E-002 27954.38 <-- SCF

2 -2.07463762E+004 1.76493285E-004 27983.69 <-- SCF

3 -2.07462542E+004 -4.06591773E-003 28013.03 <-- SCF

4 -2.07459727E+004 -9.38344691E-003 28041.58 <-- SCF

5 -2.07460821E+004 3.64612008E-003 28071.28 <-- SCF

6 -2.07461100E+004 9.31845182E-004 28100.16 <-- SCF

7 -2.07460789E+004 -1.03637953E-003 28127.98 <-- SCF

8 -2.07460578E+004 -7.05341603E-004 28156.02 <-- SCF

9 -2.07460464E+004 -3.78489512E-004 28184.08 <-- SCF

10 -2.07460495E+004 1.01951125E-004 28212.48 <-- SCF

11 -2.07460621E+004 4.22316750E-004 28239.73 <-- SCF

12 -2.07460660E+004 1.29344876E-004 28263.03 <-- SCF

13 -2.07460641E+004 -6.22754312E-005 28287.97 <-- SCF

14 -2.07460565E+004 -2.53917425E-004 28314.70 <-- SCF

15 -2.07460563E+004 -9.33583546E-006 28336.86 <-- SCF

16 -2.07460544E+004 -6.20621425E-005 28364.48 <-- SCF

17 -2.07460552E+004 2.80322146E-005 28387.02 <-- SCF

18 -2.07460550E+004 -7.91650398E-006 28408.66 <-- SCF

19 -2.07460546E+004 -1.44491053E-005 28433.58 <-- SCF

20 -2.07460547E+004 3.73108011E-006 28454.98 <-- SCF

21 -2.07460547E+004 1.00959657E-006 28476.34 <-- SCF

22 -2.07460547E+004 2.24010914E-007 28497.22 <-- SCF

23 -2.07460547E+004 -7.07211449E-007 28518.48 <-- SCF

24 -2.07460547E+004 7.83580196E-008 28539.64 <-- SCF

25 -2.07460547E+004 -1.18800240E-007 28560.17 <-- SCF

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

Final energy = -20746.05468641 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00640 -0.01441 -0.01595 \*

\* Se 2 0.01169 0.00044 0.02208 \*

\* Se 3 0.00949 0.00877 -0.00626 \*

\* Se 4 0.00247 -0.01016 0.00755 \*

\* Se 5 -0.00130 -0.01506 0.00110 \*

\* Se 6 0.01211 0.01080 0.00006 \*

\* Se 7 0.00997 0.01321 0.01122 \*

\* Se 8 -0.00618 -0.00943 -0.01235 \*

\* Se 9 0.01070 -0.00374 -0.01561 \*

\* Se 10 0.00256 0.00071 -0.00094 \*

\* Se 11 -0.00649 0.00285 0.00770 \*

\* Se 12 0.00147 -0.00142 0.00851 \*

\* Se 13 -0.00164 -0.01436 -0.01990 \*

\* Se 14 0.01067 0.00793 0.02325 \*

\* Se 15 0.00578 0.01360 -0.01208 \*

\* Se 16 -0.00387 -0.01208 0.00906 \*

\* Se 17 -0.00535 -0.01033 -0.00417 \*

\* Se 18 0.00469 0.00981 -0.00243 \*

\* Se 19 0.00137 0.01376 0.01082 \*

\* Se 20 -0.00903 -0.00156 -0.01116 \*

\* Nb 1 -0.03792 -0.00669 0.01382 \*

\* Nb 2 0.02727 0.00632 -0.01419 \*

\* Nb 3 -0.00070 -0.00561 0.00847 \*

\* Nb 4 0.00396 -0.00097 -0.01169 \*

\* Nb 5 -0.02896 -0.00494 0.01136 \*

\* Nb 6 -0.00648 0.01422 -0.01122 \*

\* Nb 7 -0.00957 -0.01154 0.01113 \*

\* Nb 8 0.01973 0.00579 -0.01139 \*

\* Nb 9 -0.01265 0.00434 0.01162 \*

\* Nb 10 -0.01019 0.00973 -0.00841 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.007078 0.006783 0.014477 \*

\* y 0.006783 0.012906 -0.012201 \*

\* z 0.014477 -0.012201 -0.010525 \*

\* \*

\* Pressure: -0.0032 \*

\* \*

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

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

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

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

| previous | 0.000000 | 3.039E-006 | -20746.054801 | <-- min BFGS

| trial step | 1.000000 | 4.470E-007 | -20746.054746 | <-- min BFGS

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

BFGS: finished iteration 20 with enthalpy= -2.07460547E+004 eV

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

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

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

| dE/ion | 1.827339E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 4.090703E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.891892E-004 | 5.000000E-004 | A | Yes | <-- BFGS

| Smax | 1.447703E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

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

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

Starting BFGS iteration 21 ...

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

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

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

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

| previous | 0.000000 | 1.067E-006 | -20746.054746 | <-- 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)

14.8780221 -8.5736164 -0.0037196 0.4214047 -0.0015766 0.0001594

0.0129154 3.4520348 -0.0004860 1.0466182 1.8162239 0.0005532

-0.0049441 -0.0011288 13.0588806 0.0001590 0.0000671 0.4811428

Lattice parameters(A) Cell Angles

a = 17.171559 alpha = 90.013099

b = 3.452059 beta = 90.028733

c = 13.058882 gamma = 119.738781

Current cell volume = 672.142868 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 0.066779 0.665526 0.122810 x

x Se 2 0.133805 0.335366 0.622355 x

x Se 3 0.133470 0.334826 0.877497 x

x Se 4 0.066621 0.665174 0.377283 x

x Se 5 0.266494 0.665549 0.122375 x

x Se 6 0.333320 0.335539 0.622418 x

x Se 7 0.333127 0.335078 0.877476 x

x Se 8 0.266329 0.665216 0.377681 x

x Se 9 0.466869 0.665959 0.122916 x

x Se 10 0.533392 0.334320 0.622771 x

x Se 11 0.533118 0.334048 0.877062 x

x Se 12 0.466596 0.665671 0.377254 x

x Se 13 0.666872 0.664903 0.122540 x

x Se 14 0.733675 0.334795 0.622301 x

x Se 15 0.733509 0.334460 0.877641 x

x Se 16 0.666680 0.664444 0.377567 x

x Se 17 0.866552 0.665195 0.122508 x

x Se 18 0.933383 0.334849 0.622724 x

x Se 19 0.933220 0.334496 0.877184 x

x Se 20 0.866218 0.664641 0.377639 x

x Nb 1 -0.000362 -0.000415 0.250028 x

x Nb 2 0.000364 0.000463 0.749973 x

x Nb 3 0.199847 0.000821 0.249988 x

x Nb 4 0.200217 0.000038 0.750013 x

x Nb 5 0.399447 -0.000543 0.249997 x

x Nb 6 0.399922 -0.000129 0.749964 x

x Nb 7 0.600039 0.000028 0.250037 x

x Nb 8 0.600568 0.000596 0.750003 x

x Nb 9 0.799798 -0.000050 0.249986 x

x Nb 10 0.800133 -0.000866 0.750008 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460542E+004 28962.91 <-- SCF

1 -2.07460605E+004 2.08525635E-004 28982.45 <-- SCF

2 -2.07460612E+004 2.57080657E-005 29009.45 <-- SCF

3 -2.07460946E+004 1.11158994E-003 29038.86 <-- SCF

4 -2.07460397E+004 -1.83010463E-003 29068.20 <-- SCF

5 -2.07460471E+004 2.47533783E-004 29095.67 <-- SCF

6 -2.07460523E+004 1.72185486E-004 29122.62 <-- SCF

7 -2.07460547E+004 8.09233639E-005 29145.92 <-- SCF

8 -2.07460554E+004 2.41635745E-005 29168.12 <-- SCF

9 -2.07460557E+004 7.79657954E-006 29189.70 <-- SCF

10 -2.07460557E+004 4.10926652E-007 29211.47 <-- SCF

11 -2.07460555E+004 -6.60168682E-006 29233.34 <-- SCF

12 -2.07460553E+004 -6.19343889E-006 29254.91 <-- SCF

13 -2.07460549E+004 -1.18005737E-005 29277.12 <-- SCF

14 -2.07460547E+004 -7.18611907E-006 29299.27 <-- SCF

15 -2.07460546E+004 -4.58576637E-006 29321.27 <-- SCF

16 -2.07460546E+004 -7.37640175E-007 29343.38 <-- SCF

17 -2.07460546E+004 2.18393062E-006 29364.88 <-- SCF

18 -2.07460547E+004 2.76445589E-006 29386.14 <-- SCF

19 -2.07460548E+004 1.78405402E-006 29407.38 <-- SCF

20 -2.07460547E+004 -7.77995569E-007 29428.69 <-- SCF

21 -2.07460547E+004 -2.90544667E-007 29449.91 <-- SCF

22 -2.07460547E+004 -4.41506963E-008 29470.98 <-- SCF

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

Final energy = -20746.05472740 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00295 -0.01436 -0.01409 \*

\* Se 2 0.00863 -0.00041 0.01613 \*

\* Se 3 0.00715 0.00819 -0.00024 \*

\* Se 4 -0.00037 -0.00982 0.00567 \*

\* Se 5 -0.00457 -0.01262 0.00493 \*

\* Se 6 0.00805 0.00995 -0.00658 \*

\* Se 7 0.00653 0.01242 0.01760 \*

\* Se 8 -0.00920 -0.00681 -0.01621 \*

\* Se 9 0.00897 -0.00336 -0.01163 \*

\* Se 10 -0.00177 0.00035 -0.00712 \*

\* Se 11 -0.01035 0.00292 0.01390 \*

\* Se 12 0.00039 -0.00078 0.00446 \*

\* Se 13 -0.00549 -0.01194 -0.01620 \*

\* Se 14 0.00801 0.00700 0.01663 \*

\* Se 15 0.00350 0.01292 -0.00539 \*

\* Se 16 -0.00717 -0.00961 0.00519 \*

\* Se 17 -0.00926 -0.00858 0.00059 \*

\* Se 18 0.00007 0.00958 -0.00844 \*

\* Se 19 -0.00278 0.01395 0.01659 \*

\* Se 20 -0.01207 0.00028 -0.01603 \*

\* Nb 1 -0.03058 -0.00544 0.01381 \*

\* Nb 2 0.03417 0.00480 -0.01372 \*

\* Nb 3 0.00021 -0.00872 0.00832 \*

\* Nb 4 0.00592 -0.00038 -0.01150 \*

\* Nb 5 -0.01794 -0.00551 0.01142 \*

\* Nb 6 0.00832 0.01350 -0.01087 \*

\* Nb 7 -0.00516 -0.01356 0.01100 \*

\* Nb 8 0.01869 0.00606 -0.01145 \*

\* Nb 9 -0.00599 0.00105 0.01135 \*

\* Nb 10 0.00111 0.00895 -0.00813 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.001473 0.007916 0.011334 \*

\* y 0.007916 -0.000495 -0.013191 \*

\* z 0.011334 -0.013191 -0.006572 \*

\* \*

\* Pressure: 0.0019 \*

\* \*

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

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

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

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

| previous | 0.000000 | 1.067E-006 | -20746.054746 | <-- min BFGS

| trial step | 1.000000 | 4.542E-007 | -20746.054778 | <-- min BFGS

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

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BFGS: improving iteration 21 with line minimization (lambda= 1.740775)

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Unit Cell

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

14.8777971 -8.5731052 -0.0039017 0.4214102 -0.0015782 0.0001654

0.0129275 3.4518528 -0.0005043 1.0466247 1.8163160 0.0005771

-0.0051304 -0.0011930 13.0599405 0.0001663 0.0000697 0.4811037

Lattice parameters(A) Cell Angles

a = 17.171109 alpha = 90.013689

b = 3.451877 beta = 90.029908

c = 13.059942 gamma = 119.737465

Current cell volume = 672.153180 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 0.066777 0.665506 0.122822 x

x Se 2 0.133810 0.335392 0.622363 x

x Se 3 0.133473 0.334846 0.877488 x

x Se 4 0.066620 0.665154 0.377272 x

x Se 5 0.266496 0.665524 0.122382 x

x Se 6 0.333320 0.335569 0.622427 x

x Se 7 0.333126 0.335105 0.877465 x

x Se 8 0.266330 0.665194 0.377673 x

x Se 9 0.466866 0.665939 0.122929 x

x Se 10 0.533397 0.334339 0.622782 x

x Se 11 0.533121 0.334069 0.877049 x

x Se 12 0.466592 0.665653 0.377244 x

x Se 13 0.666873 0.664877 0.122550 x

x Se 14 0.733673 0.334817 0.622309 x

x Se 15 0.733508 0.334485 0.877633 x

x Se 16 0.666681 0.664416 0.377558 x

x Se 17 0.866550 0.665175 0.122517 x

x Se 18 0.933386 0.334871 0.622735 x

x Se 19 0.933222 0.334517 0.877171 x

x Se 20 0.866213 0.664616 0.377632 x

x Nb 1 -0.000366 -0.000427 0.250029 x

x Nb 2 0.000367 0.000474 0.749973 x

x Nb 3 0.199843 0.000821 0.249988 x

x Nb 4 0.200222 0.000040 0.750013 x

x Nb 5 0.399443 -0.000551 0.249997 x

x Nb 6 0.399919 -0.000129 0.749964 x

x Nb 7 0.600040 0.000027 0.250037 x

x Nb 8 0.600570 0.000602 0.750003 x

x Nb 9 0.799792 -0.000054 0.249986 x

x Nb 10 0.800136 -0.000866 0.750008 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460538E+004 29871.12 <-- SCF

1 -2.07460979E+004 1.46903442E-003 29890.83 <-- SCF

2 -2.07460992E+004 4.32933737E-005 29918.19 <-- SCF

3 -2.07462521E+004 5.09733891E-003 29947.77 <-- SCF

4 -2.07460188E+004 -7.77539337E-003 29976.45 <-- SCF

5 -2.07460263E+004 2.49048293E-004 30005.14 <-- SCF

6 -2.07460477E+004 7.14561624E-004 30033.11 <-- SCF

7 -2.07460544E+004 2.21705005E-004 30057.88 <-- SCF

8 -2.07460573E+004 9.64642502E-005 30080.33 <-- SCF

9 -2.07460590E+004 5.69824863E-005 30102.16 <-- SCF

10 -2.07460593E+004 9.44432285E-006 30124.84 <-- SCF

11 -2.07460583E+004 -3.05378369E-005 30148.39 <-- SCF

12 -2.07460576E+004 -2.56460639E-005 30170.11 <-- SCF

13 -2.07460575E+004 -1.68147948E-006 30191.31 <-- SCF

14 -2.07460582E+004 2.19353578E-005 30212.58 <-- SCF

15 -2.07460604E+004 7.48424167E-005 30235.52 <-- SCF

16 -2.07460577E+004 -9.24434276E-005 30258.64 <-- SCF

17 -2.07460557E+004 -6.65590111E-005 30285.19 <-- SCF

18 -2.07460552E+004 -1.48571455E-005 30306.97 <-- SCF

19 -2.07460548E+004 -1.23882649E-005 30329.98 <-- SCF

20 -2.07460551E+004 1.02573257E-005 30350.94 <-- SCF

21 -2.07460557E+004 1.87492701E-005 30373.61 <-- SCF

22 -2.07460558E+004 2.63857085E-006 30394.95 <-- SCF

23 -2.07460567E+004 3.12958090E-005 30417.91 <-- SCF

24 -2.07460567E+004 -2.13341159E-006 30439.09 <-- SCF

25 -2.07460565E+004 -6.63203656E-006 30460.41 <-- SCF

26 -2.07460566E+004 5.96000526E-006 30481.56 <-- SCF

27 -2.07460561E+004 -1.82908639E-005 30503.22 <-- SCF

28 -2.07460567E+004 1.92782961E-005 30524.52 <-- SCF

29 -2.07460564E+004 -1.04708164E-005 30545.64 <-- SCF

30 -2.07460563E+004 -6.70897916E-007 30566.12 <-- SCF

31 -2.07460560E+004 -1.21181747E-005 30587.44 <-- SCF

32 -2.07460564E+004 1.43999941E-005 30608.69 <-- SCF

33 -2.07460561E+004 -1.02497746E-005 30629.67 <-- SCF

34 -2.07460556E+004 -1.62008304E-005 30658.34 <-- SCF

35 -2.07460553E+004 -1.21418605E-005 30680.66 <-- SCF

36 -2.07460548E+004 -1.57408570E-005 30703.17 <-- SCF

37 -2.07460547E+004 -2.63435142E-006 30724.69 <-- SCF

38 -2.07460544E+004 -9.36962298E-006 30749.16 <-- SCF

39 -2.07460548E+004 1.16741434E-005 30771.30 <-- SCF

40 -2.07460549E+004 3.00997531E-006 30793.02 <-- SCF

41 -2.07460548E+004 -1.52546476E-006 30814.22 <-- SCF

42 -2.07460550E+004 6.26103075E-006 30836.34 <-- SCF

43 -2.07460550E+004 -1.50499106E-006 30857.61 <-- SCF

44 -2.07460547E+004 -8.13771067E-006 30879.50 <-- SCF

45 -2.07460547E+004 -4.87488025E-007 30900.78 <-- SCF

46 -2.07460547E+004 5.41019889E-007 30922.05 <-- SCF

47 -2.07460547E+004 -3.37941865E-007 30943.38 <-- SCF

48 -2.07460547E+004 5.02242735E-007 30964.41 <-- SCF

49 -2.07460547E+004 7.12298011E-008 30985.53 <-- SCF

50 -2.07460547E+004 7.47521471E-008 31006.67 <-- SCF

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

Final energy = -20746.05472395 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00258 -0.01347 -0.01757 \*

\* Se 2 0.00631 -0.00098 0.01792 \*

\* Se 3 0.00539 0.00770 -0.00189 \*

\* Se 4 -0.00042 -0.00863 0.00898 \*

\* Se 5 -0.00512 -0.01126 0.00310 \*

\* Se 6 0.00710 0.00928 -0.00668 \*

\* Se 7 0.00613 0.01180 0.01780 \*

\* Se 8 -0.00924 -0.00533 -0.01440 \*

\* Se 9 0.00883 -0.00272 -0.01352 \*

\* Se 10 -0.00294 0.00042 -0.00718 \*

\* Se 11 -0.01090 0.00303 0.01414 \*

\* Se 12 0.00078 0.00002 0.00609 \*

\* Se 13 -0.00794 -0.01069 -0.01928 \*

\* Se 14 0.00712 0.00589 0.01830 \*

\* Se 15 0.00286 0.01196 -0.00725 \*

\* Se 16 -0.00894 -0.00822 0.00816 \*

\* Se 17 -0.01014 -0.00769 -0.00269 \*

\* Se 18 0.00035 0.00925 -0.00755 \*

\* Se 19 -0.00214 0.01381 0.01565 \*

\* Se 20 -0.01216 0.00134 -0.01304 \*

\* Nb 1 -0.03018 -0.00795 0.01388 \*

\* Nb 2 0.03681 0.00503 -0.01397 \*

\* Nb 3 0.00491 -0.01110 0.00832 \*

\* Nb 4 0.00589 0.00092 -0.01134 \*

\* Nb 5 -0.01760 -0.00691 0.01164 \*

\* Nb 6 0.00881 0.01251 -0.01116 \*

\* Nb 7 -0.00398 -0.01419 0.01106 \*

\* Nb 8 0.02128 0.00614 -0.01127 \*

\* Nb 9 -0.00456 -0.00030 0.01167 \*

\* Nb 10 0.00111 0.01032 -0.00795 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.005688 0.006991 0.009259 \*

\* y 0.006991 -0.010075 -0.013790 \*

\* z 0.009259 -0.013790 -0.007959 \*

\* \*

\* Pressure: 0.0079 \*

\* \*

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

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

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

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

| previous | 0.000000 | 1.067E-006 | -20746.054746 | <-- min BFGS

| trial step | 1.000000 | 4.542E-007 | -20746.054778 | <-- min BFGS

| line step | 1.740775 | 1.260E-007 | -20746.054774 | <-- min BFGS

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

BFGS: finished iteration 21 with enthalpy= -2.07460548E+004 eV

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

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

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

| dE/ion | 9.282312E-007 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 3.968916E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.312420E-004 | 5.000000E-004 | A | Yes | <-- BFGS

| Smax | 1.378995E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

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

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

Starting BFGS iteration 22 ...

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

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

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

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

| previous | 0.000000 | 1.776E-006 | -20746.054774 | <-- 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)

14.8778989 -8.5731272 -0.0041483 0.4214109 -0.0015720 0.0001691

0.0128768 3.4517738 -0.0004628 1.0466530 1.8163728 0.0005660

-0.0052439 -0.0010477 13.0596183 0.0001710 0.0000639 0.4811156

Lattice parameters(A) Cell Angles

a = 17.171209 alpha = 90.012364

b = 3.451798 beta = 90.031481

c = 13.059619 gamma = 119.738196

Current cell volume = 672.120153 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.066776 0.665477 0.122815 x

x Se 2 0.133815 0.335414 0.622362 x

x Se 3 0.133477 0.334872 0.877492 x

x Se 4 0.066619 0.665129 0.377277 x

x Se 5 0.266497 0.665489 0.122378 x

x Se 6 0.333322 0.335605 0.622422 x

x Se 7 0.333127 0.335144 0.877473 x

x Se 8 0.266332 0.665167 0.377674 x

x Se 9 0.466864 0.665922 0.122924 x

x Se 10 0.533401 0.334355 0.622778 x

x Se 11 0.533124 0.334087 0.877053 x

x Se 12 0.466587 0.665637 0.377249 x

x Se 13 0.666873 0.664840 0.122541 x

x Se 14 0.733672 0.334844 0.622310 x

x Se 15 0.733507 0.334520 0.877636 x

x Se 16 0.666680 0.664381 0.377564 x

x Se 17 0.866545 0.665148 0.122511 x

x Se 18 0.933388 0.334899 0.622731 x

x Se 19 0.933225 0.334549 0.877177 x

x Se 20 0.866207 0.664592 0.377634 x

x Nb 1 -0.000376 -0.000467 0.250033 x

x Nb 2 0.000375 0.000512 0.749969 x

x Nb 3 0.199841 0.000809 0.249991 x

x Nb 4 0.200228 0.000050 0.750010 x

x Nb 5 0.399437 -0.000580 0.250000 x

x Nb 6 0.399917 -0.000109 0.749960 x

x Nb 7 0.600041 0.000006 0.250041 x

x Nb 8 0.600575 0.000628 0.750000 x

x Nb 9 0.799785 -0.000066 0.249989 x

x Nb 10 0.800137 -0.000853 0.750006 x

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460545E+004 31406.33 <-- SCF

1 -2.07460578E+004 1.08393666E-004 31426.11 <-- SCF

2 -2.07460582E+004 1.51678415E-005 31449.97 <-- SCF

3 -2.07460630E+004 1.59748796E-004 31479.42 <-- SCF

4 -2.07460537E+004 -3.09752421E-004 31508.22 <-- SCF

5 -2.07460545E+004 2.43473776E-005 31535.47 <-- SCF

6 -2.07460548E+004 1.05403008E-005 31559.09 <-- SCF

7 -2.07460548E+004 1.41203425E-006 31580.89 <-- SCF

8 -2.07460548E+004 -3.97109090E-007 31602.69 <-- SCF

9 -2.07460548E+004 -8.58290064E-007 31624.23 <-- SCF

10 -2.07460548E+004 -4.49887358E-007 31645.78 <-- SCF

11 -2.07460548E+004 1.59492730E-007 31667.66 <-- SCF

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

Final energy = -20746.05476392 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00303 -0.01366 -0.01632 \*

\* Se 2 0.00775 -0.00114 0.01605 \*

\* Se 3 0.00752 0.00713 -0.00136 \*

\* Se 4 0.00020 -0.00927 0.00925 \*

\* Se 5 -0.00358 -0.01011 0.00395 \*

\* Se 6 0.00814 0.00803 -0.00760 \*

\* Se 7 0.00734 0.01024 0.01730 \*

\* Se 8 -0.00784 -0.00466 -0.01374 \*

\* Se 9 0.00920 -0.00235 -0.01285 \*

\* Se 10 -0.00214 0.00000 -0.00747 \*

\* Se 11 -0.00990 0.00227 0.01323 \*

\* Se 12 0.00143 -0.00009 0.00664 \*

\* Se 13 -0.00810 -0.00971 -0.01766 \*

\* Se 14 0.00879 0.00512 0.01690 \*

\* Se 15 0.00454 0.01073 -0.00708 \*

\* Se 16 -0.00908 -0.00760 0.00791 \*

\* Se 17 -0.00994 -0.00677 -0.00121 \*

\* Se 18 -0.00064 0.00879 -0.00751 \*

\* Se 19 -0.00292 0.01299 0.01423 \*

\* Se 20 -0.01133 0.00183 -0.01309 \*

\* Nb 1 -0.03293 -0.00728 0.01408 \*

\* Nb 2 0.03558 0.00673 -0.01390 \*

\* Nb 3 0.00298 -0.01174 0.00796 \*

\* Nb 4 0.00488 0.00098 -0.01124 \*

\* Nb 5 -0.01658 -0.00825 0.01141 \*

\* Nb 6 0.00805 0.01570 -0.01102 \*

\* Nb 7 -0.00690 -0.01550 0.01114 \*

\* Nb 8 0.02061 0.00733 -0.01134 \*

\* Nb 9 -0.00861 -0.00153 0.01119 \*

\* Nb 10 0.00047 0.01177 -0.00785 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.003930 0.004379 0.008276 \*

\* y 0.004379 -0.012330 -0.012040 \*

\* z 0.008276 -0.012040 -0.008023 \*

\* \*

\* Pressure: 0.0081 \*

\* \*

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

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

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

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

| previous | 0.000000 | 1.776E-006 | -20746.054774 | <-- min BFGS

| trial step | 1.000000 | 1.728E-006 | -20746.054817 | <-- min BFGS

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

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

BFGS: improving iteration 22 with line minimization (lambda= 36.902427)

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Unit Cell

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

14.8815549 -8.5739146 -0.0130018 0.4214349 -0.0013509 0.0003014

0.0110550 3.4489368 0.0010287 1.0476694 1.8184164 0.0001674

-0.0093188 0.0041680 13.0480504 0.0003373 -0.0001447 0.4815424

Lattice parameters(A) Cell Angles

a = 17.174774 alpha = 89.964740

b = 3.448955 beta = 90.087968

c = 13.048054 gamma = 119.764478

Current cell volume = 670.934605 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 0.066725 0.664434 0.122587 x

x Se 2 0.134013 0.336207 0.622355 x

x Se 3 0.133640 0.335816 0.877624 x

x Se 4 0.066572 0.664229 0.377446 x

x Se 5 0.266536 0.664221 0.122220 x

x Se 6 0.333373 0.336923 0.622245 x

x Se 7 0.333183 0.336532 0.877742 x

x Se 8 0.266385 0.664189 0.377709 x

x Se 9 0.466780 0.665316 0.122738 x

x Se 10 0.533568 0.334924 0.622622 x

x Se 11 0.533228 0.334726 0.877215 x

x Se 12 0.466435 0.665084 0.377424 x

x Se 13 0.666864 0.663536 0.122235 x

x Se 14 0.733626 0.335810 0.622337 x

x Se 15 0.733479 0.335779 0.877731 x

x Se 16 0.666672 0.663132 0.377782 x

x Se 17 0.866379 0.664168 0.122322 x

x Se 18 0.933486 0.335881 0.622578 x

x Se 19 0.933338 0.335682 0.877386 x

x Se 20 0.865985 0.663735 0.377705 x

x Nb 1 -0.000716 -0.001893 0.250180 x

x Nb 2 0.000692 0.001878 0.749817 x

x Nb 3 0.199742 0.000363 0.250080 x

x Nb 4 0.200429 0.000386 0.749896 x

x Nb 5 0.399200 -0.001631 0.250111 x

x Nb 6 0.399834 0.000592 0.749839 x

x Nb 7 0.600061 -0.000730 0.250159 x

x Nb 8 0.600759 0.001566 0.749891 x

x Nb 9 0.799535 -0.000467 0.250105 x

x Nb 10 0.800194 -0.000388 0.749919 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07458539E+004 32071.11 <-- SCF

1 -2.07463412E+004 1.62459198E-002 32088.95 <-- SCF

2 -2.07463848E+004 1.45268917E-003 32120.62 <-- SCF

3 -2.07461566E+004 -7.60889922E-003 32150.03 <-- SCF

4 -2.07460638E+004 -3.09096564E-003 32178.94 <-- SCF

5 -2.07460578E+004 -2.00120686E-004 32207.75 <-- SCF

6 -2.07460550E+004 -9.35357349E-005 32237.03 <-- SCF

7 -2.07460540E+004 -3.27007283E-005 32266.06 <-- SCF

8 -2.07460542E+004 6.02177387E-006 32294.41 <-- SCF

9 -2.07460542E+004 5.28453576E-007 32319.20 <-- SCF

10 -2.07460542E+004 -8.18518738E-007 32342.66 <-- SCF

11 -2.07460543E+004 1.46430156E-006 32364.52 <-- SCF

12 -2.07460543E+004 1.75558909E-007 32385.97 <-- SCF

13 -2.07460543E+004 1.28018375E-007 32407.34 <-- SCF

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

Final energy = -20746.05426630 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.01089 0.00004 0.02835 \*

\* Se 2 -0.00820 -0.01292 -0.01975 \*

\* Se 3 0.01614 -0.02465 -0.01681 \*

\* Se 4 -0.00212 -0.00961 0.00877 \*

\* Se 5 -0.02159 0.03803 0.02464 \*

\* Se 6 0.01587 -0.01939 -0.01959 \*

\* Se 7 0.02511 -0.03140 -0.01828 \*

\* Se 8 -0.02449 0.02318 0.01539 \*

\* Se 9 0.00193 0.00969 0.01586 \*

\* Se 10 -0.01443 0.00653 -0.01626 \*

\* Se 11 -0.00776 -0.00994 -0.01047 \*

\* Se 12 0.00914 -0.00649 0.01101 \*

\* Se 13 -0.03319 0.03492 0.02879 \*

\* Se 14 0.02035 -0.02002 -0.02498 \*

\* Se 15 0.01797 -0.03479 -0.01452 \*

\* Se 16 -0.02407 0.02335 0.00833 \*

\* Se 17 -0.01872 0.02823 0.02732 \*

\* Se 18 -0.00767 0.00870 -0.01354 \*

\* Se 19 0.00152 -0.00101 -0.02308 \*

\* Se 20 0.00752 0.01773 0.00768 \*

\* Nb 1 -0.00086 -0.02733 -0.02988 \*

\* Nb 2 0.00956 0.02515 0.03046 \*

\* Nb 3 0.00062 -0.04963 -0.02920 \*

\* Nb 4 0.00508 0.03479 0.03423 \*

\* Nb 5 0.02227 -0.02501 -0.02521 \*

\* Nb 6 0.01910 0.03288 0.02512 \*

\* Nb 7 -0.00368 -0.03749 -0.02480 \*

\* Nb 8 -0.01317 0.02265 0.02452 \*

\* Nb 9 0.00585 -0.03989 -0.03376 \*

\* Nb 10 0.01279 0.04372 0.02965 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.049400 -0.079857 -0.036633 \*

\* y -0.079857 -0.121506 0.054994 \*

\* z -0.036633 0.054994 -0.002756 \*

\* \*

\* Pressure: 0.0579 \*

\* \*

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

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

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

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

| previous | 0.000000 | 1.776E-006 | -20746.054774 | <-- min BFGS

| trial step | 1.000000 | 1.728E-006 | -20746.054817 | <-- min BFGS

| line step | 36.902427 | -2.745E-006 | -20746.054262 | <-- min BFGS

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

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

BFGS: improving iteration 22 with quad minimization (lambda= 14.869675)

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Unit Cell

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

14.8793113 -8.5734314 -0.0075686 0.4214201 -0.0014867 0.0002202

0.0121730 3.4506778 0.0001134 1.0470454 1.8171617 0.0004122

-0.0068181 0.0009672 13.0551494 0.0002352 -0.0000166 0.4812804

Lattice parameters(A) Cell Angles

a = 17.172585 alpha = 89.993978

b = 3.450699 beta = 90.053299

c = 13.055151 gamma = 119.748342

Current cell volume = 671.662115 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.066756 0.665074 0.122727 x

x Se 2 0.133892 0.335720 0.622360 x

x Se 3 0.133540 0.335237 0.877543 x

x Se 4 0.066601 0.664781 0.377342 x

x Se 5 0.266512 0.664999 0.122317 x

x Se 6 0.333341 0.336114 0.622354 x

x Se 7 0.333149 0.335680 0.877577 x

x Se 8 0.266352 0.664789 0.377688 x

x Se 9 0.466831 0.665688 0.122852 x

x Se 10 0.533466 0.334575 0.622718 x

x Se 11 0.533164 0.334334 0.877116 x

x Se 12 0.466529 0.665424 0.377317 x

x Se 13 0.666870 0.664336 0.122423 x

x Se 14 0.733654 0.335217 0.622320 x

x Se 15 0.733496 0.335007 0.877672 x

x Se 16 0.666677 0.663899 0.377648 x

x Se 17 0.866481 0.664769 0.122438 x

x Se 18 0.933426 0.335278 0.622672 x

x Se 19 0.933269 0.334986 0.877258 x

x Se 20 0.866121 0.664261 0.377662 x

x Nb 1 -0.000507 -0.001018 0.250089 x

x Nb 2 0.000498 0.001040 0.749910 x

x Nb 3 0.199803 0.000636 0.250025 x

x Nb 4 0.200306 0.000180 0.749966 x

x Nb 5 0.399345 -0.000986 0.250043 x

x Nb 6 0.399885 0.000162 0.749914 x

x Nb 7 0.600049 -0.000278 0.250086 x

x Nb 8 0.600646 0.000990 0.749958 x

x Nb 9 0.799688 -0.000221 0.250034 x

x Nb 10 0.800159 -0.000674 0.749972 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07459791E+004 32805.23 <-- SCF

1 -2.07461677E+004 6.28542057E-003 32823.53 <-- SCF

2 -2.07461838E+004 5.37067619E-004 32855.50 <-- SCF

3 -2.07461027E+004 -2.70460669E-003 32885.05 <-- SCF

4 -2.07460573E+004 -1.51171206E-003 32914.33 <-- SCF

5 -2.07460570E+004 -1.06767960E-005 32943.59 <-- SCF

6 -2.07460556E+004 -4.52787305E-005 32973.00 <-- SCF

7 -2.07460550E+004 -2.03130661E-005 33001.58 <-- SCF

8 -2.07460551E+004 2.51575401E-006 33029.03 <-- SCF

9 -2.07460551E+004 -1.87729142E-007 33051.78 <-- SCF

10 -2.07460551E+004 -1.42085589E-007 33075.91 <-- SCF

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

Final energy = -20746.05510311 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00481 -0.00516 0.00067 \*

\* Se 2 0.00215 -0.00617 0.00229 \*

\* Se 3 0.01172 -0.00585 -0.00515 \*

\* Se 4 -0.00305 -0.00701 0.00758 \*

\* Se 5 -0.01066 0.00957 0.01307 \*

\* Se 6 0.00893 -0.00228 -0.00738 \*

\* Se 7 0.01217 -0.00574 0.00149 \*

\* Se 8 -0.01498 0.00708 -0.00578 \*

\* Se 9 0.00707 0.00283 -0.00239 \*

\* Se 10 -0.00792 0.00248 -0.01067 \*

\* Se 11 -0.01035 -0.00315 0.00588 \*

\* Se 12 0.00474 -0.00270 0.00691 \*

\* Se 13 -0.01709 0.00802 0.00235 \*

\* Se 14 0.01308 -0.00595 0.00295 \*

\* Se 15 0.00912 -0.00827 -0.01006 \*

\* Se 16 -0.01364 0.00453 0.00335 \*

\* Se 17 -0.01332 0.00686 0.00961 \*

\* Se 18 -0.00317 0.00750 -0.00934 \*

\* Se 19 -0.00099 0.00565 0.00130 \*

\* Se 20 -0.00358 0.00807 -0.00725 \*

\* Nb 1 -0.01738 -0.01405 -0.00464 \*

\* Nb 2 0.02258 0.01160 0.00494 \*

\* Nb 3 0.00752 -0.02537 -0.00754 \*

\* Nb 4 0.00395 0.01477 0.00787 \*

\* Nb 5 -0.00103 -0.01187 -0.00445 \*

\* Nb 6 0.01005 0.01704 0.00514 \*

\* Nb 7 -0.00040 -0.02019 -0.00467 \*

\* Nb 8 0.00710 0.01158 0.00434 \*

\* Nb 9 0.00050 -0.01627 -0.00778 \*

\* Nb 10 0.00168 0.02245 0.00740 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.008203 -0.029689 -0.010886 \*

\* y -0.029689 -0.041766 0.017311 \*

\* z -0.010886 0.017311 0.008508 \*

\* \*

\* Pressure: 0.0138 \*

\* \*

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

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

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

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

| previous | 0.000000 | 1.776E-006 | -20746.054774 | <-- min BFGS

| trial step | 1.000000 | 1.728E-006 | -20746.054817 | <-- min BFGS

| line step | 36.902427 | -2.745E-006 | -20746.054262 | <-- min BFGS

| quad step | 14.869675 | -1.449E-007 | -20746.055129 | <-- min BFGS

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

BFGS: finished iteration 22 with enthalpy= -2.07460551E+004 eV

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

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

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

| dE/ion | 1.182965E-005 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.751685E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.473277E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.176628E-002 | 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 | 7.014E-006 | -20746.055129 | <-- 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)

14.8771361 -8.5734507 -0.0051313 0.4214545 -0.0015338 0.0001797

0.0125603 3.4513514 -0.0002337 1.0469290 1.8166901 0.0004816

-0.0055674 -0.0002521 13.0530418 0.0001844 0.0000319 0.4813580

Lattice parameters(A) Cell Angles

a = 17.170709 alpha = 90.005076

b = 3.451374 beta = 90.037743

c = 13.053043 gamma = 119.745630

Current cell volume = 671.629915 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 0.066749 0.665038 0.122698 x

x Se 2 0.133902 0.335701 0.622374 x

x Se 3 0.133554 0.335239 0.877547 x

x Se 4 0.066597 0.664748 0.377360 x

x Se 5 0.266511 0.664984 0.122316 x

x Se 6 0.333348 0.336151 0.622332 x

x Se 7 0.333161 0.335712 0.877612 x

x Se 8 0.266354 0.664781 0.377676 x

x Se 9 0.466826 0.665706 0.122826 x

x Se 10 0.533473 0.334566 0.622701 x

x Se 11 0.533171 0.334315 0.877141 x

x Se 12 0.466521 0.665431 0.377333 x

x Se 13 0.666860 0.664309 0.122386 x

x Se 14 0.733653 0.335225 0.622337 x

x Se 15 0.733498 0.335022 0.877668 x

x Se 16 0.666672 0.663866 0.377672 x

x Se 17 0.866467 0.664764 0.122431 x

x Se 18 0.933433 0.335316 0.622653 x

x Se 19 0.933279 0.335027 0.877287 x

x Se 20 0.866110 0.664275 0.377652 x

x Nb 1 -0.000530 -0.001194 0.250106 x

x Nb 2 0.000521 0.001214 0.749894 x

x Nb 3 0.199810 0.000537 0.250035 x

x Nb 4 0.200303 0.000265 0.749953 x

x Nb 5 0.399331 -0.001139 0.250056 x

x Nb 6 0.399879 0.000300 0.749900 x

x Nb 7 0.600051 -0.000416 0.250099 x

x Nb 8 0.600659 0.001141 0.749945 x

x Nb 9 0.799689 -0.000309 0.250047 x

x Nb 10 0.800150 -0.000576 0.749963 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460518E+004 33479.33 <-- SCF

1 -2.07460625E+004 3.55787781E-004 33497.97 <-- SCF

2 -2.07460636E+004 3.66344643E-005 33527.53 <-- SCF

3 -2.07460638E+004 6.06081408E-006 33557.14 <-- SCF

4 -2.07460543E+004 -3.16442293E-004 33586.31 <-- SCF

5 -2.07460557E+004 4.76580812E-005 33615.09 <-- SCF

6 -2.07460555E+004 -7.18356501E-006 33642.70 <-- SCF

7 -2.07460552E+004 -7.88651960E-006 33666.03 <-- SCF

8 -2.07460552E+004 -8.15966228E-007 33688.88 <-- SCF

9 -2.07460552E+004 -1.07216137E-007 33711.22 <-- SCF

10 -2.07460552E+004 4.18812693E-007 33733.25 <-- SCF

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

Final energy = -20746.05522654 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00252 -0.01223 0.00649 \*

\* Se 2 0.00774 -0.00286 -0.00708 \*

\* Se 3 0.01458 -0.00025 -0.00384 \*

\* Se 4 -0.00369 -0.01060 0.00804 \*

\* Se 5 -0.00816 0.00398 0.00998 \*

\* Se 6 0.01154 -0.00075 -0.01119 \*

\* Se 7 0.01148 -0.00054 -0.00242 \*

\* Se 8 -0.01531 0.00437 0.00402 \*

\* Se 9 0.00565 -0.00169 -0.00041 \*

\* Se 10 -0.00425 0.00473 -0.01472 \*

\* Se 11 -0.00945 0.00182 0.00342 \*

\* Se 12 0.00064 -0.00440 0.01087 \*

\* Se 13 -0.01448 0.00201 0.00572 \*

\* Se 14 0.01392 -0.00274 -0.00859 \*

\* Se 15 0.00709 -0.00227 -0.00574 \*

\* Se 16 -0.01473 0.00227 0.00675 \*

\* Se 17 -0.01290 0.00135 0.00796 \*

\* Se 18 -0.00085 0.01034 -0.01150 \*

\* Se 19 -0.00146 0.01186 -0.00364 \*

\* Se 20 -0.00611 0.00494 0.00164 \*

\* Nb 1 -0.01811 -0.01005 -0.00732 \*

\* Nb 2 0.02314 0.00900 0.00829 \*

\* Nb 3 -0.00052 -0.02055 -0.00990 \*

\* Nb 4 0.00925 0.01030 0.01120 \*

\* Nb 5 0.00039 -0.01049 -0.00586 \*

\* Nb 6 0.00622 0.01734 0.00723 \*

\* Nb 7 -0.00335 -0.01979 -0.00602 \*

\* Nb 8 -0.00002 0.00802 0.00625 \*

\* Nb 9 -0.00540 -0.01145 -0.01027 \*

\* Nb 10 0.00969 0.01835 0.01062 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.032749 -0.008553 0.002698 \*

\* y -0.008553 -0.033525 0.004474 \*

\* z 0.002698 0.004474 -0.018183 \*

\* \*

\* Pressure: 0.0282 \*

\* \*

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

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

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

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

| previous | 0.000000 | 7.014E-006 | -20746.055129 | <-- min BFGS

| trial step | 1.000000 | 3.195E-006 | -20746.055263 | <-- min BFGS

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

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

BFGS: improving iteration 23 with line minimization (lambda= 1.836567)

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Unit Cell

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

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

14.8753165 -8.5734669 -0.0030923 0.4214834 -0.0015732 0.0001459

0.0128843 3.4519148 -0.0005241 1.0468317 1.8162957 0.0005397

-0.0045212 -0.0012722 13.0512786 0.0001419 0.0000726 0.4814230

Lattice parameters(A) Cell Angles

a = 17.169141 alpha = 90.014358

b = 3.451939 beta = 90.024727

c = 13.051279 gamma = 119.743365

Current cell volume = 671.602910 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.066742 0.665009 0.122673 x

x Se 2 0.133910 0.335686 0.622386 x

x Se 3 0.133565 0.335241 0.877550 x

x Se 4 0.066593 0.664719 0.377376 x

x Se 5 0.266509 0.664972 0.122315 x

x Se 6 0.333354 0.336182 0.622314 x

x Se 7 0.333171 0.335739 0.877641 x

x Se 8 0.266355 0.664774 0.377665 x

x Se 9 0.466821 0.665721 0.122804 x

x Se 10 0.533480 0.334559 0.622687 x

x Se 11 0.533176 0.334300 0.877162 x

x Se 12 0.466515 0.665437 0.377347 x

x Se 13 0.666852 0.664286 0.122356 x

x Se 14 0.733653 0.335233 0.622351 x

x Se 15 0.733500 0.335035 0.877665 x

x Se 16 0.666669 0.663839 0.377692 x

x Se 17 0.866455 0.664760 0.122424 x

x Se 18 0.933438 0.335348 0.622638 x

x Se 19 0.933288 0.335060 0.877312 x

x Se 20 0.866100 0.664287 0.377643 x

x Nb 1 -0.000550 -0.001342 0.250120 x

x Nb 2 0.000540 0.001361 0.749880 x

x Nb 3 0.199815 0.000454 0.250043 x

x Nb 4 0.200300 0.000337 0.749942 x

x Nb 5 0.399319 -0.001267 0.250067 x

x Nb 6 0.399875 0.000415 0.749889 x

x Nb 7 0.600053 -0.000532 0.250110 x

x Nb 8 0.600669 0.001266 0.749934 x

x Nb 9 0.799689 -0.000383 0.250059 x

x Nb 10 0.800142 -0.000494 0.749955 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -2.07460529E+004 34134.69 <-- SCF

1 -2.07460582E+004 1.76194298E-004 34152.03 <-- SCF

2 -2.07460588E+004 2.13838038E-005 34181.59 <-- SCF

3 -2.07460596E+004 2.65143336E-005 34210.92 <-- SCF

4 -2.07460530E+004 -2.20626919E-004 34240.00 <-- SCF

5 -2.07460543E+004 4.22235594E-005 34266.45 <-- SCF

6 -2.07460553E+004 3.50721056E-005 34294.12 <-- SCF

7 -2.07460558E+004 1.72130971E-005 34317.59 <-- SCF

8 -2.07460558E+004 -4.18986552E-007 34339.69 <-- SCF

9 -2.07460558E+004 -8.09959534E-007 34361.31 <-- SCF

10 -2.07460559E+004 4.25038866E-006 34383.06 <-- SCF

11 -2.07460554E+004 -1.68159747E-005 34406.50 <-- SCF

12 -2.07460552E+004 -6.17092147E-006 34427.98 <-- SCF

13 -2.07460551E+004 -3.95787978E-006 34452.03 <-- SCF

14 -2.07460553E+004 5.05935588E-006 34473.61 <-- SCF

15 -2.07460553E+004 2.48780747E-006 34495.03 <-- SCF

16 -2.07460554E+004 5.49073912E-007 34516.30 <-- SCF

17 -2.07460553E+004 -8.06205582E-007 34537.64 <-- SCF

18 -2.07460553E+004 -1.83561981E-006 34558.75 <-- SCF

19 -2.07460552E+004 -2.20977384E-006 34580.53 <-- SCF

20 -2.07460552E+004 1.10779545E-006 34602.77 <-- SCF

21 -2.07460553E+004 2.69053716E-006 34624.25 <-- SCF

22 -2.07460554E+004 1.26493098E-006 34645.66 <-- SCF

23 -2.07460553E+004 -9.19233518E-007 34667.03 <-- SCF

24 -2.07460553E+004 -3.61177923E-007 34688.34 <-- SCF

25 -2.07460553E+004 -4.42477109E-007 34709.52 <-- SCF

26 -2.07460553E+004 2.88515177E-008 34730.89 <-- SCF

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

Final energy = -20746.05531539 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00223 -0.01605 0.01317 \*

\* Se 2 0.00594 0.00007 -0.01691 \*

\* Se 3 0.00994 0.00403 0.00160 \*

\* Se 4 -0.00551 -0.01173 0.00510 \*

\* Se 5 -0.00899 0.00012 0.01159 \*

\* Se 6 0.01305 0.00102 -0.01172 \*

\* Se 7 0.00970 0.00432 -0.00532 \*

\* Se 8 -0.01884 0.00261 0.00615 \*

\* Se 9 0.00571 -0.00659 0.00599 \*

\* Se 10 -0.00255 0.00710 -0.01524 \*

\* Se 11 -0.00945 0.00616 0.00158 \*

\* Se 12 -0.00072 -0.00733 0.00738 \*

\* Se 13 -0.01417 -0.00243 0.01423 \*

\* Se 14 0.01678 -0.00141 -0.01762 \*

\* Se 15 0.00704 0.00116 0.00004 \*

\* Se 16 -0.01742 0.00081 0.00223 \*

\* Se 17 -0.01227 -0.00303 0.00958 \*

\* Se 18 0.00030 0.01163 -0.01100 \*

\* Se 19 -0.00259 0.01580 -0.00739 \*

\* Se 20 -0.00766 0.00199 0.00495 \*

\* Nb 1 -0.00870 -0.00144 -0.01366 \*

\* Nb 2 0.01445 0.00072 0.01419 \*

\* Nb 3 -0.00111 -0.01192 -0.01426 \*

\* Nb 4 0.01035 0.00059 0.01658 \*

\* Nb 5 0.00502 0.00015 -0.01136 \*

\* Nb 6 0.01186 0.00628 0.01166 \*

\* Nb 7 -0.00100 -0.00815 -0.01123 \*

\* Nb 8 -0.00255 -0.00079 0.01135 \*

\* Nb 9 -0.00652 -0.00199 -0.01642 \*

\* Nb 10 0.01212 0.00828 0.01477 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.036939 0.009941 0.014767 \*

\* y 0.009941 -0.005691 -0.005754 \*

\* z 0.014767 -0.005754 -0.022574 \*

\* \*

\* Pressure: 0.0217 \*

\* \*

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

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

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

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

| previous | 0.000000 | 7.014E-006 | -20746.055129 | <-- min BFGS

| trial step | 1.000000 | 3.195E-006 | -20746.055263 | <-- min BFGS

| line step | 1.836567 | -2.078E-006 | -20746.055363 | <-- min BFGS

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

BFGS: finished iteration 23 with enthalpy= -2.07460554E+004 eV

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

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

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.817149E-006 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 2.436796E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.065434E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.693939E-002 | 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 | 1.879E-006 | -20746.055363 | <-- 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)

14.8767060 -8.5739531 -0.0043740 0.4214575 -0.0015496 0.0001676

0.0126913 3.4517763 -0.0003471 1.0468689 1.8164269 0.0005070

-0.0051920 -0.0006512 13.0527560 0.0001691 0.0000478 0.4813686

Lattice parameters(A) Cell Angles

a = 17.170587 alpha = 90.008704

b = 3.451800 beta = 90.032914

c = 13.052757 gamma = 119.745650

Current cell volume = 671.693110 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 0.066739 0.664971 0.122685 x

x Se 2 0.133917 0.335721 0.622383 x

x Se 3 0.133569 0.335273 0.877547 x

x Se 4 0.066590 0.664688 0.377369 x

x Se 5 0.266513 0.664931 0.122316 x

x Se 6 0.333354 0.336222 0.622318 x

x Se 7 0.333169 0.335784 0.877632 x

x Se 8 0.266357 0.664743 0.377667 x

x Se 9 0.466815 0.665680 0.122816 x

x Se 10 0.533489 0.334593 0.622693 x

x Se 11 0.533182 0.334343 0.877150 x

x Se 12 0.466506 0.665404 0.377341 x

x Se 13 0.666855 0.664243 0.122365 x

x Se 14 0.733650 0.335262 0.622349 x

x Se 15 0.733497 0.335075 0.877665 x

x Se 16 0.666669 0.663799 0.377687 x

x Se 17 0.866451 0.664727 0.122427 x

x Se 18 0.933443 0.335380 0.622645 x

x Se 19 0.933292 0.335099 0.877300 x

x Se 20 0.866092 0.664251 0.377646 x

x Nb 1 -0.000552 -0.001351 0.250117 x

x Nb 2 0.000542 0.001369 0.749883 x

x Nb 3 0.199809 0.000454 0.250041 x

x Nb 4 0.200310 0.000342 0.749945 x

x Nb 5 0.399317 -0.001268 0.250064 x

x Nb 6 0.399871 0.000410 0.749892 x

x Nb 7 0.600058 -0.000526 0.250108 x

x Nb 8 0.600669 0.001264 0.749937 x

x Nb 9 0.799679 -0.000391 0.250055 x

x Nb 10 0.800148 -0.000493 0.749957 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460504E+004 35134.89 <-- SCF

1 -2.07462422E+004 6.39538097E-003 35155.22 <-- SCF

2 -2.07462457E+004 1.16730608E-004 35183.28 <-- SCF

3 -2.07463016E+004 1.86288493E-003 35212.94 <-- SCF

4 -2.07459847E+004 -1.05652574E-002 35241.89 <-- SCF

5 -2.07460420E+004 1.91205095E-003 35271.95 <-- SCF

6 -2.07460800E+004 1.26399259E-003 35300.95 <-- SCF

7 -2.07460760E+004 -1.32226999E-004 35328.12 <-- SCF

8 -2.07460590E+004 -5.65234699E-004 35355.52 <-- SCF

9 -2.07460517E+004 -2.45994924E-004 35383.16 <-- SCF

10 -2.07460528E+004 3.80122545E-005 35409.91 <-- SCF

11 -2.07460561E+004 1.08649711E-004 35434.30 <-- SCF

12 -2.07460585E+004 8.21229435E-005 35457.62 <-- SCF

13 -2.07460582E+004 -1.10856895E-005 35480.89 <-- SCF

14 -2.07460568E+004 -4.62163665E-005 35505.23 <-- SCF

15 -2.07460559E+004 -2.84374847E-005 35527.80 <-- SCF

16 -2.07460557E+004 -7.39382673E-006 35549.27 <-- SCF

17 -2.07460550E+004 -2.25532781E-005 35574.47 <-- SCF

18 -2.07460554E+004 1.13863392E-005 35600.36 <-- SCF

19 -2.07460556E+004 8.48908413E-006 35621.81 <-- SCF

20 -2.07460553E+004 -1.28904042E-005 35645.77 <-- SCF

21 -2.07460552E+004 -1.17280943E-006 35667.86 <-- SCF

22 -2.07460553E+004 1.76845796E-006 35689.38 <-- SCF

23 -2.07460553E+004 1.53883293E-006 35710.81 <-- SCF

24 -2.07460553E+004 -8.16442226E-008 35732.05 <-- SCF

25 -2.07460553E+004 -7.81085330E-007 35754.27 <-- SCF

26 -2.07460553E+004 1.08028964E-006 35775.50 <-- SCF

27 -2.07460553E+004 -2.09189033E-006 35797.39 <-- SCF

28 -2.07460553E+004 3.79495607E-007 35818.77 <-- SCF

29 -2.07460553E+004 6.32840534E-008 35840.14 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05527949 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00175 -0.01424 0.01265 \*

\* Se 2 0.00426 -0.00060 -0.01058 \*

\* Se 3 0.01066 0.00217 -0.00284 \*

\* Se 4 -0.00355 -0.01159 0.00445 \*

\* Se 5 -0.00993 0.00308 0.01205 \*

\* Se 6 0.01314 -0.00029 -0.00935 \*

\* Se 7 0.01173 0.00114 -0.00617 \*

\* Se 8 -0.01847 0.00395 0.00449 \*

\* Se 9 0.00662 -0.00462 0.00460 \*

\* Se 10 -0.00424 0.00688 -0.01271 \*

\* Se 11 -0.00976 0.00440 0.00021 \*

\* Se 12 0.00148 -0.00697 0.00767 \*

\* Se 13 -0.01452 0.00055 0.01281 \*

\* Se 14 0.01671 -0.00272 -0.01117 \*

\* Se 15 0.00837 -0.00169 -0.00508 \*

\* Se 16 -0.01584 0.00195 0.00238 \*

\* Se 17 -0.01283 -0.00062 0.00945 \*

\* Se 18 -0.00057 0.01112 -0.00947 \*

\* Se 19 -0.00192 0.01366 -0.00753 \*

\* Se 20 -0.00587 0.00306 0.00327 \*

\* Nb 1 -0.01287 -0.00411 -0.01190 \*

\* Nb 2 0.01748 0.00279 0.01228 \*

\* Nb 3 -0.00199 -0.01630 -0.01305 \*

\* Nb 4 0.00787 0.00464 0.01475 \*

\* Nb 5 0.00329 -0.00288 -0.00982 \*

\* Nb 6 0.01112 0.00969 0.01013 \*

\* Nb 7 -0.00317 -0.01158 -0.00980 \*

\* Nb 8 -0.00044 0.00157 0.00961 \*

\* Nb 9 -0.00456 -0.00647 -0.01455 \*

\* Nb 10 0.00955 0.01404 0.01323 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.025301 0.001295 0.007316 \*

\* y 0.001295 -0.007137 0.000917 \*

\* z 0.007316 0.000917 -0.006026 \*

\* \*

\* Pressure: 0.0128 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.879E-006 | -20746.055363 | <-- min BFGS

| trial step | 1.000000 | 8.257E-007 | -20746.055325 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 24 with line minimization (lambda= 1.783614)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8777948 -8.5743341 -0.0053784 0.4214373 -0.0015311 0.0001846

0.0125401 3.4516678 -0.0002085 1.0468981 1.8165297 0.0004814

-0.0057177 -0.0001646 13.0539136 0.0001904 0.0000284 0.4813259

Lattice parameters(A) Cell Angles

a = 17.171721 alpha = 90.004274

b = 3.451691 beta = 90.039328

c = 13.053915 gamma = 119.747441

Current cell volume = 671.763784 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 0.066737 0.664942 0.122694 x

x Se 2 0.133923 0.335749 0.622380 x

x Se 3 0.133572 0.335299 0.877545 x

x Se 4 0.066587 0.664664 0.377363 x

x Se 5 0.266515 0.664900 0.122317 x

x Se 6 0.333354 0.336253 0.622321 x

x Se 7 0.333167 0.335819 0.877625 x

x Se 8 0.266359 0.664720 0.377669 x

x Se 9 0.466810 0.665647 0.122826 x

x Se 10 0.533496 0.334619 0.622698 x

x Se 11 0.533187 0.334376 0.877141 x

x Se 12 0.466500 0.665378 0.377336 x

x Se 13 0.666857 0.664208 0.122372 x

x Se 14 0.733647 0.335285 0.622347 x

x Se 15 0.733494 0.335106 0.877664 x

x Se 16 0.666669 0.663768 0.377684 x

x Se 17 0.866448 0.664701 0.122430 x

x Se 18 0.933446 0.335405 0.622651 x

x Se 19 0.933295 0.335129 0.877291 x

x Se 20 0.866086 0.664222 0.377648 x

x Nb 1 -0.000553 -0.001357 0.250114 x

x Nb 2 0.000543 0.001376 0.749885 x

x Nb 3 0.199805 0.000454 0.250039 x

x Nb 4 0.200317 0.000345 0.749948 x

x Nb 5 0.399316 -0.001268 0.250062 x

x Nb 6 0.399867 0.000407 0.749893 x

x Nb 7 0.600061 -0.000521 0.250106 x

x Nb 8 0.600669 0.001262 0.749939 x

x Nb 9 0.799671 -0.000396 0.250052 x

x Nb 10 0.800153 -0.000492 0.749959 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460545E+004 36243.73 <-- SCF

1 -2.07460845E+004 9.98009241E-004 36263.53 <-- SCF

2 -2.07460854E+004 3.07356795E-005 36290.58 <-- SCF

3 -2.07462239E+004 4.61844302E-003 36320.19 <-- SCF

4 -2.07460227E+004 -6.70702317E-003 36349.27 <-- SCF

5 -2.07460243E+004 5.36482620E-005 36377.95 <-- SCF

6 -2.07460404E+004 5.36720283E-004 36405.59 <-- SCF

7 -2.07460476E+004 2.38632287E-004 36428.33 <-- SCF

8 -2.07460528E+004 1.75034079E-004 36450.27 <-- SCF

9 -2.07460561E+004 1.07785552E-004 36474.03 <-- SCF

10 -2.07460573E+004 4.06849323E-005 36497.11 <-- SCF

11 -2.07460573E+004 1.82947917E-008 36520.52 <-- SCF

12 -2.07460563E+004 -3.31068581E-005 36543.69 <-- SCF

13 -2.07460554E+004 -3.13655233E-005 36568.84 <-- SCF

14 -2.07460552E+004 -6.04655053E-006 36590.62 <-- SCF

15 -2.07460551E+004 -3.10718177E-006 36614.70 <-- SCF

16 -2.07460553E+004 6.48409153E-006 36636.12 <-- SCF

17 -2.07460554E+004 3.00243595E-006 36657.55 <-- SCF

18 -2.07460553E+004 -1.18710093E-006 36678.89 <-- SCF

19 -2.07460553E+004 -2.04975345E-006 36700.72 <-- SCF

20 -2.07460553E+004 6.28090347E-007 36722.17 <-- SCF

21 -2.07460553E+004 2.04780213E-007 36743.45 <-- SCF

22 -2.07460553E+004 6.33491216E-008 36764.80 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05530525 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00248 -0.01259 0.01354 \*

\* Se 2 0.00148 -0.00185 -0.00768 \*

\* Se 3 0.00983 -0.00014 -0.00448 \*

\* Se 4 -0.00297 -0.01118 0.00264 \*

\* Se 5 -0.01147 0.00539 0.01374 \*

\* Se 6 0.01327 -0.00106 -0.00847 \*

\* Se 7 0.01342 -0.00113 -0.00595 \*

\* Se 8 -0.01882 0.00501 0.00186 \*

\* Se 9 0.00660 -0.00371 0.00565 \*

\* Se 10 -0.00703 0.00648 -0.01201 \*

\* Se 11 -0.01140 0.00265 0.00040 \*

\* Se 12 0.00264 -0.00732 0.00572 \*

\* Se 13 -0.01610 0.00333 0.01323 \*

\* Se 14 0.01622 -0.00412 -0.00816 \*

\* Se 15 0.00900 -0.00441 -0.00730 \*

\* Se 16 -0.01579 0.00337 0.00090 \*

\* Se 17 -0.01384 0.00051 0.01110 \*

\* Se 18 -0.00201 0.01123 -0.00923 \*

\* Se 19 -0.00223 0.01242 -0.00673 \*

\* Se 20 -0.00496 0.00319 0.00025 \*

\* Nb 1 -0.01428 -0.00514 -0.01099 \*

\* Nb 2 0.01913 0.00377 0.01132 \*

\* Nb 3 0.00131 -0.01933 -0.01236 \*

\* Nb 4 0.00845 0.00816 0.01380 \*

\* Nb 5 0.00339 -0.00270 -0.00896 \*

\* Nb 6 0.01516 0.01041 0.00937 \*

\* Nb 7 -0.00335 -0.01403 -0.00915 \*

\* Nb 8 -0.00131 0.00465 0.00890 \*

\* Nb 9 -0.00277 -0.00790 -0.01367 \*

\* Nb 10 0.01091 0.01605 0.01268 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.016652 -0.004976 0.001633 \*

\* y -0.004976 -0.008339 0.005734 \*

\* z 0.001633 0.005734 0.007150 \*

\* \*

\* Pressure: 0.0059 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.879E-006 | -20746.055363 | <-- min BFGS

| trial step | 1.000000 | 8.257E-007 | -20746.055325 | <-- min BFGS

| line step | 1.783614 | 2.828E-008 | -20746.055349 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 24 with enthalpy= -2.07460553E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 4.610784E-007 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 2.317743E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.821889E-004 | 5.000000E-004 | A | Yes | <-- BFGS

| Smax | 1.665247E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 25 ...

================================================================================

Writing analysis data to 2H-Nb1Se2-7.castep\_bin

Writing model to 2H-Nb1Se2-7.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.031E-006 | -20746.055349 | <-- 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)

14.8784273 -8.5748420 -0.0052477 0.4214215 -0.0015274 0.0001815

0.0125111 3.4518204 -0.0002136 1.0468745 1.8164583 0.0004761

-0.0056220 -0.0001816 13.0548091 0.0001865 0.0000291 0.4812929

Lattice parameters(A) Cell Angles

a = 17.172523 alpha = 90.004431

b = 3.451843 beta = 90.038489

c = 13.054810 gamma = 119.748346

Current cell volume = 671.864843 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 0.066732 0.664888 0.122700 x

x Se 2 0.133934 0.335775 0.622394 x

x Se 3 0.133583 0.335335 0.877536 x

x Se 4 0.066583 0.664616 0.377357 x

x Se 5 0.266515 0.664853 0.122327 x

x Se 6 0.333359 0.336311 0.622323 x

x Se 7 0.333172 0.335879 0.877625 x

x Se 8 0.266359 0.664683 0.377656 x

x Se 9 0.466805 0.665622 0.122833 x

x Se 10 0.533504 0.334643 0.622704 x

x Se 11 0.533192 0.334401 0.877134 x

x Se 12 0.466491 0.665353 0.377331 x

x Se 13 0.666853 0.664152 0.122372 x

x Se 14 0.733647 0.335321 0.622362 x

x Se 15 0.733494 0.335152 0.877652 x

x Se 16 0.666666 0.663714 0.377682 x

x Se 17 0.866437 0.664663 0.122438 x

x Se 18 0.933452 0.335454 0.622656 x

x Se 19 0.933302 0.335185 0.877285 x

x Se 20 0.866074 0.664194 0.377636 x

x Nb 1 -0.000569 -0.001446 0.250119 x

x Nb 2 0.000558 0.001464 0.749880 x

x Nb 3 0.199803 0.000410 0.250041 x

x Nb 4 0.200324 0.000385 0.749945 x

x Nb 5 0.399307 -0.001336 0.250065 x

x Nb 6 0.399863 0.000467 0.749889 x

x Nb 7 0.600064 -0.000581 0.250110 x

x Nb 8 0.600677 0.001326 0.749936 x

x Nb 9 0.799663 -0.000438 0.250055 x

x Nb 10 0.800155 -0.000446 0.749957 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460532E+004 37164.25 <-- SCF

1 -2.07461384E+004 2.84208440E-003 37184.23 <-- SCF

2 -2.07461406E+004 7.12129099E-005 37212.27 <-- SCF

3 -2.07462982E+004 5.25426856E-003 37241.78 <-- SCF

4 -2.07460069E+004 -9.70877282E-003 37270.67 <-- SCF

5 -2.07460204E+004 4.48561623E-004 37300.33 <-- SCF

6 -2.07460511E+004 1.02476037E-003 37328.88 <-- SCF

7 -2.07460582E+004 2.36501897E-004 37354.53 <-- SCF

8 -2.07460614E+004 1.06121513E-004 37380.45 <-- SCF

9 -2.07460600E+004 -4.69675585E-005 37406.84 <-- SCF

10 -2.07460578E+004 -7.34725229E-005 37431.16 <-- SCF

11 -2.07460557E+004 -7.08655567E-005 37456.31 <-- SCF

12 -2.07460548E+004 -2.99051881E-005 37480.19 <-- SCF

13 -2.07460547E+004 -2.21644153E-006 37506.06 <-- SCF

14 -2.07460560E+004 4.40996718E-005 37529.88 <-- SCF

15 -2.07460563E+004 1.02177139E-005 37551.28 <-- SCF

16 -2.07460562E+004 -4.63848008E-006 37573.00 <-- SCF

17 -2.07460554E+004 -2.74559429E-005 37596.91 <-- SCF

18 -2.07460554E+004 4.76302994E-007 37618.22 <-- SCF

19 -2.07460553E+004 -1.80610658E-006 37639.77 <-- SCF

20 -2.07460554E+004 1.93625189E-006 37661.05 <-- SCF

21 -2.07460553E+004 -3.47491457E-006 37682.95 <-- SCF

22 -2.07460553E+004 6.18839936E-007 37704.31 <-- SCF

23 -2.07460553E+004 1.18606479E-007 37725.38 <-- SCF

24 -2.07460553E+004 1.28819282E-006 37746.73 <-- SCF

25 -2.07460553E+004 -1.55215985E-006 37768.28 <-- SCF

26 -2.07460554E+004 2.69297562E-006 37791.41 <-- SCF

27 -2.07460554E+004 2.36238863E-006 37812.75 <-- SCF

28 -2.07460555E+004 1.86999573E-006 37834.33 <-- SCF

29 -2.07460554E+004 -2.99748407E-006 37855.75 <-- SCF

30 -2.07460553E+004 -2.03116199E-006 37877.09 <-- SCF

31 -2.07460553E+004 -1.84344996E-006 37898.50 <-- SCF

32 -2.07460553E+004 -5.42436128E-007 37919.86 <-- SCF

33 -2.07460553E+004 -3.38632145E-008 37941.75 <-- SCF

34 -2.07460553E+004 7.97207194E-007 37963.09 <-- SCF

35 -2.07460553E+004 6.74402732E-007 37984.50 <-- SCF

36 -2.07460553E+004 7.05609595E-007 38005.83 <-- SCF

37 -2.07460553E+004 -3.60609736E-007 38026.94 <-- SCF

38 -2.07460553E+004 -3.83217282E-007 38048.00 <-- SCF

39 -2.07460553E+004 4.24636970E-007 38069.11 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05533020 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00328 -0.01210 0.01266 \*

\* Se 2 0.00158 -0.00028 -0.00721 \*

\* Se 3 0.01013 0.00089 -0.00647 \*

\* Se 4 -0.00404 -0.01077 0.00467 \*

\* Se 5 -0.01165 0.00593 0.01167 \*

\* Se 6 0.01174 -0.00159 -0.00605 \*

\* Se 7 0.01158 -0.00165 -0.00966 \*

\* Se 8 -0.01952 0.00526 0.00511 \*

\* Se 9 0.00663 -0.00317 0.00533 \*

\* Se 10 -0.00753 0.00698 -0.00937 \*

\* Se 11 -0.01195 0.00306 -0.00338 \*

\* Se 12 0.00256 -0.00694 0.00710 \*

\* Se 13 -0.01718 0.00397 0.01272 \*

\* Se 14 0.01620 -0.00375 -0.00809 \*

\* Se 15 0.00855 -0.00427 -0.00857 \*

\* Se 16 -0.01727 0.00390 0.00253 \*

\* Se 17 -0.01383 0.00083 0.00960 \*

\* Se 18 -0.00300 0.01089 -0.00623 \*

\* Se 19 -0.00339 0.01214 -0.01100 \*

\* Se 20 -0.00462 0.00291 0.00313 \*

\* Nb 1 -0.01170 -0.00569 -0.01203 \*

\* Nb 2 0.01948 0.00363 0.01263 \*

\* Nb 3 0.00152 -0.01872 -0.01308 \*

\* Nb 4 0.00992 0.00549 0.01502 \*

\* Nb 5 0.00490 -0.00349 -0.00991 \*

\* Nb 6 0.01515 0.01053 0.01034 \*

\* Nb 7 -0.00272 -0.01332 -0.00991 \*

\* Nb 8 0.00148 0.00231 0.00976 \*

\* Nb 9 -0.00160 -0.00791 -0.01470 \*

\* Nb 10 0.01186 0.01494 0.01342 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.004786 -0.006133 0.002541 \*

\* y -0.006133 0.004656 0.006373 \*

\* z 0.002541 0.006373 0.014460 \*

\* \*

\* Pressure: -0.0048 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.031E-006 | -20746.055349 | <-- min BFGS

| trial step | 1.000000 | 6.937E-007 | -20746.055372 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 25 with line minimization (lambda= 3.056002)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8797277 -8.5758863 -0.0049789 0.4213889 -0.0015199 0.0001751

0.0124515 3.4521340 -0.0002240 1.0468258 1.8163115 0.0004651

-0.0054252 -0.0002165 13.0566503 0.0001787 0.0000306 0.4812250

Lattice parameters(A) Cell Angles

a = 17.174171 alpha = 90.004754

b = 3.452157 beta = 90.036762

c = 13.056651 gamma = 119.750207

Current cell volume = 672.072650 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 0.664777 0.122711 x

x Se 2 0.133956 0.335828 0.622421 x

x Se 3 0.133603 0.335409 0.877516 x

x Se 4 0.066574 0.664519 0.377345 x

x Se 5 0.266515 0.664758 0.122349 x

x Se 6 0.333367 0.336430 0.622328 x

x Se 7 0.333182 0.336002 0.877624 x

x Se 8 0.266359 0.664608 0.377629 x

x Se 9 0.466794 0.665571 0.122847 x

x Se 10 0.533522 0.334693 0.622715 x

x Se 11 0.533203 0.334451 0.877120 x

x Se 12 0.466473 0.665300 0.377319 x

x Se 13 0.666846 0.664037 0.122373 x

x Se 14 0.733647 0.335395 0.622392 x

x Se 15 0.733494 0.335246 0.877628 x

x Se 16 0.666660 0.663601 0.377678 x

x Se 17 0.866415 0.664583 0.122456 x

x Se 18 0.933464 0.335556 0.622667 x

x Se 19 0.933316 0.335301 0.877275 x

x Se 20 0.866048 0.664134 0.377612 x

x Nb 1 -0.000600 -0.001628 0.250130 x

x Nb 2 0.000590 0.001646 0.749869 x

x Nb 3 0.199799 0.000320 0.250045 x

x Nb 4 0.200339 0.000466 0.749939 x

x Nb 5 0.399287 -0.001475 0.250073 x

x Nb 6 0.399855 0.000592 0.749881 x

x Nb 7 0.600071 -0.000703 0.250119 x

x Nb 8 0.600693 0.001459 0.749928 x

x Nb 9 0.799645 -0.000523 0.250061 x

x Nb 10 0.800158 -0.000352 0.749953 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460516E+004 38472.53 <-- SCF

1 -2.07461305E+004 2.63277137E-003 38492.12 <-- SCF

2 -2.07461335E+004 9.78484771E-005 38521.17 <-- SCF

3 -2.07462844E+004 5.03124787E-003 38551.03 <-- SCF

4 -2.07460109E+004 -9.11716783E-003 38579.89 <-- SCF

5 -2.07460235E+004 4.20512752E-004 38609.47 <-- SCF

6 -2.07460516E+004 9.36888378E-004 38639.33 <-- SCF

7 -2.07460585E+004 2.30478515E-004 38666.39 <-- SCF

8 -2.07460615E+004 9.81471218E-005 38692.20 <-- SCF

9 -2.07460610E+004 -1.61190536E-005 38716.59 <-- SCF

10 -2.07460599E+004 -3.66000796E-005 38739.64 <-- SCF

11 -2.07460589E+004 -3.34977298E-005 38762.28 <-- SCF

12 -2.07460588E+004 -2.35714501E-006 38783.67 <-- SCF

13 -2.07460593E+004 1.63726475E-005 38805.17 <-- SCF

14 -2.07460633E+004 1.34291599E-004 38830.09 <-- SCF

15 -2.07460609E+004 -8.24631978E-005 38852.83 <-- SCF

16 -2.07460553E+004 -1.85183841E-004 38880.41 <-- SCF

17 -2.07460564E+004 3.49769922E-005 38903.48 <-- SCF

18 -2.07460564E+004 2.51448482E-006 38926.11 <-- SCF

19 -2.07460566E+004 6.48741238E-006 38948.56 <-- SCF

20 -2.07460561E+004 -1.80565129E-005 38970.41 <-- SCF

21 -2.07460575E+004 4.61116785E-005 38996.25 <-- SCF

22 -2.07460563E+004 -3.78581351E-005 39019.52 <-- SCF

23 -2.07460559E+004 -1.31636814E-005 39041.25 <-- SCF

24 -2.07460555E+004 -1.55569568E-005 39064.38 <-- SCF

25 -2.07460550E+004 -1.48873727E-005 39090.12 <-- SCF

26 -2.07460552E+004 6.84702351E-006 39111.67 <-- SCF

27 -2.07460553E+004 3.47739345E-006 39133.25 <-- SCF

28 -2.07460554E+004 2.91771393E-006 39154.61 <-- SCF

29 -2.07460554E+004 7.06601912E-007 39175.97 <-- SCF

30 -2.07460554E+004 -6.03296777E-007 39197.09 <-- SCF

31 -2.07460555E+004 1.98765960E-006 39218.53 <-- SCF

32 -2.07460556E+004 4.60327250E-006 39240.25 <-- SCF

33 -2.07460557E+004 4.20108273E-006 39265.05 <-- SCF

34 -2.07460558E+004 2.74620575E-006 39287.23 <-- SCF

35 -2.07460559E+004 2.34924051E-006 39308.91 <-- SCF

36 -2.07460559E+004 -4.60207632E-008 39330.36 <-- SCF

37 -2.07460558E+004 -1.81924448E-006 39351.67 <-- SCF

38 -2.07460557E+004 -3.52925097E-006 39373.00 <-- SCF

39 -2.07460557E+004 -2.62148173E-006 39394.34 <-- SCF

40 -2.07460557E+004 -1.51098517E-007 39415.53 <-- SCF

41 -2.07460556E+004 -1.67842365E-006 39436.83 <-- SCF

42 -2.07460555E+004 -1.87165791E-006 39458.28 <-- SCF

43 -2.07460556E+004 2.87959880E-006 39479.52 <-- SCF

44 -2.07460557E+004 2.16480562E-006 39500.97 <-- SCF

45 -2.07460557E+004 -8.27533419E-007 39522.06 <-- SCF

46 -2.07460556E+004 -3.25481630E-006 39543.00 <-- SCF

47 -2.07460557E+004 4.94351176E-006 39564.47 <-- SCF

48 -2.07460553E+004 -1.38874789E-005 39587.17 <-- SCF

49 -2.07460553E+004 -6.15065257E-007 39608.55 <-- SCF

50 -2.07460554E+004 2.72263239E-006 39630.19 <-- SCF

51 -2.07460553E+004 -2.52894482E-006 39651.92 <-- SCF

52 -2.07460554E+004 2.92915913E-006 39673.27 <-- SCF

53 -2.07460554E+004 -4.20583250E-007 39695.12 <-- SCF

54 -2.07460554E+004 2.90703573E-007 39716.59 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05538004 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00280 -0.01127 0.01388 \*

\* Se 2 0.00141 0.00158 -0.00964 \*

\* Se 3 0.01046 0.00166 -0.00687 \*

\* Se 4 -0.00384 -0.00995 0.00590 \*

\* Se 5 -0.01139 0.00772 0.00947 \*

\* Se 6 0.01314 -0.00199 -0.00351 \*

\* Se 7 0.01257 -0.00203 -0.01457 \*

\* Se 8 -0.02006 0.00651 0.00968 \*

\* Se 9 0.01036 -0.00314 0.00744 \*

\* Se 10 -0.00761 0.00809 -0.00654 \*

\* Se 11 -0.01180 0.00381 -0.00805 \*

\* Se 12 0.00637 -0.00721 0.00716 \*

\* Se 13 -0.01747 0.00568 0.01478 \*

\* Se 14 0.01850 -0.00417 -0.01072 \*

\* Se 15 0.01017 -0.00514 -0.00798 \*

\* Se 16 -0.01830 0.00562 0.00300 \*

\* Se 17 -0.01229 0.00080 0.01003 \*

\* Se 18 -0.00306 0.01126 -0.00314 \*

\* Se 19 -0.00363 0.01244 -0.01620 \*

\* Se 20 -0.00213 0.00172 0.00562 \*

\* Nb 1 -0.01330 -0.00523 -0.01462 \*

\* Nb 2 0.01338 0.00282 0.01485 \*

\* Nb 3 -0.00258 -0.01790 -0.01519 \*

\* Nb 4 0.01054 0.00338 0.01750 \*

\* Nb 5 0.00737 -0.00422 -0.01214 \*

\* Nb 6 0.01537 0.00730 0.01197 \*

\* Nb 7 -0.00399 -0.01163 -0.01177 \*

\* Nb 8 -0.00541 0.00021 0.01210 \*

\* Nb 9 -0.00355 -0.00828 -0.01777 \*

\* Nb 10 0.01358 0.01154 0.01535 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.009351 -0.006809 0.004015 \*

\* y -0.006809 0.024464 0.006952 \*

\* z 0.004015 0.006952 0.030908 \*

\* \*

\* Pressure: -0.0216 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.031E-006 | -20746.055349 | <-- min BFGS

| trial step | 1.000000 | 6.937E-007 | -20746.055372 | <-- min BFGS

| line step | 3.056002 | -2.738E-008 | -20746.055429 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 25 with enthalpy= -2.07460554E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.658415E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 2.361723E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 9.072522E-004 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.090810E-002 | 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 | 1.150E-006 | -20746.055429 | <-- 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)

14.8794434 -8.5752433 -0.0047273 0.4213895 -0.0015330 0.0001748

0.0125583 3.4520632 -0.0003196 1.0467703 1.8163166 0.0005113

-0.0054196 -0.0005519 13.0566509 0.0001782 0.0000439 0.4812250

Lattice parameters(A) Cell Angles

a = 17.173603 alpha = 90.007813

b = 3.452086 beta = 90.035168

c = 13.056652 gamma = 119.747044

Current cell volume = 672.057962 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 0.066722 0.664752 0.122717 x

x Se 2 0.133959 0.335842 0.622425 x

x Se 3 0.133608 0.335429 0.877510 x

x Se 4 0.066574 0.664494 0.377342 x

x Se 5 0.266512 0.664740 0.122356 x

x Se 6 0.333371 0.336456 0.622330 x

x Se 7 0.333186 0.336026 0.877620 x

x Se 8 0.266355 0.664586 0.377623 x

x Se 9 0.466797 0.665569 0.122851 x

x Se 10 0.533521 0.334702 0.622716 x

x Se 11 0.533201 0.334451 0.877116 x

x Se 12 0.466473 0.665290 0.377317 x

x Se 13 0.666843 0.664014 0.122377 x

x Se 14 0.733651 0.335417 0.622397 x

x Se 15 0.733497 0.335265 0.877621 x

x Se 16 0.666656 0.663576 0.377675 x

x Se 17 0.866410 0.664562 0.122462 x

x Se 18 0.933463 0.335579 0.622669 x

x Se 19 0.933316 0.335325 0.877270 x

x Se 20 0.866045 0.664120 0.377606 x

x Nb 1 -0.000610 -0.001661 0.250130 x

x Nb 2 0.000600 0.001678 0.749869 x

x Nb 3 0.199797 0.000300 0.250043 x

x Nb 4 0.200344 0.000478 0.749940 x

x Nb 5 0.399283 -0.001491 0.250073 x

x Nb 6 0.399858 0.000618 0.749881 x

x Nb 7 0.600069 -0.000727 0.250118 x

x Nb 8 0.600697 0.001474 0.749929 x

x Nb 9 0.799641 -0.000534 0.250060 x

x Nb 10 0.800161 -0.000329 0.749955 x

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------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460518E+004 40120.14 <-- SCF

1 -2.07462092E+004 5.24859437E-003 40140.36 <-- SCF

2 -2.07462132E+004 1.31589924E-004 40167.95 <-- SCF

3 -2.07463322E+004 3.96591847E-003 40197.91 <-- SCF

4 -2.07459876E+004 -1.14846742E-002 40226.77 <-- SCF

5 -2.07460198E+004 1.07387252E-003 40256.91 <-- SCF

6 -2.07460653E+004 1.51447398E-003 40285.95 <-- SCF

7 -2.07460738E+004 2.83304448E-004 40312.20 <-- SCF

8 -2.07460726E+004 -4.08180313E-005 40338.52 <-- SCF

9 -2.07460656E+004 -2.33127917E-004 40364.88 <-- SCF

10 -2.07460573E+004 -2.76945182E-004 40391.62 <-- SCF

11 -2.07460529E+004 -1.43946910E-004 40419.31 <-- SCF

12 -2.07460570E+004 1.37019503E-004 40446.20 <-- SCF

13 -2.07460588E+004 5.87208853E-005 40471.09 <-- SCF

14 -2.07460563E+004 -8.34634824E-005 40497.77 <-- SCF

15 -2.07460549E+004 -4.55833040E-005 40524.55 <-- SCF

16 -2.07460553E+004 1.35351763E-005 40546.19 <-- SCF

17 -2.07460554E+004 2.34063903E-006 40567.61 <-- SCF

18 -2.07460553E+004 -2.97931498E-006 40589.58 <-- SCF

19 -2.07460553E+004 1.27885455E-007 40611.48 <-- SCF

20 -2.07460553E+004 4.63037533E-007 40632.81 <-- SCF

21 -2.07460554E+004 9.41702885E-007 40654.25 <-- SCF

22 -2.07460554E+004 3.00551252E-008 40675.47 <-- SCF

23 -2.07460554E+004 -3.83133240E-008 40696.50 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05537014 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00318 -0.01203 0.01500 \*

\* Se 2 0.00273 0.00046 -0.01473 \*

\* Se 3 0.01173 0.00123 -0.00144 \*

\* Se 4 -0.00414 -0.00988 0.00404 \*

\* Se 5 -0.01087 0.00677 0.01157 \*

\* Se 6 0.01213 -0.00355 -0.00627 \*

\* Se 7 0.01140 -0.00274 -0.01108 \*

\* Se 8 -0.01935 0.00636 0.00702 \*

\* Se 9 0.00922 -0.00456 0.00915 \*

\* Se 10 -0.00725 0.00747 -0.00977 \*

\* Se 11 -0.01163 0.00410 -0.00450 \*

\* Se 12 0.00534 -0.00768 0.00498 \*

\* Se 13 -0.01799 0.00532 0.01573 \*

\* Se 14 0.01865 -0.00527 -0.01542 \*

\* Se 15 0.01034 -0.00546 -0.00270 \*

\* Se 16 -0.01869 0.00612 0.00150 \*

\* Se 17 -0.01145 -0.00027 0.01081 \*

\* Se 18 -0.00348 0.01024 -0.00592 \*

\* Se 19 -0.00415 0.01224 -0.01284 \*

\* Se 20 -0.00128 0.00119 0.00447 \*

\* Nb 1 -0.01078 -0.00421 -0.01406 \*

\* Nb 2 0.01293 0.00210 0.01477 \*

\* Nb 3 -0.00279 -0.01772 -0.01448 \*

\* Nb 4 0.01043 0.00556 0.01667 \*

\* Nb 5 0.00880 -0.00093 -0.01152 \*

\* Nb 6 0.01329 0.00735 0.01160 \*

\* Nb 7 -0.00462 -0.01142 -0.01127 \*

\* Nb 8 -0.00163 0.00108 0.01110 \*

\* Nb 9 -0.00437 -0.00636 -0.01681 \*

\* Nb 10 0.01064 0.01447 0.01438 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.010661 -0.001932 0.003595 \*

\* y -0.001932 0.023925 0.003890 \*

\* z 0.003595 0.003890 0.025982 \*

\* \*

\* Pressure: -0.0202 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.150E-006 | -20746.055429 | <-- min BFGS

| trial step | 1.000000 | 1.001E-006 | -20746.055405 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 26 with line minimization (lambda= 7.719713)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8775327 -8.5709227 -0.0030365 0.4213934 -0.0016208 0.0001734

0.0132763 3.4515872 -0.0009619 1.0463970 1.8163510 0.0008216

-0.0053820 -0.0028053 13.0566550 0.0001751 0.0001334 0.4812248

Lattice parameters(A) Cell Angles

a = 17.169790 alpha = 90.028368

b = 3.451613 beta = 90.024452

c = 13.056656 gamma = 119.725786

Current cell volume = 671.959208 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 0.066719 0.664585 0.122752 x

x Se 2 0.133979 0.335939 0.622457 x

x Se 3 0.133636 0.335564 0.877474 x

x Se 4 0.066570 0.664326 0.377326 x

x Se 5 0.266494 0.664618 0.122405 x

x Se 6 0.333392 0.336635 0.622342 x

x Se 7 0.333209 0.336189 0.877595 x

x Se 8 0.266327 0.664438 0.377586 x

x Se 9 0.466811 0.665554 0.122880 x

x Se 10 0.533516 0.334761 0.622723 x

x Se 11 0.533183 0.334454 0.877092 x

x Se 12 0.466475 0.665221 0.377304 x

x Se 13 0.666818 0.663859 0.122407 x

x Se 14 0.733677 0.335566 0.622430 x

x Se 15 0.733513 0.335390 0.877576 x

x Se 16 0.666633 0.663405 0.377657 x

x Se 17 0.866378 0.664422 0.122504 x

x Se 18 0.933463 0.335736 0.622682 x

x Se 19 0.933316 0.335482 0.877239 x

x Se 20 0.866021 0.664024 0.377568 x

x Nb 1 -0.000673 -0.001876 0.250129 x

x Nb 2 0.000666 0.001890 0.749870 x

x Nb 3 0.199788 0.000163 0.250033 x

x Nb 4 0.200375 0.000556 0.749949 x

x Nb 5 0.399256 -0.001598 0.250071 x

x Nb 6 0.399879 0.000793 0.749882 x

x Nb 7 0.600058 -0.000887 0.250118 x

x Nb 8 0.600724 0.001578 0.749930 x

x Nb 9 0.799614 -0.000607 0.250051 x

x Nb 10 0.800182 -0.000179 0.749966 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460489E+004 41097.44 <-- SCF

1 -2.07461394E+004 3.01722602E-003 41116.92 <-- SCF

2 -2.07461429E+004 1.16422406E-004 41147.34 <-- SCF

3 -2.07463057E+004 5.42470082E-003 41177.12 <-- SCF

4 -2.07460081E+004 -9.91956745E-003 41206.38 <-- SCF

5 -2.07460166E+004 2.82647084E-004 41236.50 <-- SCF

6 -2.07460472E+004 1.02286521E-003 41265.94 <-- SCF

7 -2.07460582E+004 3.65891593E-004 41294.55 <-- SCF

8 -2.07460613E+004 1.03929347E-004 41321.45 <-- SCF

9 -2.07460598E+004 -5.28111064E-005 41348.03 <-- SCF

10 -2.07460575E+004 -7.64644868E-005 41373.23 <-- SCF

11 -2.07460557E+004 -5.81070648E-005 41397.45 <-- SCF

12 -2.07460548E+004 -3.20005400E-005 41424.53 <-- SCF

13 -2.07460557E+004 3.03625974E-005 41447.41 <-- SCF

14 -2.07460560E+004 1.06886675E-005 41469.47 <-- SCF

15 -2.07460557E+004 -8.42583524E-006 41491.25 <-- SCF

16 -2.07460554E+004 -1.29833179E-005 41516.09 <-- SCF

17 -2.07460554E+004 1.79919965E-006 41537.42 <-- SCF

18 -2.07460554E+004 8.08880082E-007 41558.91 <-- SCF

19 -2.07460554E+004 2.25314032E-007 41580.03 <-- SCF

20 -2.07460554E+004 -3.97366063E-007 41601.56 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05542467 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00516 -0.01385 0.00626 \*

\* Se 2 0.00315 -0.00221 -0.02160 \*

\* Se 3 0.01161 0.00336 0.00845 \*

\* Se 4 -0.00551 -0.00607 0.00849 \*

\* Se 5 -0.01041 0.00440 -0.00479 \*

\* Se 6 0.01199 -0.00761 -0.01109 \*

\* Se 7 0.01132 -0.00089 -0.00252 \*

\* Se 8 -0.01805 0.00952 0.01912 \*

\* Se 9 0.00580 -0.00835 0.00312 \*

\* Se 10 -0.00543 0.00556 -0.01113 \*

\* Se 11 -0.00943 0.00879 -0.00089 \*

\* Se 12 0.00227 -0.00493 0.00906 \*

\* Se 13 -0.01739 0.00300 0.00492 \*

\* Se 14 0.01526 -0.00819 -0.02250 \*

\* Se 15 0.00779 -0.00298 0.00857 \*

\* Se 16 -0.01817 0.00978 0.00832 \*

\* Se 17 -0.01301 -0.00182 -0.00455 \*

\* Se 18 -0.00111 0.00646 -0.00917 \*

\* Se 19 -0.00143 0.01415 -0.00531 \*

\* Se 20 -0.00329 0.00411 0.01697 \*

\* Nb 1 -0.00315 -0.00461 -0.01176 \*

\* Nb 2 0.00965 0.00209 0.01203 \*

\* Nb 3 -0.00232 -0.01391 -0.01040 \*

\* Nb 4 0.01263 0.00500 0.01312 \*

\* Nb 5 0.01528 -0.00149 -0.00897 \*

\* Nb 6 0.00828 0.00516 0.00855 \*

\* Nb 7 -0.00380 -0.00773 -0.00817 \*

\* Nb 8 -0.00699 -0.00117 0.00861 \*

\* Nb 9 -0.00409 -0.00697 -0.01313 \*

\* Nb 10 0.01372 0.01141 0.01040 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.017636 0.022727 0.002203 \*

\* y 0.022727 -0.010446 -0.019558 \*

\* z 0.002203 -0.019558 -0.026978 \*

\* \*

\* Pressure: 0.0184 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.150E-006 | -20746.055429 | <-- min BFGS

| trial step | 1.000000 | 1.001E-006 | -20746.055405 | <-- min BFGS

| line step | 7.719713 | -8.888E-008 | -20746.055465 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 26 with enthalpy= -2.07460555E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.211253E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 2.839529E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.146446E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.697789E-002 | 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 | 4.565E-006 | -20746.055465 | <-- 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)

14.8794397 -8.5714305 -0.0044459 0.4213528 -0.0015974 0.0002047

0.0130855 3.4514608 -0.0008810 1.0463967 1.8164754 0.0008608

-0.0063519 -0.0025277 13.0555067 0.0002141 0.0001220 0.4812672

Lattice parameters(A) Cell Angles

a = 17.171697 alpha = 90.025824

b = 3.451486 beta = 90.033452

c = 13.055508 gamma = 119.727237

Current cell volume = 671.940167 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 0.066709 0.664462 0.122748 x

x Se 2 0.133997 0.335978 0.622438 x

x Se 3 0.133658 0.335636 0.877483 x

x Se 4 0.066559 0.664221 0.377346 x

x Se 5 0.266490 0.664548 0.122402 x

x Se 6 0.333408 0.336732 0.622315 x

x Se 7 0.333223 0.336295 0.877609 x

x Se 8 0.266317 0.664373 0.377602 x

x Se 9 0.466805 0.665506 0.122872 x

x Se 10 0.533529 0.334814 0.622698 x

x Se 11 0.533188 0.334496 0.877103 x

x Se 12 0.466460 0.665162 0.377327 x

x Se 13 0.666803 0.663760 0.122396 x

x Se 14 0.733686 0.335631 0.622413 x

x Se 15 0.733516 0.335461 0.877581 x

x Se 16 0.666616 0.663314 0.377682 x

x Se 17 0.866354 0.664347 0.122498 x

x Se 18 0.933473 0.335836 0.622659 x

x Se 19 0.933326 0.335601 0.877244 x

x Se 20 0.866000 0.663985 0.377584 x

x Nb 1 -0.000698 -0.002033 0.250122 x

x Nb 2 0.000693 0.002045 0.749877 x

x Nb 3 0.199784 0.000044 0.250023 x

x Nb 4 0.200394 0.000648 0.749961 x

x Nb 5 0.399251 -0.001687 0.250065 x

x Nb 6 0.399879 0.000921 0.749888 x

x Nb 7 0.600063 -0.001007 0.250112 x

x Nb 8 0.600727 0.001661 0.749937 x

x Nb 9 0.799597 -0.000700 0.250040 x

x Nb 10 0.800193 -0.000050 0.749977 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460535E+004 42005.44 <-- SCF

1 -2.07460665E+004 4.34037082E-004 42024.47 <-- SCF

2 -2.07460675E+004 3.27545910E-005 42053.75 <-- SCF

3 -2.07461353E+004 2.25843353E-003 42083.78 <-- SCF

4 -2.07460321E+004 -3.43866583E-003 42113.22 <-- SCF

5 -2.07460366E+004 1.49919029E-004 42141.38 <-- SCF

6 -2.07460458E+004 3.05429605E-004 42169.84 <-- SCF

7 -2.07460530E+004 2.40652162E-004 42197.27 <-- SCF

8 -2.07460565E+004 1.17633391E-004 42223.80 <-- SCF

9 -2.07460589E+004 7.82041219E-005 42247.23 <-- SCF

10 -2.07460596E+004 2.47196076E-005 42269.69 <-- SCF

11 -2.07460600E+004 1.43240133E-005 42291.55 <-- SCF

12 -2.07460601E+004 2.02778545E-006 42313.02 <-- SCF

13 -2.07460602E+004 4.18590327E-006 42334.47 <-- SCF

14 -2.07460602E+004 -2.38632806E-007 42355.80 <-- SCF

15 -2.07460610E+004 2.63226122E-005 42377.75 <-- SCF

16 -2.07460633E+004 7.52098819E-005 42401.53 <-- SCF

17 -2.07460633E+004 2.16302011E-006 42423.30 <-- SCF

18 -2.07460638E+004 1.63808372E-005 42445.06 <-- SCF

19 -2.07460638E+004 -5.94967941E-007 42466.62 <-- SCF

20 -2.07460623E+004 -5.07661775E-005 42488.52 <-- SCF

21 -2.07460616E+004 -2.13226577E-005 42510.05 <-- SCF

22 -2.07460639E+004 7.57916838E-005 42532.16 <-- SCF

23 -2.07460623E+004 -5.21451938E-005 42553.89 <-- SCF

24 -2.07460638E+004 4.98025617E-005 42575.39 <-- SCF

25 -2.07460733E+004 3.14765324E-004 42601.89 <-- SCF

26 -2.07460728E+004 -1.76042029E-005 42623.55 <-- SCF

27 -2.07460769E+004 1.38918642E-004 42647.41 <-- SCF

28 -2.07460707E+004 -2.07474924E-004 42672.19 <-- SCF

29 -2.07460670E+004 -1.24544041E-004 42696.11 <-- SCF

30 -2.07460696E+004 8.92418558E-005 42717.94 <-- SCF

31 -2.07460685E+004 -3.65663329E-005 42739.41 <-- SCF

32 -2.07460623E+004 -2.08821626E-004 42765.38 <-- SCF

33 -2.07460640E+004 5.59993214E-005 42790.75 <-- SCF

34 -2.07460619E+004 -6.69750138E-005 42817.52 <-- SCF

35 -2.07460580E+004 -1.30910858E-004 42844.22 <-- SCF

36 -2.07460580E+004 -4.23445530E-007 42866.08 <-- SCF

37 -2.07460610E+004 9.85507453E-005 42891.05 <-- SCF

38 -2.07460633E+004 7.76187910E-005 42917.72 <-- SCF

39 -2.07460571E+004 -2.06209599E-004 42944.39 <-- SCF

40 -2.07460552E+004 -6.45363463E-005 42969.34 <-- SCF

41 -2.07460589E+004 1.25000679E-004 42995.45 <-- SCF

42 -2.07460576E+004 -4.32076912E-005 43018.05 <-- SCF

43 -2.07460555E+004 -7.18830017E-005 43044.91 <-- SCF

44 -2.07460554E+004 -1.34907811E-006 43066.88 <-- SCF

45 -2.07460555E+004 2.03174420E-006 43089.75 <-- SCF

46 -2.07460555E+004 1.89242117E-006 43111.30 <-- SCF

47 -2.07460555E+004 1.69229143E-007 43132.77 <-- SCF

48 -2.07460556E+004 1.40776284E-007 43154.05 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05555038 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00569 -0.01313 0.00405 \*

\* Se 2 0.00206 -0.00142 -0.01883 \*

\* Se 3 0.01352 0.00327 0.01040 \*

\* Se 4 -0.00394 -0.00652 0.00580 \*

\* Se 5 -0.00938 0.00487 -0.00489 \*

\* Se 6 0.00893 -0.00745 -0.00454 \*

\* Se 7 0.01111 -0.00159 -0.00442 \*

\* Se 8 -0.01458 0.00901 0.01467 \*

\* Se 9 0.00502 -0.00828 0.00195 \*

\* Se 10 -0.00537 0.00694 -0.00844 \*

\* Se 11 -0.00679 0.00943 -0.00021 \*

\* Se 12 0.00381 -0.00564 0.00685 \*

\* Se 13 -0.01681 0.00309 0.00437 \*

\* Se 14 0.01410 -0.00794 -0.01899 \*

\* Se 15 0.00894 -0.00369 0.00970 \*

\* Se 16 -0.01475 0.00903 0.00442 \*

\* Se 17 -0.01181 -0.00141 -0.00476 \*

\* Se 18 -0.00294 0.00684 -0.00418 \*

\* Se 19 -0.00102 0.01333 -0.00524 \*

\* Se 20 0.00129 0.00344 0.01278 \*

\* Nb 1 -0.00363 -0.00328 -0.00814 \*

\* Nb 2 0.00807 0.00185 0.00862 \*

\* Nb 3 -0.00571 -0.01195 -0.00671 \*

\* Nb 4 0.01451 0.00300 0.00877 \*

\* Nb 5 0.01241 -0.00031 -0.00562 \*

\* Nb 6 0.00727 0.00208 0.00528 \*

\* Nb 7 -0.00490 -0.00479 -0.00523 \*

\* Nb 8 -0.00540 -0.00345 0.00535 \*

\* Nb 9 -0.00726 -0.00509 -0.00924 \*

\* Nb 10 0.00893 0.00979 0.00645 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.000287 0.017718 -0.008174 \*

\* y 0.017718 -0.011661 -0.017192 \*

\* z -0.008174 -0.017192 -0.018528 \*

\* \*

\* Pressure: 0.0102 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 4.565E-006 | -20746.055465 | <-- min BFGS

| trial step | 1.000000 | 3.165E-006 | -20746.055567 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 27 with line minimization (lambda= 3.260636)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8837507 -8.5725785 -0.0076319 0.4212612 -0.0015445 0.0002755

0.0126540 3.4511749 -0.0006982 1.0463959 1.8167566 0.0009494

-0.0085446 -0.0019001 13.0529106 0.0003023 0.0000963 0.4813630

Lattice parameters(A) Cell Angles

a = 17.176006 alpha = 90.020070

b = 3.451198 beta = 90.053797

c = 13.052914 gamma = 119.730519

Current cell volume = 671.897033 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 0.066685 0.664184 0.122740 x

x Se 2 0.134037 0.336067 0.622395 x

x Se 3 0.133706 0.335798 0.877503 x

x Se 4 0.066534 0.663985 0.377392 x

x Se 5 0.266481 0.664389 0.122395 x

x Se 6 0.333443 0.336951 0.622253 x

x Se 7 0.333257 0.336534 0.877640 x

x Se 8 0.266295 0.664225 0.377638 x

x Se 9 0.466791 0.665398 0.122853 x

x Se 10 0.533559 0.334936 0.622640 x

x Se 11 0.533198 0.334593 0.877127 x

x Se 12 0.466428 0.665029 0.377379 x

x Se 13 0.666769 0.663537 0.122372 x

x Se 14 0.733705 0.335778 0.622374 x

x Se 15 0.733523 0.335623 0.877592 x

x Se 16 0.666579 0.663108 0.377737 x

x Se 17 0.866299 0.664178 0.122484 x

x Se 18 0.933495 0.336062 0.622609 x

x Se 19 0.933349 0.335870 0.877257 x

x Se 20 0.865952 0.663897 0.377619 x

x Nb 1 -0.000756 -0.002389 0.250107 x

x Nb 2 0.000754 0.002395 0.749892 x

x Nb 3 0.199773 -0.000227 0.249999 x

x Nb 4 0.200435 0.000858 0.749988 x

x Nb 5 0.399240 -0.001888 0.250051 x

x Nb 6 0.399881 0.001212 0.749900 x

x Nb 7 0.600075 -0.001278 0.250100 x

x Nb 8 0.600735 0.001848 0.749951 x

x Nb 9 0.799559 -0.000912 0.250013 x

x Nb 10 0.800220 0.000240 0.750002 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460460E+004 43556.38 <-- SCF

1 -2.07460667E+004 6.87429092E-004 43574.36 <-- SCF

2 -2.07460687E+004 6.65090779E-005 43604.91 <-- SCF

3 -2.07460656E+004 -1.03305073E-004 43634.59 <-- SCF

4 -2.07460540E+004 -3.84200611E-004 43663.80 <-- SCF

5 -2.07460568E+004 9.35211660E-005 43694.34 <-- SCF

6 -2.07460564E+004 -1.58877846E-005 43723.41 <-- SCF

7 -2.07460556E+004 -2.63456781E-005 43749.12 <-- SCF

8 -2.07460555E+004 -3.28412351E-006 43775.12 <-- SCF

9 -2.07460556E+004 4.20348891E-006 43797.38 <-- SCF

10 -2.07460557E+004 2.93155861E-006 43819.78 <-- SCF

11 -2.07460557E+004 9.57345966E-007 43841.39 <-- SCF

12 -2.07460557E+004 -5.09737851E-007 43862.92 <-- SCF

13 -2.07460557E+004 -3.22927708E-007 43884.05 <-- SCF

14 -2.07460557E+004 -6.43842838E-007 43905.36 <-- SCF

15 -2.07460557E+004 -2.11693943E-007 43926.42 <-- SCF

16 -2.07460557E+004 5.95930765E-007 43948.34 <-- SCF

17 -2.07460557E+004 -2.79558140E-007 43969.52 <-- SCF

18 -2.07460557E+004 -3.59047893E-007 43990.20 <-- SCF

19 -2.07460557E+004 9.04541093E-009 44011.78 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05566338 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00598 -0.01259 0.00292 \*

\* Se 2 -0.00397 -0.00074 -0.01028 \*

\* Se 3 0.01430 0.00200 0.01203 \*

\* Se 4 0.00086 -0.00888 -0.00388 \*

\* Se 5 -0.01059 0.00567 -0.00736 \*

\* Se 6 0.00372 -0.00742 0.00567 \*

\* Se 7 0.01216 -0.00330 -0.00444 \*

\* Se 8 -0.01080 0.00775 0.00708 \*

\* Se 9 0.00387 -0.01011 0.00246 \*

\* Se 10 -0.00905 0.00942 -0.00199 \*

\* Se 11 -0.00534 0.01018 0.00039 \*

\* Se 12 0.00813 -0.00928 -0.00066 \*

\* Se 13 -0.01743 0.00375 0.00408 \*

\* Se 14 0.01084 -0.00765 -0.00980 \*

\* Se 15 0.01036 -0.00547 0.01049 \*

\* Se 16 -0.00897 0.00790 -0.00529 \*

\* Se 17 -0.01305 -0.00110 -0.00770 \*

\* Se 18 -0.00665 0.00874 0.00392 \*

\* Se 19 -0.00007 0.01227 -0.00231 \*

\* Se 20 0.00730 0.00137 0.00582 \*

\* Nb 1 -0.00632 -0.00131 -0.00108 \*

\* Nb 2 0.00783 0.00055 0.00132 \*

\* Nb 3 -0.01026 -0.00786 0.00156 \*

\* Nb 4 0.01426 0.00268 0.00015 \*

\* Nb 5 0.01058 0.00371 0.00092 \*

\* Nb 6 0.01388 -0.00106 -0.00176 \*

\* Nb 7 -0.01196 0.00013 0.00165 \*

\* Nb 8 -0.00549 -0.00386 -0.00136 \*

\* Nb 9 -0.00750 -0.00266 -0.00084 \*

\* Nb 10 0.01534 0.00717 -0.00169 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.039517 0.006501 -0.030530 \*

\* y 0.006501 -0.009230 -0.011715 \*

\* z -0.030530 -0.011715 -0.003544 \*

\* \*

\* Pressure: -0.0089 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 4.565E-006 | -20746.055465 | <-- min BFGS

| trial step | 1.000000 | 3.165E-006 | -20746.055567 | <-- min BFGS

| line step | 3.260636 | 3.572E-007 | -20746.055678 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 27 with enthalpy= -2.07460557E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 7.079410E-006 | 5.000000E-006 | eV | No | <-- BFGS

| |F|max | 1.879117E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.673444E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.951738E-002 | 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 | 2.059E-006 | -20746.055678 | <-- 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)

14.8842905 -8.5724824 -0.0076837 0.4212431 -0.0015495 0.0002739

0.0126951 3.4512082 -0.0006522 1.0463291 1.8167269 0.0009229

-0.0084911 -0.0017387 13.0498621 0.0003003 0.0000899 0.4814754

Lattice parameters(A) Cell Angles

a = 17.176426 alpha = 90.018598

b = 3.451232 beta = 90.054126

c = 13.049865 gamma = 119.728663

Current cell volume = 671.775471 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 0.066686 0.664117 0.122726 x

x Se 2 0.134038 0.336075 0.622376 x

x Se 3 0.133717 0.335849 0.877518 x

x Se 4 0.066534 0.663931 0.377418 x

x Se 5 0.266469 0.664359 0.122388 x

x Se 6 0.333456 0.336988 0.622229 x

x Se 7 0.333271 0.336580 0.877655 x

x Se 8 0.266276 0.664186 0.377655 x

x Se 9 0.466804 0.665407 0.122833 x

x Se 10 0.533548 0.334941 0.622608 x

x Se 11 0.533183 0.334575 0.877150 x

x Se 12 0.466437 0.665017 0.377408 x

x Se 13 0.666752 0.663493 0.122360 x

x Se 14 0.733722 0.335820 0.622354 x

x Se 15 0.733534 0.335656 0.877602 x

x Se 16 0.666564 0.663073 0.377758 x

x Se 17 0.866287 0.664126 0.122473 x

x Se 18 0.933490 0.336106 0.622581 x

x Se 19 0.933345 0.335927 0.877273 x

x Se 20 0.865950 0.663892 0.377634 x

x Nb 1 -0.000781 -0.002459 0.250102 x

x Nb 2 0.000781 0.002462 0.749898 x

x Nb 3 0.199771 -0.000294 0.249990 x

x Nb 4 0.200447 0.000887 0.749997 x

x Nb 5 0.399237 -0.001897 0.250046 x

x Nb 6 0.399897 0.001283 0.749905 x

x Nb 7 0.600064 -0.001342 0.250096 x

x Nb 8 0.600740 0.001858 0.749955 x

x Nb 9 0.799551 -0.000934 0.250004 x

x Nb 10 0.800230 0.000317 0.750010 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460543E+004 44412.66 <-- SCF

1 -2.07460585E+004 1.41159694E-004 44431.12 <-- SCF

2 -2.07460590E+004 1.59292623E-005 44460.28 <-- SCF

3 -2.07460583E+004 -2.52800146E-005 44489.66 <-- SCF

4 -2.07460550E+004 -1.07846923E-004 44518.72 <-- SCF

5 -2.07460561E+004 3.60727098E-005 44545.92 <-- SCF

6 -2.07460560E+004 -1.72517089E-006 44572.23 <-- SCF

7 -2.07460558E+004 -9.36270049E-006 44595.09 <-- SCF

8 -2.07460556E+004 -5.36584598E-006 44619.11 <-- SCF

9 -2.07460557E+004 1.90613221E-006 44641.33 <-- SCF

10 -2.07460557E+004 1.39841797E-006 44663.00 <-- SCF

11 -2.07460557E+004 7.55305734E-007 44684.30 <-- SCF

12 -2.07460557E+004 7.26252102E-008 44705.89 <-- SCF

13 -2.07460557E+004 -1.42502603E-007 44727.23 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05572734 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00692 -0.01171 0.00130 \*

\* Se 2 -0.00301 -0.00148 -0.00926 \*

\* Se 3 0.01403 0.00037 0.01390 \*

\* Se 4 -0.00010 -0.00896 -0.00615 \*

\* Se 5 -0.00932 0.00533 -0.01216 \*

\* Se 6 0.00338 -0.00660 0.00744 \*

\* Se 7 0.01163 -0.00289 -0.00289 \*

\* Se 8 -0.00925 0.00692 0.00828 \*

\* Se 9 0.00104 -0.01040 0.00136 \*

\* Se 10 -0.00570 0.00970 -0.00030 \*

\* Se 11 -0.00230 0.01055 0.00102 \*

\* Se 12 0.00513 -0.00950 -0.00198 \*

\* Se 13 -0.01616 0.00350 0.00150 \*

\* Se 14 0.00837 -0.00699 -0.00866 \*

\* Se 15 0.00809 -0.00538 0.01286 \*

\* Se 16 -0.00774 0.00731 -0.00610 \*

\* Se 17 -0.01393 -0.00012 -0.01192 \*

\* Se 18 -0.00452 0.00949 0.00590 \*

\* Se 19 0.00192 0.01208 -0.00041 \*

\* Se 20 0.00518 0.00132 0.00727 \*

\* Nb 1 -0.00497 -0.00256 0.00078 \*

\* Nb 2 0.00526 0.00119 -0.00071 \*

\* Nb 3 -0.01031 -0.00725 0.00391 \*

\* Nb 4 0.01484 0.00379 -0.00198 \*

\* Nb 5 0.01281 0.00365 0.00256 \*

\* Nb 6 0.01319 -0.00193 -0.00367 \*

\* Nb 7 -0.00955 -0.00001 0.00366 \*

\* Nb 8 -0.00699 -0.00303 -0.00303 \*

\* Nb 9 -0.01031 -0.00256 0.00160 \*

\* Nb 10 0.01620 0.00618 -0.00412 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.036677 0.008004 -0.029588 \*

\* y 0.008004 -0.012136 -0.010127 \*

\* z -0.029588 -0.010127 -0.026190 \*

\* \*

\* Pressure: 0.0005 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 2.059E-006 | -20746.055678 | <-- min BFGS

| trial step | 1.000000 | 9.329E-007 | -20746.055740 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 28 with line minimization (lambda= 1.828799)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8847379 -8.5724028 -0.0077267 0.4212281 -0.0015536 0.0002725

0.0127292 3.4512357 -0.0006140 1.0462737 1.8167022 0.0009008

-0.0084467 -0.0016049 13.0473355 0.0002987 0.0000846 0.4815687

Lattice parameters(A) Cell Angles

a = 17.176774 alpha = 90.017377

b = 3.451259 beta = 90.054400

c = 13.047338 gamma = 119.727124

Current cell volume = 671.674709 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 0.066686 0.664062 0.122715 x

x Se 2 0.134039 0.336082 0.622359 x

x Se 3 0.133726 0.335892 0.877530 x

x Se 4 0.066535 0.663887 0.377440 x

x Se 5 0.266459 0.664335 0.122383 x

x Se 6 0.333467 0.337019 0.622209 x

x Se 7 0.333283 0.336619 0.877667 x

x Se 8 0.266261 0.664153 0.377669 x

x Se 9 0.466814 0.665416 0.122816 x

x Se 10 0.533539 0.334946 0.622582 x

x Se 11 0.533171 0.334560 0.877169 x

x Se 12 0.466444 0.665008 0.377431 x

x Se 13 0.666738 0.663456 0.122350 x

x Se 14 0.733737 0.335854 0.622338 x

x Se 15 0.733543 0.335682 0.877610 x

x Se 16 0.666552 0.663044 0.377775 x

x Se 17 0.866276 0.664083 0.122464 x

x Se 18 0.933486 0.336143 0.622558 x

x Se 19 0.933341 0.335975 0.877286 x

x Se 20 0.865948 0.663888 0.377646 x

x Nb 1 -0.000801 -0.002516 0.250097 x

x Nb 2 0.000802 0.002516 0.749902 x

x Nb 3 0.199769 -0.000351 0.249983 x

x Nb 4 0.200457 0.000911 0.750004 x

x Nb 5 0.399234 -0.001905 0.250043 x

x Nb 6 0.399911 0.001341 0.749908 x

x Nb 7 0.600056 -0.001395 0.250092 x

x Nb 8 0.600744 0.001867 0.749958 x

x Nb 9 0.799545 -0.000953 0.249997 x

x Nb 10 0.800238 0.000381 0.750018 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460543E+004 45128.36 <-- SCF

1 -2.07460841E+004 9.90438096E-004 45147.55 <-- SCF

2 -2.07460854E+004 4.42985929E-005 45175.89 <-- SCF

3 -2.07462186E+004 4.44084255E-003 45205.77 <-- SCF

4 -2.07460233E+004 -6.51010977E-003 45234.67 <-- SCF

5 -2.07460247E+004 4.60865593E-005 45263.31 <-- SCF

6 -2.07460416E+004 5.65013062E-004 45291.83 <-- SCF

7 -2.07460536E+004 3.97535259E-004 45318.52 <-- SCF

8 -2.07460590E+004 1.80670210E-004 45344.12 <-- SCF

9 -2.07460605E+004 5.04983217E-005 45368.05 <-- SCF

10 -2.07460598E+004 -2.47533090E-005 45391.38 <-- SCF

11 -2.07460585E+004 -4.06580000E-005 45414.30 <-- SCF

12 -2.07460571E+004 -4.76138565E-005 45438.06 <-- SCF

13 -2.07460558E+004 -4.19809984E-005 45462.30 <-- SCF

14 -2.07460549E+004 -3.09339532E-005 45488.81 <-- SCF

15 -2.07460560E+004 3.73953659E-005 45512.97 <-- SCF

16 -2.07460562E+004 4.18891188E-006 45534.88 <-- SCF

17 -2.07460557E+004 -1.55483732E-005 45559.59 <-- SCF

18 -2.07460557E+004 -4.00424063E-007 45580.94 <-- SCF

19 -2.07460557E+004 7.26361718E-007 45602.72 <-- SCF

20 -2.07460557E+004 8.42930355E-007 45623.94 <-- SCF

21 -2.07460557E+004 1.22908612E-007 45645.02 <-- SCF

22 -2.07460557E+004 4.60485023E-008 45665.66 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05573889 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00690 -0.01177 0.00031 \*

\* Se 2 -0.00186 -0.00174 -0.00949 \*

\* Se 3 0.01433 -0.00063 0.01653 \*

\* Se 4 -0.00012 -0.00974 -0.00829 \*

\* Se 5 -0.00816 0.00515 -0.01561 \*

\* Se 6 0.00306 -0.00653 0.00798 \*

\* Se 7 0.01132 -0.00307 -0.00070 \*

\* Se 8 -0.00808 0.00635 0.00888 \*

\* Se 9 -0.00066 -0.01120 -0.00005 \*

\* Se 10 -0.00199 0.00998 0.00051 \*

\* Se 11 0.00121 0.01087 0.00214 \*

\* Se 12 0.00307 -0.01025 -0.00230 \*

\* Se 13 -0.01381 0.00276 -0.00027 \*

\* Se 14 0.00753 -0.00674 -0.00842 \*

\* Se 15 0.00740 -0.00556 0.01551 \*

\* Se 16 -0.00558 0.00637 -0.00693 \*

\* Se 17 -0.01366 0.00072 -0.01543 \*

\* Se 18 -0.00177 0.00951 0.00704 \*

\* Se 19 0.00467 0.01133 0.00168 \*

\* Se 20 0.00434 0.00128 0.00852 \*

\* Nb 1 -0.00244 -0.00239 0.00269 \*

\* Nb 2 0.00175 0.00307 -0.00280 \*

\* Nb 3 -0.01230 -0.00615 0.00658 \*

\* Nb 4 0.01299 0.00390 -0.00472 \*

\* Nb 5 0.01337 0.00397 0.00442 \*

\* Nb 6 0.01105 -0.00191 -0.00582 \*

\* Nb 7 -0.01182 0.00149 0.00552 \*

\* Nb 8 -0.00971 -0.00288 -0.00472 \*

\* Nb 9 -0.01014 -0.00226 0.00392 \*

\* Nb 10 0.01292 0.00605 -0.00666 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.041781 0.009624 -0.028636 \*

\* y 0.009624 -0.006452 -0.008903 \*

\* z -0.028636 -0.008903 -0.033333 \*

\* \*

\* Pressure: -0.0007 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 2.059E-006 | -20746.055678 | <-- min BFGS

| trial step | 1.000000 | 9.329E-007 | -20746.055740 | <-- min BFGS

| line step | 1.828799 | 3.193E-007 | -20746.055742 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 28 with enthalpy= -2.07460557E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.124571E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 2.188000E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 8.358437E-004 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.178102E-002 | 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 | 1.261E-006 | -20746.055742 | <-- 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)

14.8847188 -8.5725888 -0.0071136 0.4212283 -0.0015540 0.0002554

0.0127334 3.4513164 -0.0005969 1.0462725 1.8166585 0.0008495

-0.0079143 -0.0015428 13.0460723 0.0002775 0.0000823 0.4816153

Lattice parameters(A) Cell Angles

a = 17.176850 alpha = 90.016812

b = 3.451340 beta = 90.050467

c = 13.046075 gamma = 119.727630

Current cell volume = 671.625027 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 0.066682 0.663982 0.122707 x

x Se 2 0.134046 0.336113 0.622348 x

x Se 3 0.133740 0.335951 0.877540 x

x Se 4 0.066533 0.663821 0.377453 x

x Se 5 0.266454 0.664280 0.122376 x

x Se 6 0.333475 0.337080 0.622195 x

x Se 7 0.333293 0.336690 0.877678 x

x Se 8 0.266253 0.664103 0.377678 x

x Se 9 0.466815 0.665388 0.122806 x

x Se 10 0.533540 0.334977 0.622565 x

x Se 11 0.533169 0.334584 0.877181 x

x Se 12 0.466442 0.664974 0.377446 x

x Se 13 0.666727 0.663388 0.122340 x

x Se 14 0.733744 0.335904 0.622328 x

x Se 15 0.733548 0.335737 0.877617 x

x Se 16 0.666543 0.662986 0.377788 x

x Se 17 0.866262 0.664023 0.122455 x

x Se 18 0.933487 0.336205 0.622543 x

x Se 19 0.933345 0.336051 0.877295 x

x Se 20 0.865939 0.663859 0.377656 x

x Nb 1 -0.000823 -0.002602 0.250098 x

x Nb 2 0.000825 0.002601 0.749902 x

x Nb 3 0.199763 -0.000413 0.249981 x

x Nb 4 0.200471 0.000952 0.750007 x

x Nb 5 0.399227 -0.001942 0.250043 x

x Nb 6 0.399917 0.001407 0.749908 x

x Nb 7 0.600052 -0.001458 0.250093 x

x Nb 8 0.600750 0.001902 0.749958 x

x Nb 9 0.799532 -0.000990 0.249994 x

x Nb 10 0.800248 0.000448 0.750020 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460550E+004 46065.36 <-- SCF

1 -2.07460628E+004 2.60639578E-004 46084.59 <-- SCF

2 -2.07460635E+004 2.10759285E-005 46111.81 <-- SCF

3 -2.07461142E+004 1.69095644E-003 46141.48 <-- SCF

4 -2.07460367E+004 -2.58275559E-003 46170.70 <-- SCF

5 -2.07460416E+004 1.63377797E-004 46198.03 <-- SCF

6 -2.07460488E+004 2.41569154E-004 46225.61 <-- SCF

7 -2.07460546E+004 1.91576840E-004 46251.16 <-- SCF

8 -2.07460565E+004 6.50890903E-005 46276.31 <-- SCF

9 -2.07460578E+004 4.08926883E-005 46299.06 <-- SCF

10 -2.07460579E+004 2.86054000E-006 46320.91 <-- SCF

11 -2.07460575E+004 -1.07138122E-005 46343.02 <-- SCF

12 -2.07460573E+004 -8.78900460E-006 46364.61 <-- SCF

13 -2.07460571E+004 -5.47560503E-006 46386.11 <-- SCF

14 -2.07460570E+004 -5.30038281E-006 46407.47 <-- SCF

15 -2.07460566E+004 -1.04772209E-005 46429.41 <-- SCF

16 -2.07460560E+004 -2.01094204E-005 46452.53 <-- SCF

17 -2.07460554E+004 -2.06059366E-005 46479.17 <-- SCF

18 -2.07460558E+004 1.41606554E-005 46500.91 <-- SCF

19 -2.07460559E+004 3.15593756E-006 46522.38 <-- SCF

20 -2.07460557E+004 -6.68360843E-006 46547.28 <-- SCF

21 -2.07460558E+004 1.38145878E-006 46568.73 <-- SCF

22 -2.07460558E+004 -6.84367038E-007 46590.64 <-- SCF

23 -2.07460558E+004 1.91198381E-007 46612.16 <-- SCF

24 -2.07460558E+004 2.58590601E-007 46633.50 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05576927 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00775 -0.01097 0.00010 \*

\* Se 2 -0.00081 -0.00224 -0.00833 \*

\* Se 3 0.01355 -0.00179 0.01609 \*

\* Se 4 -0.00225 -0.00955 -0.00947 \*

\* Se 5 -0.00713 0.00592 -0.01523 \*

\* Se 6 0.00331 -0.00720 0.00954 \*

\* Se 7 0.01000 -0.00397 -0.00143 \*

\* Se 8 -0.00814 0.00656 0.00781 \*

\* Se 9 -0.00176 -0.01063 -0.00009 \*

\* Se 10 -0.00006 0.00990 0.00198 \*

\* Se 11 0.00163 0.01054 0.00159 \*

\* Se 12 0.00084 -0.01001 -0.00319 \*

\* Se 13 -0.01331 0.00333 -0.00049 \*

\* Se 14 0.00805 -0.00695 -0.00747 \*

\* Se 15 0.00648 -0.00634 0.01531 \*

\* Se 16 -0.00634 0.00659 -0.00761 \*

\* Se 17 -0.01255 0.00223 -0.01517 \*

\* Se 18 -0.00050 0.00919 0.00904 \*

\* Se 19 0.00436 0.01045 0.00093 \*

\* Se 20 0.00406 0.00199 0.00762 \*

\* Nb 1 0.00134 -0.00372 0.00348 \*

\* Nb 2 -0.00083 0.00410 -0.00343 \*

\* Nb 3 -0.01171 -0.00439 0.00762 \*

\* Nb 4 0.01272 0.00450 -0.00583 \*

\* Nb 5 0.01430 0.00244 0.00514 \*

\* Nb 6 0.00890 -0.00210 -0.00668 \*

\* Nb 7 -0.00837 0.00271 0.00647 \*

\* Nb 8 -0.01131 -0.00222 -0.00567 \*

\* Nb 9 -0.00965 -0.00333 0.00529 \*

\* Nb 10 0.01292 0.00498 -0.00790 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.038339 0.009003 -0.022761 \*

\* y 0.009003 -0.005047 -0.007526 \*

\* z -0.022761 -0.007526 -0.039527 \*

\* \*

\* Pressure: 0.0021 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.261E-006 | -20746.055742 | <-- min BFGS

| trial step | 1.000000 | 8.127E-007 | -20746.055780 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 29 with line minimization (lambda= 2.811643)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8846843 -8.5729258 -0.0060028 0.4212287 -0.0015549 0.0002243

0.0127410 3.4514627 -0.0005659 1.0462703 1.8165792 0.0007566

-0.0069498 -0.0014303 13.0437837 0.0002392 0.0000781 0.4816997

Lattice parameters(A) Cell Angles

a = 17.176988 alpha = 90.015789

b = 3.451486 beta = 90.043341

c = 13.043786 gamma = 119.728546

Current cell volume = 671.535008 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066674 0.663839 0.122693 x

x Se 2 0.134060 0.336169 0.622328 x

x Se 3 0.133765 0.336057 0.877560 x

x Se 4 0.066528 0.663702 0.377477 x

x Se 5 0.266445 0.664182 0.122364 x

x Se 6 0.333489 0.337190 0.622170 x

x Se 7 0.333312 0.336819 0.877698 x

x Se 8 0.266240 0.664012 0.377695 x

x Se 9 0.466817 0.665339 0.122788 x

x Se 10 0.533543 0.335032 0.622534 x

x Se 11 0.533166 0.334628 0.877201 x

x Se 12 0.466438 0.664913 0.377474 x

x Se 13 0.666708 0.663264 0.122322 x

x Se 14 0.733756 0.335994 0.622310 x

x Se 15 0.733557 0.335837 0.877631 x

x Se 16 0.666528 0.662879 0.377812 x

x Se 17 0.866235 0.663914 0.122439 x

x Se 18 0.933489 0.336317 0.622518 x

x Se 19 0.933351 0.336188 0.877311 x

x Se 20 0.865923 0.663805 0.377673 x

x Nb 1 -0.000862 -0.002759 0.250098 x

x Nb 2 0.000865 0.002753 0.749902 x

x Nb 3 0.199752 -0.000526 0.249977 x

x Nb 4 0.200498 0.001025 0.750011 x

x Nb 5 0.399216 -0.002008 0.250043 x

x Nb 6 0.399928 0.001527 0.749907 x

x Nb 7 0.600045 -0.001571 0.250094 x

x Nb 8 0.600761 0.001966 0.749958 x

x Nb 9 0.799507 -0.001059 0.249990 x

x Nb 10 0.800266 0.000571 0.750025 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460535E+004 47037.30 <-- SCF

1 -2.07460629E+004 3.10674262E-004 47055.94 <-- SCF

2 -2.07460641E+004 3.98915893E-005 47085.19 <-- SCF

3 -2.07460855E+004 7.15715153E-004 47114.80 <-- SCF

4 -2.07460437E+004 -1.39490683E-003 47144.16 <-- SCF

5 -2.07460512E+004 2.51703377E-004 47171.80 <-- SCF

6 -2.07460562E+004 1.64233917E-004 47200.59 <-- SCF

7 -2.07460568E+004 2.31477694E-005 47226.67 <-- SCF

8 -2.07460567E+004 -5.72153043E-006 47250.59 <-- SCF

9 -2.07460562E+004 -1.67678673E-005 47273.62 <-- SCF

10 -2.07460558E+004 -1.11654971E-005 47296.33 <-- SCF

11 -2.07460556E+004 -6.61139168E-006 47319.36 <-- SCF

12 -2.07460557E+004 2.06952275E-006 47340.94 <-- SCF

13 -2.07460557E+004 1.34150607E-006 47362.59 <-- SCF

14 -2.07460558E+004 1.16149468E-006 47384.39 <-- SCF

15 -2.07460558E+004 4.99979577E-007 47405.81 <-- SCF

16 -2.07460558E+004 2.28210341E-007 47427.25 <-- SCF

17 -2.07460558E+004 8.11527565E-009 47448.56 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05579832 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00689 -0.00958 -0.00084 \*

\* Se 2 0.00027 -0.00313 -0.00636 \*

\* Se 3 0.01174 -0.00395 0.01523 \*

\* Se 4 -0.00396 -0.00928 -0.01091 \*

\* Se 5 -0.00581 0.00801 -0.01682 \*

\* Se 6 0.00520 -0.00832 0.01203 \*

\* Se 7 0.00938 -0.00561 -0.00239 \*

\* Se 8 -0.00932 0.00771 0.00790 \*

\* Se 9 -0.00255 -0.01037 -0.00091 \*

\* Se 10 0.00351 0.01091 0.00467 \*

\* Se 11 0.00296 0.01106 0.00051 \*

\* Se 12 -0.00242 -0.01025 -0.00395 \*

\* Se 13 -0.01160 0.00509 -0.00095 \*

\* Se 14 0.00887 -0.00812 -0.00545 \*

\* Se 15 0.00491 -0.00842 0.01470 \*

\* Se 16 -0.00732 0.00791 -0.00875 \*

\* Se 17 -0.01112 0.00455 -0.01680 \*

\* Se 18 0.00276 0.00943 0.01184 \*

\* Se 19 0.00509 0.00961 0.00058 \*

\* Se 20 0.00238 0.00286 0.00811 \*

\* Nb 1 0.00536 -0.00520 0.00419 \*

\* Nb 2 -0.00343 0.00470 -0.00425 \*

\* Nb 3 -0.01121 -0.00536 0.00905 \*

\* Nb 4 0.00929 0.00588 -0.00723 \*

\* Nb 5 0.01641 0.00176 0.00619 \*

\* Nb 6 0.00818 -0.00330 -0.00784 \*

\* Nb 7 -0.00742 0.00296 0.00765 \*

\* Nb 8 -0.01469 -0.00231 -0.00665 \*

\* Nb 9 -0.00859 -0.00490 0.00680 \*

\* Nb 10 0.01002 0.00570 -0.00935 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.039417 0.008769 -0.012002 \*

\* y 0.008769 0.006972 -0.005125 \*

\* z -0.012002 -0.005125 -0.040707 \*

\* \*

\* Pressure: -0.0019 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.261E-006 | -20746.055742 | <-- min BFGS

| trial step | 1.000000 | 8.127E-007 | -20746.055780 | <-- min BFGS

| line step | 2.811643 | 2.684E-007 | -20746.055804 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 29 with enthalpy= -2.07460558E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.083293E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 2.065106E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 9.741957E-004 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 4.070742E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 30 ...

================================================================================

Writing analysis data to 2H-Nb1Se2-7.castep\_bin

Writing model to 2H-Nb1Se2-7.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.502E-006 | -20746.055804 | <-- 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)

14.8831346 -8.5735375 -0.0046945 0.4212774 -0.0015463 0.0001835

0.0126694 3.4515804 -0.0004649 1.0464302 1.8165383 0.0006050

-0.0056870 -0.0010692 13.0457941 0.0001889 0.0000642 0.4816255

Lattice parameters(A) Cell Angles

a = 17.175950 alpha = 90.012505

b = 3.451604 beta = 90.034958

c = 13.045795 gamma = 119.734091

Current cell volume = 671.583749 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 0.066669 0.663755 0.122709 x

x Se 2 0.134065 0.336185 0.622329 x

x Se 3 0.133780 0.336111 0.877557 x

x Se 4 0.066526 0.663636 0.377465 x

x Se 5 0.266436 0.664153 0.122370 x

x Se 6 0.333497 0.337223 0.622179 x

x Se 7 0.333324 0.336870 0.877685 x

x Se 8 0.266227 0.663982 0.377692 x

x Se 9 0.466819 0.665304 0.122801 x

x Se 10 0.533542 0.335069 0.622538 x

x Se 11 0.533163 0.334659 0.877191 x

x Se 12 0.466438 0.664874 0.377467 x

x Se 13 0.666694 0.663211 0.122335 x

x Se 14 0.733768 0.336024 0.622312 x

x Se 15 0.733565 0.335865 0.877626 x

x Se 16 0.666517 0.662844 0.377801 x

x Se 17 0.866219 0.663862 0.122444 x

x Se 18 0.933489 0.336375 0.622527 x

x Se 19 0.933354 0.336263 0.877297 x

x Se 20 0.865919 0.663792 0.377669 x

x Nb 1 -0.000877 -0.002820 0.250096 x

x Nb 2 0.000881 0.002815 0.749904 x

x Nb 3 0.199744 -0.000594 0.249975 x

x Nb 4 0.200513 0.001076 0.750015 x

x Nb 5 0.399218 -0.002007 0.250043 x

x Nb 6 0.399938 0.001583 0.749907 x

x Nb 7 0.600038 -0.001624 0.250094 x

x Nb 8 0.600761 0.001970 0.749958 x

x Nb 9 0.799496 -0.001101 0.249986 x

x Nb 10 0.800279 0.000646 0.750027 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460549E+004 47852.91 <-- SCF

1 -2.07460628E+004 2.63147305E-004 47871.88 <-- SCF

2 -2.07460635E+004 2.56302406E-005 47899.69 <-- SCF

3 -2.07461081E+004 1.48544683E-003 47929.20 <-- SCF

4 -2.07460373E+004 -2.35985108E-003 47958.45 <-- SCF

5 -2.07460457E+004 2.78832083E-004 47986.05 <-- SCF

6 -2.07460525E+004 2.28977737E-004 48013.73 <-- SCF

7 -2.07460558E+004 1.08566338E-004 48038.00 <-- SCF

8 -2.07460566E+004 2.78180434E-005 48061.28 <-- SCF

9 -2.07460570E+004 1.28289076E-005 48083.34 <-- SCF

10 -2.07460569E+004 -3.00730617E-006 48104.89 <-- SCF

11 -2.07460565E+004 -1.45827389E-005 48127.48 <-- SCF

12 -2.07460562E+004 -8.27591805E-006 48149.22 <-- SCF

13 -2.07460559E+004 -1.19458503E-005 48172.38 <-- SCF

14 -2.07460559E+004 -8.72539283E-007 48193.67 <-- SCF

15 -2.07460559E+004 1.99594812E-006 48215.00 <-- SCF

16 -2.07460558E+004 -2.73049379E-006 48236.59 <-- SCF

17 -2.07460558E+004 -4.61383500E-007 48258.11 <-- SCF

18 -2.07460558E+004 4.13688700E-007 48279.45 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05584032 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00745 -0.00738 -0.00149 \*

\* Se 2 0.00216 -0.00272 -0.00438 \*

\* Se 3 0.00938 -0.00512 0.01446 \*

\* Se 4 -0.00799 -0.00860 -0.01189 \*

\* Se 5 -0.00335 0.00803 -0.01384 \*

\* Se 6 0.00558 -0.00808 0.01161 \*

\* Se 7 0.00624 -0.00671 -0.00098 \*

\* Se 8 -0.00921 0.00666 0.00378 \*

\* Se 9 -0.00339 -0.00925 0.00072 \*

\* Se 10 0.00617 0.01021 0.00535 \*

\* Se 11 0.00215 0.00966 0.00036 \*

\* Se 12 -0.00645 -0.00986 -0.00616 \*

\* Se 13 -0.01001 0.00537 -0.00013 \*

\* Se 14 0.00803 -0.00726 -0.00401 \*

\* Se 15 0.00146 -0.00869 0.01425 \*

\* Se 16 -0.00916 0.00688 -0.01070 \*

\* Se 17 -0.01048 0.00549 -0.01446 \*

\* Se 18 0.00538 0.00823 0.01153 \*

\* Se 19 0.00405 0.00691 0.00226 \*

\* Se 20 -0.00098 0.00220 0.00449 \*

\* Nb 1 0.00654 -0.00657 0.00506 \*

\* Nb 2 0.00439 0.00728 -0.00484 \*

\* Nb 3 -0.00658 -0.00574 0.00966 \*

\* Nb 4 0.00771 0.00565 -0.00828 \*

\* Nb 5 0.01597 0.00089 0.00708 \*

\* Nb 6 0.00912 -0.00067 -0.00875 \*

\* Nb 7 -0.00229 0.00391 0.00850 \*

\* Nb 8 -0.01463 -0.00159 -0.00727 \*

\* Nb 9 -0.00994 -0.00577 0.00759 \*

\* Nb 10 0.00758 0.00665 -0.00952 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.025036 0.006037 0.002113 \*

\* y 0.006037 0.011142 -0.000452 \*

\* z 0.002113 -0.000452 -0.027668 \*

\* \*

\* Pressure: -0.0028 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.502E-006 | -20746.055804 | <-- min BFGS

| trial step | 1.000000 | 2.340E-006 | -20746.055853 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 30 with line minimization (lambda= 3.015021)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8800119 -8.5747702 -0.0020582 0.4213756 -0.0015290 0.0001014

0.0125253 3.4518175 -0.0002616 1.0467527 1.8164560 0.0002996

-0.0031424 -0.0003417 13.0498450 0.0000874 0.0000362 0.4814759

Lattice parameters(A) Cell Angles

a = 17.173859 alpha = 90.005892

b = 3.451840 beta = 90.018072

c = 13.049845 gamma = 119.745265

Current cell volume = 671.681848 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066658 0.663586 0.122740 x

x Se 2 0.134075 0.336219 0.622330 x

x Se 3 0.133810 0.336218 0.877553 x

x Se 4 0.066520 0.663502 0.377443 x

x Se 5 0.266418 0.664095 0.122383 x

x Se 6 0.333513 0.337289 0.622197 x

x Se 7 0.333347 0.336972 0.877660 x

x Se 8 0.266202 0.663920 0.377686 x

x Se 9 0.466824 0.665233 0.122827 x

x Se 10 0.533539 0.335143 0.622546 x

x Se 11 0.533155 0.334722 0.877170 x

x Se 12 0.466439 0.664796 0.377453 x

x Se 13 0.666665 0.663104 0.122362 x

x Se 14 0.733791 0.336085 0.622314 x

x Se 15 0.733581 0.335922 0.877618 x

x Se 16 0.666496 0.662773 0.377780 x

x Se 17 0.866187 0.663757 0.122455 x

x Se 18 0.933488 0.336493 0.622547 x

x Se 19 0.933358 0.336415 0.877270 x

x Se 20 0.865909 0.663767 0.377661 x

x Nb 1 -0.000906 -0.002943 0.250091 x

x Nb 2 0.000914 0.002939 0.749909 x

x Nb 3 0.199727 -0.000733 0.249971 x

x Nb 4 0.200544 0.001178 0.750022 x

x Nb 5 0.399223 -0.002005 0.250041 x

x Nb 6 0.399959 0.001696 0.749906 x

x Nb 7 0.600025 -0.001729 0.250094 x

x Nb 8 0.600760 0.001977 0.749960 x

x Nb 9 0.799472 -0.001187 0.249978 x

x Nb 10 0.800306 0.000797 0.750031 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460505E+004 48682.86 <-- SCF

1 -2.07461537E+004 3.43778101E-003 48702.72 <-- SCF

2 -2.07461571E+004 1.14720544E-004 48733.36 <-- SCF

3 -2.07463082E+004 5.03651305E-003 48763.45 <-- SCF

4 -2.07460063E+004 -1.00641957E-002 48792.52 <-- SCF

5 -2.07460206E+004 4.76737612E-004 48822.66 <-- SCF

6 -2.07460524E+004 1.05931219E-003 48852.30 <-- SCF

7 -2.07460619E+004 3.16598090E-004 48880.12 <-- SCF

8 -2.07460626E+004 2.29922271E-005 48907.38 <-- SCF

9 -2.07460595E+004 -1.00925644E-004 48934.33 <-- SCF

10 -2.07460567E+004 -9.35689079E-005 48959.30 <-- SCF

11 -2.07460554E+004 -4.35504757E-005 48985.31 <-- SCF

12 -2.07460555E+004 1.49225707E-006 49010.70 <-- SCF

13 -2.07460560E+004 1.72655212E-005 49032.86 <-- SCF

14 -2.07460562E+004 8.72835287E-006 49054.72 <-- SCF

15 -2.07460561E+004 -5.26347881E-006 49076.67 <-- SCF

16 -2.07460559E+004 -6.65635598E-006 49099.69 <-- SCF

17 -2.07460559E+004 9.94027944E-009 49121.22 <-- SCF

18 -2.07460559E+004 3.61364775E-008 49142.67 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05588434 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00423 -0.00260 -0.00454 \*

\* Se 2 0.00693 -0.00230 0.00447 \*

\* Se 3 0.00595 -0.00787 0.00829 \*

\* Se 4 -0.01203 -0.00705 -0.01184 \*

\* Se 5 0.00109 0.00863 -0.01313 \*

\* Se 6 0.00982 -0.00711 0.01441 \*

\* Se 7 0.00358 -0.00839 -0.00169 \*

\* Se 8 -0.01004 0.00493 0.00095 \*

\* Se 9 -0.00123 -0.00683 -0.00053 \*

\* Se 10 0.01392 0.00905 0.00916 \*

\* Se 11 0.00295 0.00694 -0.00234 \*

\* Se 12 -0.01138 -0.00904 -0.00589 \*

\* Se 13 -0.00503 0.00702 -0.00376 \*

\* Se 14 0.00968 -0.00602 0.00547 \*

\* Se 15 -0.00202 -0.00975 0.00668 \*

\* Se 16 -0.01100 0.00588 -0.00892 \*

\* Se 17 -0.00504 0.00706 -0.01504 \*

\* Se 18 0.01283 0.00742 0.01506 \*

\* Se 19 0.00418 0.00296 0.00181 \*

\* Se 20 -0.00436 0.00041 0.00248 \*

\* Nb 1 0.00682 -0.00800 0.00692 \*

\* Nb 2 -0.00549 0.00815 -0.00693 \*

\* Nb 3 -0.00428 -0.00349 0.01150 \*

\* Nb 4 -0.00008 0.00839 -0.01126 \*

\* Nb 5 0.01558 -0.00073 0.00887 \*

\* Nb 6 0.00190 -0.00321 -0.01041 \*

\* Nb 7 -0.00232 0.00405 0.01026 \*

\* Nb 8 -0.01582 0.00183 -0.00944 \*

\* Nb 9 -0.00218 -0.00511 0.01079 \*

\* Nb 10 0.00131 0.00479 -0.01140 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.007616 0.001481 0.030854 \*

\* y 0.001481 0.024555 0.009418 \*

\* z 0.030854 0.009418 0.001689 \*

\* \*

\* Pressure: -0.0062 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.502E-006 | -20746.055804 | <-- min BFGS

| trial step | 1.000000 | 2.340E-006 | -20746.055853 | <-- min BFGS

| line step | 3.015021 | -5.858E-007 | -20746.055919 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 30 with enthalpy= -2.07460559E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 3.836978E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 2.113272E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 9.824809E-004 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.085390E-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 | 2.223E-006 | -20746.055919 | <-- 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)

14.8801629 -8.5742712 -0.0037599 0.4213804 -0.0015134 0.0001493

0.0123962 3.4513961 -0.0003126 1.0468315 1.8167166 0.0004448

-0.0046257 -0.0005302 13.0512500 0.0001465 0.0000431 0.4814241

Lattice parameters(A) Cell Angles

a = 17.173741 alpha = 90.007589

b = 3.451418 beta = 90.028977

c = 13.051251 gamma = 119.745688

Current cell volume = 671.664548 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 0.066651 0.663547 0.122746 x

x Se 2 0.134088 0.336231 0.622338 x

x Se 3 0.133819 0.336225 0.877544 x

x Se 4 0.066511 0.663460 0.377439 x

x Se 5 0.266422 0.664079 0.122392 x

x Se 6 0.333520 0.337330 0.622196 x

x Se 7 0.333350 0.337006 0.877660 x

x Se 8 0.266203 0.663904 0.377678 x

x Se 9 0.466814 0.665210 0.122834 x

x Se 10 0.533555 0.335172 0.622551 x

x Se 11 0.533165 0.334747 0.877162 x

x Se 12 0.466424 0.664766 0.377449 x

x Se 13 0.666663 0.663073 0.122362 x

x Se 14 0.733790 0.336099 0.622323 x

x Se 15 0.733577 0.335937 0.877607 x

x Se 16 0.666490 0.662735 0.377782 x

x Se 17 0.866178 0.663747 0.122462 x

x Se 18 0.933499 0.336538 0.622552 x

x Se 19 0.933368 0.336457 0.877263 x

x Se 20 0.865895 0.663752 0.377655 x

x Nb 1 -0.000911 -0.003031 0.250092 x

x Nb 2 0.000918 0.003026 0.749908 x

x Nb 3 0.199729 -0.000787 0.249971 x

x Nb 4 0.200546 0.001236 0.750022 x

x Nb 5 0.399222 -0.002077 0.250041 x

x Nb 6 0.399949 0.001760 0.749905 x

x Nb 7 0.600035 -0.001791 0.250095 x

x Nb 8 0.600760 0.002044 0.749959 x

x Nb 9 0.799469 -0.001249 0.249978 x

x Nb 10 0.800304 0.000852 0.750032 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460548E+004 49546.23 <-- SCF

1 -2.07460676E+004 4.27966053E-004 49565.25 <-- SCF

2 -2.07460692E+004 5.31056402E-005 49593.92 <-- SCF

3 -2.07461354E+004 2.20793312E-003 49623.42 <-- SCF

4 -2.07460314E+004 -3.46705615E-003 49652.59 <-- SCF

5 -2.07460369E+004 1.80665689E-004 49680.80 <-- SCF

6 -2.07460458E+004 2.99150334E-004 49709.11 <-- SCF

7 -2.07460531E+004 2.43482703E-004 49735.09 <-- SCF

8 -2.07460564E+004 1.09164691E-004 49759.69 <-- SCF

9 -2.07460584E+004 6.63375782E-005 49782.61 <-- SCF

10 -2.07460591E+004 2.27680902E-005 49804.91 <-- SCF

11 -2.07460589E+004 -5.78690120E-006 49826.38 <-- SCF

12 -2.07460587E+004 -8.43857788E-006 49848.06 <-- SCF

13 -2.07460585E+004 -3.86117263E-006 49869.36 <-- SCF

14 -2.07460586E+004 3.35523554E-006 49890.62 <-- SCF

15 -2.07460595E+004 2.83406771E-005 49912.03 <-- SCF

16 -2.07460608E+004 4.24840411E-005 49934.02 <-- SCF

17 -2.07460597E+004 -3.51650428E-005 49955.39 <-- SCF

18 -2.07460574E+004 -7.77846184E-005 49980.34 <-- SCF

19 -2.07460569E+004 -1.52469046E-005 50002.06 <-- SCF

20 -2.07460556E+004 -4.40909935E-005 50027.19 <-- SCF

21 -2.07460554E+004 -5.23892871E-006 50051.62 <-- SCF

22 -2.07460557E+004 1.01754358E-005 50073.33 <-- SCF

23 -2.07460559E+004 4.30608232E-006 50094.69 <-- SCF

24 -2.07460559E+004 1.70997875E-006 50116.42 <-- SCF

25 -2.07460559E+004 4.09301184E-007 50137.83 <-- SCF

26 -2.07460559E+004 4.20201194E-007 50159.09 <-- SCF

27 -2.07460559E+004 -2.05758505E-007 50180.70 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05593998 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00341 -0.00456 -0.00254 \*

\* Se 2 0.00447 -0.00066 0.00113 \*

\* Se 3 0.00820 -0.00562 0.01192 \*

\* Se 4 -0.00768 -0.00859 -0.01388 \*

\* Se 5 -0.00031 0.00778 -0.01021 \*

\* Se 6 0.00820 -0.00735 0.01418 \*

\* Se 7 0.00613 -0.00810 -0.00140 \*

\* Se 8 -0.00797 0.00430 -0.00163 \*

\* Se 9 0.00047 -0.00818 0.00267 \*

\* Se 10 0.00933 0.01040 0.00818 \*

\* Se 11 0.00239 0.00860 -0.00139 \*

\* Se 12 -0.00570 -0.01053 -0.00887 \*

\* Se 13 -0.00698 0.00561 -0.00100 \*

\* Se 14 0.01036 -0.00572 0.00118 \*

\* Se 15 0.00193 -0.00874 0.01124 \*

\* Se 16 -0.00895 0.00496 -0.01160 \*

\* Se 17 -0.00452 0.00547 -0.01208 \*

\* Se 18 0.00881 0.00765 0.01348 \*

\* Se 19 0.00403 0.00380 0.00358 \*

\* Se 20 0.00115 -0.00099 -0.00019 \*

\* Nb 1 0.00551 -0.00454 0.00698 \*

\* Nb 2 -0.00693 0.00585 -0.00691 \*

\* Nb 3 -0.01081 -0.00056 0.01116 \*

\* Nb 4 0.00339 0.00457 -0.01115 \*

\* Nb 5 0.01524 0.00218 0.00887 \*

\* Nb 6 0.00305 -0.00378 -0.01051 \*

\* Nb 7 -0.00967 0.00762 0.01022 \*

\* Nb 8 -0.01572 -0.00121 -0.00968 \*

\* Nb 9 -0.00706 -0.00256 0.01020 \*

\* Nb 10 0.00302 0.00291 -0.01194 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.008411 -0.002343 0.013930 \*

\* y -0.002343 0.004632 0.006388 \*

\* z 0.013930 0.006388 0.010876 \*

\* \*

\* Pressure: -0.0024 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 2.223E-006 | -20746.055919 | <-- min BFGS

| trial step | 1.000000 | 5.195E-007 | -20746.055962 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 31 with enthalpy= -2.07460560E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.411547E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 1.850351E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.363841E-004 | 5.000000E-004 | A | Yes | <-- BFGS

| Smax | 1.392997E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 32 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.146E-007 | -20746.055962 | <-- 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)

14.8796952 -8.5738792 -0.0044675 0.4213946 -0.0015119 0.0001685

0.0123827 3.4512166 -0.0003220 1.0468733 1.8168151 0.0004976

-0.0052205 -0.0005666 13.0517566 0.0001701 0.0000443 0.4814054

Lattice parameters(A) Cell Angles

a = 17.173140 alpha = 90.007915

b = 3.451239 beta = 90.033520

c = 13.051758 gamma = 119.745547

Current cell volume = 671.633090 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 0.663536 0.122751 x

x Se 2 0.134089 0.336225 0.622336 x

x Se 3 0.133821 0.336221 0.877544 x

x Se 4 0.066508 0.663446 0.377435 x

x Se 5 0.266420 0.664095 0.122393 x

x Se 6 0.333524 0.337323 0.622198 x

x Se 7 0.333353 0.336998 0.877656 x

x Se 8 0.266198 0.663909 0.377679 x

x Se 9 0.466815 0.665207 0.122838 x

x Se 10 0.533556 0.335183 0.622552 x

x Se 11 0.533164 0.334749 0.877160 x

x Se 12 0.466422 0.664755 0.377448 x

x Se 13 0.666659 0.663079 0.122367 x

x Se 14 0.733794 0.336094 0.622322 x

x Se 15 0.733578 0.335922 0.877607 x

x Se 16 0.666485 0.662740 0.377780 x

x Se 17 0.866176 0.663752 0.122463 x

x Se 18 0.933501 0.336550 0.622555 x

x Se 19 0.933368 0.336465 0.877259 x

x Se 20 0.865894 0.663760 0.377655 x

x Nb 1 -0.000909 -0.003041 0.250089 x

x Nb 2 0.000917 0.003037 0.749911 x

x Nb 3 0.199728 -0.000811 0.249969 x

x Nb 4 0.200546 0.001256 0.750025 x

x Nb 5 0.399227 -0.002069 0.250040 x

x Nb 6 0.399951 0.001775 0.749907 x

x Nb 7 0.600034 -0.001804 0.250094 x

x Nb 8 0.600755 0.002039 0.749961 x

x Nb 9 0.799469 -0.001268 0.249975 x

x Nb 10 0.800306 0.000876 0.750033 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460557E+004 50580.58 <-- SCF

1 -2.07460595E+004 1.24510950E-004 50600.25 <-- SCF

2 -2.07460599E+004 1.36154034E-005 50623.41 <-- SCF

3 -2.07460882E+004 9.43375767E-004 50653.11 <-- SCF

4 -2.07460428E+004 -1.51172338E-003 50682.41 <-- SCF

5 -2.07460468E+004 1.30284611E-004 50709.38 <-- SCF

6 -2.07460510E+004 1.40831891E-004 50735.69 <-- SCF

7 -2.07460536E+004 8.85696675E-005 50757.98 <-- SCF

8 -2.07460548E+004 3.96308073E-005 50780.30 <-- SCF

9 -2.07460558E+004 3.29010100E-005 50802.52 <-- SCF

10 -2.07460564E+004 2.04800730E-005 50824.75 <-- SCF

11 -2.07460567E+004 1.01460999E-005 50846.69 <-- SCF

12 -2.07460568E+004 3.58966336E-006 50868.45 <-- SCF

13 -2.07460570E+004 5.96843711E-006 50890.12 <-- SCF

14 -2.07460571E+004 3.04165332E-006 50911.53 <-- SCF

15 -2.07460570E+004 -3.16116241E-006 50933.02 <-- SCF

16 -2.07460569E+004 -4.62759492E-006 50954.44 <-- SCF

17 -2.07460566E+004 -1.04362415E-005 50976.28 <-- SCF

18 -2.07460565E+004 -5.53190534E-007 50997.61 <-- SCF

19 -2.07460566E+004 1.50560926E-006 51018.80 <-- SCF

20 -2.07460563E+004 -1.00748353E-005 51040.58 <-- SCF

21 -2.07460565E+004 5.56360480E-006 51062.03 <-- SCF

22 -2.07460565E+004 7.15894190E-007 51083.89 <-- SCF

23 -2.07460561E+004 -1.12317106E-005 51105.83 <-- SCF

24 -2.07460560E+004 -4.19019045E-006 51127.36 <-- SCF

25 -2.07460559E+004 -5.14340814E-006 51149.88 <-- SCF

26 -2.07460559E+004 1.73392220E-006 51171.31 <-- SCF

27 -2.07460559E+004 8.49250428E-007 51192.77 <-- SCF

28 -2.07460559E+004 4.94573965E-007 51214.11 <-- SCF

29 -2.07460560E+004 4.00930069E-007 51235.62 <-- SCF

30 -2.07460560E+004 4.24547153E-007 51256.98 <-- SCF

31 -2.07460560E+004 1.39137617E-007 51278.39 <-- SCF

32 -2.07460560E+004 1.37044297E-007 51299.61 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05598220 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00463 -0.00218 -0.00417 \*

\* Se 2 0.00102 -0.00032 0.00245 \*

\* Se 3 0.00615 -0.00482 0.01135 \*

\* Se 4 -0.00747 -0.00563 -0.01302 \*

\* Se 5 -0.00173 0.00622 -0.00964 \*

\* Se 6 0.00564 -0.00493 0.01105 \*

\* Se 7 0.00514 -0.00563 0.00253 \*

\* Se 8 -0.00771 0.00318 -0.00315 \*

\* Se 9 -0.00075 -0.00710 0.00286 \*

\* Se 10 0.00814 0.01044 0.00899 \*

\* Se 11 0.00270 0.00915 -0.00178 \*

\* Se 12 -0.00539 -0.00861 -0.01027 \*

\* Se 13 -0.00805 0.00592 -0.00216 \*

\* Se 14 0.00681 -0.00416 0.00192 \*

\* Se 15 0.00031 -0.00723 0.01113 \*

\* Se 16 -0.00805 0.00558 -0.01120 \*

\* Se 17 -0.00682 0.00435 -0.01022 \*

\* Se 18 0.00774 0.00827 0.01355 \*

\* Se 19 0.00378 0.00434 0.00423 \*

\* Se 20 0.00036 -0.00145 -0.00312 \*

\* Nb 1 0.00335 -0.01438 0.00766 \*

\* Nb 2 -0.01770 0.00579 -0.00866 \*

\* Nb 3 -0.00763 0.00043 0.01209 \*

\* Nb 4 0.02045 0.00320 -0.01175 \*

\* Nb 5 0.00901 -0.00246 0.01013 \*

\* Nb 6 -0.00246 -0.00613 -0.01087 \*

\* Nb 7 -0.00526 0.00602 0.01126 \*

\* Nb 8 -0.01079 -0.00174 -0.01033 \*

\* Nb 9 -0.00240 0.00035 0.01136 \*

\* Nb 10 0.01624 0.00355 -0.01221 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.031110 0.003970 0.007216 \*

\* y 0.003970 -0.005120 0.005516 \*

\* z 0.007216 0.005516 0.031625 \*

\* \*

\* Pressure: 0.0015 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.146E-007 | -20746.055962 | <-- min BFGS

| trial step | 1.000000 | 1.157E-007 | -20746.056023 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 32 with enthalpy= -2.07460560E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.052786E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 2.380256E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.056652E-004 | 5.000000E-004 | A | Yes | <-- BFGS

| Smax | 3.162519E-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 | 3.093E-006 | -20746.056023 | <-- 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)

14.8798859 -8.5730262 -0.0077956 0.4214097 -0.0014766 0.0002603

0.0120904 3.4503714 -0.0003945 1.0470631 1.8173482 0.0007643

-0.0080619 -0.0008427 13.0489039 0.0002834 0.0000541 0.4815108

Lattice parameters(A) Cell Angles

a = 17.172881 alpha = 90.010374

b = 3.450393 beta = 90.054834

c = 13.048906 gamma = 119.747562

Current cell volume = 671.297786 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 0.066627 0.663356 0.122740 x

x Se 2 0.134115 0.336248 0.622293 x

x Se 3 0.133857 0.336279 0.877578 x

x Se 4 0.066481 0.663270 0.377459 x

x Se 5 0.266415 0.664072 0.122370 x

x Se 6 0.333554 0.337407 0.622162 x

x Se 7 0.333380 0.337088 0.877679 x

x Se 8 0.266178 0.663860 0.377717 x

x Se 9 0.466801 0.665116 0.122823 x

x Se 10 0.533586 0.335307 0.622515 x

x Se 11 0.533178 0.334839 0.877179 x

x Se 12 0.466393 0.664631 0.377481 x

x Se 13 0.666630 0.662988 0.122346 x

x Se 14 0.733813 0.336142 0.622281 x

x Se 15 0.733582 0.335944 0.877635 x

x Se 16 0.666451 0.662655 0.377813 x

x Se 17 0.866138 0.663695 0.122435 x

x Se 18 0.933525 0.336716 0.622528 x

x Se 19 0.933388 0.336636 0.877274 x

x Se 20 0.865867 0.663744 0.377692 x

x Nb 1 -0.000926 -0.003269 0.250078 x

x Nb 2 0.000934 0.003256 0.749922 x

x Nb 3 0.199717 -0.001034 0.249960 x

x Nb 4 0.200571 0.001451 0.750038 x

x Nb 5 0.399247 -0.002157 0.250033 x

x Nb 6 0.399951 0.001964 0.749910 x

x Nb 7 0.600040 -0.001982 0.250090 x

x Nb 8 0.600734 0.002120 0.749967 x

x Nb 9 0.799448 -0.001456 0.249961 x

x Nb 10 0.800325 0.001111 0.750043 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460497E+004 51699.02 <-- SCF

1 -2.07460646E+004 4.94914356E-004 51717.80 <-- SCF

2 -2.07460658E+004 4.05392652E-005 51748.67 <-- SCF

3 -2.07460625E+004 -1.08822092E-004 51778.58 <-- SCF

4 -2.07460554E+004 -2.38572899E-004 51807.75 <-- SCF

5 -2.07460563E+004 3.12109180E-005 51837.55 <-- SCF

6 -2.07460561E+004 -6.15876661E-006 51864.66 <-- SCF

7 -2.07460560E+004 -5.16114310E-006 51889.00 <-- SCF

8 -2.07460559E+004 -1.06861397E-006 51912.03 <-- SCF

9 -2.07460559E+004 2.71696228E-007 51934.16 <-- SCF

10 -2.07460559E+004 -1.10434488E-008 51955.92 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05593765 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00440 -0.00652 -0.01189 \*

\* Se 2 -0.00424 0.00131 0.00675 \*

\* Se 3 0.00752 -0.00334 0.01173 \*

\* Se 4 -0.00025 -0.00947 -0.01040 \*

\* Se 5 -0.00275 0.00311 -0.01385 \*

\* Se 6 -0.00073 -0.00321 0.01655 \*

\* Se 7 0.00631 -0.00289 0.00126 \*

\* Se 8 -0.00096 0.00104 -0.00367 \*

\* Se 9 -0.00190 -0.01121 -0.00590 \*

\* Se 10 0.00189 0.01273 0.00809 \*

\* Se 11 0.00458 0.01192 0.00320 \*

\* Se 12 0.00150 -0.01204 -0.00514 \*

\* Se 13 -0.00785 0.00118 -0.00734 \*

\* Se 14 0.00238 -0.00226 0.00878 \*

\* Se 15 0.00322 -0.00436 0.00869 \*

\* Se 16 -0.00040 0.00164 -0.01046 \*

\* Se 17 -0.00694 0.00264 -0.01604 \*

\* Se 18 0.00079 0.01008 0.01262 \*

\* Se 19 0.00408 0.00723 0.00994 \*

\* Se 20 0.00648 -0.00324 -0.00224 \*

\* Nb 1 -0.00444 -0.00113 0.01081 \*

\* Nb 2 0.00082 0.00088 -0.01074 \*

\* Nb 3 -0.01271 0.00564 0.01513 \*

\* Nb 4 0.00488 -0.00099 -0.01620 \*

\* Nb 5 0.00859 0.00552 0.01274 \*

\* Nb 6 0.01309 -0.01215 -0.01386 \*

\* Nb 7 -0.01159 0.01314 0.01350 \*

\* Nb 8 -0.00492 -0.00536 -0.01268 \*

\* Nb 9 -0.00695 0.00360 0.01582 \*

\* Nb 10 0.00492 -0.00348 -0.01521 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.024065 -0.005290 -0.022651 \*

\* y -0.005290 -0.047497 0.001081 \*

\* z -0.022651 0.001081 0.001082 \*

\* \*

\* Pressure: 0.0235 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.093E-006 | -20746.056023 | <-- min BFGS

| trial step | 1.000000 | -3.874E-006 | -20746.055946 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 33 with line minimization (lambda= 0.443923)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8797798 -8.5735005 -0.0059449 0.4214013 -0.0014962 0.0002092

0.0122529 3.4508414 -0.0003542 1.0469575 1.8170517 0.0006160

-0.0064818 -0.0006892 13.0504902 0.0002204 0.0000486 0.4814522

Lattice parameters(A) Cell Angles

a = 17.173025 alpha = 90.009007

b = 3.450863 beta = 90.042981

c = 13.050492 gamma = 119.746441

Current cell volume = 671.484239 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 0.066639 0.663456 0.122746 x

x Se 2 0.134100 0.336235 0.622317 x

x Se 3 0.133837 0.336247 0.877559 x

x Se 4 0.066496 0.663368 0.377446 x

x Se 5 0.266418 0.664085 0.122383 x

x Se 6 0.333537 0.337360 0.622182 x

x Se 7 0.333365 0.337038 0.877667 x

x Se 8 0.266189 0.663887 0.377696 x

x Se 9 0.466809 0.665167 0.122831 x

x Se 10 0.533569 0.335238 0.622535 x

x Se 11 0.533170 0.334789 0.877168 x

x Se 12 0.466409 0.664700 0.377462 x

x Se 13 0.666646 0.663038 0.122358 x

x Se 14 0.733803 0.336116 0.622304 x

x Se 15 0.733580 0.335932 0.877619 x

x Se 16 0.666470 0.662702 0.377794 x

x Se 17 0.866159 0.663727 0.122451 x

x Se 18 0.933512 0.336624 0.622543 x

x Se 19 0.933377 0.336541 0.877266 x

x Se 20 0.865882 0.663753 0.377672 x

x Nb 1 -0.000917 -0.003142 0.250084 x

x Nb 2 0.000925 0.003134 0.749916 x

x Nb 3 0.199723 -0.000910 0.249965 x

x Nb 4 0.200557 0.001343 0.750031 x

x Nb 5 0.399236 -0.002108 0.250037 x

x Nb 6 0.399951 0.001859 0.749908 x

x Nb 7 0.600037 -0.001883 0.250092 x

x Nb 8 0.600746 0.002075 0.749963 x

x Nb 9 0.799460 -0.001351 0.249969 x

x Nb 10 0.800314 0.000981 0.750037 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460540E+004 52359.86 <-- SCF

1 -2.07460598E+004 1.94388361E-004 52378.72 <-- SCF

2 -2.07460604E+004 2.19524258E-005 52408.08 <-- SCF

3 -2.07460617E+004 4.00961485E-005 52437.67 <-- SCF

4 -2.07460545E+004 -2.38417367E-004 52466.80 <-- SCF

5 -2.07460560E+004 4.94499411E-005 52494.70 <-- SCF

6 -2.07460564E+004 1.23515654E-005 52521.17 <-- SCF

7 -2.07460561E+004 -8.43277557E-006 52544.28 <-- SCF

8 -2.07460559E+004 -6.89110955E-006 52568.33 <-- SCF

9 -2.07460559E+004 1.26301276E-006 52589.98 <-- SCF

10 -2.07460559E+004 5.73398084E-007 52611.48 <-- SCF

11 -2.07460560E+004 3.37911754E-007 52633.17 <-- SCF

12 -2.07460560E+004 -4.81296542E-008 52654.55 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05595679 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00412 -0.00543 -0.00659 \*

\* Se 2 -0.00041 0.00032 0.00511 \*

\* Se 3 0.00784 -0.00439 0.01053 \*

\* Se 4 -0.00359 -0.00869 -0.01269 \*

\* Se 5 -0.00270 0.00522 -0.01213 \*

\* Se 6 0.00316 -0.00481 0.01545 \*

\* Se 7 0.00620 -0.00493 -0.00034 \*

\* Se 8 -0.00511 0.00274 -0.00262 \*

\* Se 9 -0.00223 -0.01005 -0.00056 \*

\* Se 10 0.00436 0.01166 0.00867 \*

\* Se 11 0.00258 0.01055 0.00006 \*

\* Se 12 -0.00324 -0.01119 -0.00790 \*

\* Se 13 -0.00798 0.00337 -0.00373 \*

\* Se 14 0.00621 -0.00382 0.00593 \*

\* Se 15 0.00295 -0.00634 0.00891 \*

\* Se 16 -0.00468 0.00336 -0.01158 \*

\* Se 17 -0.00601 0.00380 -0.01387 \*

\* Se 18 0.00402 0.00905 0.01377 \*

\* Se 19 0.00365 0.00580 0.00584 \*

\* Se 20 0.00389 -0.00208 -0.00150 \*

\* Nb 1 0.00349 -0.00257 0.00904 \*

\* Nb 2 -0.00193 0.00258 -0.00912 \*

\* Nb 3 -0.00971 0.00258 0.01351 \*

\* Nb 4 0.00411 0.00127 -0.01399 \*

\* Nb 5 0.01174 0.00445 0.01113 \*

\* Nb 6 0.00945 -0.00921 -0.01218 \*

\* Nb 7 -0.01102 0.01046 0.01220 \*

\* Nb 8 -0.01128 -0.00382 -0.01117 \*

\* Nb 9 -0.00690 0.00137 0.01360 \*

\* Nb 10 0.00728 -0.00125 -0.01380 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.020129 -0.003278 -0.006689 \*

\* y -0.003278 -0.025681 0.003465 \*

\* z -0.006689 0.003465 0.004717 \*

\* \*

\* Pressure: 0.0137 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.093E-006 | -20746.056023 | <-- min BFGS

| trial step | 1.000000 | -3.874E-006 | -20746.055946 | <-- min BFGS

| line step | 0.443923 | -9.958E-007 | -20746.055991 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 33 with enthalpy= -2.07460560E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.061767E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 1.948609E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.190915E-004 | 5.000000E-004 | A | Yes | <-- BFGS

| Smax | 2.568065E-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 | 1.095E-006 | -20746.055991 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 34 with trial guess (lambda= 1.000000)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8799731 -8.5739163 -0.0053606 0.4213973 -0.0014935 0.0001946

0.0122313 3.4509695 -0.0003652 1.0469596 1.8169908 0.0005847

-0.0060303 -0.0007253 13.0508501 0.0002024 0.0000502 0.4814389

Lattice parameters(A) Cell Angles

a = 17.173400 alpha = 90.009342

b = 3.450991 beta = 90.039233

c = 13.050851 gamma = 119.747689

Current cell volume = 671.534014 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 0.066638 0.663427 0.122749 x

x Se 2 0.134103 0.336243 0.622324 x

x Se 3 0.133843 0.336265 0.877558 x

x Se 4 0.066495 0.663340 0.377438 x

x Se 5 0.266415 0.664075 0.122385 x

x Se 6 0.333540 0.337373 0.622190 x

x Se 7 0.333370 0.337055 0.877663 x

x Se 8 0.266185 0.663874 0.377689 x

x Se 9 0.466810 0.665152 0.122835 x

x Se 10 0.533570 0.335258 0.622541 x

x Se 11 0.533169 0.334804 0.877165 x

x Se 12 0.466409 0.664681 0.377456 x

x Se 13 0.666641 0.663019 0.122360 x

x Se 14 0.733807 0.336129 0.622311 x

x Se 15 0.733583 0.335941 0.877617 x

x Se 16 0.666467 0.662687 0.377787 x

x Se 17 0.866153 0.663709 0.122451 x

x Se 18 0.933513 0.336651 0.622551 x

x Se 19 0.933378 0.336569 0.877263 x

x Se 20 0.865881 0.663745 0.377665 x

x Nb 1 -0.000923 -0.003168 0.250088 x

x Nb 2 0.000931 0.003159 0.749912 x

x Nb 3 0.199720 -0.000929 0.249969 x

x Nb 4 0.200562 0.001358 0.750026 x

x Nb 5 0.399236 -0.002108 0.250041 x

x Nb 6 0.399955 0.001873 0.749904 x

x Nb 7 0.600032 -0.001898 0.250097 x

x Nb 8 0.600746 0.002076 0.749959 x

x Nb 9 0.799455 -0.001363 0.249973 x

x Nb 10 0.800318 0.001001 0.750033 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460558E+004 53058.27 <-- SCF

1 -2.07460600E+004 1.42475755E-004 53077.84 <-- SCF

2 -2.07460603E+004 8.95131650E-006 53101.61 <-- SCF

3 -2.07460966E+004 1.20863078E-003 53131.16 <-- SCF

4 -2.07460411E+004 -1.85002210E-003 53160.42 <-- SCF

5 -2.07460451E+004 1.33430123E-004 53187.62 <-- SCF

6 -2.07460489E+004 1.26575986E-004 53213.47 <-- SCF

7 -2.07460516E+004 9.20125236E-005 53236.23 <-- SCF

8 -2.07460544E+004 9.17095902E-005 53259.05 <-- SCF

9 -2.07460561E+004 5.84204587E-005 53281.22 <-- SCF

10 -2.07460569E+004 2.60665952E-005 53302.98 <-- SCF

11 -2.07460574E+004 1.64504309E-005 53324.98 <-- SCF

12 -2.07460576E+004 5.28763036E-006 53347.00 <-- SCF

13 -2.07460575E+004 -5.82477936E-007 53368.67 <-- SCF

14 -2.07460577E+004 4.28183116E-006 53390.36 <-- SCF

15 -2.07460577E+004 2.01295361E-006 53411.94 <-- SCF

16 -2.07460582E+004 1.67736678E-005 53433.59 <-- SCF

17 -2.07460577E+004 -1.93854272E-005 53454.94 <-- SCF

18 -2.07460571E+004 -1.73409159E-005 53477.12 <-- SCF

19 -2.07460569E+004 -6.80301934E-006 53498.62 <-- SCF

20 -2.07460569E+004 -1.14744644E-006 53519.91 <-- SCF

21 -2.07460566E+004 -8.53855773E-006 53541.67 <-- SCF

22 -2.07460565E+004 -4.09681694E-006 53563.31 <-- SCF

23 -2.07460562E+004 -9.01545521E-006 53586.09 <-- SCF

24 -2.07460562E+004 -8.55087388E-007 53607.58 <-- SCF

25 -2.07460563E+004 1.22302354E-006 53628.98 <-- SCF

26 -2.07460562E+004 -6.62121028E-007 53650.31 <-- SCF

27 -2.07460562E+004 -1.40963342E-006 53671.72 <-- SCF

28 -2.07460562E+004 1.65670324E-006 53692.97 <-- SCF

29 -2.07460562E+004 -3.16629630E-006 53714.28 <-- SCF

30 -2.07460563E+004 3.93413875E-006 53735.89 <-- SCF

31 -2.07460563E+004 -9.79758307E-008 53757.33 <-- SCF

32 -2.07460562E+004 -2.06469862E-006 53778.31 <-- SCF

33 -2.07460563E+004 2.19579779E-006 53798.88 <-- SCF

34 -2.07460565E+004 6.87623914E-006 53820.38 <-- SCF

35 -2.07460562E+004 -9.50361887E-006 53841.81 <-- SCF

36 -2.07460567E+004 1.73748613E-005 53868.08 <-- SCF

37 -2.07460567E+004 -3.91357410E-007 53890.17 <-- SCF

38 -2.07460564E+004 -8.96947961E-006 53911.97 <-- SCF

39 -2.07460563E+004 -3.54613096E-006 53933.66 <-- SCF

40 -2.07460560E+004 -9.48221091E-006 53955.72 <-- SCF

41 -2.07460559E+004 -3.46954917E-006 53978.97 <-- SCF

42 -2.07460559E+004 -2.55657272E-007 54000.88 <-- SCF

43 -2.07460559E+004 -1.71074977E-007 54022.27 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05592520 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00334 -0.00433 -0.00460 \*

\* Se 2 0.00109 0.00009 0.00490 \*

\* Se 3 0.00754 -0.00502 0.00881 \*

\* Se 4 -0.00366 -0.00737 -0.01246 \*

\* Se 5 -0.00240 0.00515 -0.01201 \*

\* Se 6 0.00261 -0.00477 0.01531 \*

\* Se 7 0.00427 -0.00470 -0.00199 \*

\* Se 8 -0.00567 0.00290 -0.00137 \*

\* Se 9 -0.00383 -0.00899 0.00181 \*

\* Se 10 0.00484 0.01149 0.00755 \*

\* Se 11 0.00187 0.01043 -0.00113 \*

\* Se 12 -0.00559 -0.01006 -0.00802 \*

\* Se 13 -0.00626 0.00375 0.00035 \*

\* Se 14 0.00584 -0.00384 0.00437 \*

\* Se 15 0.00155 -0.00651 0.00831 \*

\* Se 16 -0.00399 0.00384 -0.01321 \*

\* Se 17 -0.00857 0.00457 -0.00813 \*

\* Se 18 0.00316 0.00876 0.00947 \*

\* Se 19 0.00142 0.00579 0.00733 \*

\* Se 20 -0.00025 -0.00160 -0.00504 \*

\* Nb 1 0.00881 -0.00504 0.00781 \*

\* Nb 2 -0.00681 0.00028 -0.00777 \*

\* Nb 3 -0.01083 0.00168 0.01156 \*

\* Nb 4 0.00900 0.00341 -0.01111 \*

\* Nb 5 0.01492 0.00381 0.00988 \*

\* Nb 6 0.00675 -0.01154 -0.01062 \*

\* Nb 7 -0.00581 0.00944 0.01055 \*

\* Nb 8 -0.01030 -0.00449 -0.01031 \*

\* Nb 9 -0.00789 0.00071 0.01288 \*

\* Nb 10 0.01153 0.00219 -0.01313 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.021191 -0.002930 -0.001737 \*

\* y -0.002930 -0.019945 0.003802 \*

\* z -0.001737 0.003802 -0.000169 \*

\* \*

\* Pressure: 0.0138 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.095E-006 | -20746.055991 | <-- min BFGS

| trial step | 1.000000 | 9.641E-007 | -20746.055949 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 34 with line minimization (lambda= 8.337157)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8813911 -8.5769670 -0.0010733 0.4213683 -0.0014737 0.0000876

0.0120725 3.4519098 -0.0004464 1.0469745 1.8165439 0.0003557

-0.0027169 -0.0009904 13.0534905 0.0000705 0.0000620 0.4813414

Lattice parameters(A) Cell Angles

a = 17.176151 alpha = 90.011799

b = 3.451931 beta = 90.011742

c = 13.053491 gamma = 119.756838

Current cell volume = 671.899231 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 0.066626 0.663213 0.122769 x

x Se 2 0.134118 0.336303 0.622373 x

x Se 3 0.133886 0.336400 0.877550 x

x Se 4 0.066488 0.663133 0.377381 x

x Se 5 0.266393 0.663999 0.122398 x

x Se 6 0.333562 0.337469 0.622249 x

x Se 7 0.333403 0.337183 0.877639 x

x Se 8 0.266152 0.663773 0.377642 x

x Se 9 0.466820 0.665047 0.122865 x

x Se 10 0.533572 0.335403 0.622581 x

x Se 11 0.533161 0.334913 0.877138 x

x Se 12 0.466409 0.664543 0.377413 x

x Se 13 0.666605 0.662876 0.122378 x

x Se 14 0.733841 0.336225 0.622363 x

x Se 15 0.733605 0.336011 0.877599 x

x Se 16 0.666441 0.662578 0.377735 x

x Se 17 0.866113 0.663578 0.122456 x

x Se 18 0.933518 0.336853 0.622607 x

x Se 19 0.933388 0.336775 0.877245 x

x Se 20 0.865870 0.663691 0.377620 x

x Nb 1 -0.000970 -0.003358 0.250117 x

x Nb 2 0.000977 0.003339 0.749883 x

x Nb 3 0.199693 -0.001072 0.250000 x

x Nb 4 0.200598 0.001470 0.749994 x

x Nb 5 0.399234 -0.002108 0.250072 x

x Nb 6 0.399981 0.001980 0.749869 x

x Nb 7 0.600001 -0.002006 0.250131 x

x Nb 8 0.600749 0.002083 0.749927 x

x Nb 9 0.799421 -0.001448 0.250004 x

x Nb 10 0.800343 0.001153 0.750002 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460460E+004 54423.08 <-- SCF

1 -2.07461824E+004 4.54450898E-003 54442.33 <-- SCF

2 -2.07461874E+004 1.68285415E-004 54472.89 <-- SCF

3 -2.07462978E+004 3.68067884E-003 54502.42 <-- SCF

4 -2.07460012E+004 -9.88584572E-003 54531.27 <-- SCF

5 -2.07460286E+004 9.13088766E-004 54561.09 <-- SCF

6 -2.07460633E+004 1.15554577E-003 54591.25 <-- SCF

7 -2.07460660E+004 9.09163221E-005 54620.55 <-- SCF

8 -2.07460630E+004 -9.96876952E-005 54647.84 <-- SCF

9 -2.07460590E+004 -1.35650228E-004 54673.95 <-- SCF

10 -2.07460564E+004 -8.69821448E-005 54699.08 <-- SCF

11 -2.07460546E+004 -5.74128700E-005 54726.22 <-- SCF

12 -2.07460561E+004 5.00579653E-005 54751.62 <-- SCF

13 -2.07460568E+004 2.29603605E-005 54773.70 <-- SCF

14 -2.07460565E+004 -1.17604333E-005 54797.02 <-- SCF

15 -2.07460562E+004 -9.87581591E-006 54819.06 <-- SCF

16 -2.07460561E+004 -1.75363746E-006 54840.64 <-- SCF

17 -2.07460561E+004 -4.31498213E-007 54861.94 <-- SCF

18 -2.07460560E+004 -3.43157356E-006 54883.41 <-- SCF

19 -2.07460561E+004 1.82913836E-006 54904.66 <-- SCF

20 -2.07460560E+004 -1.91682433E-006 54928.22 <-- SCF

21 -2.07460561E+004 2.17919446E-006 54949.45 <-- SCF

22 -2.07460561E+004 1.49100376E-006 54970.92 <-- SCF

23 -2.07460560E+004 -3.12795761E-006 54992.25 <-- SCF

24 -2.07460560E+004 -1.56953904E-006 55013.80 <-- SCF

25 -2.07460560E+004 -2.77512976E-007 55035.28 <-- SCF

26 -2.07460560E+004 4.57826403E-007 55056.95 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05598764 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00143 0.00027 -0.00320 \*

\* Se 2 0.00665 0.00112 -0.00438 \*

\* Se 3 0.00284 -0.00617 0.00275 \*

\* Se 4 -0.01005 -0.00206 -0.00115 \*

\* Se 5 0.00365 0.00574 -0.00460 \*

\* Se 6 0.00880 -0.00599 0.00239 \*

\* Se 7 0.00143 -0.00635 -0.00417 \*

\* Se 8 -0.00572 0.00309 0.00590 \*

\* Se 9 0.00123 -0.00662 0.00428 \*

\* Se 10 0.01144 0.00694 0.00150 \*

\* Se 11 0.00127 0.00695 -0.00566 \*

\* Se 12 -0.00852 -0.00664 0.00008 \*

\* Se 13 -0.00259 0.00535 0.00098 \*

\* Se 14 0.00786 -0.00390 -0.00451 \*

\* Se 15 -0.00210 -0.00667 0.00300 \*

\* Se 16 -0.00940 0.00519 0.00052 \*

\* Se 17 0.00027 0.00571 -0.00458 \*

\* Se 18 0.01045 0.00258 0.00437 \*

\* Se 19 0.00098 0.00046 0.00004 \*

\* Se 20 -0.00247 -0.00253 0.00599 \*

\* Nb 1 0.00236 -0.00663 -0.00430 \*

\* Nb 2 -0.00627 0.00715 0.00437 \*

\* Nb 3 -0.00474 0.00116 0.00033 \*

\* Nb 4 -0.00010 0.00453 -0.00067 \*

\* Nb 5 0.01094 -0.00072 0.00027 \*

\* Nb 6 0.00383 -0.00749 -0.00083 \*

\* Nb 7 -0.00588 0.00688 0.00069 \*

\* Nb 8 -0.01214 0.00193 -0.00009 \*

\* Nb 9 -0.00294 -0.00267 0.00084 \*

\* Nb 10 0.00033 -0.00060 -0.00017 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.001090 -0.012464 0.032028 \*

\* y -0.012464 0.032622 0.005834 \*

\* z 0.032028 0.005834 0.012287 \*

\* \*

\* Pressure: -0.0153 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.095E-006 | -20746.055991 | <-- min BFGS

| trial step | 1.000000 | 9.641E-007 | -20746.055949 | <-- min BFGS

| line step | 8.337157 | -4.855E-007 | -20746.056035 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 34 with enthalpy= -2.07460560E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.443939E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 1.346369E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.132183E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.262237E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 35 ...

================================================================================

Writing analysis data to 2H-Nb1Se2-7.castep\_bin

Writing model to 2H-Nb1Se2-7.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.879E-006 | -20746.056035 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: starting iteration 35 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8807880 -8.5754653 -0.0032344 0.4213787 -0.0014855 0.0001490

0.0121675 3.4514763 -0.0005189 1.0469487 1.8167434 0.0005455

-0.0046210 -0.0012560 13.0518572 0.0001460 0.0000719 0.4814017

Lattice parameters(A) Cell Angles

a = 17.174879 alpha = 90.014198

b = 3.451498 beta = 90.025613

c = 13.051858 gamma = 119.751899

Current cell volume = 671.714128 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 0.066623 0.663178 0.122759 x

x Se 2 0.134119 0.336297 0.622342 x

x Se 3 0.133893 0.336397 0.877575 x

x Se 4 0.066480 0.663087 0.377396 x

x Se 5 0.266389 0.664032 0.122378 x

x Se 6 0.333574 0.337457 0.622234 x

x Se 7 0.333411 0.337168 0.877647 x

x Se 8 0.266139 0.663776 0.377670 x

x Se 9 0.466822 0.665030 0.122852 x

x Se 10 0.533575 0.335444 0.622560 x

x Se 11 0.533158 0.334929 0.877153 x

x Se 12 0.466406 0.664502 0.377433 x

x Se 13 0.666593 0.662885 0.122371 x

x Se 14 0.733854 0.336223 0.622332 x

x Se 15 0.733608 0.335978 0.877623 x

x Se 16 0.666427 0.662585 0.377748 x

x Se 17 0.866106 0.663584 0.122435 x

x Se 18 0.933523 0.336892 0.622591 x

x Se 19 0.933388 0.336802 0.877256 x

x Se 20 0.865871 0.663704 0.377647 x

x Nb 1 -0.000967 -0.003376 0.250108 x

x Nb 2 0.000974 0.003354 0.749892 x

x Nb 3 0.199688 -0.001131 0.249995 x

x Nb 4 0.200605 0.001517 0.750001 x

x Nb 5 0.399251 -0.002071 0.250067 x

x Nb 6 0.399989 0.002005 0.749873 x

x Nb 7 0.599997 -0.002026 0.250127 x

x Nb 8 0.600733 0.002048 0.749932 x

x Nb 9 0.799418 -0.001487 0.249996 x

x Nb 10 0.800353 0.001216 0.750007 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460547E+004 55461.16 <-- SCF

1 -2.07460582E+004 1.16949757E-004 55479.45 <-- SCF

2 -2.07460586E+004 1.27649543E-005 55508.86 <-- SCF

3 -2.07460569E+004 -5.71666358E-005 55538.28 <-- SCF

4 -2.07460561E+004 -2.62303641E-005 55566.72 <-- SCF

5 -2.07460561E+004 9.01906191E-007 55592.55 <-- SCF

6 -2.07460561E+004 -1.30635252E-006 55615.19 <-- SCF

7 -2.07460561E+004 -5.25078896E-007 55636.97 <-- SCF

8 -2.07460561E+004 7.83070787E-008 55658.64 <-- SCF

9 -2.07460561E+004 -3.47119887E-008 55679.31 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05609085 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00244 -0.00064 -0.00591 \*

\* Se 2 0.00366 0.00091 0.00017 \*

\* Se 3 0.00365 -0.00538 0.00184 \*

\* Se 4 -0.00638 -0.00192 -0.00151 \*

\* Se 5 0.00215 0.00335 -0.00334 \*

\* Se 6 0.00443 -0.00423 0.00242 \*

\* Se 7 0.00196 -0.00372 -0.00109 \*

\* Se 8 -0.00173 0.00165 0.00161 \*

\* Se 9 -0.00158 -0.00730 0.00062 \*

\* Se 10 0.00840 0.00656 0.00039 \*

\* Se 11 0.00303 0.00781 -0.00179 \*

\* Se 12 -0.00649 -0.00613 0.00101 \*

\* Se 13 -0.00372 0.00234 -0.00102 \*

\* Se 14 0.00273 -0.00249 -0.00004 \*

\* Se 15 -0.00199 -0.00426 0.00152 \*

\* Se 16 -0.00558 0.00296 -0.00040 \*

\* Se 17 -0.00206 0.00507 -0.00412 \*

\* Se 18 0.00705 0.00265 0.00319 \*

\* Se 19 0.00242 0.00161 0.00432 \*

\* Se 20 -0.00120 -0.00221 0.00220 \*

\* Nb 1 0.00336 -0.00723 -0.00346 \*

\* Nb 2 -0.00211 0.00676 0.00328 \*

\* Nb 3 -0.00664 0.00264 0.00125 \*

\* Nb 4 0.00262 0.00215 -0.00235 \*

\* Nb 5 0.01155 -0.00033 0.00157 \*

\* Nb 6 0.00462 -0.00870 -0.00201 \*

\* Nb 7 -0.00684 0.00949 0.00174 \*

\* Nb 8 -0.01069 0.00102 -0.00126 \*

\* Nb 9 -0.00535 -0.00085 0.00258 \*

\* Nb 10 0.00314 -0.00159 -0.00143 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.000789 -0.007368 0.012536 \*

\* y -0.007368 0.017764 0.001296 \*

\* z 0.012536 0.001296 0.014799 \*

\* \*

\* Pressure: -0.0111 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.879E-006 | -20746.056035 | <-- min BFGS

| trial step | 1.000000 | 2.242E-006 | -20746.056122 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 35 with line minimization (lambda= 2.369150)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8799623 -8.5734093 -0.0061934 0.4213931 -0.0015016 0.0002332

0.0122975 3.4508828 -0.0006181 1.0469134 1.8170166 0.0008054

-0.0072279 -0.0016196 13.0496210 0.0002496 0.0000853 0.4814843

Lattice parameters(A) Cell Angles

a = 17.173138 alpha = 90.017486

b = 3.450905 beta = 90.044610

c = 13.049623 gamma = 119.745134

Current cell volume = 671.460690 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 0.066617 0.663130 0.122745 x

x Se 2 0.134121 0.336288 0.622300 x

x Se 3 0.133902 0.336393 0.877610 x

x Se 4 0.066470 0.663025 0.377416 x

x Se 5 0.266384 0.664077 0.122350 x

x Se 6 0.333589 0.337441 0.622213 x

x Se 7 0.333422 0.337148 0.877660 x

x Se 8 0.266121 0.663779 0.377709 x

x Se 9 0.466826 0.665007 0.122835 x

x Se 10 0.533579 0.335500 0.622530 x

x Se 11 0.533153 0.334951 0.877174 x

x Se 12 0.466402 0.664447 0.377459 x

x Se 13 0.666577 0.662897 0.122360 x

x Se 14 0.733871 0.336219 0.622289 x

x Se 15 0.733612 0.335933 0.877656 x

x Se 16 0.666407 0.662594 0.377767 x

x Se 17 0.866096 0.663592 0.122405 x

x Se 18 0.933529 0.336945 0.622570 x

x Se 19 0.933389 0.336839 0.877272 x

x Se 20 0.865871 0.663721 0.377684 x

x Nb 1 -0.000962 -0.003401 0.250095 x

x Nb 2 0.000970 0.003375 0.749905 x

x Nb 3 0.199681 -0.001211 0.249988 x

x Nb 4 0.200614 0.001581 0.750011 x

x Nb 5 0.399275 -0.002019 0.250059 x

x Nb 6 0.400001 0.002039 0.749879 x

x Nb 7 0.599990 -0.002053 0.250121 x

x Nb 8 0.600712 0.001999 0.749938 x

x Nb 9 0.799413 -0.001541 0.249985 x

x Nb 10 0.800367 0.001303 0.750013 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460536E+004 56080.56 <-- SCF

1 -2.07460598E+004 2.04905676E-004 56098.69 <-- SCF

2 -2.07460604E+004 2.13462502E-005 56128.69 <-- SCF

3 -2.07460574E+004 -1.00473913E-004 56157.97 <-- SCF

4 -2.07460562E+004 -4.08330442E-005 56186.48 <-- SCF

5 -2.07460562E+004 -4.02243396E-007 56213.05 <-- SCF

6 -2.07460561E+004 -1.50844906E-006 56237.19 <-- SCF

7 -2.07460561E+004 -6.90561821E-007 56259.22 <-- SCF

8 -2.07460561E+004 -7.59930836E-008 56280.77 <-- SCF

9 -2.07460561E+004 1.64776662E-007 56302.30 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05610568 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00415 -0.00292 -0.00977 \*

\* Se 2 -0.00035 0.00020 0.00594 \*

\* Se 3 0.00523 -0.00479 -0.00005 \*

\* Se 4 -0.00143 -0.00279 -0.00118 \*

\* Se 5 0.00119 -0.00026 -0.00106 \*

\* Se 6 -0.00068 -0.00208 0.00322 \*

\* Se 7 0.00378 -0.00041 0.00145 \*

\* Se 8 0.00473 -0.00055 -0.00422 \*

\* Se 9 -0.00567 -0.00862 -0.00281 \*

\* Se 10 0.00604 0.00625 0.00012 \*

\* Se 11 0.00742 0.00920 0.00146 \*

\* Se 12 -0.00401 -0.00567 0.00131 \*

\* Se 13 -0.00399 -0.00115 -0.00382 \*

\* Se 14 -0.00348 -0.00053 0.00714 \*

\* Se 15 -0.00085 -0.00095 -0.00224 \*

\* Se 16 0.00114 0.00073 -0.00095 \*

\* Se 17 -0.00411 0.00428 -0.00350 \*

\* Se 18 0.00306 0.00324 0.00289 \*

\* Se 19 0.00510 0.00361 0.00794 \*

\* Se 20 0.00194 -0.00175 -0.00242 \*

\* Nb 1 -0.00124 -0.00521 -0.00119 \*

\* Nb 2 0.00131 0.00564 0.00084 \*

\* Nb 3 -0.00585 0.00602 0.00367 \*

\* Nb 4 0.00404 -0.00011 -0.00543 \*

\* Nb 5 0.00644 0.00058 0.00406 \*

\* Nb 6 0.00763 -0.01093 -0.00434 \*

\* Nb 7 -0.00957 0.01178 0.00407 \*

\* Nb 8 -0.00724 -0.00012 -0.00345 \*

\* Nb 9 -0.00711 0.00155 0.00588 \*

\* Nb 10 0.00069 -0.00425 -0.00353 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.013635 -0.000689 -0.015220 \*

\* y -0.000689 -0.016700 -0.005062 \*

\* z -0.015220 -0.005062 0.003802 \*

\* \*

\* Pressure: 0.0088 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.879E-006 | -20746.056035 | <-- min BFGS

| trial step | 1.000000 | 2.242E-006 | -20746.056122 | <-- min BFGS

| line step | 2.369150 | -9.116E-007 | -20746.056137 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 35 with enthalpy= -2.07460561E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 3.415511E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 1.571539E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.100178E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.669966E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 36 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.732E-006 | -20746.056137 | <-- 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)

14.8798834 -8.5741916 -0.0048846 0.4213966 -0.0014991 0.0002009

0.0122776 3.4511592 -0.0006479 1.0469340 1.8168770 0.0007391

-0.0062290 -0.0017191 13.0498787 0.0002097 0.0000896 0.4814747

Lattice parameters(A) Cell Angles

a = 17.173460 alpha = 90.018401

b = 3.451181 beta = 90.036224

c = 13.049880 gamma = 119.747874

Current cell volume = 671.522035 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 0.066607 0.662988 0.122746 x

x Se 2 0.134136 0.336335 0.622304 x

x Se 3 0.133929 0.336477 0.877620 x

x Se 4 0.066461 0.662891 0.377403 x

x Se 5 0.266376 0.664018 0.122342 x

x Se 6 0.333603 0.337517 0.622225 x

x Se 7 0.333441 0.337243 0.877660 x

x Se 8 0.266107 0.663711 0.377704 x

x Se 9 0.466824 0.664927 0.122839 x

x Se 10 0.533589 0.335599 0.622533 x

x Se 11 0.533156 0.335033 0.877171 x

x Se 12 0.466394 0.664352 0.377455 x

x Se 13 0.666557 0.662797 0.122358 x

x Se 14 0.733885 0.336285 0.622296 x

x Se 15 0.733620 0.335990 0.877662 x

x Se 16 0.666391 0.662512 0.377758 x

x Se 17 0.866070 0.663510 0.122394 x

x Se 18 0.933537 0.337076 0.622583 x

x Se 19 0.933399 0.336977 0.877273 x

x Se 20 0.865858 0.663677 0.377681 x

x Nb 1 -0.000989 -0.003537 0.250105 x

x Nb 2 0.000997 0.003507 0.749895 x

x Nb 3 0.199664 -0.001316 0.249999 x

x Nb 4 0.200639 0.001668 0.750000 x

x Nb 5 0.399276 -0.002042 0.250071 x

x Nb 6 0.400012 0.002122 0.749865 x

x Nb 7 0.599978 -0.002134 0.250135 x

x Nb 8 0.600711 0.002024 0.749926 x

x Nb 9 0.799388 -0.001617 0.249995 x

x Nb 10 0.800384 0.001413 0.750002 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460546E+004 56706.08 <-- SCF

1 -2.07460585E+004 1.28752673E-004 56724.39 <-- SCF

2 -2.07460589E+004 1.26577107E-005 56753.12 <-- SCF

3 -2.07460587E+004 -6.45218201E-006 56782.98 <-- SCF

4 -2.07460558E+004 -9.68197153E-005 56812.19 <-- SCF

5 -2.07460563E+004 1.76482950E-005 56839.56 <-- SCF

6 -2.07460563E+004 -2.40423450E-006 56864.92 <-- SCF

7 -2.07460561E+004 -3.78781981E-006 56887.27 <-- SCF

8 -2.07460561E+004 -3.35648906E-007 56909.50 <-- SCF

9 -2.07460561E+004 2.43496527E-007 56931.61 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05613391 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00180 -0.00075 -0.00827 \*

\* Se 2 0.00160 -0.00016 0.00656 \*

\* Se 3 0.00361 -0.00602 -0.00724 \*

\* Se 4 -0.00136 -0.00029 0.00250 \*

\* Se 5 0.00393 0.00041 0.00353 \*

\* Se 6 0.00091 -0.00401 0.00059 \*

\* Se 7 0.00314 -0.00239 -0.00239 \*

\* Se 8 0.00611 -0.00019 -0.00258 \*

\* Se 9 -0.00357 -0.00697 -0.00134 \*

\* Se 10 0.00631 0.00415 -0.00158 \*

\* Se 11 0.00619 0.00733 -0.00126 \*

\* Se 12 -0.00353 -0.00378 0.00417 \*

\* Se 13 -0.00174 0.00058 -0.00052 \*

\* Se 14 -0.00272 -0.00113 0.00542 \*

\* Se 15 -0.00111 -0.00180 -0.00690 \*

\* Se 16 0.00081 0.00234 0.00193 \*

\* Se 17 -0.00068 0.00536 0.00204 \*

\* Se 18 0.00407 0.00038 0.00012 \*

\* Se 19 0.00386 0.00118 0.00507 \*

\* Se 20 0.00137 -0.00153 -0.00172 \*

\* Nb 1 -0.00714 -0.00621 -0.00029 \*

\* Nb 2 0.00624 0.00696 0.00120 \*

\* Nb 3 -0.00998 0.00609 0.00363 \*

\* Nb 4 0.00321 0.00062 -0.00584 \*

\* Nb 5 0.00567 -0.00151 0.00464 \*

\* Nb 6 0.00468 -0.00803 -0.00501 \*

\* Nb 7 -0.00975 0.00978 0.00438 \*

\* Nb 8 -0.00619 0.00216 -0.00412 \*

\* Nb 9 -0.01126 0.00158 0.00592 \*

\* Nb 10 -0.00089 -0.00417 -0.00262 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.020877 -0.001614 -0.006124 \*

\* y -0.001614 -0.011074 -0.005118 \*

\* z -0.006124 -0.005118 -0.001017 \*

\* \*

\* Pressure: 0.0110 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.732E-006 | -20746.056137 | <-- min BFGS

| trial step | 1.000000 | 1.175E-006 | -20746.056152 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 36 with line minimization (lambda= 3.111582)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8797169 -8.5758433 -0.0021211 0.4214042 -0.0014938 0.0001328

0.0122358 3.4517429 -0.0007109 1.0469774 1.8165823 0.0005990

-0.0041198 -0.0019291 13.0504230 0.0001255 0.0000987 0.4814546

Lattice parameters(A) Cell Angles

a = 17.174140 alpha = 90.020334

b = 3.451765 beta = 90.018518

c = 13.050424 gamma = 119.753658

Current cell volume = 671.651545 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 0.066585 0.662688 0.122747 x

x Se 2 0.134166 0.336436 0.622313 x

x Se 3 0.133987 0.336655 0.877643 x

x Se 4 0.066443 0.662607 0.377375 x

x Se 5 0.266358 0.663893 0.122327 x

x Se 6 0.333633 0.337679 0.622249 x

x Se 7 0.333480 0.337441 0.877660 x

x Se 8 0.266077 0.663567 0.377694 x

x Se 9 0.466820 0.664756 0.122849 x

x Se 10 0.533610 0.335807 0.622540 x

x Se 11 0.533161 0.335208 0.877166 x

x Se 12 0.466375 0.664150 0.377444 x

x Se 13 0.666515 0.662585 0.122352 x

x Se 14 0.733916 0.336424 0.622310 x

x Se 15 0.733638 0.336109 0.877674 x

x Se 16 0.666358 0.662337 0.377740 x

x Se 17 0.866014 0.663336 0.122370 x

x Se 18 0.933554 0.337353 0.622609 x

x Se 19 0.933420 0.337267 0.877274 x

x Se 20 0.865832 0.663583 0.377674 x

x Nb 1 -0.001046 -0.003824 0.250126 x

x Nb 2 0.001053 0.003787 0.749873 x

x Nb 3 0.199628 -0.001539 0.250023 x

x Nb 4 0.200692 0.001850 0.749977 x

x Nb 5 0.399277 -0.002091 0.250096 x

x Nb 6 0.400034 0.002297 0.749836 x

x Nb 7 0.599953 -0.002305 0.250164 x

x Nb 8 0.600709 0.002075 0.749901 x

x Nb 9 0.799336 -0.001779 0.250017 x

x Nb 10 0.800421 0.001646 0.749978 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460497E+004 57332.55 <-- SCF

1 -2.07460636E+004 4.64363330E-004 57350.47 <-- SCF

2 -2.07460647E+004 3.85280398E-005 57380.66 <-- SCF

3 -2.07460617E+004 -1.00927420E-004 57410.48 <-- SCF

4 -2.07460555E+004 -2.07631802E-004 57439.81 <-- SCF

5 -2.07460563E+004 2.66581756E-005 57469.02 <-- SCF

6 -2.07460563E+004 -3.20547613E-007 57495.41 <-- SCF

7 -2.07460562E+004 -4.10648323E-006 57518.88 <-- SCF

8 -2.07460561E+004 -2.77503592E-006 57544.09 <-- SCF

9 -2.07460561E+004 5.02201384E-007 57566.16 <-- SCF

10 -2.07460561E+004 -1.41266410E-007 57587.64 <-- SCF

11 -2.07460561E+004 -1.11387515E-007 57609.50 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05608399 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00012 0.00332 -0.00533 \*

\* Se 2 0.00223 -0.00010 0.00402 \*

\* Se 3 -0.00369 -0.00806 -0.01590 \*

\* Se 4 -0.00481 0.00430 0.00875 \*

\* Se 5 0.00445 0.00153 0.01354 \*

\* Se 6 0.00346 -0.00470 -0.00833 \*

\* Se 7 -0.00011 -0.00324 -0.00456 \*

\* Se 8 0.00277 0.00051 -0.00192 \*

\* Se 9 -0.00421 -0.00548 0.00103 \*

\* Se 10 0.01045 0.00260 -0.00627 \*

\* Se 11 0.00571 0.00622 -0.00411 \*

\* Se 12 -0.00884 -0.00187 0.00923 \*

\* Se 13 0.00124 0.00206 0.00348 \*

\* Se 14 -0.00145 -0.00115 0.00322 \*

\* Se 15 -0.00370 -0.00232 -0.01572 \*

\* Se 16 -0.00171 0.00371 0.00890 \*

\* Se 17 0.00477 0.00773 0.01230 \*

\* Se 18 0.00748 -0.00364 -0.00652 \*

\* Se 19 0.00203 -0.00212 0.00240 \*

\* Se 20 -0.00141 -0.00116 -0.00094 \*

\* Nb 1 -0.00103 -0.00735 -0.01243 \*

\* Nb 2 -0.00067 0.00798 0.01281 \*

\* Nb 3 0.00036 0.00725 -0.00894 \*

\* Nb 4 -0.00790 0.00020 0.00570 \*

\* Nb 5 -0.00087 -0.00458 -0.00534 \*

\* Nb 6 0.00504 -0.01097 0.00640 \*

\* Nb 7 -0.00560 0.01095 -0.00649 \*

\* Nb 8 -0.00131 0.00446 0.00621 \*

\* Nb 9 0.00258 0.00041 -0.00465 \*

\* Nb 10 -0.00513 -0.00650 0.00947 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.007797 -0.004039 0.015123 \*

\* y -0.004039 0.030144 -0.003882 \*

\* z 0.015123 -0.003882 0.018170 \*

\* \*

\* Pressure: -0.0135 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.732E-006 | -20746.056137 | <-- min BFGS

| trial step | 1.000000 | 1.175E-006 | -20746.056152 | <-- min BFGS

| line step | 3.111582 | -2.030E-006 | -20746.056123 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 36 with quad minimization (lambda= 1.774230)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8798224 -8.5747972 -0.0038714 0.4213994 -0.0014971 0.0001760

0.0122623 3.4513732 -0.0006710 1.0469499 1.8167690 0.0006877

-0.0054556 -0.0017961 13.0500783 0.0001788 0.0000930 0.4814673

Lattice parameters(A) Cell Angles

a = 17.173709 alpha = 90.019110

b = 3.451395 beta = 90.029732

c = 13.050080 gamma = 119.749995

Current cell volume = 671.569525 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 0.066599 0.662878 0.122746 x

x Se 2 0.134147 0.336372 0.622307 x

x Se 3 0.133950 0.336542 0.877629 x

x Se 4 0.066454 0.662787 0.377393 x

x Se 5 0.266369 0.663972 0.122337 x

x Se 6 0.333614 0.337577 0.622233 x

x Se 7 0.333455 0.337315 0.877660 x

x Se 8 0.266096 0.663658 0.377701 x

x Se 9 0.466823 0.664864 0.122843 x

x Se 10 0.533597 0.335675 0.622535 x

x Se 11 0.533158 0.335097 0.877169 x

x Se 12 0.466387 0.664278 0.377451 x

x Se 13 0.666542 0.662719 0.122356 x

x Se 14 0.733897 0.336336 0.622301 x

x Se 15 0.733627 0.336034 0.877666 x

x Se 16 0.666379 0.662448 0.377752 x

x Se 17 0.866049 0.663446 0.122385 x

x Se 18 0.933543 0.337177 0.622592 x

x Se 19 0.933407 0.337083 0.877273 x

x Se 20 0.865849 0.663642 0.377678 x

x Nb 1 -0.001010 -0.003642 0.250113 x

x Nb 2 0.001018 0.003610 0.749887 x

x Nb 3 0.199651 -0.001398 0.250008 x

x Nb 4 0.200659 0.001735 0.749992 x

x Nb 5 0.399276 -0.002060 0.250080 x

x Nb 6 0.400020 0.002186 0.749854 x

x Nb 7 0.599969 -0.002197 0.250145 x

x Nb 8 0.600710 0.002042 0.749917 x

x Nb 9 0.799369 -0.001676 0.250003 x

x Nb 10 0.800398 0.001499 0.749993 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460535E+004 58013.19 <-- SCF

1 -2.07460598E+004 2.08635283E-004 58031.19 <-- SCF

2 -2.07460604E+004 1.83931308E-005 58060.30 <-- SCF

3 -2.07460589E+004 -4.90621933E-005 58090.12 <-- SCF

4 -2.07460559E+004 -9.92236650E-005 58119.17 <-- SCF

5 -2.07460563E+004 1.26889112E-005 58147.44 <-- SCF

6 -2.07460563E+004 -1.35026543E-006 58173.00 <-- SCF

7 -2.07460562E+004 -2.45933759E-006 58195.25 <-- SCF

8 -2.07460561E+004 -9.48413780E-007 58218.47 <-- SCF

9 -2.07460562E+004 9.70508514E-008 58240.42 <-- SCF

10 -2.07460562E+004 1.11875682E-007 58261.95 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05615613 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00192 0.00085 -0.00760 \*

\* Se 2 0.00071 -0.00010 0.00524 \*

\* Se 3 -0.00015 -0.00692 -0.00891 \*

\* Se 4 -0.00327 0.00142 0.00429 \*

\* Se 5 0.00166 0.00093 0.00646 \*

\* Se 6 0.00124 -0.00345 -0.00278 \*

\* Se 7 0.00132 -0.00190 -0.00203 \*

\* Se 8 0.00227 0.00011 -0.00259 \*

\* Se 9 -0.00487 -0.00687 -0.00132 \*

\* Se 10 0.00868 0.00427 -0.00220 \*

\* Se 11 0.00667 0.00751 -0.00243 \*

\* Se 12 -0.00662 -0.00363 0.00593 \*

\* Se 13 -0.00051 0.00085 -0.00065 \*

\* Se 14 -0.00169 -0.00097 0.00567 \*

\* Se 15 -0.00174 -0.00192 -0.01013 \*

\* Se 16 0.00015 0.00251 0.00513 \*

\* Se 17 0.00154 0.00633 0.00464 \*

\* Se 18 0.00533 -0.00066 -0.00216 \*

\* Se 19 0.00314 0.00035 0.00510 \*

\* Se 20 0.00065 -0.00145 -0.00122 \*

\* Nb 1 0.00246 -0.00504 -0.00680 \*

\* Nb 2 -0.00338 0.00547 0.00693 \*

\* Nb 3 -0.00224 0.00839 -0.00314 \*

\* Nb 4 -0.00517 -0.00073 0.00059 \*

\* Nb 5 0.00112 -0.00150 -0.00141 \*

\* Nb 6 0.00669 -0.01191 0.00145 \*

\* Nb 7 -0.00730 0.01200 -0.00160 \*

\* Nb 8 -0.00248 0.00174 0.00204 \*

\* Nb 9 0.00137 0.00176 0.00004 \*

\* Nb 10 -0.00365 -0.00746 0.00347 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.014484 -0.002637 0.002169 \*

\* y -0.002637 0.006032 -0.003860 \*

\* z 0.002169 -0.003860 0.007357 \*

\* \*

\* Pressure: 0.0004 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.732E-006 | -20746.056137 | <-- min BFGS

| trial step | 1.000000 | 1.175E-006 | -20746.056152 | <-- min BFGS

| line step | 3.111582 | -2.030E-006 | -20746.056123 | <-- min BFGS

| quad step | 1.774230 | -6.023E-007 | -20746.056170 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 36 with enthalpy= -2.07460562E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.101877E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 1.413512E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 8.602645E-004 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.448414E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 37 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 7.593E-007 | -20746.056170 | <-- 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)

14.8806258 -8.5748219 -0.0042215 0.4213760 -0.0014983 0.0001826

0.0122726 3.4514018 -0.0006353 1.0468860 1.8167510 0.0006868

-0.0056622 -0.0016706 13.0495882 0.0001873 0.0000880 0.4814854

Lattice parameters(A) Cell Angles

a = 17.174417 alpha = 90.017969

b = 3.451424 beta = 90.031961

c = 13.049590 gamma = 119.748559

Current cell volume = 671.587197 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 0.066610 0.663028 0.122741 x

x Se 2 0.134127 0.336317 0.622309 x

x Se 3 0.133923 0.336446 0.877625 x

x Se 4 0.066464 0.662920 0.377393 x

x Se 5 0.266376 0.664058 0.122335 x

x Se 6 0.333599 0.337464 0.622239 x

x Se 7 0.333437 0.337191 0.877656 x

x Se 8 0.266108 0.663742 0.377702 x

x Se 9 0.466827 0.664927 0.122839 x

x Se 10 0.533585 0.335600 0.622543 x

x Se 11 0.533154 0.335037 0.877170 x

x Se 12 0.466400 0.664355 0.377446 x

x Se 13 0.666560 0.662840 0.122358 x

x Se 14 0.733885 0.336253 0.622300 x

x Se 15 0.733620 0.335948 0.877667 x

x Se 16 0.666395 0.662558 0.377747 x

x Se 17 0.866078 0.663544 0.122387 x

x Se 18 0.933534 0.337049 0.622594 x

x Se 19 0.933395 0.336938 0.877277 x

x Se 20 0.865870 0.663696 0.377679 x

x Nb 1 -0.000976 -0.003464 0.250110 x

x Nb 2 0.000983 0.003435 0.749890 x

x Nb 3 0.199662 -0.001266 0.250008 x

x Nb 4 0.200633 0.001631 0.749991 x

x Nb 5 0.399284 -0.001975 0.250077 x

x Nb 6 0.400016 0.002051 0.749859 x

x Nb 7 0.599971 -0.002067 0.250141 x

x Nb 8 0.600703 0.001960 0.749920 x

x Nb 9 0.799393 -0.001577 0.250005 x

x Nb 10 0.800381 0.001358 0.749993 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460544E+004 58665.78 <-- SCF

1 -2.07460608E+004 2.13794200E-004 58684.30 <-- SCF

2 -2.07460615E+004 2.22466018E-005 58712.86 <-- SCF

3 -2.07460655E+004 1.36265289E-004 58742.55 <-- SCF

4 -2.07460546E+004 -3.66378912E-004 58771.75 <-- SCF

5 -2.07460560E+004 4.80901503E-005 58799.47 <-- SCF

6 -2.07460564E+004 1.29572945E-005 58825.25 <-- SCF

7 -2.07460563E+004 -3.12686197E-006 58848.27 <-- SCF

8 -2.07460562E+004 -2.70981158E-006 58870.28 <-- SCF

9 -2.07460562E+004 -1.90340079E-006 58892.97 <-- SCF

10 -2.07460561E+004 -4.14756602E-007 58915.52 <-- SCF

11 -2.07460561E+004 2.03497100E-007 58937.48 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05614781 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00321 0.00011 -0.00676 \*

\* Se 2 -0.00045 -0.00036 0.00408 \*

\* Se 3 0.00015 -0.00643 -0.00761 \*

\* Se 4 -0.00389 0.00089 0.00423 \*

\* Se 5 0.00115 0.00080 0.00676 \*

\* Se 6 -0.00023 -0.00295 -0.00396 \*

\* Se 7 0.00020 -0.00156 -0.00111 \*

\* Se 8 0.00225 0.00018 -0.00273 \*

\* Se 9 -0.00472 -0.00628 -0.00065 \*

\* Se 10 0.00805 0.00364 -0.00374 \*

\* Se 11 0.00626 0.00674 -0.00152 \*

\* Se 12 -0.00630 -0.00321 0.00569 \*

\* Se 13 -0.00076 0.00067 -0.00056 \*

\* Se 14 -0.00099 -0.00108 0.00507 \*

\* Se 15 -0.00052 -0.00182 -0.00974 \*

\* Se 16 0.00027 0.00221 0.00524 \*

\* Se 17 0.00010 0.00600 0.00418 \*

\* Se 18 0.00485 0.00001 -0.00204 \*

\* Se 19 0.00341 0.00117 0.00405 \*

\* Se 20 0.00073 -0.00096 -0.00107 \*

\* Nb 1 -0.00099 -0.00698 -0.00589 \*

\* Nb 2 -0.00186 0.00670 0.00634 \*

\* Nb 3 -0.00385 0.00459 -0.00284 \*

\* Nb 4 -0.00292 0.00026 0.00062 \*

\* Nb 5 -0.00225 -0.00294 -0.00090 \*

\* Nb 6 0.00853 -0.00829 0.00126 \*

\* Nb 7 -0.00723 0.00879 -0.00133 \*

\* Nb 8 0.00389 0.00352 0.00151 \*

\* Nb 9 0.00075 0.00070 0.00018 \*

\* Nb 10 -0.00044 -0.00412 0.00325 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.006402 -0.003666 -0.000327 \*

\* y -0.003666 0.006529 -0.003838 \*

\* z -0.000327 -0.003838 0.002143 \*

\* \*

\* Pressure: -0.0008 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 7.593E-007 | -20746.056170 | <-- min BFGS

| trial step | 1.000000 | 8.844E-008 | -20746.056167 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 37 with enthalpy= -2.07460562E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 9.021004E-008 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 1.196164E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.025486E-004 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 6.529225E-003 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 38 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.853E-007 | -20746.056167 | <-- 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)

14.8810214 -8.5745693 -0.0046151 0.4213636 -0.0015005 0.0001926

0.0122906 3.4513333 -0.0006308 1.0468451 1.8167817 0.0007096

-0.0059716 -0.0016564 13.0495982 0.0001996 0.0000873 0.4814851

Lattice parameters(A) Cell Angles

a = 17.174634 alpha = 90.017838

b = 3.451355 beta = 90.034483

c = 13.049600 gamma = 119.746865

Current cell volume = 671.594191 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 0.066611 0.663046 0.122742 x

x Se 2 0.134126 0.336312 0.622313 x

x Se 3 0.133919 0.336433 0.877618 x

x Se 4 0.066465 0.662937 0.377394 x

x Se 5 0.266378 0.664063 0.122342 x

x Se 6 0.333597 0.337459 0.622238 x

x Se 7 0.333435 0.337183 0.877654 x

x Se 8 0.266111 0.663749 0.377698 x

x Se 9 0.466827 0.664937 0.122841 x

x Se 10 0.533585 0.335589 0.622544 x

x Se 11 0.533155 0.335028 0.877168 x

x Se 12 0.466399 0.664367 0.377446 x

x Se 13 0.666563 0.662851 0.122361 x

x Se 14 0.733883 0.336247 0.622304 x

x Se 15 0.733619 0.335943 0.877660 x

x Se 16 0.666397 0.662565 0.377748 x

x Se 17 0.866082 0.663557 0.122393 x

x Se 18 0.933534 0.337033 0.622593 x

x Se 19 0.933395 0.336922 0.877275 x

x Se 20 0.865870 0.663700 0.377675 x

x Nb 1 -0.000974 -0.003457 0.250108 x

x Nb 2 0.000981 0.003429 0.749892 x

x Nb 3 0.199665 -0.001253 0.250005 x

x Nb 4 0.200628 0.001619 0.749993 x

x Nb 5 0.399282 -0.001985 0.250075 x

x Nb 6 0.400014 0.002045 0.749861 x

x Nb 7 0.599973 -0.002061 0.250139 x

x Nb 8 0.600705 0.001970 0.749922 x

x Nb 9 0.799397 -0.001569 0.250003 x

x Nb 10 0.800378 0.001342 0.749996 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460561E+004 59341.61 <-- SCF

1 -2.07460567E+004 2.13766604E-005 59360.38 <-- SCF

2 -2.07460568E+004 2.33309937E-006 59382.38 <-- SCF

3 -2.07460574E+004 1.93249126E-005 59411.36 <-- SCF

4 -2.07460561E+004 -4.33953194E-005 59439.78 <-- SCF

5 -2.07460561E+004 3.11035258E-006 59463.00 <-- SCF

6 -2.07460562E+004 2.55305326E-007 59485.00 <-- SCF

7 -2.07460562E+004 -1.09700691E-007 59506.12 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05615038 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00276 -0.00114 -0.00694 \*

\* Se 2 0.00055 0.00011 0.00345 \*

\* Se 3 0.00238 -0.00557 -0.00551 \*

\* Se 4 -0.00270 -0.00037 0.00341 \*

\* Se 5 0.00199 0.00032 0.00498 \*

\* Se 6 0.00151 -0.00253 -0.00283 \*

\* Se 7 0.00282 -0.00109 -0.00075 \*

\* Se 8 0.00335 -0.00019 -0.00225 \*

\* Se 9 -0.00416 -0.00664 -0.00097 \*

\* Se 10 0.00755 0.00421 -0.00365 \*

\* Se 11 0.00625 0.00724 -0.00071 \*

\* Se 12 -0.00523 -0.00362 0.00527 \*

\* Se 13 -0.00224 0.00019 -0.00105 \*

\* Se 14 -0.00173 -0.00069 0.00421 \*

\* Se 15 -0.00091 -0.00129 -0.00743 \*

\* Se 16 -0.00045 0.00177 0.00441 \*

\* Se 17 -0.00252 0.00528 0.00253 \*

\* Se 18 0.00401 0.00101 -0.00175 \*

\* Se 19 0.00325 0.00216 0.00497 \*

\* Se 20 -0.00067 -0.00131 -0.00067 \*

\* Nb 1 -0.00169 -0.00579 -0.00742 \*

\* Nb 2 -0.00131 0.00633 0.00735 \*

\* Nb 3 -0.00027 0.00714 -0.00409 \*

\* Nb 4 -0.00375 -0.00058 0.00106 \*

\* Nb 5 -0.00159 -0.00322 -0.00204 \*

\* Nb 6 0.00763 -0.01017 0.00222 \*

\* Nb 7 -0.00628 0.00988 -0.00231 \*

\* Nb 8 0.00234 0.00347 0.00265 \*

\* Nb 9 0.00067 0.00097 -0.00051 \*

\* Nb 10 -0.00605 -0.00589 0.00439 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.004701 -0.002492 -0.004071 \*

\* y -0.002492 0.000117 -0.003952 \*

\* z -0.004071 -0.003952 -0.003258 \*

\* \*

\* Pressure: 0.0026 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.853E-007 | -20746.056167 | <-- min BFGS

| trial step | 1.000000 | 9.890E-008 | -20746.056178 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 38 with line minimization (lambda= 2.144946)

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

14.8814743 -8.5742802 -0.0050658 0.4213493 -0.0015030 0.0002041

0.0123113 3.4512549 -0.0006258 1.0467982 1.8168169 0.0007358

-0.0063259 -0.0016401 13.0496096 0.0002138 0.0000865 0.4814847

Lattice parameters(A) Cell Angles

a = 17.174882 alpha = 90.017689

b = 3.451277 beta = 90.037371

c = 13.049611 gamma = 119.744927

Current cell volume = 671.602197 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 0.066613 0.663067 0.122744 x

x Se 2 0.134125 0.336306 0.622318 x

x Se 3 0.133915 0.336417 0.877610 x

x Se 4 0.066465 0.662956 0.377395 x

x Se 5 0.266379 0.664069 0.122349 x

x Se 6 0.333595 0.337453 0.622237 x

x Se 7 0.333432 0.337172 0.877652 x

x Se 8 0.266113 0.663757 0.377693 x

x Se 9 0.466826 0.664948 0.122843 x

x Se 10 0.533585 0.335575 0.622545 x

x Se 11 0.533155 0.335016 0.877165 x

x Se 12 0.466399 0.664380 0.377445 x

x Se 13 0.666566 0.662863 0.122363 x

x Se 14 0.733880 0.336239 0.622308 x

x Se 15 0.733617 0.335938 0.877652 x

x Se 16 0.666400 0.662573 0.377748 x

x Se 17 0.866086 0.663571 0.122401 x

x Se 18 0.933534 0.337016 0.622593 x

x Se 19 0.933394 0.336904 0.877272 x

x Se 20 0.865870 0.663704 0.377671 x

x Nb 1 -0.000972 -0.003449 0.250105 x

x Nb 2 0.000979 0.003422 0.749895 x

x Nb 3 0.199669 -0.001237 0.250002 x

x Nb 4 0.200623 0.001606 0.749995 x

x Nb 5 0.399280 -0.001996 0.250073 x

x Nb 6 0.400012 0.002039 0.749864 x

x Nb 7 0.599975 -0.002054 0.250136 x

x Nb 8 0.600708 0.001981 0.749925 x

x Nb 9 0.799401 -0.001561 0.250001 x

x Nb 10 0.800373 0.001324 0.749999 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460560E+004 59908.20 <-- SCF

1 -2.07460598E+004 1.28342852E-004 59928.47 <-- SCF

2 -2.07460603E+004 1.54354813E-005 59951.48 <-- SCF

3 -2.07460654E+004 1.70599531E-004 59981.11 <-- SCF

4 -2.07460548E+004 -3.54618769E-004 60010.23 <-- SCF

5 -2.07460559E+004 3.86896594E-005 60038.16 <-- SCF

6 -2.07460563E+004 1.20021265E-005 60062.12 <-- SCF

7 -2.07460563E+004 -2.63326763E-007 60084.27 <-- SCF

8 -2.07460562E+004 -2.65334948E-006 60106.83 <-- SCF

9 -2.07460561E+004 -1.32813666E-006 60128.92 <-- SCF

10 -2.07460561E+004 -1.89287892E-007 60150.88 <-- SCF

11 -2.07460561E+004 1.44279037E-007 60172.86 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05614864 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00278 -0.00123 -0.00739 \*

\* Se 2 0.00152 0.00000 0.00311 \*

\* Se 3 0.00462 -0.00535 -0.00433 \*

\* Se 4 -0.00191 -0.00046 0.00323 \*

\* Se 5 0.00161 0.00007 0.00175 \*

\* Se 6 -0.00014 -0.00261 -0.00122 \*

\* Se 7 0.00214 -0.00111 -0.00146 \*

\* Se 8 0.00373 -0.00031 -0.00008 \*

\* Se 9 -0.00522 -0.00678 -0.00204 \*

\* Se 10 0.00475 0.00440 -0.00368 \*

\* Se 11 0.00424 0.00744 -0.00019 \*

\* Se 12 -0.00545 -0.00377 0.00588 \*

\* Se 13 -0.00154 -0.00007 -0.00127 \*

\* Se 14 -0.00283 -0.00045 0.00298 \*

\* Se 15 -0.00134 -0.00093 -0.00525 \*

\* Se 16 0.00110 0.00154 0.00374 \*

\* Se 17 -0.00147 0.00453 0.00066 \*

\* Se 18 0.00579 0.00120 -0.00113 \*

\* Se 19 0.00594 0.00231 0.00498 \*

\* Se 20 0.00168 -0.00169 0.00043 \*

\* Nb 1 -0.00088 -0.00534 -0.00487 \*

\* Nb 2 0.00375 0.00570 0.00494 \*

\* Nb 3 -0.00332 0.00698 -0.00146 \*

\* Nb 4 -0.00194 -0.00043 -0.00095 \*

\* Nb 5 0.00015 -0.00177 0.00009 \*

\* Nb 6 0.00221 -0.01013 0.00013 \*

\* Nb 7 -0.00978 0.00991 -0.00021 \*

\* Nb 8 -0.00322 0.00202 0.00045 \*

\* Nb 9 -0.00308 0.00220 0.00145 \*

\* Nb 10 0.00169 -0.00587 0.00171 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.000462 -0.001409 -0.006871 \*

\* y -0.001409 -0.000469 -0.004449 \*

\* z -0.006871 -0.004449 -0.004215 \*

\* \*

\* Pressure: 0.0014 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.853E-007 | -20746.056167 | <-- min BFGS

| trial step | 1.000000 | 9.890E-008 | -20746.056178 | <-- min BFGS

| line step | 2.144946 | -6.238E-008 | -20746.056170 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 38 with enthalpy= -2.07460562E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 8.528014E-008 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 1.392838E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.344699E-004 | 5.000000E-004 | A | Yes | <-- BFGS

| Smax | 6.870973E-003 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 39 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 2.138E-007 | -20746.056170 | <-- 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)

14.8815017 -8.5743482 -0.0048923 0.4213490 -0.0015022 0.0001985

0.0123047 3.4512705 -0.0006104 1.0468010 1.8168107 0.0007143

-0.0061535 -0.0015852 13.0495841 0.0002069 0.0000844 0.4814856

Lattice parameters(A) Cell Angles

a = 17.174940 alpha = 90.017189

b = 3.451292 beta = 90.036256

c = 13.049586 gamma = 119.745188

Current cell volume = 671.604422 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 0.066609 0.663031 0.122743 x

x Se 2 0.134130 0.336322 0.622316 x

x Se 3 0.133922 0.336436 0.877613 x

x Se 4 0.066462 0.662923 0.377394 x

x Se 5 0.266379 0.664050 0.122347 x

x Se 6 0.333598 0.337475 0.622236 x

x Se 7 0.333436 0.337199 0.877653 x

x Se 8 0.266112 0.663739 0.377695 x

x Se 9 0.466823 0.664920 0.122843 x

x Se 10 0.533590 0.335604 0.622544 x

x Se 11 0.533159 0.335046 0.877165 x

x Se 12 0.466394 0.664352 0.377446 x

x Se 13 0.666563 0.662835 0.122361 x

x Se 14 0.733882 0.336256 0.622308 x

x Se 15 0.733618 0.335956 0.877655 x

x Se 16 0.666397 0.662550 0.377750 x

x Se 17 0.866079 0.663553 0.122397 x

x Se 18 0.933538 0.337050 0.622593 x

x Se 19 0.933398 0.336940 0.877273 x

x Se 20 0.865866 0.663689 0.377673 x

x Nb 1 -0.000977 -0.003485 0.250106 x

x Nb 2 0.000984 0.003458 0.749894 x

x Nb 3 0.199664 -0.001259 0.250004 x

x Nb 4 0.200629 0.001626 0.749994 x

x Nb 5 0.399279 -0.002008 0.250075 x

x Nb 6 0.400014 0.002056 0.749862 x

x Nb 7 0.599973 -0.002070 0.250138 x

x Nb 8 0.600707 0.001992 0.749923 x

x Nb 9 0.799394 -0.001580 0.250002 x

x Nb 10 0.800378 0.001346 0.749997 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460561E+004 60575.98 <-- SCF

1 -2.07460565E+004 1.41729494E-005 60594.81 <-- SCF

2 -2.07460566E+004 2.42343695E-006 60616.45 <-- SCF

3 -2.07460576E+004 3.57566849E-005 60645.47 <-- SCF

4 -2.07460554E+004 -7.35704217E-005 60673.88 <-- SCF

5 -2.07460558E+004 1.16000153E-005 60696.55 <-- SCF

6 -2.07460561E+004 1.00813763E-005 60718.75 <-- SCF

7 -2.07460562E+004 3.26750079E-006 60740.70 <-- SCF

8 -2.07460562E+004 1.08120049E-006 60762.50 <-- SCF

9 -2.07460562E+004 1.25250553E-007 60783.88 <-- SCF

10 -2.07460562E+004 -4.96641608E-007 60805.23 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05620360 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00230 -0.00012 -0.00845 \*

\* Se 2 -0.00008 0.00002 0.00444 \*

\* Se 3 0.00240 -0.00547 -0.00647 \*

\* Se 4 -0.00206 0.00044 0.00502 \*

\* Se 5 0.00215 0.00100 0.00216 \*

\* Se 6 -0.00004 -0.00308 -0.00099 \*

\* Se 7 0.00180 -0.00185 -0.00262 \*

\* Se 8 0.00381 0.00036 0.00035 \*

\* Se 9 -0.00341 -0.00590 -0.00327 \*

\* Se 10 0.00613 0.00403 -0.00303 \*

\* Se 11 0.00557 0.00667 -0.00130 \*

\* Se 12 -0.00395 -0.00328 0.00741 \*

\* Se 13 -0.00145 0.00110 -0.00186 \*

\* Se 14 -0.00291 -0.00085 0.00465 \*

\* Se 15 -0.00157 -0.00156 -0.00784 \*

\* Se 16 0.00067 0.00246 0.00511 \*

\* Se 17 -0.00139 0.00511 0.00090 \*

\* Se 18 0.00396 0.00044 -0.00049 \*

\* Se 19 0.00379 0.00141 0.00360 \*

\* Se 20 0.00097 -0.00128 0.00089 \*

\* Nb 1 -0.00267 -0.00622 -0.00447 \*

\* Nb 2 -0.00056 0.00635 0.00462 \*

\* Nb 3 -0.00246 0.00577 -0.00073 \*

\* Nb 4 0.00325 -0.00034 -0.00161 \*

\* Nb 5 -0.00204 -0.00259 0.00106 \*

\* Nb 6 0.00890 -0.00950 -0.00076 \*

\* Nb 7 -0.00759 0.00893 0.00070 \*

\* Nb 8 -0.00178 0.00212 -0.00021 \*

\* Nb 9 -0.00548 0.00145 0.00204 \*

\* Nb 10 -0.00165 -0.00562 0.00115 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.002489 -0.001873 -0.004973 \*

\* y -0.001873 0.001912 -0.003510 \*

\* z -0.004973 -0.003510 -0.001432 \*

\* \*

\* Pressure: -0.0010 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 2.138E-007 | -20746.056170 | <-- min BFGS

| trial step | 1.000000 | 1.706E-007 | -20746.056229 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 39 with line minimization (lambda= 4.947061)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8816097 -8.5746166 -0.0042073 0.4213478 -0.0014990 0.0001765

0.0122787 3.4513319 -0.0005496 1.0468120 1.8167862 0.0006295

-0.0054727 -0.0013684 13.0494835 0.0001799 0.0000760 0.4814893

Lattice parameters(A) Cell Angles

a = 17.175167 alpha = 90.015218

b = 3.451354 beta = 90.031856

c = 13.049485 gamma = 119.746221

Current cell volume = 671.613201 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 0.066596 0.662889 0.122737 x

x Se 2 0.134148 0.336383 0.622310 x

x Se 3 0.133948 0.336511 0.877625 x

x Se 4 0.066451 0.662793 0.377392 x

x Se 5 0.266377 0.663977 0.122335 x

x Se 6 0.333609 0.337560 0.622235 x

x Se 7 0.333449 0.337304 0.877657 x

x Se 8 0.266108 0.663670 0.377701 x

x Se 9 0.466811 0.664806 0.122844 x

x Se 10 0.533611 0.335720 0.622538 x

x Se 11 0.533172 0.335164 0.877164 x

x Se 12 0.466376 0.664240 0.377452 x

x Se 13 0.666549 0.662724 0.122354 x

x Se 14 0.733886 0.336322 0.622305 x

x Se 15 0.733620 0.336025 0.877663 x

x Se 16 0.666386 0.662460 0.377754 x

x Se 17 0.866054 0.663481 0.122383 x

x Se 18 0.933551 0.337183 0.622596 x

x Se 19 0.933413 0.337084 0.877279 x

x Se 20 0.865850 0.663629 0.377681 x

x Nb 1 -0.000999 -0.003627 0.250109 x

x Nb 2 0.001007 0.003600 0.749891 x

x Nb 3 0.199645 -0.001346 0.250009 x

x Nb 4 0.200653 0.001705 0.749987 x

x Nb 5 0.399279 -0.002052 0.250081 x

x Nb 6 0.400018 0.002121 0.749853 x

x Nb 7 0.599966 -0.002135 0.250146 x

x Nb 8 0.600706 0.002034 0.749916 x

x Nb 9 0.799367 -0.001659 0.250008 x

x Nb 10 0.800395 0.001434 0.749992 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460530E+004 61208.56 <-- SCF

1 -2.07461575E+004 3.48317067E-003 61228.69 <-- SCF

2 -2.07461602E+004 9.04390511E-005 61257.47 <-- SCF

3 -2.07463168E+004 5.21880302E-003 61287.38 <-- SCF

4 -2.07460032E+004 -1.04516556E-002 61316.23 <-- SCF

5 -2.07460189E+004 5.21437127E-004 61346.05 <-- SCF

6 -2.07460527E+004 1.12777138E-003 61374.67 <-- SCF

7 -2.07460618E+004 3.04455990E-004 61401.36 <-- SCF

8 -2.07460641E+004 7.66690847E-005 61427.78 <-- SCF

9 -2.07460602E+004 -1.30958156E-004 61454.36 <-- SCF

10 -2.07460562E+004 -1.33787689E-004 61480.59 <-- SCF

11 -2.07460555E+004 -2.35300498E-005 61505.98 <-- SCF

12 -2.07460558E+004 9.31792675E-006 61529.64 <-- SCF

13 -2.07460566E+004 2.83166448E-005 61554.03 <-- SCF

14 -2.07460567E+004 3.12858612E-006 61575.44 <-- SCF

15 -2.07460563E+004 -1.38996323E-005 61598.75 <-- SCF

16 -2.07460561E+004 -6.60648609E-006 61621.62 <-- SCF

17 -2.07460561E+004 8.36795484E-007 61642.98 <-- SCF

18 -2.07460562E+004 1.16934731E-006 61664.39 <-- SCF

19 -2.07460562E+004 1.93678708E-007 61685.78 <-- SCF

20 -2.07460562E+004 -3.30696709E-007 61707.30 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05616317 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00110 0.00069 -0.00711 \*

\* Se 2 0.00026 -0.00012 0.00320 \*

\* Se 3 0.00071 -0.00668 -0.00740 \*

\* Se 4 -0.00268 0.00060 0.00549 \*

\* Se 5 0.00218 0.00246 0.00833 \*

\* Se 6 0.00166 -0.00399 -0.00348 \*

\* Se 7 0.00168 -0.00369 -0.00257 \*

\* Se 8 0.00214 0.00094 -0.00331 \*

\* Se 9 -0.00265 -0.00506 -0.00193 \*

\* Se 10 0.00626 0.00399 -0.00513 \*

\* Se 11 0.00412 0.00552 -0.00015 \*

\* Se 12 -0.00462 -0.00350 0.00705 \*

\* Se 13 -0.00152 0.00269 0.00110 \*

\* Se 14 -0.00082 -0.00157 0.00381 \*

\* Se 15 -0.00149 -0.00316 -0.00932 \*

\* Se 16 -0.00100 0.00310 0.00446 \*

\* Se 17 0.00082 0.00648 0.00653 \*

\* Se 18 0.00324 -0.00026 -0.00326 \*

\* Se 19 0.00099 0.00001 0.00456 \*

\* Se 20 0.00141 -0.00087 -0.00267 \*

\* Nb 1 -0.00424 -0.00618 -0.00666 \*

\* Nb 2 0.00041 0.00653 0.00691 \*

\* Nb 3 -0.00141 0.00490 -0.00368 \*

\* Nb 4 -0.00080 0.00007 0.00102 \*

\* Nb 5 -0.00069 -0.00320 -0.00125 \*

\* Nb 6 0.00803 -0.00871 0.00172 \*

\* Nb 7 -0.00774 0.00871 -0.00169 \*

\* Nb 8 -0.00106 0.00339 0.00193 \*

\* Nb 9 -0.00062 0.00068 -0.00038 \*

\* Nb 10 -0.00146 -0.00380 0.00389 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.004592 -0.003200 0.001773 \*

\* y -0.003200 0.008282 -0.000128 \*

\* z 0.001773 -0.000128 0.005214 \*

\* \*

\* Pressure: -0.0060 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 2.138E-007 | -20746.056170 | <-- min BFGS

| trial step | 1.000000 | 1.706E-007 | -20746.056229 | <-- min BFGS

| line step | 4.947061 | 1.472E-008 | -20746.056184 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 39 with enthalpy= -2.07460562E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 4.810498E-007 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 1.196853E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 5.637480E-004 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 8.282283E-003 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 40 ...

================================================================================

Writing analysis data to 2H-Nb1Se2-7.castep\_bin

Writing model to 2H-Nb1Se2-7.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.106E-007 | -20746.056184 | <-- 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)

14.8817902 -8.5740851 -0.0044228 0.4213407 -0.0015024 0.0001794

0.0123063 3.4511682 -0.0005075 1.0467793 1.8168641 0.0006163

-0.0055607 -0.0012224 13.0483433 0.0001835 0.0000702 0.4815314

Lattice parameters(A) Cell Angles

a = 17.175059 alpha = 90.013881

b = 3.451190 beta = 90.033232

c = 13.048345 gamma = 119.743916

Current cell volume = 671.533862 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 0.066586 0.662782 0.122724 x

x Se 2 0.134160 0.336415 0.622300 x

x Se 3 0.133968 0.336553 0.877635 x

x Se 4 0.066441 0.662694 0.377404 x

x Se 5 0.266373 0.663940 0.122328 x

x Se 6 0.333621 0.337613 0.622222 x

x Se 7 0.333464 0.337371 0.877667 x

x Se 8 0.266100 0.663626 0.377711 x

x Se 9 0.466805 0.664730 0.122835 x

x Se 10 0.533624 0.335806 0.622520 x

x Se 11 0.533178 0.335241 0.877173 x

x Se 12 0.466363 0.664156 0.377470 x

x Se 13 0.666533 0.662653 0.122342 x

x Se 14 0.733895 0.336365 0.622297 x

x Se 15 0.733623 0.336060 0.877668 x

x Se 16 0.666373 0.662403 0.377769 x

x Se 17 0.866035 0.663441 0.122371 x

x Se 18 0.933562 0.337283 0.622585 x

x Se 19 0.933424 0.337192 0.877291 x

x Se 20 0.865839 0.663598 0.377693 x

x Nb 1 -0.001019 -0.003753 0.250105 x

x Nb 2 0.001027 0.003727 0.749895 x

x Nb 3 0.199634 -0.001425 0.250008 x

x Nb 4 0.200668 0.001770 0.749988 x

x Nb 5 0.399280 -0.002092 0.250083 x

x Nb 6 0.400028 0.002184 0.749850 x

x Nb 7 0.599956 -0.002197 0.250149 x

x Nb 8 0.600704 0.002074 0.749915 x

x Nb 9 0.799350 -0.001725 0.250008 x

x Nb 10 0.800406 0.001513 0.749994 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460553E+004 62108.64 <-- SCF

1 -2.07460581E+004 9.11547710E-005 62126.95 <-- SCF

2 -2.07460584E+004 1.05071861E-005 62155.23 <-- SCF

3 -2.07460587E+004 1.04973676E-005 62184.91 <-- SCF

4 -2.07460558E+004 -9.56305890E-005 62214.02 <-- SCF

5 -2.07460563E+004 1.52566550E-005 62240.77 <-- SCF

6 -2.07460563E+004 2.14225004E-007 62264.69 <-- SCF

7 -2.07460562E+004 -2.64290639E-006 62286.75 <-- SCF

8 -2.07460562E+004 -7.87876555E-007 62308.78 <-- SCF

9 -2.07460562E+004 2.30234262E-008 62330.86 <-- SCF

10 -2.07460562E+004 2.30114644E-007 62352.77 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05618288 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00012 0.00156 -0.00669 \*

\* Se 2 -0.00051 -0.00020 0.00406 \*

\* Se 3 -0.00053 -0.00705 -0.00802 \*

\* Se 4 -0.00155 0.00096 0.00450 \*

\* Se 5 0.00272 0.00274 0.00764 \*

\* Se 6 0.00118 -0.00373 -0.00259 \*

\* Se 7 0.00124 -0.00397 -0.00327 \*

\* Se 8 0.00306 0.00072 -0.00318 \*

\* Se 9 -0.00319 -0.00415 -0.00363 \*

\* Se 10 0.00493 0.00390 -0.00579 \*

\* Se 11 0.00343 0.00482 0.00141 \*

\* Se 12 -0.00431 -0.00319 0.00776 \*

\* Se 13 -0.00176 0.00380 0.00113 \*

\* Se 14 -0.00271 -0.00125 0.00410 \*

\* Se 15 -0.00284 -0.00335 -0.00911 \*

\* Se 16 -0.00119 0.00365 0.00436 \*

\* Se 17 0.00169 0.00666 0.00689 \*

\* Se 18 0.00160 0.00020 -0.00378 \*

\* Se 19 -0.00069 0.00001 0.00557 \*

\* Se 20 0.00175 -0.00100 -0.00330 \*

\* Nb 1 -0.00746 -0.00746 -0.00682 \*

\* Nb 2 0.00653 0.00657 0.00713 \*

\* Nb 3 -0.00197 0.00404 -0.00356 \*

\* Nb 4 0.00406 0.00091 0.00082 \*

\* Nb 5 0.00033 -0.00412 -0.00066 \*

\* Nb 6 0.00919 -0.00876 0.00113 \*

\* Nb 7 -0.00817 0.00654 -0.00110 \*

\* Nb 8 -0.00191 0.00458 0.00133 \*

\* Nb 9 -0.00318 0.00017 -0.00022 \*

\* Nb 10 0.00037 -0.00360 0.00390 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.013508 -0.001777 0.001151 \*

\* y -0.001777 0.009057 0.001391 \*

\* z 0.001151 0.001391 0.010800 \*

\* \*

\* Pressure: -0.0111 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.106E-007 | -20746.056184 | <-- min BFGS

| trial step | 1.000000 | 7.805E-007 | -20746.056199 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 40 with line minimization (lambda= -3.594428)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8809609 -8.5765273 -0.0034325 0.4213730 -0.0014867 0.0001662

0.0121794 3.4519203 -0.0007009 1.0469296 1.8165063 0.0006770

-0.0051566 -0.0018933 13.0535820 0.0001670 0.0000971 0.4813381

Lattice parameters(A) Cell Angles

a = 17.175559 alpha = 90.020024

b = 3.451942 beta = 90.026911

c = 13.053583 gamma = 119.754507

Current cell volume = 671.898397 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 0.066632 0.663274 0.122786 x

x Se 2 0.134104 0.336267 0.622347 x

x Se 3 0.133875 0.336361 0.877587 x

x Se 4 0.066487 0.663151 0.377350 x

x Se 5 0.266390 0.664112 0.122362 x

x Se 6 0.333563 0.337369 0.622282 x

x Se 7 0.333398 0.337064 0.877624 x

x Se 8 0.266138 0.663829 0.377664 x

x Se 9 0.466832 0.665080 0.122877 x

x Se 10 0.533562 0.335410 0.622604 x

x Se 11 0.533150 0.334884 0.877131 x

x Se 12 0.466421 0.664541 0.377387 x

x Se 13 0.666604 0.662980 0.122395 x

x Se 14 0.733855 0.336168 0.622334 x

x Se 15 0.733606 0.335898 0.877644 x

x Se 16 0.666434 0.662662 0.377701 x

x Se 17 0.866124 0.663624 0.122427 x

x Se 18 0.933513 0.336821 0.622635 x

x Se 19 0.933376 0.336696 0.877233 x

x Se 20 0.865889 0.663740 0.377639 x

x Nb 1 -0.000930 -0.003171 0.250122 x

x Nb 2 0.000935 0.003143 0.749877 x

x Nb 3 0.199686 -0.001060 0.250014 x

x Nb 4 0.200600 0.001470 0.749987 x

x Nb 5 0.399275 -0.001906 0.250075 x

x Nb 6 0.399983 0.001891 0.749863 x

x Nb 7 0.600000 -0.001914 0.250137 x

x Nb 8 0.600713 0.001890 0.749922 x

x Nb 9 0.799428 -0.001422 0.250008 x

x Nb 10 0.800354 0.001149 0.749986 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460378E+004 62755.20 <-- SCF

1 -2.07460882E+004 1.68011032E-003 62773.58 <-- SCF

2 -2.07460931E+004 1.64058310E-004 62805.09 <-- SCF

3 -2.07460875E+004 -1.87833314E-004 62834.64 <-- SCF

4 -2.07460525E+004 -1.16644133E-003 62863.84 <-- SCF

5 -2.07460567E+004 1.39164734E-004 62893.67 <-- SCF

6 -2.07460569E+004 8.45213806E-006 62922.53 <-- SCF

7 -2.07460564E+004 -1.86933107E-005 62949.97 <-- SCF

8 -2.07460560E+004 -1.23660788E-005 62976.86 <-- SCF

9 -2.07460560E+004 7.94881237E-007 62999.48 <-- SCF

10 -2.07460561E+004 4.63438769E-007 63021.45 <-- SCF

11 -2.07460560E+004 -9.09027810E-008 63043.33 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05604925 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00386 0.00039 -0.00678 \*

\* Se 2 0.00299 -0.00076 0.00282 \*

\* Se 3 0.00426 -0.00605 -0.00821 \*

\* Se 4 -0.00580 0.00198 0.00742 \*

\* Se 5 0.00064 0.00200 0.00642 \*

\* Se 6 0.00400 -0.00482 -0.00401 \*

\* Se 7 0.00347 -0.00268 -0.00243 \*

\* Se 8 -0.00054 0.00217 -0.00013 \*

\* Se 9 -0.00163 -0.00632 0.00238 \*

\* Se 10 0.00644 0.00334 -0.00155 \*

\* Se 11 0.00285 0.00705 -0.00593 \*

\* Se 12 -0.00497 -0.00256 0.00479 \*

\* Se 13 -0.00370 0.00193 -0.00119 \*

\* Se 14 0.00124 -0.00290 0.00364 \*

\* Se 15 -0.00064 -0.00285 -0.01072 \*

\* Se 16 -0.00360 0.00420 0.00710 \*

\* Se 17 -0.00289 0.00552 0.00422 \*

\* Se 18 0.00608 -0.00086 -0.00366 \*

\* Se 19 0.00340 0.00107 0.00259 \*

\* Se 20 -0.00129 -0.00069 0.00054 \*

\* Nb 1 -0.00201 -0.00900 -0.00775 \*

\* Nb 2 0.00200 0.00853 0.00837 \*

\* Nb 3 -0.00014 0.00193 -0.00466 \*

\* Nb 4 -0.00169 0.00300 0.00244 \*

\* Nb 5 0.00343 -0.00300 -0.00239 \*

\* Nb 6 0.00575 -0.00699 0.00294 \*

\* Nb 7 -0.00671 0.00677 -0.00290 \*

\* Nb 8 -0.00454 0.00308 0.00320 \*

\* Nb 9 0.00025 -0.00171 -0.00170 \*

\* Nb 10 -0.00278 -0.00178 0.00514 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.006108 -0.009240 0.004563 \*

\* y -0.009240 0.032652 -0.005448 \*

\* z 0.004563 -0.005448 0.017285 \*

\* \*

\* Pressure: -0.0187 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.106E-007 | -20746.056184 | <-- min BFGS

| trial step | 1.000000 | 7.805E-007 | -20746.056199 | <-- min BFGS

| line step | -3.594428 | 1.310E-006 | -20746.056083 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 40 with quad minimization (lambda= 4.863340)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8824876 -8.5720315 -0.0052556 0.4213136 -0.0015156 0.0001905

0.0124130 3.4505358 -0.0003449 1.0466530 1.8171652 0.0005652

-0.0059005 -0.0006583 13.0439383 0.0001974 0.0000474 0.4816940

Lattice parameters(A) Cell Angles

a = 17.174638 alpha = 90.008712

b = 3.450558 beta = 90.038549

c = 13.043940 gamma = 119.735010

Current cell volume = 671.227369 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 0.066547 0.662369 0.122671 x

x Se 2 0.134207 0.336540 0.622261 x

x Se 3 0.134046 0.336714 0.877675 x

x Se 4 0.066402 0.662310 0.377449 x

x Se 5 0.266359 0.663795 0.122298 x

x Se 6 0.333670 0.337819 0.622171 x

x Se 7 0.333519 0.337630 0.877703 x

x Se 8 0.266067 0.663456 0.377750 x

x Se 9 0.466783 0.664435 0.122799 x

x Se 10 0.533676 0.336139 0.622450 x

x Se 11 0.533201 0.335542 0.877208 x

x Se 12 0.466314 0.663833 0.377541 x

x Se 13 0.666474 0.662379 0.122298 x

x Se 14 0.733929 0.336531 0.622266 x

x Se 15 0.733638 0.336197 0.877689 x

x Se 16 0.666322 0.662186 0.377826 x

x Se 17 0.865959 0.663287 0.122324 x

x Se 18 0.933603 0.337673 0.622543 x

x Se 19 0.933464 0.337610 0.877341 x

x Se 20 0.865796 0.663478 0.377738 x

x Nb 1 -0.001094 -0.004243 0.250091 x

x Nb 2 0.001104 0.004219 0.749910 x

x Nb 3 0.199589 -0.001732 0.250003 x

x Nb 4 0.200724 0.002022 0.749988 x

x Nb 5 0.399283 -0.002249 0.250090 x

x Nb 6 0.400066 0.002431 0.749839 x

x Nb 7 0.599920 -0.002435 0.250159 x

x Nb 8 0.600696 0.002228 0.749909 x

x Nb 9 0.799285 -0.001980 0.250009 x

x Nb 10 0.800450 0.001819 0.750000 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07459956E+004 63444.22 <-- SCF

1 -2.07461507E+004 5.17122131E-003 63462.58 <-- SCF

2 -2.07461649E+004 4.73171611E-004 63494.52 <-- SCF

3 -2.07461320E+004 -1.09673954E-003 63524.59 <-- SCF

4 -2.07460490E+004 -2.76781411E-003 63553.75 <-- SCF

5 -2.07460608E+004 3.92383137E-004 63583.80 <-- SCF

6 -2.07460588E+004 -6.69073456E-005 63613.06 <-- SCF

7 -2.07460565E+004 -7.61249175E-005 63642.52 <-- SCF

8 -2.07460561E+004 -1.18823464E-005 63671.05 <-- SCF

9 -2.07460561E+004 -1.55468544E-006 63697.81 <-- SCF

10 -2.07460561E+004 2.47233020E-006 63722.27 <-- SCF

11 -2.07460562E+004 7.17883772E-007 63744.34 <-- SCF

12 -2.07460562E+004 3.28281760E-007 63766.66 <-- SCF

13 -2.07460562E+004 1.66059774E-007 63788.30 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05618237 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00416 0.00208 -0.00662 \*

\* Se 2 -0.00543 0.00106 0.00638 \*

\* Se 3 -0.00701 -0.00738 -0.00914 \*

\* Se 4 0.00305 -0.00047 0.00229 \*

\* Se 5 0.00134 0.00333 0.00921 \*

\* Se 6 -0.00015 -0.00340 -0.00134 \*

\* Se 7 0.00060 -0.00557 -0.00423 \*

\* Se 8 0.00279 -0.00056 -0.00638 \*

\* Se 9 -0.00395 -0.00367 -0.00725 \*

\* Se 10 0.00224 0.00549 -0.00532 \*

\* Se 11 0.00363 0.00441 0.00482 \*

\* Se 12 -0.00241 -0.00469 0.00757 \*

\* Se 13 0.00181 0.00470 0.00461 \*

\* Se 14 -0.00221 0.00070 0.00601 \*

\* Se 15 -0.00090 -0.00325 -0.00924 \*

\* Se 16 0.00293 0.00261 0.00071 \*

\* Se 17 0.00600 0.00825 0.00926 \*

\* Se 18 -0.00080 0.00027 -0.00071 \*

\* Se 19 -0.00249 -0.00182 0.00481 \*

\* Se 20 0.00415 -0.00085 -0.00641 \*

\* Nb 1 -0.00057 -0.00022 -0.00527 \*

\* Nb 2 -0.00153 0.00126 0.00511 \*

\* Nb 3 -0.00495 0.00926 -0.00237 \*

\* Nb 4 -0.00290 -0.00519 -0.00058 \*

\* Nb 5 -0.00427 -0.00254 0.00012 \*

\* Nb 6 0.00934 -0.01209 0.00037 \*

\* Nb 7 -0.00835 0.01203 -0.00023 \*

\* Nb 8 0.00586 0.00149 0.00038 \*

\* Nb 9 -0.00174 0.00344 0.00106 \*

\* Nb 10 0.00178 -0.00869 0.00237 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.000602 0.004227 -0.002270 \*

\* y 0.004227 -0.034082 0.007384 \*

\* z -0.002270 0.007384 -0.018946 \*

\* \*

\* Pressure: 0.0179 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 6.106E-007 | -20746.056184 | <-- min BFGS

| trial step | 1.000000 | 7.805E-007 | -20746.056199 | <-- min BFGS

| line step | -3.594428 | 1.310E-006 | -20746.056083 | <-- min BFGS

| quad step | 4.863340 | -9.230E-007 | -20746.056189 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 40 with enthalpy= -2.07460562E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.530667E-007 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 1.528558E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.968786E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 3.408209E-002 | 2.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 41 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.455E-006 | -20746.056189 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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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)

14.8830163 -8.5734213 -0.0045678 0.4213006 -0.0015119 0.0001769

0.0123849 3.4510412 -0.0004137 1.0466371 1.8169076 0.0005643

-0.0054825 -0.0008940 13.0465045 0.0001807 0.0000571 0.4815992

Lattice parameters(A) Cell Angles

a = 17.175790 alpha = 90.010880

b = 3.451063 beta = 90.034141

c = 13.046506 gamma = 119.738644

Current cell volume = 671.478470 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 0.066577 0.662704 0.122699 x

x Se 2 0.134167 0.336422 0.622298 x

x Se 3 0.133985 0.336550 0.877637 x

x Se 4 0.066431 0.662618 0.377421 x

x Se 5 0.266369 0.663940 0.122328 x

x Se 6 0.333634 0.337622 0.622207 x

x Se 7 0.333479 0.337397 0.877676 x

x Se 8 0.266091 0.663612 0.377716 x

x Se 9 0.466801 0.664652 0.122820 x

x Se 10 0.533636 0.335896 0.622498 x

x Se 11 0.533183 0.335324 0.877186 x

x Se 12 0.466352 0.664072 0.377495 x

x Se 13 0.666517 0.662619 0.122329 x

x Se 14 0.733905 0.336378 0.622296 x

x Se 15 0.733628 0.336056 0.877663 x

x Se 16 0.666360 0.662389 0.377787 x

x Se 17 0.866021 0.663447 0.122364 x

x Se 18 0.933573 0.337366 0.622571 x

x Se 19 0.933433 0.337277 0.877313 x

x Se 20 0.865836 0.663591 0.377700 x

x Nb 1 -0.001034 -0.003872 0.250096 x

x Nb 2 0.001043 0.003848 0.749905 x

x Nb 3 0.199624 -0.001473 0.250005 x

x Nb 4 0.200672 0.001810 0.749986 x

x Nb 5 0.399283 -0.002123 0.250085 x

x Nb 6 0.400046 0.002212 0.749848 x

x Nb 7 0.599937 -0.002226 0.250151 x

x Nb 8 0.600700 0.002107 0.749914 x

x Nb 9 0.799341 -0.001769 0.250010 x

x Nb 10 0.800411 0.001554 0.749997 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460484E+004 64189.23 <-- SCF

1 -2.07460694E+004 7.02775348E-004 64207.47 <-- SCF

2 -2.07460719E+004 8.26078013E-005 64237.45 <-- SCF

3 -2.07460781E+004 2.04516452E-004 64267.28 <-- SCF

4 -2.07460514E+004 -8.88545331E-004 64296.69 <-- SCF

5 -2.07460564E+004 1.65345734E-004 64326.56 <-- SCF

6 -2.07460574E+004 3.39844547E-005 64355.56 <-- SCF

7 -2.07460566E+004 -2.64669316E-005 64383.14 <-- SCF

8 -2.07460562E+004 -1.46753292E-005 64408.14 <-- SCF

9 -2.07460560E+004 -4.23751052E-006 64431.80 <-- SCF

10 -2.07460561E+004 2.21773258E-006 64454.11 <-- SCF

11 -2.07460562E+004 3.63878677E-006 64476.23 <-- SCF

12 -2.07460563E+004 2.73040407E-006 64498.27 <-- SCF

13 -2.07460563E+004 8.69626062E-007 64520.08 <-- SCF

14 -2.07460563E+004 -1.98155525E-007 64541.89 <-- SCF

15 -2.07460563E+004 1.11878548E-006 64563.80 <-- SCF

16 -2.07460563E+004 -6.25579292E-007 64585.59 <-- SCF

17 -2.07460563E+004 -1.11671712E-006 64606.75 <-- SCF

18 -2.07460562E+004 -2.20393575E-006 64628.31 <-- SCF

19 -2.07460562E+004 4.80697625E-007 64649.45 <-- SCF

20 -2.07460562E+004 -1.61226061E-007 64670.09 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05622653 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00175 0.00107 -0.00670 \*

\* Se 2 -0.00129 0.00127 0.00432 \*

\* Se 3 -0.00157 -0.00564 -0.00724 \*

\* Se 4 -0.00001 -0.00032 0.00369 \*

\* Se 5 0.00219 0.00266 0.00434 \*

\* Se 6 0.00086 -0.00175 -0.00022 \*

\* Se 7 0.00083 -0.00293 -0.00476 \*

\* Se 8 0.00227 0.00003 -0.00123 \*

\* Se 9 -0.00213 -0.00375 -0.00501 \*

\* Se 10 0.00490 0.00485 -0.00379 \*

\* Se 11 0.00363 0.00472 0.00110 \*

\* Se 12 -0.00331 -0.00385 0.00764 \*

\* Se 13 0.00093 0.00322 0.00204 \*

\* Se 14 -0.00216 0.00075 0.00366 \*

\* Se 15 -0.00221 -0.00199 -0.00701 \*

\* Se 16 0.00111 0.00210 0.00278 \*

\* Se 17 0.00203 0.00638 0.00373 \*

\* Se 18 0.00157 0.00115 -0.00044 \*

\* Se 19 -0.00056 0.00020 0.00307 \*

\* Se 20 0.00146 -0.00121 -0.00075 \*

\* Nb 1 -0.00425 -0.00343 -0.00566 \*

\* Nb 2 0.00118 0.00199 0.00567 \*

\* Nb 3 -0.00084 0.00471 -0.00273 \*

\* Nb 4 -0.00290 -0.00172 0.00041 \*

\* Nb 5 -0.00199 -0.00262 -0.00088 \*

\* Nb 6 0.01369 -0.01170 0.00078 \*

\* Nb 7 -0.00611 0.00797 -0.00100 \*

\* Nb 8 -0.00110 0.00114 0.00118 \*

\* Nb 9 -0.00771 0.00323 0.00008 \*

\* Nb 10 -0.00025 -0.00655 0.00292 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.018956 0.002834 0.001666 \*

\* y 0.002834 -0.001414 0.004448 \*

\* z 0.001666 0.004448 -0.004745 \*

\* \*

\* Pressure: -0.0043 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.455E-006 | -20746.056189 | <-- min BFGS

| trial step | 1.000000 | -3.660E-009 | -20746.056235 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 41 with enthalpy= -2.07460562E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 1.526937E-006 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 1.802072E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.189368E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 1.895595E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 42 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.907E-007 | -20746.056235 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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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)

14.8829375 -8.5733103 -0.0044010 0.4213022 -0.0015131 0.0001701

0.0123944 3.4510134 -0.0003767 1.0466359 1.8169194 0.0005292

-0.0052706 -0.0007638 13.0457951 0.0001723 0.0000520 0.4816254

Lattice parameters(A) Cell Angles

a = 17.175666 alpha = 90.009691

b = 3.451036 beta = 90.033065

c = 13.045796 gamma = 119.738295

Current cell volume = 671.434057 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 0.066579 0.662727 0.122686 x

x Se 2 0.134161 0.336402 0.622297 x

x Se 3 0.133981 0.336518 0.877639 x

x Se 4 0.066432 0.662638 0.377428 x

x Se 5 0.266368 0.663973 0.122325 x

x Se 6 0.333633 0.337583 0.622204 x

x Se 7 0.333479 0.337361 0.877679 x

x Se 8 0.266091 0.663637 0.377719 x

x Se 9 0.466803 0.664651 0.122810 x

x Se 10 0.533634 0.335900 0.622491 x

x Se 11 0.533181 0.335327 0.877193 x

x Se 12 0.466355 0.664073 0.377504 x

x Se 13 0.666516 0.662651 0.122324 x

x Se 14 0.733907 0.336354 0.622295 x

x Se 15 0.733629 0.336023 0.877664 x

x Se 16 0.666361 0.662425 0.377792 x

x Se 17 0.866025 0.663481 0.122359 x

x Se 18 0.933572 0.337350 0.622566 x

x Se 19 0.933431 0.337257 0.877324 x

x Se 20 0.865843 0.663611 0.377703 x

x Nb 1 -0.001030 -0.003854 0.250093 x

x Nb 2 0.001038 0.003828 0.749908 x

x Nb 3 0.199625 -0.001448 0.250005 x

x Nb 4 0.200665 0.001789 0.749984 x

x Nb 5 0.399286 -0.002101 0.250086 x

x Nb 6 0.400054 0.002177 0.749847 x

x Nb 7 0.599929 -0.002194 0.250152 x

x Nb 8 0.600697 0.002086 0.749913 x

x Nb 9 0.799345 -0.001750 0.250013 x

x Nb 10 0.800409 0.001524 0.749997 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460547E+004 65069.89 <-- SCF

1 -2.07461268E+004 2.40202022E-003 65090.00 <-- SCF

2 -2.07461290E+004 7.40247839E-005 65116.78 <-- SCF

3 -2.07462950E+004 5.53410721E-003 65146.48 <-- SCF

4 -2.07460129E+004 -9.40371702E-003 65175.50 <-- SCF

5 -2.07460167E+004 1.26332970E-004 65205.27 <-- SCF

6 -2.07460429E+004 8.73963941E-004 65234.33 <-- SCF

7 -2.07460588E+004 5.30098741E-004 65259.83 <-- SCF

8 -2.07460634E+004 1.51437856E-004 65286.53 <-- SCF

9 -2.07460609E+004 -8.30148822E-005 65313.17 <-- SCF

10 -2.07460586E+004 -7.73490912E-005 65337.44 <-- SCF

11 -2.07460562E+004 -7.73752157E-005 65363.06 <-- SCF

12 -2.07460554E+004 -2.89431985E-005 65389.84 <-- SCF

13 -2.07460563E+004 3.03271388E-005 65413.45 <-- SCF

14 -2.07460568E+004 1.80957610E-005 65435.38 <-- SCF

15 -2.07460569E+004 4.10531200E-006 65457.47 <-- SCF

16 -2.07460564E+004 -1.95242492E-005 65480.98 <-- SCF

17 -2.07460562E+004 -5.57984340E-006 65502.77 <-- SCF

18 -2.07460562E+004 3.74286437E-007 65524.11 <-- SCF

19 -2.07460562E+004 4.36579721E-007 65545.48 <-- SCF

20 -2.07460562E+004 -3.05056530E-008 65566.97 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05620711 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00053 0.00048 -0.00407 \*

\* Se 2 -0.00262 0.00243 0.00085 \*

\* Se 3 -0.00365 -0.00428 -0.00416 \*

\* Se 4 -0.00133 -0.00103 0.00175 \*

\* Se 5 0.00072 0.00218 0.00605 \*

\* Se 6 0.00002 -0.00146 -0.00182 \*

\* Se 7 -0.00096 -0.00298 -0.00372 \*

\* Se 8 0.00059 -0.00063 -0.00278 \*

\* Se 9 -0.00485 -0.00307 -0.00251 \*

\* Se 10 0.00325 0.00528 -0.00615 \*

\* Se 11 0.00125 0.00487 0.00316 \*

\* Se 12 -0.00645 -0.00353 0.00528 \*

\* Se 13 0.00043 0.00248 0.00526 \*

\* Se 14 -0.00366 0.00159 0.00078 \*

\* Se 15 -0.00415 -0.00121 -0.00455 \*

\* Se 16 0.00002 0.00100 0.00008 \*

\* Se 17 -0.00091 0.00651 0.00516 \*

\* Se 18 0.00015 0.00180 -0.00213 \*

\* Se 19 -0.00250 0.00075 0.00404 \*

\* Se 20 -0.00206 -0.00082 -0.00202 \*

\* Nb 1 0.00132 -0.00416 -0.00580 \*

\* Nb 2 0.00681 0.00042 0.00601 \*

\* Nb 3 -0.00065 0.00614 -0.00277 \*

\* Nb 4 0.00237 -0.00363 0.00101 \*

\* Nb 5 0.00219 -0.00335 -0.00119 \*

\* Nb 6 0.01225 -0.01017 0.00120 \*

\* Nb 7 -0.00387 0.00860 -0.00110 \*

\* Nb 8 0.00339 0.00047 0.00156 \*

\* Nb 9 -0.00199 0.00145 -0.00050 \*

\* Nb 10 0.00439 -0.00611 0.00308 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.012407 0.001197 0.004535 \*

\* y 0.001197 -0.008401 0.005809 \*

\* z 0.004535 0.005809 -0.015198 \*

\* \*

\* Pressure: 0.0037 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.907E-007 | -20746.056235 | <-- min BFGS

| trial step | 1.000000 | 1.585E-007 | -20746.056221 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 42 with line minimization (lambda= 1.682569)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8828836 -8.5732346 -0.0042872 0.4213032 -0.0015139 0.0001655

0.0124009 3.4509943 -0.0003514 1.0466350 1.8169274 0.0005053

-0.0051259 -0.0006749 13.0453108 0.0001667 0.0000484 0.4816433

Lattice parameters(A) Cell Angles

a = 17.175581 alpha = 90.008880

b = 3.451017 beta = 90.032330

c = 13.045312 gamma = 119.738057

Current cell volume = 671.403742 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 0.066580 0.662744 0.122677 x

x Se 2 0.134156 0.336389 0.622297 x

x Se 3 0.133979 0.336496 0.877641 x

x Se 4 0.066433 0.662651 0.377433 x

x Se 5 0.266368 0.663995 0.122323 x

x Se 6 0.333633 0.337556 0.622202 x

x Se 7 0.333480 0.337336 0.877681 x

x Se 8 0.266090 0.663654 0.377721 x

x Se 9 0.466805 0.664651 0.122804 x

x Se 10 0.533632 0.335902 0.622486 x

x Se 11 0.533180 0.335329 0.877199 x

x Se 12 0.466358 0.664073 0.377510 x

x Se 13 0.666516 0.662673 0.122320 x

x Se 14 0.733908 0.336337 0.622294 x

x Se 15 0.733630 0.336000 0.877665 x

x Se 16 0.666361 0.662450 0.377795 x

x Se 17 0.866029 0.663505 0.122356 x

x Se 18 0.933571 0.337339 0.622562 x

x Se 19 0.933429 0.337243 0.877331 x

x Se 20 0.865849 0.663625 0.377705 x

x Nb 1 -0.001027 -0.003842 0.250091 x

x Nb 2 0.001035 0.003814 0.749910 x

x Nb 3 0.199625 -0.001431 0.250005 x

x Nb 4 0.200661 0.001776 0.749983 x

x Nb 5 0.399289 -0.002087 0.250087 x

x Nb 6 0.400059 0.002153 0.749847 x

x Nb 7 0.599924 -0.002172 0.250152 x

x Nb 8 0.600695 0.002072 0.749912 x

x Nb 9 0.799348 -0.001736 0.250014 x

x Nb 10 0.800407 0.001504 0.749997 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460525E+004 65967.55 <-- SCF

1 -2.07462161E+004 5.45332001E-003 65987.89 <-- SCF

2 -2.07462193E+004 1.08077483E-004 66015.33 <-- SCF

3 -2.07462946E+004 2.50952028E-003 66044.73 <-- SCF

4 -2.07459924E+004 -1.00725804E-002 66073.56 <-- SCF

5 -2.07460345E+004 1.40285968E-003 66103.66 <-- SCF

6 -2.07460710E+004 1.21541720E-003 66132.39 <-- SCF

7 -2.07460684E+004 -8.50954047E-005 66159.28 <-- SCF

8 -2.07460609E+004 -2.52774037E-004 66186.02 <-- SCF

9 -2.07460567E+004 -1.39713999E-004 66212.38 <-- SCF

10 -2.07460547E+004 -6.45638265E-005 66238.47 <-- SCF

11 -2.07460560E+004 4.06818475E-005 66265.41 <-- SCF

12 -2.07460579E+004 6.57843789E-005 66288.62 <-- SCF

13 -2.07460580E+004 1.24698927E-006 66310.36 <-- SCF

14 -2.07460574E+004 -1.75838000E-005 66332.80 <-- SCF

15 -2.07460566E+004 -2.65053962E-005 66356.05 <-- SCF

16 -2.07460569E+004 6.95836462E-006 66377.39 <-- SCF

17 -2.07460562E+004 -2.29422704E-005 66402.11 <-- SCF

18 -2.07460562E+004 4.63432170E-008 66425.62 <-- SCF

19 -2.07460563E+004 4.10056707E-006 66447.14 <-- SCF

20 -2.07460564E+004 5.26681513E-006 66468.75 <-- SCF

21 -2.07460565E+004 1.91387616E-006 66490.31 <-- SCF

22 -2.07460564E+004 -3.77264345E-006 66511.61 <-- SCF

23 -2.07460562E+004 -5.53760494E-006 66533.47 <-- SCF

24 -2.07460563E+004 1.35315049E-006 66554.59 <-- SCF

25 -2.07460563E+004 -2.68570272E-007 66575.31 <-- SCF

26 -2.07460562E+004 -4.55031048E-007 66595.97 <-- SCF

27 -2.07460562E+004 -6.70406450E-007 66617.97 <-- SCF

28 -2.07460562E+004 -6.57708969E-007 66639.34 <-- SCF

29 -2.07460562E+004 3.09436622E-007 66660.80 <-- SCF

30 -2.07460562E+004 3.63924194E-007 66682.17 <-- SCF

31 -2.07460562E+004 2.15879861E-007 66703.66 <-- SCF

32 -2.07460562E+004 5.39121670E-008 66725.16 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05623052 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00105 -0.00006 -0.00315 \*

\* Se 2 0.00008 0.00124 -0.00063 \*

\* Se 3 -0.00131 -0.00546 -0.00274 \*

\* Se 4 -0.00144 -0.00163 0.00124 \*

\* Se 5 0.00351 0.00130 0.00624 \*

\* Se 6 -0.00013 -0.00081 -0.00205 \*

\* Se 7 -0.00161 -0.00257 -0.00361 \*

\* Se 8 0.00291 -0.00159 -0.00284 \*

\* Se 9 -0.00357 -0.00306 -0.00296 \*

\* Se 10 0.00625 0.00424 -0.00641 \*

\* Se 11 0.00394 0.00359 0.00345 \*

\* Se 12 -0.00574 -0.00367 0.00584 \*

\* Se 13 0.00176 0.00231 0.00519 \*

\* Se 14 -0.00186 0.00157 0.00010 \*

\* Se 15 -0.00248 -0.00139 -0.00365 \*

\* Se 16 0.00044 0.00059 0.00042 \*

\* Se 17 0.00180 0.00559 0.00548 \*

\* Se 18 0.00168 0.00181 -0.00140 \*

\* Se 19 -0.00124 0.00060 0.00311 \*

\* Se 20 0.00012 -0.00163 -0.00193 \*

\* Nb 1 -0.00130 -0.00255 -0.00600 \*

\* Nb 2 -0.00069 0.00276 0.00593 \*

\* Nb 3 -0.00450 0.00585 -0.00328 \*

\* Nb 4 0.00347 -0.00334 0.00114 \*

\* Nb 5 -0.00094 -0.00323 -0.00117 \*

\* Nb 6 0.00677 -0.00890 0.00118 \*

\* Nb 7 -0.00778 0.00835 -0.00136 \*

\* Nb 8 0.00072 0.00306 0.00140 \*

\* Nb 9 -0.00397 0.00305 -0.00082 \*

\* Nb 10 0.00407 -0.00602 0.00326 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.016232 0.001862 0.006139 \*

\* y 0.001862 -0.006027 0.006463 \*

\* z 0.006139 0.006463 -0.012710 \*

\* \*

\* Pressure: 0.0008 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 3.907E-007 | -20746.056235 | <-- min BFGS

| trial step | 1.000000 | 1.585E-007 | -20746.056221 | <-- min BFGS

| line step | 1.682569 | 1.338E-007 | -20746.056249 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 42 with enthalpy= -2.07460562E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 4.575540E-007 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 1.149384E-002 | 1.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.619995E-004 | 5.000000E-004 | A | Yes | <-- BFGS

| Smax | 1.623195E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 43 ...

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+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 7.307E-007 | -20746.056249 | <-- 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)

14.8823636 -8.5726164 -0.0042549 0.4213108 -0.0015265 0.0001610

0.0125037 3.4509254 -0.0002961 1.0465991 1.8169327 0.0004671

-0.0049880 -0.0004805 13.0446832 0.0001612 0.0000407 0.4816664

Lattice parameters(A) Cell Angles

a = 17.174822 alpha = 90.007106

b = 3.450948 beta = 90.032126

c = 13.044684 gamma = 119.735426

Current cell volume = 671.346044 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 0.066577 0.662756 0.122659 x

x Se 2 0.134153 0.336375 0.622293 x

x Se 3 0.133978 0.336439 0.877640 x

x Se 4 0.066429 0.662656 0.377441 x

x Se 5 0.266371 0.664038 0.122321 x

x Se 6 0.333632 0.337506 0.622197 x

x Se 7 0.333480 0.337294 0.877680 x

x Se 8 0.266095 0.663687 0.377726 x

x Se 9 0.466798 0.664595 0.122795 x

x Se 10 0.533641 0.335957 0.622476 x

x Se 11 0.533188 0.335393 0.877203 x

x Se 12 0.466350 0.664028 0.377523 x

x Se 13 0.666515 0.662707 0.122317 x

x Se 14 0.733905 0.336304 0.622291 x

x Se 15 0.733627 0.335953 0.877663 x

x Se 16 0.666362 0.662495 0.377803 x

x Se 17 0.866032 0.663566 0.122352 x

x Se 18 0.933578 0.337345 0.622558 x

x Se 19 0.933433 0.337242 0.877345 x

x Se 20 0.865856 0.663637 0.377713 x

x Nb 1 -0.001018 -0.003846 0.250080 x

x Nb 2 0.001024 0.003813 0.749921 x

x Nb 3 0.199619 -0.001395 0.250003 x

x Nb 4 0.200656 0.001761 0.749982 x

x Nb 5 0.399296 -0.002069 0.250086 x

x Nb 6 0.400070 0.002089 0.749848 x

x Nb 7 0.599910 -0.002115 0.250151 x

x Nb 8 0.600687 0.002054 0.749914 x

x Nb 9 0.799349 -0.001725 0.250017 x

x Nb 10 0.800408 0.001460 0.750000 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460555E+004 67128.66 <-- SCF

1 -2.07460710E+004 5.15438510E-004 67148.27 <-- SCF

2 -2.07460719E+004 2.94904222E-005 67174.70 <-- SCF

3 -2.07461648E+004 3.09799692E-003 67204.11 <-- SCF

4 -2.07460297E+004 -4.50356838E-003 67233.14 <-- SCF

5 -2.07460330E+004 1.09872963E-004 67261.50 <-- SCF

6 -2.07460413E+004 2.74712385E-004 67288.72 <-- SCF

7 -2.07460476E+004 2.10558613E-004 67313.05 <-- SCF

8 -2.07460524E+004 1.62592646E-004 67336.66 <-- SCF

9 -2.07460561E+004 1.22710095E-004 67360.11 <-- SCF

10 -2.07460585E+004 7.94030390E-005 67382.62 <-- SCF

11 -2.07460591E+004 1.97049587E-005 67404.34 <-- SCF

12 -2.07460590E+004 -2.74135636E-006 67426.05 <-- SCF

13 -2.07460590E+004 -1.24733513E-007 67447.67 <-- SCF

14 -2.07460588E+004 -5.92912755E-006 67469.38 <-- SCF

15 -2.07460592E+004 1.37448955E-005 67491.12 <-- SCF

16 -2.07460594E+004 6.02858871E-006 67512.84 <-- SCF

17 -2.07460608E+004 4.66147196E-005 67534.66 <-- SCF

18 -2.07460589E+004 -6.30228265E-005 67556.86 <-- SCF

19 -2.07460571E+004 -6.15551402E-005 67582.22 <-- SCF

20 -2.07460569E+004 -4.83705303E-006 67603.75 <-- SCF

21 -2.07460567E+004 -8.38660642E-006 67625.45 <-- SCF

22 -2.07460564E+004 -9.03635314E-006 67647.09 <-- SCF

23 -2.07460561E+004 -1.08314542E-005 67669.59 <-- SCF

24 -2.07460561E+004 -1.12225173E-006 67691.28 <-- SCF

25 -2.07460560E+004 -1.37122111E-006 67713.53 <-- SCF

26 -2.07460561E+004 3.35252207E-006 67735.20 <-- SCF

27 -2.07460562E+004 2.13596658E-006 67756.64 <-- SCF

28 -2.07460562E+004 5.60414344E-007 67778.09 <-- SCF

29 -2.07460562E+004 7.56540070E-007 67799.53 <-- SCF

30 -2.07460562E+004 6.00374482E-008 67821.05 <-- SCF

31 -2.07460562E+004 3.86138856E-007 67842.39 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05623961 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00278 -0.00097 -0.00411 \*

\* Se 2 0.00107 0.00183 0.00189 \*

\* Se 3 -0.00021 -0.00388 -0.00332 \*

\* Se 4 -0.00007 -0.00251 0.00192 \*

\* Se 5 0.00480 0.00100 0.00434 \*

\* Se 6 0.00104 0.00002 0.00022 \*

\* Se 7 -0.00120 -0.00238 -0.00467 \*

\* Se 8 0.00354 -0.00175 -0.00217 \*

\* Se 9 -0.00286 -0.00222 -0.00603 \*

\* Se 10 0.00729 0.00451 -0.00506 \*

\* Se 11 0.00470 0.00278 0.00356 \*

\* Se 12 -0.00531 -0.00362 0.00745 \*

\* Se 13 0.00384 0.00262 0.00395 \*

\* Se 14 -0.00141 0.00218 0.00243 \*

\* Se 15 -0.00231 -0.00082 -0.00442 \*

\* Se 16 0.00165 0.00042 0.00064 \*

\* Se 17 0.00183 0.00431 0.00240 \*

\* Se 18 0.00236 0.00262 0.00018 \*

\* Se 19 -0.00091 0.00131 0.00217 \*

\* Se 20 -0.00012 -0.00150 -0.00075 \*

\* Nb 1 -0.00503 -0.00078 -0.00595 \*

\* Nb 2 0.00147 0.00093 0.00542 \*

\* Nb 3 -0.00386 0.00434 -0.00298 \*

\* Nb 4 -0.00184 -0.00417 0.00048 \*

\* Nb 5 -0.00398 -0.00212 -0.00056 \*

\* Nb 6 0.00943 -0.00838 0.00012 \*

\* Nb 7 -0.00833 0.00626 -0.00057 \*

\* Nb 8 -0.00054 0.00124 0.00060 \*

\* Nb 9 -0.00690 0.00429 -0.00014 \*

\* Nb 10 -0.00092 -0.00555 0.00299 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.013869 0.006395 0.007990 \*

\* y 0.006395 -0.010524 0.006647 \*

\* z 0.007990 0.006647 -0.012229 \*

\* \*

\* Pressure: 0.0030 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 7.307E-007 | -20746.056249 | <-- min BFGS

| trial step | 1.000000 | 5.786E-007 | -20746.056252 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

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BFGS: improving iteration 43 with line minimization (lambda= 4.803614)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8803857 -8.5702652 -0.0041322 0.4213394 -0.0015745 0.0001442

0.0128944 3.4506632 -0.0000856 1.0464626 1.8169527 0.0003221

-0.0044637 0.0002587 13.0422960 0.0001404 0.0000114 0.4817546

Lattice parameters(A) Cell Angles

a = 17.171935 alpha = 90.000358

b = 3.450687 beta = 90.031347

c = 13.042297 gamma = 119.725420

Current cell volume = 671.126594 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 0.066566 0.662801 0.122591 x

x Se 2 0.134138 0.336323 0.622282 x

x Se 3 0.133973 0.336222 0.877638 x

x Se 4 0.066414 0.662674 0.377471 x

x Se 5 0.266385 0.664205 0.122314 x

x Se 6 0.333627 0.337315 0.622179 x

x Se 7 0.333479 0.337131 0.877677 x

x Se 8 0.266113 0.663811 0.377748 x

x Se 9 0.466771 0.664385 0.122765 x

x Se 10 0.533677 0.336165 0.622440 x

x Se 11 0.533220 0.335637 0.877219 x

x Se 12 0.466322 0.663856 0.377575 x

x Se 13 0.666513 0.662837 0.122306 x

x Se 14 0.733893 0.336178 0.622281 x

x Se 15 0.733616 0.335773 0.877655 x

x Se 16 0.666367 0.662664 0.377834 x

x Se 17 0.866047 0.663800 0.122337 x

x Se 18 0.933602 0.337369 0.622543 x

x Se 19 0.933448 0.337235 0.877396 x

x Se 20 0.865883 0.663686 0.377741 x

x Nb 1 -0.000985 -0.003862 0.250037 x

x Nb 2 0.000983 0.003808 0.749966 x

x Nb 3 0.199598 -0.001258 0.249994 x

x Nb 4 0.200636 0.001705 0.749977 x

x Nb 5 0.399326 -0.002003 0.250083 x

x Nb 6 0.400113 0.001845 0.749852 x

x Nb 7 0.599860 -0.001895 0.250146 x

x Nb 8 0.600655 0.001985 0.749920 x

x Nb 9 0.799350 -0.001683 0.250024 x

x Nb 10 0.800411 0.001291 0.750010 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460491E+004 68245.77 <-- SCF

1 -2.07460674E+004 6.10011773E-004 68264.03 <-- SCF

2 -2.07460695E+004 6.92871712E-005 68294.39 <-- SCF

3 -2.07460687E+004 -2.36156177E-005 68323.95 <-- SCF

4 -2.07460519E+004 -5.60616512E-004 68353.25 <-- SCF

5 -2.07460566E+004 1.54927385E-004 68383.14 <-- SCF

6 -2.07460582E+004 5.40612191E-005 68412.33 <-- SCF

7 -2.07460574E+004 -2.60240720E-005 68439.03 <-- SCF

8 -2.07460566E+004 -2.87103764E-005 68463.73 <-- SCF

9 -2.07460561E+004 -1.50820462E-005 68490.14 <-- SCF

10 -2.07460563E+004 7.04706488E-006 68512.19 <-- SCF

11 -2.07460563E+004 -7.11962564E-007 68533.72 <-- SCF

12 -2.07460562E+004 -1.56079227E-006 68555.59 <-- SCF

13 -2.07460563E+004 2.90343275E-007 68576.92 <-- SCF

14 -2.07460563E+004 8.60120430E-008 68598.22 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05625623 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00467 -0.00453 0.00068 \*

\* Se 2 -0.00048 0.00213 0.00031 \*

\* Se 3 -0.00089 0.00135 0.00560 \*

\* Se 4 -0.00015 -0.00665 -0.00460 \*

\* Se 5 0.00115 -0.00122 0.00376 \*

\* Se 6 0.00209 0.00400 0.00096 \*

\* Se 7 -0.00238 -0.00073 -0.00099 \*

\* Se 8 -0.00202 -0.00385 -0.00674 \*

\* Se 9 -0.00142 0.00234 -0.00996 \*

\* Se 10 0.00238 0.00203 -0.00860 \*

\* Se 11 -0.00090 -0.00272 0.01317 \*

\* Se 12 -0.00423 -0.00229 0.00517 \*

\* Se 13 0.00309 0.00169 0.00575 \*

\* Se 14 0.00039 0.00506 0.00119 \*

\* Se 15 -0.00196 0.00255 0.00292 \*

\* Se 16 -0.00182 -0.00322 -0.00506 \*

\* Se 17 -0.00243 0.00026 0.00109 \*

\* Se 18 -0.00161 0.00520 0.00041 \*

\* Se 19 -0.00632 0.00331 0.00400 \*

\* Se 20 -0.00335 -0.00002 -0.00602 \*

\* Nb 1 -0.00024 0.00316 -0.00019 \*

\* Nb 2 0.00392 -0.00253 -0.00040 \*

\* Nb 3 -0.00310 0.00263 0.00002 \*

\* Nb 4 0.00857 -0.00928 -0.00198 \*

\* Nb 5 -0.00474 -0.00410 0.00217 \*

\* Nb 6 0.00687 -0.00384 -0.00301 \*

\* Nb 7 -0.00390 0.00274 0.00274 \*

\* Nb 8 0.00752 0.00386 -0.00290 \*

\* Nb 9 -0.00496 0.00666 0.00134 \*

\* Nb 10 0.00626 -0.00400 -0.00084 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.003541 0.018886 0.015062 \*

\* y 0.018886 -0.031307 0.012270 \*

\* z 0.015062 0.012270 -0.031550 \*

\* \*

\* Pressure: 0.0221 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 7.307E-007 | -20746.056249 | <-- min BFGS

| trial step | 1.000000 | 5.786E-007 | -20746.056252 | <-- min BFGS

| line step | 4.803614 | -6.252E-007 | -20746.056250 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 43 with quad minimization (lambda= 2.828192)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8814130 -8.5714863 -0.0041960 0.4213245 -0.0015496 0.0001530

0.0126915 3.4507994 -0.0001949 1.0465335 1.8169423 0.0003974

-0.0047360 -0.0001252 13.0435358 0.0001512 0.0000267 0.4817088

Lattice parameters(A) Cell Angles

a = 17.173434 alpha = 90.003863

b = 3.450823 beta = 90.031752

c = 13.043537 gamma = 119.730617

Current cell volume = 671.240564 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 0.066572 0.662777 0.122626 x

x Se 2 0.134145 0.336350 0.622288 x

x Se 3 0.133976 0.336334 0.877639 x

x Se 4 0.066422 0.662665 0.377455 x

x Se 5 0.266378 0.664118 0.122317 x

x Se 6 0.333629 0.337414 0.622189 x

x Se 7 0.333480 0.337215 0.877679 x

x Se 8 0.266103 0.663746 0.377737 x

x Se 9 0.466785 0.664494 0.122781 x

x Se 10 0.533658 0.336057 0.622459 x

x Se 11 0.533204 0.335511 0.877211 x

x Se 12 0.466337 0.663945 0.377548 x

x Se 13 0.666514 0.662769 0.122312 x

x Se 14 0.733899 0.336243 0.622286 x

x Se 15 0.733622 0.335866 0.877659 x

x Se 16 0.666365 0.662576 0.377818 x

x Se 17 0.866039 0.663679 0.122345 x

x Se 18 0.933589 0.337357 0.622551 x

x Se 19 0.933440 0.337239 0.877369 x

x Se 20 0.865869 0.663661 0.377726 x

x Nb 1 -0.001002 -0.003854 0.250059 x

x Nb 2 0.001004 0.003811 0.749943 x

x Nb 3 0.199609 -0.001329 0.249999 x

x Nb 4 0.200646 0.001734 0.749980 x

x Nb 5 0.399311 -0.002037 0.250084 x

x Nb 6 0.400091 0.001972 0.749850 x

x Nb 7 0.599886 -0.002009 0.250149 x

x Nb 8 0.600671 0.002021 0.749917 x

x Nb 9 0.799349 -0.001705 0.250020 x

x Nb 10 0.800410 0.001379 0.750005 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460543E+004 69001.72 <-- SCF

1 -2.07460587E+004 1.46901947E-004 69019.30 <-- SCF

2 -2.07460593E+004 1.85573927E-005 69049.06 <-- SCF

3 -2.07460585E+004 -2.68804019E-005 69078.56 <-- SCF

4 -2.07460555E+004 -1.00099211E-004 69107.66 <-- SCF

5 -2.07460565E+004 3.55288325E-005 69134.95 <-- SCF

6 -2.07460567E+004 6.35762561E-006 69161.84 <-- SCF

7 -2.07460564E+004 -9.19457905E-006 69184.61 <-- SCF

8 -2.07460562E+004 -7.51768311E-006 69209.36 <-- SCF

9 -2.07460563E+004 1.29850577E-006 69230.81 <-- SCF

10 -2.07460563E+004 2.07240740E-008 69252.45 <-- SCF

11 -2.07460563E+004 1.34897045E-007 69273.97 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05625655 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00391 -0.00286 -0.00002 \*

\* Se 2 -0.00072 0.00187 -0.00020 \*

\* Se 3 -0.00121 -0.00160 0.00166 \*

\* Se 4 -0.00014 -0.00482 -0.00255 \*

\* Se 5 0.00227 0.00022 0.00578 \*

\* Se 6 0.00142 0.00141 0.00001 \*

\* Se 7 -0.00171 -0.00203 -0.00252 \*

\* Se 8 -0.00022 -0.00260 -0.00585 \*

\* Se 9 -0.00265 -0.00013 -0.00676 \*

\* Se 10 0.00445 0.00336 -0.00721 \*

\* Se 11 0.00133 0.00033 0.00845 \*

\* Se 12 -0.00526 -0.00305 0.00535 \*

\* Se 13 0.00280 0.00230 0.00563 \*

\* Se 14 -0.00037 0.00317 0.00080 \*

\* Se 15 -0.00240 0.00037 -0.00018 \*

\* Se 16 -0.00050 -0.00126 -0.00265 \*

\* Se 17 -0.00103 0.00270 0.00291 \*

\* Se 18 0.00017 0.00393 -0.00058 \*

\* Se 19 -0.00407 0.00225 0.00336 \*

\* Se 20 -0.00186 -0.00076 -0.00356 \*

\* Nb 1 -0.00063 0.00261 -0.00103 \*

\* Nb 2 0.00305 -0.00189 0.00047 \*

\* Nb 3 -0.00577 0.00193 -0.00062 \*

\* Nb 4 0.00502 -0.00643 -0.00094 \*

\* Nb 5 -0.00481 -0.00363 0.00085 \*

\* Nb 6 0.00703 -0.00239 -0.00149 \*

\* Nb 7 -0.00311 0.00178 0.00141 \*

\* Nb 8 0.00497 0.00299 -0.00143 \*

\* Nb 9 -0.00451 0.00478 0.00052 \*

\* Nb 10 0.00454 -0.00255 0.00038 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.005881 0.012193 0.011573 \*

\* y 0.012193 -0.019351 0.009741 \*

\* z 0.011573 0.009741 -0.021047 \*

\* \*

\* Pressure: 0.0115 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 7.307E-007 | -20746.056249 | <-- min BFGS

| trial step | 1.000000 | 5.786E-007 | -20746.056252 | <-- min BFGS

| line step | 4.803614 | -6.252E-007 | -20746.056250 | <-- min BFGS

| quad step | 2.828192 | -1.823E-007 | -20746.056269 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 43 with enthalpy= -2.07460563E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 6.930512E-007 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 9.117871E-003 | 1.000000E-002 | eV/A | Yes | <-- BFGS

| |dR|max | 1.046244E-003 | 5.000000E-004 | A | No | <-- BFGS

| Smax | 2.104679E-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 | 8.667E-007 | -20746.056269 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

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)

14.8818316 -8.5718248 -0.0044093 0.4213181 -0.0015400 0.0001576

0.0126138 3.4508005 -0.0001809 1.0465586 1.8169652 0.0004020

-0.0048803 -0.0000755 13.0449128 0.0001569 0.0000247 0.4816580

Lattice parameters(A) Cell Angles

a = 17.173966 alpha = 90.003413

b = 3.450824 beta = 90.033119

c = 13.044914 gamma = 119.732189

Current cell volume = 671.321849 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066565 0.662677 0.122634 x

x Se 2 0.134158 0.336389 0.622301 x

x Se 3 0.133994 0.336388 0.877630 x

x Se 4 0.066414 0.662570 0.377445 x

x Se 5 0.266373 0.664069 0.122329 x

x Se 6 0.333641 0.337483 0.622196 x

x Se 7 0.333492 0.337291 0.877671 x

x Se 8 0.266093 0.663691 0.377724 x

x Se 9 0.466783 0.664436 0.122790 x

x Se 10 0.533668 0.336128 0.622463 x

x Se 11 0.533206 0.335569 0.877201 x

x Se 12 0.466327 0.663876 0.377543 x

x Se 13 0.666501 0.662693 0.122319 x

x Se 14 0.733909 0.336297 0.622301 x

x Se 15 0.733626 0.335914 0.877646 x

x Se 16 0.666353 0.662508 0.377811 x

x Se 17 0.866021 0.663625 0.122353 x

x Se 18 0.933597 0.337453 0.622562 x

x Se 19 0.933447 0.337339 0.877362 x

x Se 20 0.865856 0.663621 0.377714 x

x Nb 1 -0.001026 -0.003975 0.250061 x

x Nb 2 0.001027 0.003926 0.749941 x

x Nb 3 0.199599 -0.001399 0.250000 x

x Nb 4 0.200663 0.001792 0.749977 x

x Nb 5 0.399305 -0.002087 0.250089 x

x Nb 6 0.400098 0.002038 0.749844 x

x Nb 7 0.599879 -0.002074 0.250154 x

x Nb 8 0.600676 0.002068 0.749913 x

x Nb 9 0.799333 -0.001759 0.250023 x

x Nb 10 0.800420 0.001453 0.750003 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -2.07460554E+004 69674.77 <-- SCF

1 -2.07460588E+004 1.12070461E-004 69693.17 <-- SCF

2 -2.07460592E+004 1.47605527E-005 69720.81 <-- SCF

3 -2.07460625E+004 1.08468612E-004 69750.34 <-- SCF

4 -2.07460544E+004 -2.69802611E-004 69779.66 <-- SCF

5 -2.07460558E+004 4.79353642E-005 69806.83 <-- SCF

6 -2.07460564E+004 2.16707888E-005 69832.95 <-- SCF

7 -2.07460564E+004 -5.52232659E-007 69854.97 <-- SCF

8 -2.07460563E+004 -3.19418829E-006 69877.33 <-- SCF

9 -2.07460563E+004 -2.42900900E-006 69899.20 <-- SCF

10 -2.07460562E+004 -9.83704267E-007 69920.97 <-- SCF

11 -2.07460562E+004 1.33015842E-007 69942.58 <-- SCF

12 -2.07460563E+004 6.65410633E-007 69964.95 <-- SCF

13 -2.07460563E+004 4.36505578E-007 69986.59 <-- SCF

14 -2.07460563E+004 1.10259597E-007 70008.00 <-- SCF

15 -2.07460563E+004 -6.96781663E-008 70029.50 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -20746.05626903 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00381 -0.00069 -0.00033 \*

\* Se 2 -0.00066 0.00184 -0.00108 \*

\* Se 3 -0.00162 -0.00185 0.00157 \*

\* Se 4 0.00035 -0.00279 -0.00159 \*

\* Se 5 0.00199 0.00082 0.00443 \*

\* Se 6 0.00078 0.00117 -0.00084 \*

\* Se 7 -0.00197 -0.00264 -0.00271 \*

\* Se 8 0.00054 -0.00216 -0.00366 \*

\* Se 9 -0.00178 0.00050 -0.00601 \*

\* Se 10 0.00354 0.00236 -0.00718 \*

\* Se 11 0.00155 -0.00081 0.00764 \*

\* Se 12 -0.00353 -0.00257 0.00540 \*

\* Se 13 0.00246 0.00303 0.00611 \*

\* Se 14 -0.00077 0.00266 -0.00061 \*

\* Se 15 -0.00176 -0.00034 0.00038 \*

\* Se 16 -0.00045 -0.00085 -0.00219 \*

\* Se 17 0.00032 0.00254 0.00362 \*

\* Se 18 -0.00118 0.00202 -0.00082 \*

\* Se 19 -0.00474 0.00022 0.00294 \*

\* Se 20 -0.00101 -0.00103 -0.00343 \*

\* Nb 1 0.00027 0.00103 -0.00310 \*

\* Nb 2 0.00029 -0.00018 0.00280 \*

\* Nb 3 -0.00531 0.00283 -0.00202 \*

\* Nb 4 0.00554 -0.00605 0.00004 \*

\* Nb 5 -0.00284 -0.00376 -0.00010 \*

\* Nb 6 0.00651 -0.00544 -0.00053 \*

\* Nb 7 -0.00564 0.00479 0.00029 \*

\* Nb 8 0.00353 0.00432 -0.00030 \*

\* Nb 9 -0.00304 0.00476 -0.00035 \*

\* Nb 10 0.00483 -0.00374 0.00162 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.010822 0.009013 0.009203 \*

\* y 0.009013 -0.014650 0.010710 \*

\* z 0.009203 0.010710 -0.011622 \*

\* \*

\* Pressure: 0.0051 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 8.667E-007 | -20746.056269 | <-- min BFGS

| trial step | 1.000000 | 3.602E-007 | -20746.056286 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 44 with enthalpy= -2.07460563E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 5.421464E-007 | 5.000000E-006 | eV | Yes | <-- BFGS

| |F|max | 8.500900E-003 | 1.000000E-002 | eV/A | Yes | <-- BFGS

| |dR|max | 4.109353E-004 | 5.000000E-004 | A | Yes | <-- BFGS

| Smax | 1.464953E-002 | 2.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

BFGS: Geometry optimization completed successfully.

================================================================================

BFGS: Final Configuration:

================================================================================

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

14.8818316 -8.5718248 -0.0044093 0.4213181 -0.0015400 0.0001576

0.0126138 3.4508005 -0.0001809 1.0465586 1.8169652 0.0004020

-0.0048803 -0.0000755 13.0449128 0.0001569 0.0000247 0.4816580

Lattice parameters(A) Cell Angles

a = 17.173966 alpha = 90.003413

b = 3.450824 beta = 90.033119

c = 13.044914 gamma = 119.732189

Current cell volume = 671.321849 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.066565 0.662677 0.122634 x

x Se 2 0.134158 0.336389 0.622301 x

x Se 3 0.133994 0.336388 0.877630 x

x Se 4 0.066414 0.662570 0.377445 x

x Se 5 0.266373 0.664069 0.122329 x

x Se 6 0.333641 0.337483 0.622196 x

x Se 7 0.333492 0.337291 0.877671 x

x Se 8 0.266093 0.663691 0.377724 x

x Se 9 0.466783 0.664436 0.122790 x

x Se 10 0.533668 0.336128 0.622463 x

x Se 11 0.533206 0.335569 0.877201 x

x Se 12 0.466327 0.663876 0.377543 x

x Se 13 0.666501 0.662693 0.122319 x

x Se 14 0.733909 0.336297 0.622301 x

x Se 15 0.733626 0.335914 0.877646 x

x Se 16 0.666353 0.662508 0.377811 x

x Se 17 0.866021 0.663625 0.122353 x

x Se 18 0.933597 0.337453 0.622562 x

x Se 19 0.933447 0.337339 0.877362 x

x Se 20 0.865856 0.663621 0.377714 x

x Nb 1 -0.001026 -0.003975 0.250061 x

x Nb 2 0.001027 0.003926 0.749941 x

x Nb 3 0.199599 -0.001399 0.250000 x

x Nb 4 0.200663 0.001792 0.749977 x

x Nb 5 0.399305 -0.002087 0.250089 x

x Nb 6 0.400098 0.002038 0.749844 x

x Nb 7 0.599879 -0.002074 0.250154 x

x Nb 8 0.600676 0.002068 0.749913 x

x Nb 9 0.799333 -0.001759 0.250023 x

x Nb 10 0.800420 0.001453 0.750003 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

BFGS: Final Enthalpy = -2.07460563E+004 eV

BFGS: Final <frequency> = 2789.90708 cm-1

BFGS: Final bulk modulus = 77.50523 GPa

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00381 -0.00069 -0.00033 \*

\* Se 2 -0.00066 0.00184 -0.00108 \*

\* Se 3 -0.00162 -0.00185 0.00157 \*

\* Se 4 0.00035 -0.00279 -0.00159 \*

\* Se 5 0.00199 0.00082 0.00443 \*

\* Se 6 0.00078 0.00117 -0.00084 \*

\* Se 7 -0.00197 -0.00264 -0.00271 \*

\* Se 8 0.00054 -0.00216 -0.00366 \*

\* Se 9 -0.00178 0.00050 -0.00601 \*

\* Se 10 0.00354 0.00236 -0.00718 \*

\* Se 11 0.00155 -0.00081 0.00764 \*

\* Se 12 -0.00353 -0.00257 0.00540 \*

\* Se 13 0.00246 0.00303 0.00611 \*

\* Se 14 -0.00077 0.00266 -0.00061 \*

\* Se 15 -0.00176 -0.00034 0.00038 \*

\* Se 16 -0.00045 -0.00085 -0.00219 \*

\* Se 17 0.00032 0.00254 0.00362 \*

\* Se 18 -0.00118 0.00202 -0.00082 \*

\* Se 19 -0.00474 0.00022 0.00294 \*

\* Se 20 -0.00101 -0.00103 -0.00343 \*

\* Nb 1 0.00027 0.00103 -0.00310 \*

\* Nb 2 0.00029 -0.00018 0.00280 \*

\* Nb 3 -0.00531 0.00283 -0.00202 \*

\* Nb 4 0.00554 -0.00605 0.00004 \*

\* Nb 5 -0.00284 -0.00376 -0.00010 \*

\* Nb 6 0.00651 -0.00544 -0.00053 \*

\* Nb 7 -0.00564 0.00479 0.00029 \*

\* Nb 8 0.00353 0.00432 -0.00030 \*

\* Nb 9 -0.00304 0.00476 -0.00035 \*

\* Nb 10 0.00483 -0.00374 0.00162 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.010822 0.009013 0.009203 \*

\* y 0.009013 -0.014650 0.010710 \*

\* z 0.009203 0.010710 -0.011622 \*

\* \*

\* Pressure: 0.0051 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Pseudo atomic calculation performed for Se 4s2 4p4

Converged in 19 iterations to a total energy of -256.4822 eV

Pseudo atomic calculation performed for Nb 4s2 4p6 4d4 5s1

Converged in 19 iterations to a total energy of -1541.3312 eV

Charge spilling parameter for spin component 1 = 0.23%

Atomic Populations (Mulliken)

-----------------------------

Species Ion s p d f Total Charge (e)

==============================================================

Se 1 1.66 4.15 0.00 0.00 5.81 0.19

Se 2 1.66 4.15 0.00 0.00 5.81 0.19

Se 3 1.66 4.15 0.00 0.00 5.81 0.19

Se 4 1.66 4.15 0.00 0.00 5.80 0.20

Se 5 1.66 4.15 0.00 0.00 5.81 0.19

Se 6 1.66 4.15 0.00 0.00 5.80 0.20

Se 7 1.66 4.15 0.00 0.00 5.81 0.19

Se 8 1.66 4.15 0.00 0.00 5.81 0.19

Se 9 1.66 4.15 0.00 0.00 5.81 0.19

Se 10 1.66 4.15 0.00 0.00 5.81 0.19

Se 11 1.66 4.15 0.00 0.00 5.81 0.19

Se 12 1.66 4.15 0.00 0.00 5.81 0.19

Se 13 1.66 4.15 0.00 0.00 5.81 0.19

Se 14 1.66 4.15 0.00 0.00 5.81 0.19

Se 15 1.66 4.15 0.00 0.00 5.81 0.19

Se 16 1.66 4.15 0.00 0.00 5.80 0.20

Se 17 1.66 4.15 0.00 0.00 5.81 0.19

Se 18 1.66 4.15 0.00 0.00 5.80 0.20

Se 19 1.66 4.15 0.00 0.00 5.81 0.19

Se 20 1.66 4.15 0.00 0.00 5.81 0.19

Nb 1 2.61 6.86 3.92 0.00 13.39 -0.39

Nb 2 2.61 6.86 3.92 0.00 13.39 -0.39

Nb 3 2.61 6.86 3.92 0.00 13.39 -0.39

Nb 4 2.61 6.86 3.93 0.00 13.39 -0.39

Nb 5 2.61 6.86 3.92 0.00 13.39 -0.39

Nb 6 2.61 6.86 3.92 0.00 13.39 -0.39

Nb 7 2.61 6.86 3.92 0.00 13.39 -0.39

Nb 8 2.61 6.86 3.92 0.00 13.39 -0.39

Nb 9 2.61 6.86 3.92 0.00 13.39 -0.39

Nb 10 2.61 6.86 3.92 0.00 13.39 -0.39

==============================================================

Bond Population Length (A)

============================================================

Se 19 -- Nb 10 -0.52 2.58686

Se 1 -- Nb 3 -0.52 2.58701

Se 7 -- Nb 4 -0.53 2.58742

Se 13 -- Nb 9 -0.53 2.58753

Se 9 -- Nb 7 -0.52 2.58762

Se 11 -- Nb 6 -0.52 2.58770

Se 3 -- Nb 2 -0.52 2.58886

Se 17 -- Nb 1 -0.52 2.58887

Se 15 -- Nb 8 -0.53 2.58908

Se 5 -- Nb 5 -0.53 2.58909

Se 18 -- Nb 10 -0.52 2.59105

Se 4 -- Nb 3 -0.52 2.59117

Se 6 -- Nb 4 -0.53 2.59163

Se 16 -- Nb 9 -0.53 2.59171

Se 2 -- Nb 4 0.31 2.59186

Se 20 -- Nb 1 -0.53 2.59207

Se 2 -- Nb 2 -0.53 2.59211

Se 20 -- Nb 9 0.31 2.59226

Se 14 -- Nb 10 0.30 2.59273

Se 8 -- Nb 3 0.30 2.59286

Se 8 -- Nb 5 -0.53 2.59301

Se 6 -- Nb 6 0.31 2.59303

Se 14 -- Nb 8 -0.53 2.59307

Se 16 -- Nb 7 0.31 2.59323

Se 3 -- Nb 4 0.29 2.59430

Se 10 -- Nb 8 0.30 2.59446

Se 12 -- Nb 5 0.30 2.59461

Se 17 -- Nb 9 0.29 2.59471

Se 12 -- Nb 7 -0.52 2.59483

Se 10 -- Nb 6 -0.52 2.59497

Se 15 -- Nb 10 0.28 2.59533

Se 5 -- Nb 3 0.28 2.59549

Se 7 -- Nb 6 0.28 2.59654

Se 13 -- Nb 7 0.28 2.59675

Se 4 -- Nb 1 0.30 2.59746

Se 18 -- Nb 2 0.30 2.59747

Se 11 -- Nb 8 0.28 2.59786

Se 9 -- Nb 5 0.28 2.59799

Se 19 -- Nb 2 0.28 2.59919

Se 1 -- Nb 1 0.28 2.59939

============================================================

Hirshfeld Analysis

------------------

Species Ion Hirshfeld Charge (e) Spin (hbar/2)

===================================================

Se 1 -0.13 0.00

Se 2 -0.13 0.00

Se 3 -0.13 0.00

Se 4 -0.13 0.00

Se 5 -0.13 0.00

Se 6 -0.13 0.00

Se 7 -0.13 0.00

Se 8 -0.13 0.00

Se 9 -0.13 0.00

Se 10 -0.13 0.00

Se 11 -0.13 0.00

Se 12 -0.13 0.00

Se 13 -0.13 0.00

Se 14 -0.13 0.00

Se 15 -0.13 0.00

Se 16 -0.13 0.00

Se 17 -0.13 0.00

Se 18 -0.13 0.00

Se 19 -0.13 0.00

Se 20 -0.13 0.00

Nb 1 0.26 0.00

Nb 2 0.26 0.00

Nb 3 0.26 0.00

Nb 4 0.26 0.00

Nb 5 0.26 0.00

Nb 6 0.26 0.00

Nb 7 0.26 0.00

Nb 8 0.26 0.00

Nb 9 0.26 0.00

Nb 10 0.26 0.00

===================================================

Writing analysis data to 2H-Nb1Se2-7.castep\_bin

Writing model to 2H-Nb1Se2-7.check

A BibTeX formatted list of references used in this run has been written to

2H-Nb1Se2-7.bib

Initialisation time = 2.31 s

Calculation time = 70415.86 s

Finalisation time = 27.48 s

Total time = 70445.66 s

Overall parallel efficiency rating: Very good (83%)

Data was distributed by:-

G-vector (2-way); efficiency rating: Very good (87%)

k-point (7-way); efficiency rating: Excellent (95%)