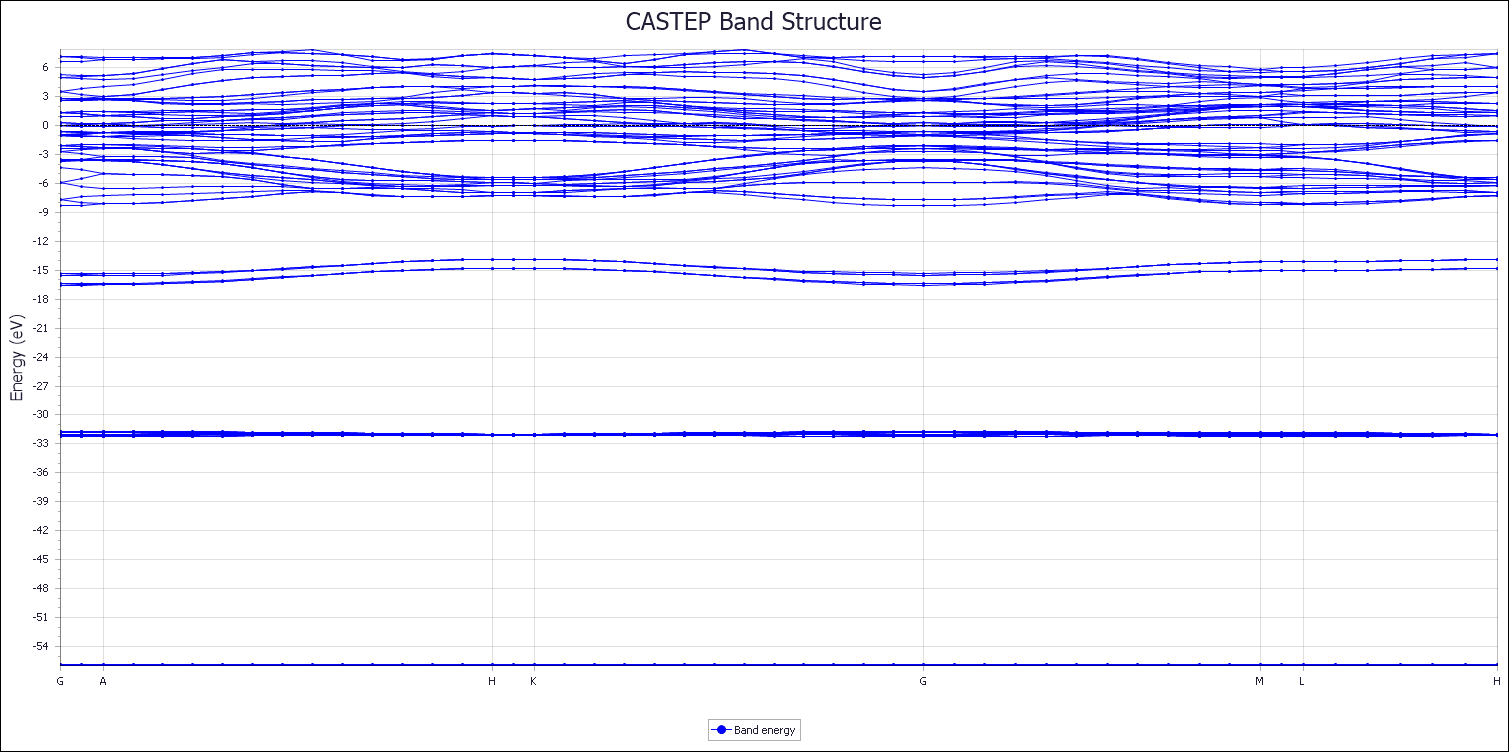
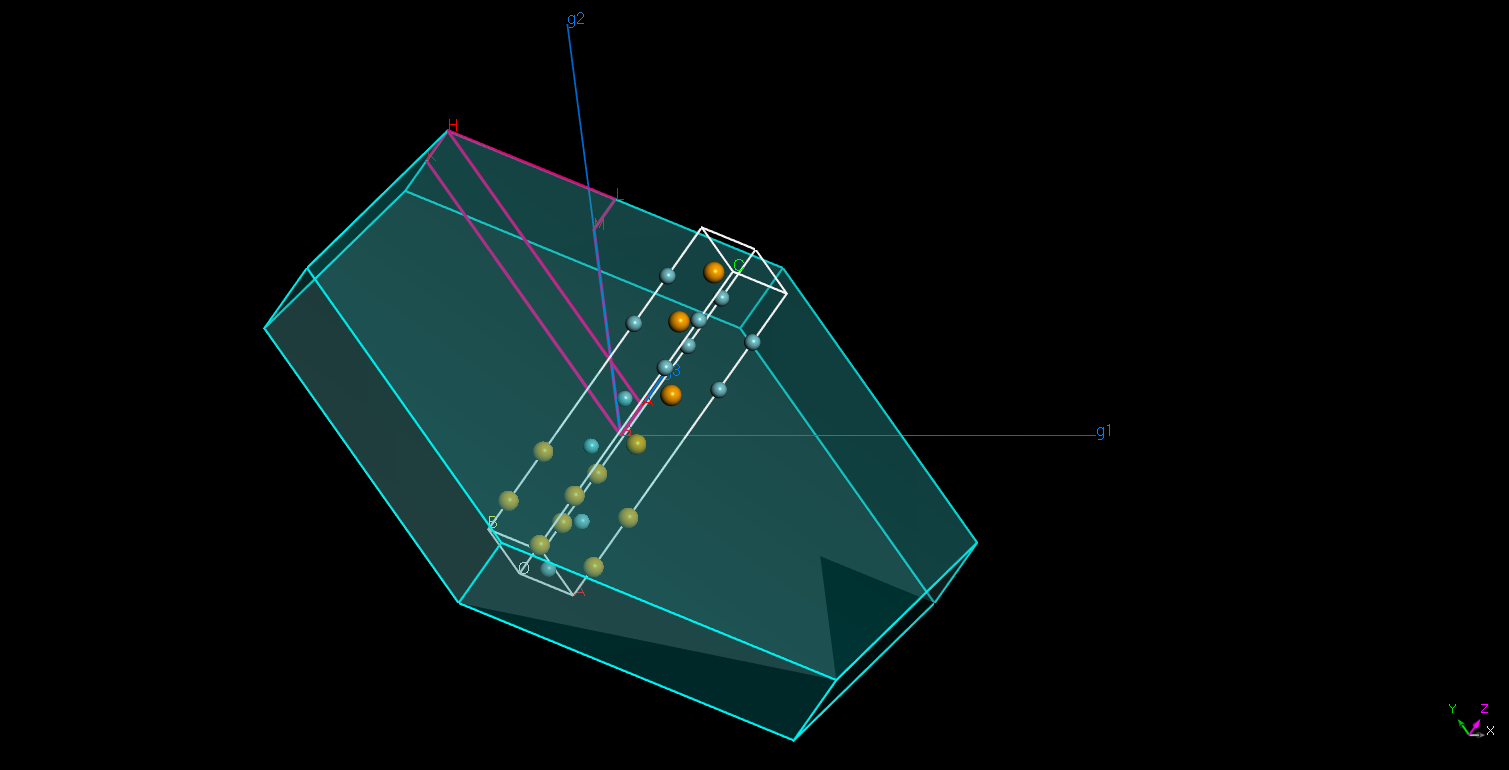
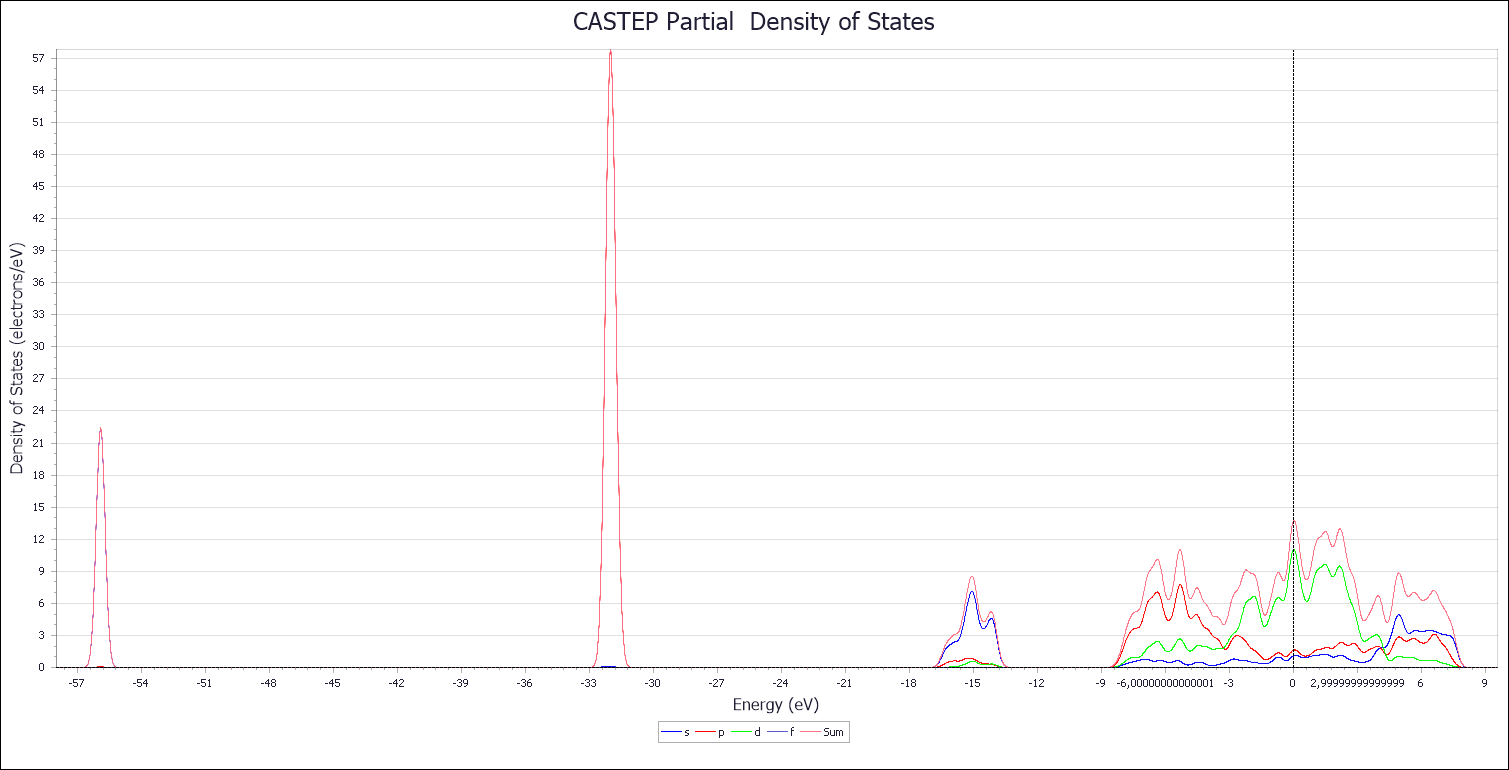
3R-Nb1.1Se2-12-US CASTEP GeomOpt

3R-Nb1.1Se2-7-US Band Structure

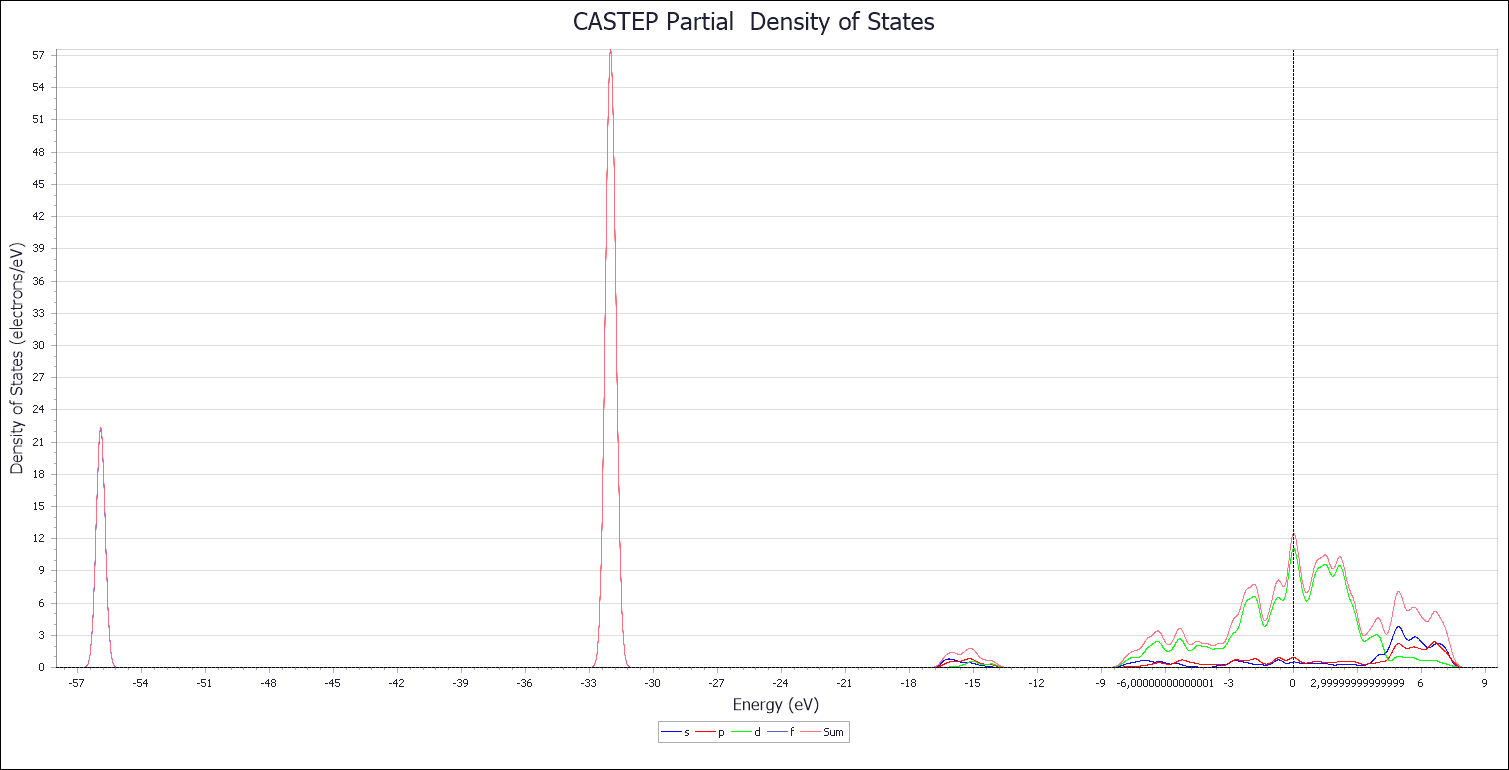




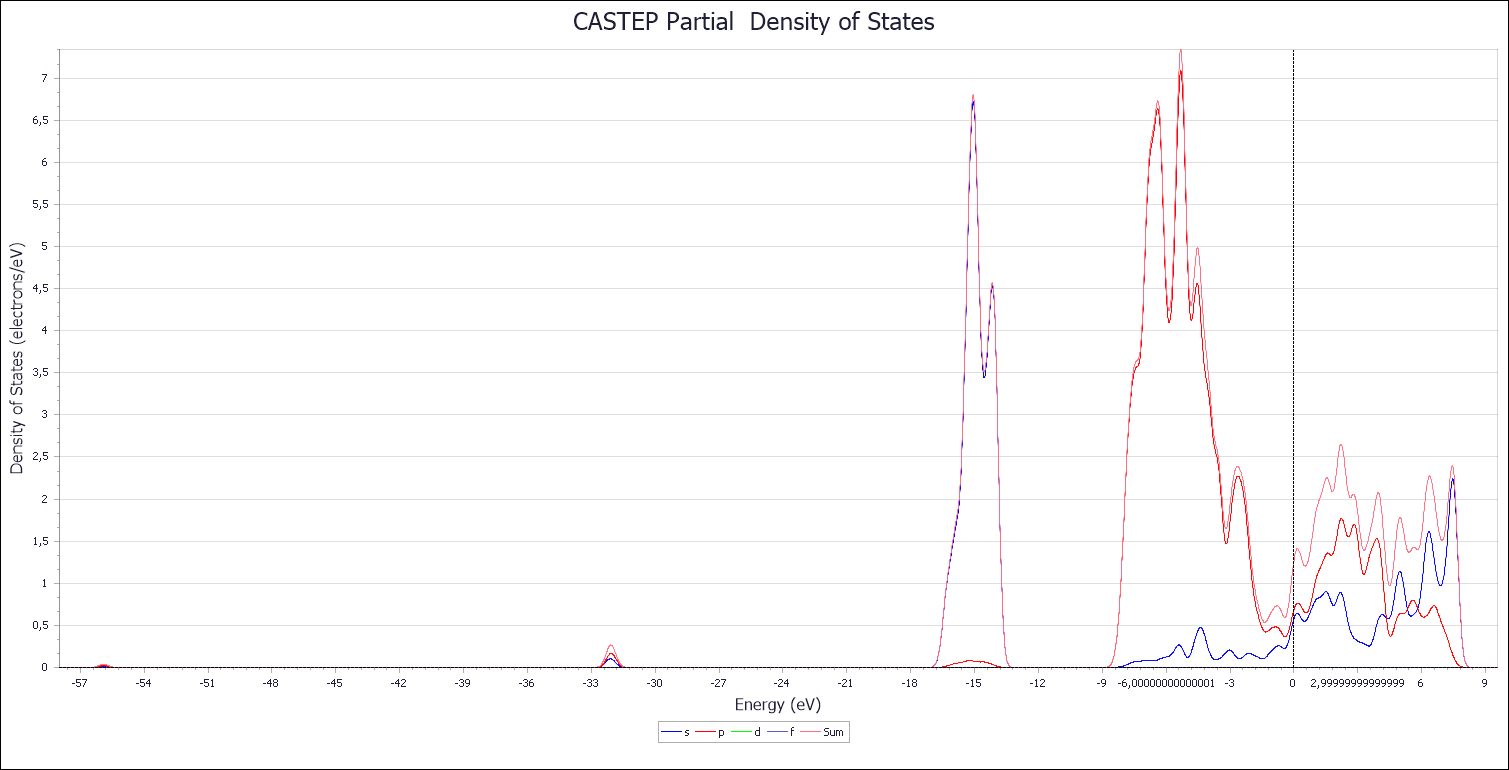
3R-Nb1.1Se2-7-US PDOS-Total



3R-Nb1.1Se2-7-US PDOS-Nb



3R-Nb1.1Se2-7-US PDOS-Se



Job started on host DESKTOP-UVBHK2J

at Sun Mar 8 09:53:27 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: |

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

| |

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| |

| Copyright (c) 2000 - 2014 |

| |

| Please cite |

| |

| "First principles methods using CASTEP" |

| |

| Zeitschrift fuer Kristallographie |

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

| |

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

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

| M. C. Payne |

| |

| in all publications arising from |

| your use of CASTEP |

| |

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

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

Code version: 6546

Intel(R) Math Kernel Library Version 11.1.2

Fundamental constants values: CODATA 2010

License checkout of MS\_castep successful

Pseudo atomic calculation performed for Se 4s2 4p4

Converged in 18 iterations to a total energy of -256.4822 eV

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

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

Calculation parallelised over 14 processes.

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

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

CASTEP calculation from Materials Studio

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

output verbosity : normal (1)

write checkpoint data to : 3R-Nb1.1Se2-7-US.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 (95328462)

data distribution : optimal for this architecture

optimization strategy : balance speed and memory

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

using functional : Perdew Burke Ernzerhof

Divergence correction : off

relativistic treatment : Koelling-Harmon

DFT+D: Semi-empirical dispersion correction : off

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

pseudopotential representation : reciprocal space

<beta|phi> representation : reciprocal space

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

plane wave basis set cut-off : 500.0000 eV

size of standard grid : 1.7500

size of fine grid : 2.1000

size of fine gmax : 24.0571 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 : 114.0

net charge of system : 0.000

net spin of system : 0.000

number of up spins : 57.00

number of down spins : 57.00

treating system as non-spin-polarized

number of bands : 57

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* 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. : 0.1000E-05 eV

eigen-energy convergence tolerance : 0.2105E-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

Partial DOS weights calculated

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* 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 : 0.1000E-04 eV/atom

max ionic |force| tolerance : 0.3000E-01 eV/A

max ionic |displacement| tolerance : 0.1000E-02 A

max |stress component| tolerance : 0.5000E-01 GPa

convergence tolerance window : 2 steps

backup results every : 5 steps

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

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Unit Cell

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

3.0025101 -1.7335000 0.0000000 2.0926442 0.0000000 0.0000000

0.0000000 3.4670000 0.0000000 1.0463221 1.8122830 0.0000000

0.0000000 0.0000000 18.8660000 0.0000000 0.0000000 0.3330428

Lattice parameters(A) Cell Angles

a = 3.467000 alpha = 90.000000

b = 3.467000 beta = 90.000000

c = 18.866000 gamma = 120.000000

Current cell volume = 196.389446 A\*\*3

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Cell Contents

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

Total number of ions in cell = 12

Total number of species in cell = 2

Max number of any one species = 6

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.423400 x

x Se 2 0.666667 0.333333 0.600600 x

x Se 3 1.333333 0.666667 0.756733 x

x Se 4 1.333333 0.666667 0.933933 x

x Se 5 1.000000 1.000000 1.090067 x

x Se 6 1.000000 1.000000 1.267267 x

x Nb 1 0.333333 0.666667 0.512100 x

x Nb 2 0.333333 0.666667 0.335000 x

x Nb 3 1.000000 1.000000 0.845433 x

x Nb 4 1.000000 1.000000 0.668333 x

x Nb 5 0.666667 1.333333 1.178767 x

x Nb 6 0.666667 1.333333 1.001667 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 5 5 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 3 primitive cells

Maximum deviation from symmetry = 0.858764E-13 ANG

Number of symmetry operations = 18

There are no ionic constraints specified or generated for this cell

Point group of crystal = 18: C3v, 3m, 3 m

Space group of crystal = 160: R3m, P 3\* -2

Set iprint > 1 for details on symmetry rotations/translations

Centre of mass is NOT constrained

Number of cell constraints= 4

Cell constraints are: 1 1 3 0 0 0

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 112.9 MB 87.0 MB |

| Electronic energy minimisation requirements 11.5 MB 0.0 MB |

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

| Approx. total storage required per process 124.4 MB 87.0 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 -7.90080132E+003 2.38 <-- SCF

1 -1.05895400E+004 2.24061560E+002 4.02 <-- SCF

2 -1.08644930E+004 2.29127440E+001 5.23 <-- SCF

3 -1.08740691E+004 7.98011121E-001 6.47 <-- SCF

4 -1.08716816E+004 -1.98954591E-001 8.55 <-- SCF

5 -1.08714779E+004 -1.69791224E-002 10.56 <-- SCF

6 -1.08713540E+004 -1.03288146E-002 12.53 <-- SCF

7 -1.08713784E+004 2.03455159E-003 14.84 <-- SCF

8 -1.08713784E+004 5.91792849E-006 16.92 <-- SCF

9 -1.08713885E+004 8.41893553E-004 18.84 <-- SCF

10 -1.08713947E+004 5.15696679E-004 20.48 <-- SCF

11 -1.08713990E+004 3.57741973E-004 22.02 <-- SCF

12 -1.08714023E+004 2.69690306E-004 23.50 <-- SCF

13 -1.08714049E+004 2.17469433E-004 25.02 <-- SCF

14 -1.08714083E+004 2.82585380E-004 26.72 <-- SCF

15 -1.08714117E+004 2.90379734E-004 28.16 <-- SCF

16 -1.08714157E+004 3.30664536E-004 29.72 <-- SCF

17 -1.08714227E+004 5.78700248E-004 31.61 <-- SCF

18 -1.08714282E+004 4.58622123E-004 33.28 <-- SCF

19 -1.08714303E+004 1.77320509E-004 34.89 <-- SCF

20 -1.08714312E+004 7.40340330E-005 36.42 <-- SCF

21 -1.08714314E+004 1.51120475E-005 37.86 <-- SCF

22 -1.08714327E+004 1.08230580E-004 39.59 <-- SCF

23 -1.08714297E+004 -2.45749193E-004 41.52 <-- SCF

24 -1.08714282E+004 -1.24252191E-004 43.56 <-- SCF

25 -1.08714285E+004 2.64227539E-005 45.36 <-- SCF

26 -1.08714284E+004 -1.07548325E-005 47.38 <-- SCF

27 -1.08714282E+004 -1.26274413E-005 49.31 <-- SCF

28 -1.08714286E+004 2.64769203E-005 51.23 <-- SCF

29 -1.08714288E+004 2.04359201E-005 52.89 <-- SCF

30 -1.08714286E+004 -2.16054539E-005 54.44 <-- SCF

31 -1.08714284E+004 -1.15870761E-005 55.95 <-- SCF

32 -1.08714280E+004 -3.33578029E-005 57.84 <-- SCF

33 -1.08714281E+004 4.38761504E-006 59.39 <-- SCF

34 -1.08714290E+004 7.50123938E-005 61.42 <-- SCF

35 -1.08714290E+004 4.03561581E-006 63.00 <-- SCF

36 -1.08714287E+004 -2.68292916E-005 64.59 <-- SCF

37 -1.08714284E+004 -2.71645398E-005 66.20 <-- SCF

38 -1.08714278E+004 -4.42092786E-005 68.19 <-- SCF

39 -1.08714279E+004 7.75981122E-006 69.84 <-- SCF

40 -1.08714279E+004 -5.86956275E-006 71.56 <-- SCF

41 -1.08714279E+004 -1.86197461E-007 72.98 <-- SCF

42 -1.08714279E+004 2.32313918E-007 74.59 <-- SCF

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

Final energy = -10871.42786019 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 -1.08714307E+004 76.16 <-- SCF

1 -1.08714296E+004 -9.73499589E-005 77.52 <-- SCF

2 -1.08714296E+004 1.35596000E-006 79.11 <-- SCF

3 -1.08714297E+004 1.40943715E-005 81.23 <-- SCF

4 -1.08714393E+004 8.00399883E-004 83.39 <-- SCF

5 -1.08714286E+004 -8.95254573E-004 85.55 <-- SCF

6 -1.08714301E+004 1.28223495E-004 87.61 <-- SCF

7 -1.08714296E+004 -4.69147949E-005 89.44 <-- SCF

8 -1.08714294E+004 -1.26271153E-005 91.27 <-- SCF

9 -1.08714294E+004 -1.91967573E-006 93.09 <-- SCF

10 -1.08714294E+004 3.85951746E-007 94.50 <-- SCF

11 -1.08714294E+004 -1.11045417E-006 95.94 <-- SCF

12 -1.08714294E+004 4.70699238E-008 97.50 <-- SCF

13 -1.08714294E+004 8.77705607E-008 98.95 <-- SCF

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

Final energy = -10871.42939788 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 -1.08714323E+004 100.45 <-- SCF

1 -1.08714309E+004 -1.10597454E-004 101.95 <-- SCF

2 -1.08714310E+004 7.57827204E-007 103.50 <-- SCF

3 -1.08714310E+004 5.88232298E-006 105.44 <-- SCF

4 -1.08714354E+004 3.63380247E-004 107.58 <-- SCF

5 -1.08714305E+004 -4.04687535E-004 109.72 <-- SCF

6 -1.08714311E+004 5.15438361E-005 111.56 <-- SCF

7 -1.08714309E+004 -1.67086584E-005 113.50 <-- SCF

8 -1.08714309E+004 -6.27849732E-006 116.12 <-- SCF

9 -1.08714309E+004 5.24212824E-007 118.83 <-- SCF

10 -1.08714309E+004 -1.80474602E-007 120.50 <-- SCF

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

Final energy = -10871.43087531 eV

(energy not corrected for finite basis set)

For future reference: finite basis dEtot/dlog(Ecut) = -0.148365eV

Total energy corrected for finite basis set = -10871.430813 eV

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

| Memory Disk |

| Model and support data 112.9 MB 87.0 MB |

| Electronic energy minimisation requirements 11.5 MB 0.0 MB |

| Geometry minimisation requirements 14.3 MB 0.0 MB |

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

| Approx. total storage required per process 138.7 MB 87.0 MB |

| |

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

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

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 1.25333 \*

\* Se 2 -0.00000 0.00000 -3.21159 \*

\* Se 3 0.00000 -0.00000 1.25333 \*

\* Se 4 -0.00000 -0.00000 -3.21159 \*

\* Se 5 0.00000 0.00000 1.25333 \*

\* Se 6 -0.00000 0.00000 -3.21159 \*

\* Nb 1 0.00000 0.00000 -0.92103 \*

\* Nb 2 0.00000 0.00000 2.87929 \*

\* Nb 3 0.00000 0.00000 -0.92103 \*

\* Nb 4 0.00000 0.00000 2.87929 \*

\* Nb 5 -0.00000 0.00000 -0.92103 \*

\* Nb 6 0.00000 -0.00000 2.87929 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -20.486843 0.000000 -0.000000 \*

\* y 0.000000 -20.486843 0.000000 \*

\* z -0.000000 0.000000 -24.129843 \*

\* \*

\* Pressure: 21.7012 \*

\* \*

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

BFGS: finished iteration 0 with enthalpy= -1.08714308E+004 eV

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

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

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

| dE/ion | 0.000000E+000 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 3.211591E+000 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 0.000000E+000 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 2.412984E+001 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 1 ...

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

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

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

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

| previous | 0.000000 | 0.045331 | -10871.430813 | <-- min BFGS

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

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

BFGS: starting iteration 1 with trial guess (lambda= 0.871822)

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

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

| Memory Disk |

| Model and support data 113.2 MB 87.0 MB |

| Electronic energy minimisation requirements 11.8 MB 0.0 MB |

| Geometry minimisation requirements 14.6 MB 0.0 MB |

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

| Approx. total storage required per process 139.6 MB 87.0 MB |

| |

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

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

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Unit Cell

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

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

3.0382617 -1.7541412 0.0000000 2.0680198 -0.0000000 -0.0000000

0.0000000 3.5082825 0.0000000 1.0340099 1.7909576 -0.0000000

0.0000000 0.0000000 19.1305886 -0.0000000 -0.0000000 0.3284366

Lattice parameters(A) Cell Angles

a = 3.508282 alpha = 90.000000

b = 3.508282 beta = 90.000000

c = 19.130589 gamma = 120.000000

Current cell volume = 203.914483 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.423466 x

x Se 2 0.666667 0.333333 0.600431 x

x Se 3 1.333333 0.666667 0.756799 x

x Se 4 1.333333 0.666667 0.933764 x

x Se 5 1.000000 1.000000 1.090133 x

x Se 6 1.000000 1.000000 1.267098 x

x Nb 1 0.333333 0.666667 0.512052 x

x Nb 2 0.333333 0.666667 0.335151 x

x Nb 3 1.000000 1.000000 0.845385 x

x Nb 4 1.000000 1.000000 0.668485 x

x Nb 5 0.666667 1.333333 1.178718 x

x Nb 6 0.666667 1.333333 1.001818 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08701162E+004 139.05 <-- SCF

1 -1.08738361E+004 3.09992519E-001 140.67 <-- SCF

2 -1.08739480E+004 9.32107790E-003 143.23 <-- SCF

3 -1.08726693E+004 -1.06556018E-001 145.50 <-- SCF

4 -1.08724153E+004 -2.11698531E-002 147.72 <-- SCF

5 -1.08723143E+004 -8.41417744E-003 149.86 <-- SCF

6 -1.08723176E+004 2.75879203E-004 152.23 <-- SCF

7 -1.08723169E+004 -5.47283268E-005 154.69 <-- SCF

8 -1.08723172E+004 2.13953369E-005 156.80 <-- SCF

9 -1.08723172E+004 -3.11027480E-006 158.75 <-- SCF

10 -1.08723172E+004 1.12171080E-006 160.41 <-- SCF

11 -1.08723172E+004 1.03884832E-006 162.11 <-- SCF

12 -1.08723172E+004 3.37849599E-007 163.64 <-- SCF

13 -1.08723172E+004 -1.94970456E-007 165.16 <-- SCF

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

Final energy = -10872.31719278 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 1.20036 \*

\* Se 2 0.00000 -0.00000 -2.81096 \*

\* Se 3 0.00000 -0.00000 1.20036 \*

\* Se 4 0.00000 -0.00000 -2.81096 \*

\* Se 5 0.00000 -0.00000 1.20036 \*

\* Se 6 0.00000 0.00000 -2.81096 \*

\* Nb 1 0.00000 0.00000 -0.91870 \*

\* Nb 2 -0.00000 -0.00000 2.52931 \*

\* Nb 3 0.00000 0.00000 -0.91870 \*

\* Nb 4 -0.00000 -0.00000 2.52931 \*

\* Nb 5 0.00000 0.00000 -0.91870 \*

\* Nb 6 0.00000 -0.00000 2.52931 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -12.540595 -0.000000 0.000000 \*

\* y -0.000000 -12.540595 -0.000000 \*

\* z 0.000000 -0.000000 -15.607821 \*

\* \*

\* Pressure: 13.5630 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.045331 | -10871.430813 | <-- min BFGS

| trial step | 0.871822 | 0.029788 | -10872.317284 | <-- min BFGS

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

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

BFGS: improving iteration 1 with line minimization (lambda= 1.307734)

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

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

| Memory Disk |

| Model and support data 115.1 MB 107.4 MB |

| Electronic energy minimisation requirements 12.5 MB 0.0 MB |

| Geometry minimisation requirements 15.4 MB 0.0 MB |

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

| Approx. total storage required per process 142.9 MB 107.4 MB |

| |

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

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

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Unit Cell

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

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

3.0561376 -1.7644619 0.0000000 2.0559236 -0.0000000 -0.0000000

0.0000000 3.5289237 0.0000000 1.0279618 1.7804820 -0.0000000

0.0000000 0.0000000 19.2628829 -0.0000000 -0.0000000 0.3261809

Lattice parameters(A) Cell Angles

a = 3.528924 alpha = 90.000000

b = 3.528924 beta = 90.000000

c = 19.262883 gamma = 120.000000

Current cell volume = 207.747810 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.423499 x

x Se 2 0.666667 0.333333 0.600347 x

x Se 3 1.333333 0.666667 0.756832 x

x Se 4 1.333333 0.666667 0.933680 x

x Se 5 1.000000 1.000000 1.090166 x

x Se 6 1.000000 1.000000 1.267013 x

x Nb 1 0.333333 0.666667 0.512027 x

x Nb 2 0.333333 0.666667 0.335227 x

x Nb 3 1.000000 1.000000 0.845361 x

x Nb 4 1.000000 1.000000 0.668560 x

x Nb 5 0.666667 1.333333 1.178694 x

x Nb 6 0.666667 1.333333 1.001894 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08721112E+004 184.33 <-- SCF

1 -1.08730274E+004 7.63537802E-002 186.20 <-- SCF

2 -1.08730547E+004 2.27512848E-003 188.64 <-- SCF

3 -1.08727504E+004 -2.53552352E-002 191.22 <-- SCF

4 -1.08726808E+004 -5.80655749E-003 194.14 <-- SCF

5 -1.08726527E+004 -2.33568353E-003 197.09 <-- SCF

6 -1.08726536E+004 7.06345187E-005 200.34 <-- SCF

7 -1.08726534E+004 -1.65848103E-005 203.00 <-- SCF

8 -1.08726534E+004 4.84250662E-006 205.17 <-- SCF

9 -1.08726534E+004 5.01402339E-007 207.56 <-- SCF

10 -1.08726534E+004 4.08734905E-008 209.38 <-- SCF

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

Final energy = -10872.65344344 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 1.16967 \*

\* Se 2 0.00000 0.00000 -2.60557 \*

\* Se 3 0.00000 0.00000 1.16967 \*

\* Se 4 0.00000 0.00000 -2.60557 \*

\* Se 5 0.00000 0.00000 1.16967 \*

\* Se 6 0.00000 -0.00000 -2.60557 \*

\* Nb 1 -0.00000 0.00000 -0.92545 \*

\* Nb 2 -0.00000 0.00000 2.36135 \*

\* Nb 3 0.00000 0.00000 -0.92545 \*

\* Nb 4 -0.00000 0.00000 2.36135 \*

\* Nb 5 0.00000 0.00000 -0.92545 \*

\* Nb 6 -0.00000 -0.00000 2.36135 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -9.315545 -0.000000 0.000000 \*

\* y -0.000000 -9.315545 -0.000000 \*

\* z 0.000000 -0.000000 -11.969618 \*

\* \*

\* Pressure: 10.2002 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.045331 | -10871.430813 | <-- min BFGS

| trial step | 0.871822 | 0.029788 | -10872.317284 | <-- min BFGS

| line step | 1.307734 | 0.023138 | -10872.653468 | <-- min BFGS

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

BFGS: finished iteration 1 with enthalpy= -1.08726535E+004 eV

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

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

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

| dE/ion | 1.018879E-001 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 2.605568E+000 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.878458E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.196962E+001 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 2 ...

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

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

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

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

| previous | 0.000000 | 0.032987 | -10872.653468 | <-- min BFGS

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

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

BFGS: starting iteration 2 with trial guess (lambda= 0.621682)

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

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

| Memory Disk |

| Model and support data 115.5 MB 107.4 MB |

| Electronic energy minimisation requirements 12.8 MB 0.0 MB |

| Geometry minimisation requirements 15.9 MB 0.0 MB |

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

| Approx. total storage required per process 144.1 MB 107.4 MB |

| |

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

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

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

Unit Cell

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

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

3.0897354 -1.7838596 0.0000000 2.0335675 -0.0000000 -0.0000000

0.0000000 3.5677191 -0.0000000 1.0167837 1.7611211 0.0000000

0.0000000 -0.0000000 19.5274715 -0.0000000 0.0000000 0.3217613

Lattice parameters(A) Cell Angles

a = 3.567719 alpha = 90.000000

b = 3.567719 beta = 90.000000

c = 19.527472 gamma = 120.000000

Current cell volume = 215.257332 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.423607 x

x Se 2 0.666667 0.333333 0.600101 x

x Se 3 1.333333 0.666667 0.756940 x

x Se 4 1.333333 0.666667 0.933434 x

x Se 5 1.000000 1.000000 1.090274 x

x Se 6 1.000000 1.000000 1.266767 x

x Nb 1 0.333333 0.666667 0.511943 x

x Nb 2 0.333333 0.666667 0.335450 x

x Nb 3 1.000000 1.000000 0.845276 x

x Nb 4 1.000000 1.000000 0.668783 x

x Nb 5 0.666667 1.333333 1.178610 x

x Nb 6 0.666667 1.333333 1.002116 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08710402E+004 232.56 <-- SCF

1 -1.08745157E+004 2.89618102E-001 234.06 <-- SCF

2 -1.08746541E+004 1.15382897E-002 236.83 <-- SCF

3 -1.08735247E+004 -9.41146664E-002 239.64 <-- SCF

4 -1.08731577E+004 -3.05855609E-002 242.25 <-- SCF

5 -1.08730595E+004 -8.18156936E-003 245.09 <-- SCF

6 -1.08730635E+004 3.31433684E-004 247.67 <-- SCF

7 -1.08730635E+004 -9.41228330E-007 250.34 <-- SCF

8 -1.08730640E+004 4.21840183E-005 252.70 <-- SCF

9 -1.08730641E+004 5.76650463E-006 255.11 <-- SCF

10 -1.08730641E+004 5.10899811E-006 257.28 <-- SCF

11 -1.08730642E+004 2.00836148E-006 259.39 <-- SCF

12 -1.08730642E+004 1.57769918E-006 261.11 <-- SCF

13 -1.08730642E+004 6.82521049E-007 262.98 <-- SCF

14 -1.08730642E+004 4.65014921E-007 264.45 <-- SCF

15 -1.08730642E+004 2.68815283E-007 266.28 <-- SCF

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

Final energy = -10873.06420025 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 1.08734 \*

\* Se 2 0.00000 0.00000 -2.25343 \*

\* Se 3 0.00000 0.00000 1.08734 \*

\* Se 4 0.00000 0.00000 -2.25343 \*

\* Se 5 0.00000 0.00000 1.08734 \*

\* Se 6 0.00000 -0.00000 -2.25343 \*

\* Nb 1 -0.00000 0.00000 -0.90647 \*

\* Nb 2 0.00000 -0.00000 2.07257 \*

\* Nb 3 -0.00000 0.00000 -0.90647 \*

\* Nb 4 -0.00000 -0.00000 2.07257 \*

\* Nb 5 -0.00000 0.00000 -0.90647 \*

\* Nb 6 0.00000 -0.00000 2.07257 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -3.307479 -0.000000 0.000000 \*

\* y -0.000000 -3.307479 0.000000 \*

\* z 0.000000 0.000000 -5.553622 \*

\* \*

\* Pressure: 4.0562 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.032987 | -10872.653468 | <-- min BFGS

| trial step | 0.621682 | 0.015880 | -10873.064176 | <-- min BFGS

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

BFGS: finished iteration 2 with enthalpy= -1.08730642E+004 eV

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

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

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

| dE/ion | 3.422570E-002 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 2.253429E+000 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.806985E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 5.553622E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 3 ...

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

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

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

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

| previous | 0.000000 | 0.010646 | -10873.064176 | <-- min BFGS

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

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

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

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

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

| Memory Disk |

| Model and support data 116.7 MB 114.5 MB |

| Electronic energy minimisation requirements 13.3 MB 0.0 MB |

| Geometry minimisation requirements 16.4 MB 0.0 MB |

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

| Approx. total storage required per process 146.4 MB 114.5 MB |

| |

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

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

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Unit Cell

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

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

3.1187417 -1.8006063 0.0000000 2.0146540 -0.0000000 -0.0000000

0.0000000 3.6012127 -0.0000000 1.0073270 1.7447415 0.0000000

0.0000000 -0.0000000 19.7878403 -0.0000000 0.0000000 0.3175276

Lattice parameters(A) Cell Angles

a = 3.601213 alpha = 90.000000

b = 3.601213 beta = 90.000000

c = 19.787840 gamma = 120.000000

Current cell volume = 222.242221 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.423777 x

x Se 2 0.666667 0.333333 0.599736 x

x Se 3 1.333333 0.666667 0.757110 x

x Se 4 1.333333 0.666667 0.933070 x

x Se 5 1.000000 1.000000 1.090443 x

x Se 6 1.000000 1.000000 1.266403 x

x Nb 1 0.333333 0.666667 0.511804 x

x Nb 2 0.333333 0.666667 0.335783 x

x Nb 3 1.000000 1.000000 0.845137 x

x Nb 4 1.000000 1.000000 0.669116 x

x Nb 5 0.666667 1.333333 1.178470 x

x Nb 6 0.666667 1.333333 1.002450 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08714586E+004 289.53 <-- SCF

1 -1.08746261E+004 2.63954314E-001 291.09 <-- SCF

2 -1.08748564E+004 1.91948379E-002 293.77 <-- SCF

3 -1.08741483E+004 -5.90069604E-002 296.16 <-- SCF

4 -1.08732548E+004 -7.44659627E-002 298.69 <-- SCF

5 -1.08732305E+004 -2.01967114E-003 302.08 <-- SCF

6 -1.08732309E+004 3.26904081E-005 305.77 <-- SCF

7 -1.08732322E+004 1.05779095E-004 308.48 <-- SCF

8 -1.08732326E+004 3.42895546E-005 311.92 <-- SCF

9 -1.08732327E+004 7.33114002E-006 314.27 <-- SCF

10 -1.08732328E+004 6.17887191E-006 316.12 <-- SCF

11 -1.08732328E+004 3.98181208E-006 318.02 <-- SCF

12 -1.08732328E+004 2.10127756E-006 320.42 <-- SCF

13 -1.08732328E+004 1.25658415E-006 323.06 <-- SCF

14 -1.08732329E+004 6.68167758E-007 325.41 <-- SCF

15 -1.08732329E+004 7.51805558E-007 327.27 <-- SCF

16 -1.08732329E+004 4.53635200E-007 329.17 <-- SCF

17 -1.08732329E+004 1.51404008E-007 331.33 <-- SCF

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

Final energy = -10873.23286712 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 0.99411 \*

\* Se 2 0.00000 0.00000 -1.90567 \*

\* Se 3 0.00000 -0.00000 0.99411 \*

\* Se 4 0.00000 -0.00000 -1.90567 \*

\* Se 5 0.00000 -0.00000 0.99411 \*

\* Se 6 0.00000 0.00000 -1.90567 \*

\* Nb 1 -0.00000 0.00000 -0.90442 \*

\* Nb 2 -0.00000 0.00000 1.81598 \*

\* Nb 3 -0.00000 0.00000 -0.90442 \*

\* Nb 4 0.00000 0.00000 1.81598 \*

\* Nb 5 -0.00000 0.00000 -0.90442 \*

\* Nb 6 0.00000 0.00000 1.81598 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 1.497664 0.000000 -0.000000 \*

\* y 0.000000 1.497664 0.000000 \*

\* z -0.000000 0.000000 -0.321971 \*

\* \*

\* Pressure: -0.8911 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.010646 | -10873.064176 | <-- min BFGS

| trial step | 1.000000 | 0.002274 | -10873.232906 | <-- min BFGS

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

BFGS: finished iteration 3 with enthalpy= -1.08732329E+004 eV

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

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

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

| dE/ion | 1.406081E-002 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.905672E+000 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.208878E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.497664E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 4 ...

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

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

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

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

| previous | 0.000000 | 0.002264 | -10873.232906 | <-- min BFGS

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

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

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

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

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

| Memory Disk |

| Model and support data 116.8 MB 114.5 MB |

| Electronic energy minimisation requirements 13.3 MB 0.0 MB |

| Geometry minimisation requirements 16.5 MB 0.0 MB |

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

| Approx. total storage required per process 146.6 MB 114.5 MB |

| |

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

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

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

Unit Cell

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

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

3.1240764 -1.8036864 0.0000000 2.0112137 -0.0000000 -0.0000000

0.0000000 3.6073727 0.0000000 1.0056069 1.7417622 -0.0000000

0.0000000 0.0000000 19.8740324 -0.0000000 -0.0000000 0.3161505

Lattice parameters(A) Cell Angles

a = 3.607373 alpha = 90.000000

b = 3.607373 beta = 90.000000

c = 19.874032 gamma = 120.000000

Current cell volume = 223.974541 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.423901 x

x Se 2 0.666667 0.333333 0.599486 x

x Se 3 1.333333 0.666667 0.757234 x

x Se 4 1.333333 0.666667 0.932819 x

x Se 5 1.000000 1.000000 1.090568 x

x Se 6 1.000000 1.000000 1.266153 x

x Nb 1 0.333333 0.666667 0.511695 x

x Nb 2 0.333333 0.666667 0.336018 x

x Nb 3 1.000000 1.000000 0.845029 x

x Nb 4 1.000000 1.000000 0.669351 x

x Nb 5 0.666667 1.333333 1.178362 x

x Nb 6 0.666667 1.333333 1.002684 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08730896E+004 357.86 <-- SCF

1 -1.08735761E+004 4.05372368E-002 359.67 <-- SCF

2 -1.08736110E+004 2.90630170E-003 362.30 <-- SCF

3 -1.08736572E+004 3.85295334E-003 365.36 <-- SCF

4 -1.08732551E+004 -3.35076353E-002 367.78 <-- SCF

5 -1.08732881E+004 2.74936047E-003 370.64 <-- SCF

6 -1.08732862E+004 -1.60024922E-004 373.08 <-- SCF

7 -1.08732862E+004 1.86711471E-006 375.48 <-- SCF

8 -1.08732863E+004 7.23171093E-006 377.61 <-- SCF

9 -1.08732863E+004 3.05648357E-006 379.73 <-- SCF

10 -1.08732864E+004 2.12409642E-006 381.64 <-- SCF

11 -1.08732864E+004 1.46761478E-006 383.55 <-- SCF

12 -1.08732864E+004 9.75412735E-007 385.55 <-- SCF

13 -1.08732864E+004 5.73398367E-007 387.42 <-- SCF

14 -1.08732864E+004 7.52934585E-007 389.16 <-- SCF

15 -1.08732864E+004 -5.68018122E-007 390.88 <-- SCF

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

Final energy = -10873.28639216 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 0.97243 \*

\* Se 2 0.00000 0.00000 -1.77304 \*

\* Se 3 -0.00000 0.00000 0.97243 \*

\* Se 4 -0.00000 0.00000 -1.77304 \*

\* Se 5 -0.00000 0.00000 0.97243 \*

\* Se 6 0.00000 0.00000 -1.77304 \*

\* Nb 1 -0.00000 0.00000 -0.91759 \*

\* Nb 2 0.00000 -0.00000 1.71821 \*

\* Nb 3 -0.00000 0.00000 -0.91759 \*

\* Nb 4 0.00000 0.00000 1.71821 \*

\* Nb 5 -0.00000 0.00000 -0.91759 \*

\* Nb 6 0.00000 0.00000 1.71821 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 2.679330 0.000000 -0.000000 \*

\* y 0.000000 2.679330 0.000000 \*

\* z -0.000000 0.000000 0.860710 \*

\* \*

\* Pressure: -2.0731 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.002264 | -10873.232906 | <-- min BFGS

| trial step | 1.000000 | 0.001677 | -10873.286465 | <-- min BFGS

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

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

BFGS: improving iteration 4 with line minimization (lambda= 3.069755)

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

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

| Memory Disk |

| Model and support data 117.4 MB 114.5 MB |

| Electronic energy minimisation requirements 13.4 MB 0.0 MB |

| Geometry minimisation requirements 16.7 MB 0.0 MB |

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

| Approx. total storage required per process 147.5 MB 114.5 MB |

| |

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

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

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

Unit Cell

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

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

3.1351180 -1.8100612 -0.0000000 2.0041304 -0.0000000 -0.0000000

0.0000000 3.6201224 0.0000000 1.0020652 1.7356278 -0.0000000

0.0000000 0.0000000 20.0524289 -0.0000000 -0.0000000 0.3133379

Lattice parameters(A) Cell Angles

a = 3.620122 alpha = 90.000000

b = 3.620122 beta = 90.000000

c = 20.052429 gamma = 120.000000

Current cell volume = 227.585264 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.424158 x

x Se 2 0.666667 0.333333 0.598968 x

x Se 3 1.333333 0.666667 0.757492 x

x Se 4 1.333333 0.666667 0.932301 x

x Se 5 1.000000 1.000000 1.090825 x

x Se 6 1.000000 1.000000 1.265634 x

x Nb 1 0.333333 0.666667 0.511471 x

x Nb 2 0.333333 0.666667 0.336503 x

x Nb 3 1.000000 1.000000 0.844804 x

x Nb 4 1.000000 1.000000 0.669837 x

x Nb 5 0.666667 1.333333 1.178137 x

x Nb 6 0.666667 1.333333 1.003170 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08725011E+004 416.00 <-- SCF

1 -1.08744604E+004 1.63272239E-001 417.72 <-- SCF

2 -1.08746181E+004 1.31462098E-002 420.31 <-- SCF

3 -1.08744841E+004 -1.11672033E-002 422.92 <-- SCF

4 -1.08733096E+004 -9.78795381E-002 425.44 <-- SCF

5 -1.08733522E+004 3.55372371E-003 427.89 <-- SCF

6 -1.08733460E+004 -5.19634786E-004 430.31 <-- SCF

7 -1.08733485E+004 2.06229238E-004 432.86 <-- SCF

8 -1.08733499E+004 1.17433119E-004 435.05 <-- SCF

9 -1.08733511E+004 1.05191435E-004 437.06 <-- SCF

10 -1.08733527E+004 1.33397113E-004 438.89 <-- SCF

11 -1.08733548E+004 1.67863764E-004 440.70 <-- SCF

12 -1.08733597E+004 4.11251001E-004 442.41 <-- SCF

13 -1.08733665E+004 5.66644569E-004 444.23 <-- SCF

14 -1.08733708E+004 3.60684065E-004 446.06 <-- SCF

15 -1.08733750E+004 3.49073418E-004 447.81 <-- SCF

16 -1.08733800E+004 4.13781631E-004 449.56 <-- SCF

17 -1.08733836E+004 2.98214507E-004 451.33 <-- SCF

18 -1.08733867E+004 2.59442778E-004 453.12 <-- SCF

19 -1.08733888E+004 1.76846318E-004 454.88 <-- SCF

20 -1.08733902E+004 1.14892472E-004 456.66 <-- SCF

21 -1.08733911E+004 8.01169830E-005 458.48 <-- SCF

22 -1.08733917E+004 4.68996756E-005 460.39 <-- SCF

23 -1.08733921E+004 3.30967387E-005 462.09 <-- SCF

24 -1.08733924E+004 2.33309961E-005 463.88 <-- SCF

25 -1.08733926E+004 1.75057705E-005 465.64 <-- SCF

26 -1.08733927E+004 1.01104212E-005 467.38 <-- SCF

27 -1.08733928E+004 8.00412757E-006 469.16 <-- SCF

28 -1.08733929E+004 4.92294219E-006 470.88 <-- SCF

29 -1.08733929E+004 3.97753121E-006 472.56 <-- SCF

30 -1.08733929E+004 3.40339335E-006 474.25 <-- SCF

31 -1.08733930E+004 2.65138155E-006 476.14 <-- SCF

32 -1.08733930E+004 -9.10904193E-007 477.92 <-- SCF

33 -1.08733931E+004 1.17708130E-005 480.14 <-- SCF

34 -1.08733931E+004 -2.63106204E-006 481.89 <-- SCF

35 -1.08733931E+004 2.72135142E-006 483.73 <-- SCF

36 -1.08733930E+004 -5.83633542E-006 486.02 <-- SCF

37 -1.08733936E+004 4.96489920E-005 488.39 <-- SCF

38 -1.08733989E+004 4.41606409E-004 490.86 <-- SCF

39 -1.08734035E+004 3.80711225E-004 493.05 <-- SCF

40 -1.08733945E+004 -7.50173531E-004 495.58 <-- SCF

41 -1.08733943E+004 -1.34850102E-005 498.61 <-- SCF

42 -1.08733931E+004 -9.98496443E-005 501.14 <-- SCF

43 -1.08733929E+004 -2.30000806E-005 503.52 <-- SCF

44 -1.08733929E+004 5.95991026E-006 505.78 <-- SCF

45 -1.08733932E+004 2.21793078E-005 508.17 <-- SCF

46 -1.08733929E+004 -2.72621279E-005 510.41 <-- SCF

47 -1.08733929E+004 4.83084100E-006 512.50 <-- SCF

48 -1.08733930E+004 4.58917520E-006 514.34 <-- SCF

49 -1.08733930E+004 -1.06182754E-006 516.17 <-- SCF

50 -1.08733929E+004 -7.26788812E-006 518.23 <-- SCF

51 -1.08733929E+004 -2.77249661E-007 520.06 <-- SCF

52 -1.08733929E+004 5.67739443E-007 521.83 <-- SCF

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

Final energy = -10873.39288878 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 1.02434 \*

\* Se 2 0.00000 0.00000 -1.74901 \*

\* Se 3 0.00000 0.00000 1.02434 \*

\* Se 4 0.00000 0.00000 -1.74901 \*

\* Se 5 0.00000 -0.00000 1.02434 \*

\* Se 6 0.00000 0.00000 -1.74901 \*

\* Nb 1 0.00000 0.00000 -1.05737 \*

\* Nb 2 -0.00000 -0.00000 1.78204 \*

\* Nb 3 0.00000 0.00000 -1.05737 \*

\* Nb 4 -0.00000 -0.00000 1.78204 \*

\* Nb 5 0.00000 0.00000 -1.05737 \*

\* Nb 6 -0.00000 0.00000 1.78204 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 6.106139 0.000000 0.000000 \*

\* y 0.000000 6.106139 0.000000 \*

\* z 0.000000 0.000000 1.268052 \*

\* \*

\* Pressure: -4.4934 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.002264 | -10873.232906 | <-- min BFGS

| trial step | 1.000000 | 0.001677 | -10873.286465 | <-- min BFGS

| line step | 3.069755 | 0.001058 | -10873.392968 | <-- min BFGS

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

BFGS: finished iteration 4 with enthalpy= -1.08733930E+004 eV

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

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

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

| dE/ion | 1.333852E-002 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.782038E+000 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.540980E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 6.106139E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 5 ...

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

Writing analysis data to 3R-Nb1.1Se2-7-US.castep\_bin

Writing model to 3R-Nb1.1Se2-7-US.check

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

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

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

| previous | 0.000000 | 0.014828 | -10873.392968 | <-- min BFGS

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

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

BFGS: starting iteration 5 with trial guess (lambda= 0.524233)

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

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

| Memory Disk |

| Model and support data 118.1 MB 114.5 MB |

| Electronic energy minimisation requirements 13.7 MB 0.0 MB |

| Geometry minimisation requirements 17.0 MB 0.0 MB |

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

| Approx. total storage required per process 148.7 MB 114.5 MB |

| |

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

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

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

Unit Cell

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

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

3.1384691 -1.8119960 -0.0000000 2.0019905 -0.0000000 -0.0000000

0.0000000 3.6239920 0.0000000 1.0009952 1.7337746 -0.0000000

0.0000000 0.0000000 20.3170175 -0.0000000 -0.0000000 0.3092573

Lattice parameters(A) Cell Angles

a = 3.623992 alpha = 90.000000

b = 3.623992 beta = 90.000000

c = 20.317018 gamma = 120.000000

Current cell volume = 231.081425 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 0.666667 0.333333 0.424641 x

x Se 2 0.666667 0.333333 0.598017 x

x Se 3 1.333333 0.666667 0.757974 x

x Se 4 1.333333 0.666667 0.931350 x

x Se 5 1.000000 1.000000 1.091308 x

x Se 6 1.000000 1.000000 1.264684 x

x Nb 1 0.333333 0.666667 0.511038 x

x Nb 2 0.333333 0.666667 0.337404 x

x Nb 3 1.000000 1.000000 0.844372 x

x Nb 4 1.000000 1.000000 0.670737 x

x Nb 5 0.666667 1.333333 1.177705 x

x Nb 6 0.666667 1.333333 1.004071 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08715009E+004 548.52 <-- SCF

1 -1.08769040E+004 4.50256270E-001 550.36 <-- SCF

2 -1.08773536E+004 3.74665354E-002 553.05 <-- SCF

3 -1.08767601E+004 -4.94558547E-002 555.55 <-- SCF

4 -1.08735577E+004 -2.66870406E-001 558.34 <-- SCF

5 -1.08735899E+004 2.68887691E-003 561.14 <-- SCF

6 -1.08735628E+004 -2.25951955E-003 564.28 <-- SCF

7 -1.08735660E+004 2.68348352E-004 567.23 <-- SCF

8 -1.08735645E+004 -1.28942047E-004 570.17 <-- SCF

9 -1.08735645E+004 5.43053683E-006 572.44 <-- SCF

10 -1.08735646E+004 2.69778623E-006 574.41 <-- SCF

11 -1.08735646E+004 1.38862520E-006 576.31 <-- SCF

12 -1.08735646E+004 7.02736024E-007 578.34 <-- SCF

13 -1.08735646E+004 3.44572069E-007 580.44 <-- SCF

14 -1.08735646E+004 1.60953104E-007 582.33 <-- SCF

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

Final energy = -10873.56461024 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.93592 \*

\* Se 2 0.00000 0.00000 -1.45045 \*

\* Se 3 0.00000 0.00000 0.93592 \*

\* Se 4 -0.00000 0.00000 -1.45045 \*

\* Se 5 0.00000 0.00000 0.93592 \*

\* Se 6 0.00000 0.00000 -1.45045 \*

\* Nb 1 -0.00000 0.00000 -1.05989 \*

\* Nb 2 -0.00000 0.00000 1.57442 \*

\* Nb 3 0.00000 0.00000 -1.05989 \*

\* Nb 4 0.00000 0.00000 1.57442 \*

\* Nb 5 0.00000 0.00000 -1.05989 \*

\* Nb 6 0.00000 0.00000 1.57442 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 8.320491 0.000000 0.000000 \*

\* y 0.000000 8.320491 -0.000000 \*

\* z 0.000000 -0.000000 3.725833 \*

\* \*

\* Pressure: -6.7889 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.014828 | -10873.392968 | <-- min BFGS

| trial step | 0.524233 | 0.009137 | -10873.564683 | <-- min BFGS

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

BFGS: finished iteration 5 with enthalpy= -1.08735647E+004 eV

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

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

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

| dE/ion | 1.430956E-002 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.574420E+000 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.932044E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 8.320491E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 6 ...

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

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

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

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

| previous | 0.000000 | 0.023048 | -10873.564683 | <-- min BFGS

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

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

BFGS: starting iteration 6 with trial guess (lambda= 0.483016)

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

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

| Memory Disk |

| Model and support data 119.5 MB 114.5 MB |

| Electronic energy minimisation requirements 13.7 MB 0.0 MB |

| Geometry minimisation requirements 17.0 MB 0.0 MB |

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

| Approx. total storage required per process 150.3 MB 114.5 MB |

| |

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

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

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

Unit Cell

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

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

3.1289541 -1.8065025 -0.0000000 2.0080785 -0.0000000 -0.0000000

0.0000000 3.6130050 0.0000000 1.0040392 1.7390470 -0.0000000

0.0000000 0.0000000 20.5816061 -0.0000000 -0.0000000 0.3052816

Lattice parameters(A) Cell Angles

a = 3.613005 alpha = 90.000000

b = 3.613005 beta = 90.000000

c = 20.581606 gamma = 120.000000

Current cell volume = 232.673548 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.425286 x

x Se 2 0.666667 0.333333 0.596764 x

x Se 3 1.333333 0.666667 0.758619 x

x Se 4 1.333333 0.666667 0.930098 x

x Se 5 1.000000 1.000000 1.091953 x

x Se 6 1.000000 1.000000 1.263431 x

x Nb 1 0.333333 0.666667 0.510451 x

x Nb 2 0.333333 0.666667 0.338599 x

x Nb 3 1.000000 1.000000 0.843784 x

x Nb 4 1.000000 1.000000 0.671932 x

x Nb 5 0.666667 1.333333 1.177118 x

x Nb 6 0.666667 1.333333 1.005266 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08706407E+004 606.53 <-- SCF

1 -1.08796116E+004 7.47573911E-001 608.30 <-- SCF

2 -1.08803651E+004 6.27955494E-002 611.06 <-- SCF

3 -1.08791140E+004 -1.04265030E-001 613.59 <-- SCF

4 -1.08738196E+004 -4.41193270E-001 616.27 <-- SCF

5 -1.08738689E+004 4.10523176E-003 619.45 <-- SCF

6 -1.08737990E+004 -5.82277747E-003 622.23 <-- SCF

7 -1.08738057E+004 5.60357765E-004 624.98 <-- SCF

8 -1.08738038E+004 -1.59585510E-004 627.53 <-- SCF

9 -1.08738043E+004 4.14084607E-005 629.98 <-- SCF

10 -1.08738046E+004 2.17167884E-005 632.22 <-- SCF

11 -1.08738047E+004 9.94013752E-006 634.22 <-- SCF

12 -1.08738048E+004 8.60867658E-006 636.30 <-- SCF

13 -1.08738050E+004 1.19033202E-005 638.09 <-- SCF

14 -1.08738052E+004 2.27654489E-005 640.03 <-- SCF

15 -1.08738058E+004 4.46625165E-005 642.39 <-- SCF

16 -1.08738068E+004 8.61454175E-005 644.45 <-- SCF

17 -1.08738088E+004 1.65528417E-004 646.34 <-- SCF

18 -1.08738122E+004 2.85569348E-004 648.12 <-- SCF

19 -1.08738172E+004 4.18250617E-004 650.11 <-- SCF

20 -1.08738232E+004 4.96105390E-004 652.03 <-- SCF

21 -1.08738292E+004 5.01066336E-004 654.03 <-- SCF

22 -1.08738341E+004 4.07916622E-004 656.12 <-- SCF

23 -1.08738372E+004 2.58578419E-004 658.22 <-- SCF

24 -1.08738393E+004 1.71565944E-004 660.31 <-- SCF

25 -1.08738405E+004 1.07416974E-004 662.41 <-- SCF

26 -1.08738412E+004 5.63698729E-005 664.56 <-- SCF

27 -1.08738416E+004 3.07928200E-005 666.48 <-- SCF

28 -1.08738418E+004 1.62663378E-005 668.22 <-- SCF

29 -1.08738419E+004 1.32431921E-005 670.25 <-- SCF

30 -1.08738420E+004 6.35427589E-006 672.14 <-- SCF

31 -1.08738421E+004 2.97889771E-006 674.73 <-- SCF

32 -1.08738421E+004 1.76692654E-006 677.08 <-- SCF

33 -1.08738421E+004 3.21746271E-006 679.05 <-- SCF

34 -1.08738421E+004 -1.16153737E-007 681.06 <-- SCF

35 -1.08738421E+004 1.34444765E-007 683.19 <-- SCF

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

Final energy = -10873.84211665 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.66296 \*

\* Se 2 0.00000 -0.00000 -1.02576 \*

\* Se 3 0.00000 0.00000 0.66296 \*

\* Se 4 0.00000 -0.00000 -1.02576 \*

\* Se 5 0.00000 0.00000 0.66296 \*

\* Se 6 0.00000 -0.00000 -1.02576 \*

\* Nb 1 -0.00000 0.00000 -0.99283 \*

\* Nb 2 0.00000 -0.00000 1.35563 \*

\* Nb 3 -0.00000 0.00000 -0.99283 \*

\* Nb 4 0.00000 -0.00000 1.35563 \*

\* Nb 5 -0.00000 0.00000 -0.99283 \*

\* Nb 6 0.00000 -0.00000 1.35563 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 9.871983 0.000000 0.000000 \*

\* y 0.000000 9.871983 0.000000 \*

\* z 0.000000 0.000000 4.753023 \*

\* \*

\* Pressure: -8.1657 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.023048 | -10873.564683 | <-- min BFGS

| trial step | 0.483016 | 0.018277 | -10873.842146 | <-- min BFGS

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

BFGS: finished iteration 6 with enthalpy= -1.08738421E+004 eV

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

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

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

| dE/ion | 2.312188E-002 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.355626E+000 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.578200E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 9.871983E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 7 ...

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

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

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

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

| previous | 0.000000 | 0.061080 | -10873.842146 | <-- min BFGS

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

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

BFGS: starting iteration 7 with trial guess (lambda= 0.229527)

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

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

| Memory Disk |

| Model and support data 121.4 MB 114.5 MB |

| Electronic energy minimisation requirements 13.7 MB 0.0 MB |

| Geometry minimisation requirements 17.0 MB 0.0 MB |

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

| Approx. total storage required per process 152.2 MB 114.5 MB |

| |

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

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

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Unit Cell

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

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

3.1083409 -1.7946014 -0.0000000 2.0213952 -0.0000000 -0.0000000

0.0000000 3.5892029 0.0000000 1.0106976 1.7505796 -0.0000000

0.0000000 0.0000000 20.8461947 -0.0000000 -0.0000000 0.3014068

Lattice parameters(A) Cell Angles

a = 3.589203 alpha = 90.000000

b = 3.589203 beta = 90.000000

c = 20.846195 gamma = 120.000000

Current cell volume = 232.569860 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 0.666667 0.333333 0.426030 x

x Se 2 0.666667 0.333333 0.595318 x

x Se 3 1.333333 0.666667 0.759363 x

x Se 4 1.333333 0.666667 0.928651 x

x Se 5 1.000000 1.000000 1.092696 x

x Se 6 1.000000 1.000000 1.261984 x

x Nb 1 0.333333 0.666667 0.509758 x

x Nb 2 0.333333 0.666667 0.339994 x

x Nb 3 1.000000 1.000000 0.843092 x

x Nb 4 1.000000 1.000000 0.673328 x

x Nb 5 0.666667 1.333333 1.176425 x

x Nb 6 0.666667 1.333333 1.006661 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08697263E+004 708.88 <-- SCF

1 -1.08831356E+004 1.11743756E+000 710.77 <-- SCF

2 -1.08842943E+004 9.65598324E-002 713.47 <-- SCF

3 -1.08825249E+004 -1.47447713E-001 717.91 <-- SCF

4 -1.08742263E+004 -6.91548241E-001 721.72 <-- SCF

5 -1.08742801E+004 4.48273683E-003 724.41 <-- SCF

6 -1.08741413E+004 -1.15691315E-002 727.08 <-- SCF

7 -1.08741519E+004 8.80422749E-004 729.75 <-- SCF

8 -1.08741476E+004 -3.50425801E-004 732.38 <-- SCF

9 -1.08741482E+004 4.47906712E-005 734.95 <-- SCF

10 -1.08741485E+004 2.41498255E-005 737.41 <-- SCF

11 -1.08741487E+004 1.47839471E-005 739.23 <-- SCF

12 -1.08741490E+004 2.87917447E-005 741.11 <-- SCF

13 -1.08741499E+004 7.46776277E-005 743.14 <-- SCF

14 -1.08741522E+004 1.96204671E-004 745.00 <-- SCF

15 -1.08741573E+004 4.17200704E-004 746.92 <-- SCF

16 -1.08741652E+004 6.58256253E-004 748.81 <-- SCF

17 -1.08741748E+004 8.03376261E-004 750.80 <-- SCF

18 -1.08741832E+004 6.98481450E-004 752.58 <-- SCF

19 -1.08741888E+004 4.65927168E-004 755.52 <-- SCF

20 -1.08741920E+004 2.72362404E-004 758.48 <-- SCF

21 -1.08741938E+004 1.44827040E-004 761.42 <-- SCF

22 -1.08741946E+004 7.19452137E-005 764.69 <-- SCF

23 -1.08741951E+004 4.28231748E-005 767.41 <-- SCF

24 -1.08741955E+004 2.84741209E-005 770.08 <-- SCF

25 -1.08741958E+004 2.39395866E-005 772.06 <-- SCF

26 -1.08741961E+004 2.71458227E-005 773.80 <-- SCF

27 -1.08741965E+004 3.34327060E-005 775.77 <-- SCF

28 -1.08741971E+004 4.87039114E-005 777.61 <-- SCF

29 -1.08741978E+004 5.59015073E-005 780.30 <-- SCF

30 -1.08741985E+004 6.28495664E-005 782.55 <-- SCF

31 -1.08741994E+004 7.57146496E-005 784.48 <-- SCF

32 -1.08742005E+004 9.13213711E-005 786.31 <-- SCF

33 -1.08742017E+004 9.65780563E-005 788.25 <-- SCF

34 -1.08742029E+004 1.04685540E-004 790.09 <-- SCF

35 -1.08742044E+004 1.18903872E-004 791.98 <-- SCF

36 -1.08742056E+004 1.02133220E-004 794.08 <-- SCF

37 -1.08742068E+004 1.02906207E-004 795.89 <-- SCF

38 -1.08742079E+004 9.40261853E-005 798.16 <-- SCF

39 -1.08742090E+004 8.91064888E-005 800.09 <-- SCF

40 -1.08742096E+004 5.21424513E-005 802.39 <-- SCF

41 -1.08742111E+004 1.20229354E-004 804.89 <-- SCF

42 -1.08742112E+004 9.25876316E-006 807.25 <-- SCF

43 -1.08742114E+004 1.88474552E-005 809.73 <-- SCF

44 -1.08742116E+004 1.23037332E-005 811.98 <-- SCF

45 -1.08742118E+004 1.69705287E-005 814.03 <-- SCF

46 -1.08742120E+004 1.49306502E-005 815.98 <-- SCF

47 -1.08742120E+004 6.77178108E-006 818.55 <-- SCF

48 -1.08742120E+004 -8.14270536E-007 821.08 <-- SCF

49 -1.08742120E+004 -2.06240961E-006 822.97 <-- SCF

50 -1.08742120E+004 -2.84635278E-006 824.84 <-- SCF

51 -1.08742120E+004 1.06405388E-006 826.67 <-- SCF

52 -1.08742121E+004 7.59705096E-006 828.53 <-- SCF

53 -1.08742119E+004 -1.18402628E-005 830.38 <-- SCF

54 -1.08742120E+004 7.93673646E-006 832.62 <-- SCF

55 -1.08742120E+004 -4.96827455E-006 834.61 <-- SCF

56 -1.08742117E+004 -2.16955745E-005 836.83 <-- SCF

57 -1.08742116E+004 -6.01345014E-006 838.88 <-- SCF

58 -1.08742116E+004 -2.86356377E-007 841.39 <-- SCF

59 -1.08742115E+004 -7.59961798E-006 843.53 <-- SCF

60 -1.08742116E+004 2.13529994E-006 845.78 <-- SCF

61 -1.08742115E+004 -2.17054918E-006 848.14 <-- SCF

62 -1.08742115E+004 -1.50835537E-006 850.39 <-- SCF

63 -1.08742115E+004 1.75114466E-007 852.55 <-- SCF

64 -1.08742115E+004 8.29805445E-008 854.41 <-- SCF

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

Final energy = -10874.21152284 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 0.55221 \*

\* Se 2 -0.00000 -0.00000 -0.70654 \*

\* Se 3 -0.00000 -0.00000 0.55221 \*

\* Se 4 0.00000 -0.00000 -0.70654 \*

\* Se 5 0.00000 0.00000 0.55221 \*

\* Se 6 -0.00000 -0.00000 -0.70654 \*

\* Nb 1 0.00000 -0.00000 -1.08300 \*

\* Nb 2 0.00000 0.00000 1.23733 \*

\* Nb 3 0.00000 -0.00000 -1.08300 \*

\* Nb 4 0.00000 0.00000 1.23733 \*

\* Nb 5 0.00000 0.00000 -1.08300 \*

\* Nb 6 -0.00000 0.00000 1.23733 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 10.349778 0.000000 -0.000000 \*

\* y 0.000000 10.349778 0.000000 \*

\* z -0.000000 0.000000 5.671215 \*

\* \*

\* Pressure: -8.7903 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.061080 | -10873.842146 | <-- min BFGS

| trial step | 0.229527 | 0.054321 | -10874.211503 | <-- min BFGS

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

BFGS: finished iteration 7 with enthalpy= -1.08742115E+004 eV

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

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

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

| dE/ion | 3.077976E-002 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.237328E+000 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.015263E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.034978E+001 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 8 ...

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

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

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

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

| previous | 0.000000 | 0.129619 | -10874.211503 | <-- min BFGS

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

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

BFGS: starting iteration 8 with trial guess (lambda= 0.125179)

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

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

| Memory Disk |

| Model and support data 123.3 MB 115.9 MB |

| Electronic energy minimisation requirements 13.7 MB 0.0 MB |

| Geometry minimisation requirements 17.0 MB 0.0 MB |

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

| Approx. total storage required per process 154.0 MB 115.9 MB |

| |

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

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

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Unit Cell

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

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

3.0802246 -1.7783685 -0.0000000 2.0398465 -0.0000000 0.0000000

0.0000000 3.5567370 0.0000000 1.0199233 1.7665589 -0.0000000

-0.0000000 0.0000000 21.1107833 0.0000000 -0.0000000 0.2976292

Lattice parameters(A) Cell Angles

a = 3.556737 alpha = 90.000000

b = 3.556737 beta = 90.000000

c = 21.110783 gamma = 120.000000

Current cell volume = 231.280211 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.426861 x

x Se 2 0.666667 0.333333 0.593713 x

x Se 3 1.333333 0.666667 0.760194 x

x Se 4 1.333333 0.666667 0.927046 x

x Se 5 1.000000 1.000000 1.093528 x

x Se 6 1.000000 1.000000 1.260380 x

x Nb 1 0.333333 0.666667 0.508967 x

x Nb 2 0.333333 0.666667 0.341559 x

x Nb 3 1.000000 1.000000 0.842301 x

x Nb 4 1.000000 1.000000 0.674892 x

x Nb 5 0.666667 1.333333 1.175634 x

x Nb 6 0.666667 1.333333 1.008225 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08687499E+004 879.47 <-- SCF

1 -1.08855589E+004 1.40075021E+000 881.22 <-- SCF

2 -1.08873285E+004 1.47468415E-001 883.95 <-- SCF

3 -1.08836220E+004 -3.08882464E-001 886.55 <-- SCF

4 -1.08747501E+004 -7.39319205E-001 889.11 <-- SCF

5 -1.08746660E+004 -7.01354531E-003 891.72 <-- SCF

6 -1.08745693E+004 -8.05332717E-003 894.41 <-- SCF

7 -1.08745744E+004 4.24561539E-004 896.95 <-- SCF

8 -1.08745708E+004 -3.00163946E-004 899.44 <-- SCF

9 -1.08746156E+004 3.73557685E-003 901.91 <-- SCF

10 -1.08746313E+004 1.30266761E-003 903.83 <-- SCF

11 -1.08746350E+004 3.12003560E-004 905.72 <-- SCF

12 -1.08746351E+004 7.02870543E-006 907.59 <-- SCF

13 -1.08746352E+004 5.27439295E-006 909.42 <-- SCF

14 -1.08746352E+004 4.35131476E-006 912.08 <-- SCF

15 -1.08746354E+004 1.21483836E-005 914.33 <-- SCF

16 -1.08746353E+004 -3.55837302E-006 916.28 <-- SCF

17 -1.08746350E+004 -2.30118220E-005 918.41 <-- SCF

18 -1.08746347E+004 -2.77382234E-005 921.09 <-- SCF

19 -1.08746347E+004 -1.56394037E-006 923.31 <-- SCF

20 -1.08746347E+004 3.80911795E-007 925.84 <-- SCF

21 -1.08746347E+004 3.74332699E-006 927.83 <-- SCF

22 -1.08746349E+004 9.62227694E-006 930.20 <-- SCF

23 -1.08746346E+004 -2.42661765E-005 932.55 <-- SCF

24 -1.08746346E+004 8.04824816E-007 934.33 <-- SCF

25 -1.08746346E+004 -2.43896629E-006 936.23 <-- SCF

26 -1.08746345E+004 -9.07932555E-007 938.14 <-- SCF

27 -1.08746345E+004 -8.25097022E-007 940.00 <-- SCF

28 -1.08746345E+004 -3.82751055E-007 941.98 <-- SCF

29 -1.08746345E+004 -4.42576180E-007 943.80 <-- SCF

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

Final energy = -10874.63452167 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 0.26776 \*

\* Se 2 0.00000 0.00000 -0.42415 \*

\* Se 3 0.00000 -0.00000 0.26776 \*

\* Se 4 0.00000 0.00000 -0.42415 \*

\* Se 5 0.00000 0.00000 0.26776 \*

\* Se 6 0.00000 0.00000 -0.42415 \*

\* Nb 1 0.00000 0.00000 -1.04510 \*

\* Nb 2 0.00000 -0.00000 1.20148 \*

\* Nb 3 0.00000 -0.00000 -1.04510 \*

\* Nb 4 0.00000 -0.00000 1.20148 \*

\* Nb 5 -0.00000 -0.00000 -1.04510 \*

\* Nb 6 0.00000 0.00000 1.20148 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 10.245769 0.000000 0.000000 \*

\* y 0.000000 10.245769 0.000000 \*

\* z 0.000000 0.000000 5.617944 \*

\* \*

\* Pressure: -8.7032 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.129619 | -10874.211503 | <-- min BFGS

| trial step | 0.125179 | 0.116531 | -10874.634499 | <-- min BFGS

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

BFGS: finished iteration 8 with enthalpy= -1.08746345E+004 eV

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

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

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

| dE/ion | 3.524972E-002 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.201483E+000 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.387862E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.024577E+001 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 9 ...

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

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

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

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

| previous | 0.000000 | 0.141409 | -10874.634499 | <-- min BFGS

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

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

BFGS: starting iteration 9 with trial guess (lambda= 0.117049)

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

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

| Memory Disk |

| Model and support data 124.9 MB 104.2 MB |

| Electronic energy minimisation requirements 13.4 MB 0.0 MB |

| Geometry minimisation requirements 16.6 MB 0.0 MB |

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

| Approx. total storage required per process 155.0 MB 104.2 MB |

| |

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

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

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Unit Cell

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

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

3.0476810 -1.7595795 -0.0000000 2.0616283 -0.0000000 0.0000000

0.0000000 3.5191589 0.0000000 1.0308141 1.7854224 -0.0000000

-0.0000000 0.0000000 21.3753719 0.0000000 -0.0000000 0.2939451

Lattice parameters(A) Cell Angles

a = 3.519159 alpha = 90.000000

b = 3.519159 beta = 90.000000

c = 21.375372 gamma = 120.000000

Current cell volume = 229.256718 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.427715 x

x Se 2 0.666667 0.333333 0.592048 x

x Se 3 1.333333 0.666667 0.761048 x

x Se 4 1.333333 0.666667 0.925382 x

x Se 5 1.000000 1.000000 1.094381 x

x Se 6 1.000000 1.000000 1.258715 x

x Nb 1 0.333333 0.666667 0.508134 x

x Nb 2 0.333333 0.666667 0.343203 x

x Nb 3 1.000000 1.000000 0.841467 x

x Nb 4 1.000000 1.000000 0.676537 x

x Nb 5 0.666667 1.333333 1.174801 x

x Nb 6 0.666667 1.333333 1.009870 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08681876E+004 968.59 <-- SCF

1 -1.08879797E+004 1.64934138E+000 970.36 <-- SCF

2 -1.08901993E+004 1.84962075E-001 973.02 <-- SCF

3 -1.08852929E+004 -4.08866842E-001 975.61 <-- SCF

4 -1.08752894E+004 -8.33622168E-001 978.17 <-- SCF

5 -1.08750687E+004 -1.83863689E-002 980.70 <-- SCF

6 -1.08749973E+004 -5.95208557E-003 983.59 <-- SCF

7 -1.08749962E+004 -9.32244244E-005 986.20 <-- SCF

8 -1.08749912E+004 -4.13689820E-004 988.70 <-- SCF

9 -1.08749916E+004 3.29320233E-005 990.97 <-- SCF

10 -1.08749916E+004 -2.24414806E-006 992.89 <-- SCF

11 -1.08749916E+004 -3.06717265E-007 995.14 <-- SCF

12 -1.08749916E+004 -2.07497765E-007 997.03 <-- SCF

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

Final energy = -10874.99160232 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 0.05223 \*

\* Se 2 -0.00000 0.00000 0.05400 \*

\* Se 3 -0.00000 0.00000 0.05223 \*

\* Se 4 -0.00000 0.00000 0.05400 \*

\* Se 5 -0.00000 -0.00000 0.05223 \*

\* Se 6 -0.00000 0.00000 0.05400 \*

\* Nb 1 0.00000 -0.00000 -0.99134 \*

\* Nb 2 -0.00000 0.00000 0.88511 \*

\* Nb 3 0.00000 -0.00000 -0.99134 \*

\* Nb 4 -0.00000 0.00000 0.88511 \*

\* Nb 5 0.00000 0.00000 -0.99134 \*

\* Nb 6 -0.00000 -0.00000 0.88511 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 9.601862 0.000000 0.000000 \*

\* y 0.000000 9.601862 -0.000000 \*

\* z 0.000000 -0.000000 6.254943 \*

\* \*

\* Pressure: -8.4862 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.141409 | -10874.634499 | <-- min BFGS

| trial step | 0.117049 | 0.102374 | -10874.991625 | <-- min BFGS

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

BFGS: finished iteration 9 with enthalpy= -1.08749916E+004 eV

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

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

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

| dE/ion | 2.976045E-002 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 9.913358E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.558497E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 9.601862E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 10 ...

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

Writing analysis data to 3R-Nb1.1Se2-7-US.castep\_bin

Writing model to 3R-Nb1.1Se2-7-US.check

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

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

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

| previous | 0.000000 | 0.041854 | -10874.991625 | <-- min BFGS

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

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

BFGS: starting iteration 10 with trial guess (lambda= 0.509228)

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

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

| Memory Disk |

| Model and support data 133.9 MB 104.2 MB |

| Electronic energy minimisation requirements 13.2 MB 0.0 MB |

| Geometry minimisation requirements 16.3 MB 0.0 MB |

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

| Approx. total storage required per process 163.5 MB 104.2 MB |

| |

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

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

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Unit Cell

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

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

2.9921033 -1.7274916 -0.0000000 2.0999226 0.0000000 0.0000000

-0.0000000 3.4549833 0.0000000 1.0499613 1.8185863 -0.0000000

-0.0000000 0.0000000 21.6399606 0.0000000 -0.0000000 0.2903511

Lattice parameters(A) Cell Angles

a = 3.454983 alpha = 90.000000

b = 3.454983 beta = 90.000000

c = 21.639961 gamma = 120.000000

Current cell volume = 223.706702 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 0.666667 0.333333 0.428816 x

x Se 2 0.666667 0.333333 0.589914 x

x Se 3 1.333333 0.666667 0.762150 x

x Se 4 1.333333 0.666667 0.923247 x

x Se 5 1.000000 1.000000 1.095483 x

x Se 6 1.000000 1.000000 1.256580 x

x Nb 1 0.333333 0.666667 0.507014 x

x Nb 2 0.333333 0.666667 0.345356 x

x Nb 3 1.000000 1.000000 0.840348 x

x Nb 4 1.000000 1.000000 0.678689 x

x Nb 5 0.666667 1.333333 1.173681 x

x Nb 6 0.666667 1.333333 1.012022 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08625161E+004 1018.95 <-- SCF

1 -1.09015027E+004 3.24887824E+000 1020.70 <-- SCF

2 -1.09052492E+004 3.12213111E-001 1022.17 <-- SCF

3 -1.08915204E+004 -1.14407244E+000 1024.77 <-- SCF

4 -1.08760627E+004 -1.28813636E+000 1027.20 <-- SCF

5 -1.08756675E+004 -3.29380568E-002 1029.83 <-- SCF

6 -1.08754524E+004 -1.79207833E-002 1032.55 <-- SCF

7 -1.08754546E+004 1.78309957E-004 1035.23 <-- SCF

8 -1.08754482E+004 -5.33274586E-004 1038.05 <-- SCF

9 -1.08754486E+004 3.77372060E-005 1040.69 <-- SCF

10 -1.08754487E+004 6.59204790E-006 1042.70 <-- SCF

11 -1.08754487E+004 -2.84139468E-006 1044.77 <-- SCF

12 -1.08754487E+004 1.93700414E-007 1046.33 <-- SCF

13 -1.08754487E+004 8.05353302E-008 1048.09 <-- SCF

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

Final energy = -10875.44866388 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 -0.37256 \*

\* Se 2 0.00000 -0.00000 0.26729 \*

\* Se 3 0.00000 -0.00000 -0.37256 \*

\* Se 4 0.00000 -0.00000 0.26729 \*

\* Se 5 0.00000 -0.00000 -0.37256 \*

\* Se 6 0.00000 -0.00000 0.26729 \*

\* Nb 1 -0.00000 0.00000 -0.53506 \*

\* Nb 2 0.00000 0.00000 0.64032 \*

\* Nb 3 -0.00000 0.00000 -0.53506 \*

\* Nb 4 0.00000 0.00000 0.64032 \*

\* Nb 5 -0.00000 -0.00000 -0.53506 \*

\* Nb 6 0.00000 0.00000 0.64032 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 6.236089 0.000000 -0.000000 \*

\* y 0.000000 6.236089 0.000000 \*

\* z -0.000000 0.000000 5.484876 \*

\* \*

\* Pressure: -5.9857 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.041854 | -10874.991625 | <-- min BFGS

| trial step | 0.509228 | 0.021254 | -10875.448596 | <-- min BFGS

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

BFGS: finished iteration 10 with enthalpy= -1.08754486E+004 eV

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

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

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

| dE/ion | 3.808096E-002 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 6.403239E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.657925E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 6.236089E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 11 ...

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

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

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

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

| previous | 0.000000 | 0.013682 | -10875.448596 | <-- min BFGS

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

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

BFGS: starting iteration 11 with trial guess (lambda= 1.000000)

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

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

| Memory Disk |

| Model and support data 137.5 MB 104.2 MB |

| Electronic energy minimisation requirements 13.0 MB 0.0 MB |

| Geometry minimisation requirements 16.0 MB 0.0 MB |

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

| Approx. total storage required per process 166.5 MB 104.2 MB |

| |

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

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

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

Unit Cell

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

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

2.9307242 -1.6920544 -0.0000000 2.1439019 0.0000000 0.0000000

-0.0000000 3.3841088 0.0000000 1.0719510 1.8566735 -0.0000000

-0.0000000 0.0000000 21.7650229 0.0000000 -0.0000000 0.2886827

Lattice parameters(A) Cell Angles

a = 3.384109 alpha = 90.000000

b = 3.384109 beta = 90.000000

c = 21.765023 gamma = 120.000000

Current cell volume = 215.863094 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.429711 x

x Se 2 0.666667 0.333333 0.588111 x

x Se 3 1.333333 0.666667 0.763044 x

x Se 4 1.333333 0.666667 0.921445 x

x Se 5 1.000000 1.000000 1.096378 x

x Se 6 1.000000 1.000000 1.254778 x

x Nb 1 0.333333 0.666667 0.506038 x

x Nb 2 0.333333 0.666667 0.347240 x

x Nb 3 1.000000 1.000000 0.839371 x

x Nb 4 1.000000 1.000000 0.680573 x

x Nb 5 0.666667 1.333333 1.172704 x

x Nb 6 0.666667 1.333333 1.013907 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08642967E+004 1070.00 <-- SCF

1 -1.08976150E+004 2.77652730E+000 1071.66 <-- SCF

2 -1.09003428E+004 2.27309047E-001 1073.20 <-- SCF

3 -1.08858656E+004 -1.20643040E+000 1075.80 <-- SCF

4 -1.08760474E+004 -8.18178903E-001 1078.30 <-- SCF

5 -1.08756891E+004 -2.98618978E-002 1080.83 <-- SCF

6 -1.08756737E+004 -1.28469077E-003 1083.44 <-- SCF

7 -1.08756748E+004 9.19869473E-005 1085.92 <-- SCF

8 -1.08756715E+004 -2.72654333E-004 1088.48 <-- SCF

9 -1.08757056E+004 2.83873166E-003 1090.86 <-- SCF

10 -1.08757101E+004 3.74454259E-004 1092.80 <-- SCF

11 -1.08757103E+004 1.52573286E-005 1094.53 <-- SCF

12 -1.08757101E+004 -9.70099415E-006 1096.33 <-- SCF

13 -1.08757156E+004 4.56584527E-004 1098.77 <-- SCF

14 -1.08757142E+004 -1.20228210E-004 1100.86 <-- SCF

15 -1.08757111E+004 -2.57836475E-004 1103.19 <-- SCF

16 -1.08757099E+004 -9.70828917E-005 1105.66 <-- SCF

17 -1.08757101E+004 1.37390990E-005 1107.55 <-- SCF

18 -1.08757097E+004 -3.00739743E-005 1109.78 <-- SCF

19 -1.08757097E+004 -4.62952330E-006 1111.84 <-- SCF

20 -1.08757097E+004 -3.96742140E-008 1113.52 <-- SCF

21 -1.08757096E+004 -2.25331291E-006 1115.34 <-- SCF

22 -1.08757096E+004 -7.48290998E-007 1117.09 <-- SCF

23 -1.08757096E+004 -1.53595807E-007 1118.81 <-- SCF

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

Final energy = -10875.70962489 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 -0.00000 -0.79153 \*

\* Se 2 -0.00000 0.00000 0.69483 \*

\* Se 3 -0.00000 0.00000 -0.79153 \*

\* Se 4 0.00000 0.00000 0.69483 \*

\* Se 5 -0.00000 0.00000 -0.79153 \*

\* Se 6 -0.00000 -0.00000 0.69483 \*

\* Nb 1 0.00000 -0.00000 -0.37314 \*

\* Nb 2 -0.00000 0.00000 0.46983 \*

\* Nb 3 0.00000 0.00000 -0.37314 \*

\* Nb 4 -0.00000 0.00000 0.46983 \*

\* Nb 5 0.00000 -0.00000 -0.37314 \*

\* Nb 6 -0.00000 0.00000 0.46983 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 1.536258 -0.000000 0.000000 \*

\* y -0.000000 1.536258 -0.000000 \*

\* z 0.000000 -0.000000 -0.175323 \*

\* \*

\* Pressure: -0.9657 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.013682 | -10875.448596 | <-- min BFGS

| trial step | 1.000000 | 0.001530 | -10875.709582 | <-- min BFGS

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

BFGS: finished iteration 11 with enthalpy= -1.08757096E+004 eV

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

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

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

| dE/ion | 2.174884E-002 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 7.915253E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.101015E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.536258E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 12 ...

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

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

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

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

| previous | 0.000000 | 0.000616 | -10875.709582 | <-- min BFGS

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

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

BFGS: starting iteration 12 with trial guess (lambda= 1.000000)

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

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

| Memory Disk |

| Model and support data 141.0 MB 104.2 MB |

| Electronic energy minimisation requirements 12.9 MB 0.0 MB |

| Geometry minimisation requirements 15.9 MB 0.0 MB |

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

| Approx. total storage required per process 169.8 MB 104.2 MB |

| |

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

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

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Unit Cell

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

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

2.9221620 -1.6871110 -0.0000000 2.1501837 0.0000000 0.0000000

-0.0000000 3.3742221 0.0000000 1.0750919 1.8621137 -0.0000000

-0.0000000 0.0000000 21.7646349 0.0000000 -0.0000000 0.2886878

Lattice parameters(A) Cell Angles

a = 3.374222 alpha = 90.000000

b = 3.374222 beta = 90.000000

c = 21.764635 gamma = 120.000000

Current cell volume = 214.599814 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.429703 x

x Se 2 0.666667 0.333333 0.588058 x

x Se 3 1.333333 0.666667 0.763036 x

x Se 4 1.333333 0.666667 0.921392 x

x Se 5 1.000000 1.000000 1.096369 x

x Se 6 1.000000 1.000000 1.254725 x

x Nb 1 0.333333 0.666667 0.505951 x

x Nb 2 0.333333 0.666667 0.347388 x

x Nb 3 1.000000 1.000000 0.839285 x

x Nb 4 1.000000 1.000000 0.680721 x

x Nb 5 0.666667 1.333333 1.172618 x

x Nb 6 0.666667 1.333333 1.014054 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08756108E+004 1140.66 <-- SCF

1 -1.08758564E+004 2.04739295E-002 1142.39 <-- SCF

2 -1.08758622E+004 4.78310552E-004 1144.89 <-- SCF

3 -1.08757340E+004 -1.06840724E-002 1147.31 <-- SCF

4 -1.08757227E+004 -9.38140911E-004 1149.86 <-- SCF

5 -1.08757225E+004 -1.70532206E-005 1152.44 <-- SCF

6 -1.08757223E+004 -2.04281660E-005 1154.75 <-- SCF

7 -1.08757309E+004 7.22967866E-004 1156.69 <-- SCF

8 -1.08757667E+004 2.98250109E-003 1158.61 <-- SCF

9 -1.08757680E+004 1.09249352E-004 1160.47 <-- SCF

10 -1.08757682E+004 1.66195243E-005 1162.30 <-- SCF

11 -1.08757683E+004 3.00709991E-006 1164.06 <-- SCF

12 -1.08757683E+004 1.18814419E-006 1165.89 <-- SCF

13 -1.08757683E+004 1.35098411E-007 1167.66 <-- SCF

14 -1.08757684E+004 7.81589712E-006 1169.83 <-- SCF

15 -1.08757687E+004 2.36576445E-005 1172.00 <-- SCF

16 -1.08757689E+004 1.54176872E-005 1174.03 <-- SCF

17 -1.08757686E+004 -1.77711312E-005 1176.23 <-- SCF

18 -1.08757693E+004 5.52464867E-005 1178.70 <-- SCF

19 -1.08757693E+004 -2.91883760E-006 1180.59 <-- SCF

20 -1.08757697E+004 3.46893678E-005 1182.75 <-- SCF

21 -1.08757741E+004 3.69939934E-004 1185.33 <-- SCF

22 -1.08757742E+004 9.39880845E-006 1187.31 <-- SCF

23 -1.08757740E+004 -1.61270469E-005 1189.34 <-- SCF

24 -1.08757775E+004 2.87799928E-004 1191.81 <-- SCF

25 -1.08757759E+004 -1.34304037E-004 1193.94 <-- SCF

26 -1.08757725E+004 -2.85362491E-004 1196.38 <-- SCF

27 -1.08757725E+004 9.60105977E-007 1198.53 <-- SCF

28 -1.08757709E+004 -1.31257823E-004 1201.09 <-- SCF

29 -1.08757677E+004 -2.69379087E-004 1203.64 <-- SCF

30 -1.08757677E+004 3.12381680E-006 1205.80 <-- SCF

31 -1.08757677E+004 2.19991482E-006 1207.48 <-- SCF

32 -1.08757684E+004 5.54977938E-005 1209.89 <-- SCF

33 -1.08757676E+004 -6.36795199E-005 1212.34 <-- SCF

34 -1.08757676E+004 6.31425223E-007 1214.28 <-- SCF

35 -1.08757676E+004 -9.20332511E-008 1216.03 <-- SCF

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

Final energy = -10875.76764004 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 -0.87301 \*

\* Se 2 -0.00000 0.00000 0.73266 \*

\* Se 3 -0.00000 0.00000 -0.87301 \*

\* Se 4 -0.00000 -0.00000 0.73266 \*

\* Se 5 0.00000 0.00000 -0.87301 \*

\* Se 6 -0.00000 0.00000 0.73266 \*

\* Nb 1 0.00000 0.00000 -0.36127 \*

\* Nb 2 -0.00000 0.00000 0.50162 \*

\* Nb 3 0.00000 0.00000 -0.36127 \*

\* Nb 4 0.00000 -0.00000 0.50162 \*

\* Nb 5 -0.00000 0.00000 -0.36127 \*

\* Nb 6 0.00000 -0.00000 0.50162 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 1.034553 0.000000 -0.000000 \*

\* y 0.000000 1.034553 -0.000000 \*

\* z -0.000000 -0.000000 -1.626593 \*

\* \*

\* Pressure: -0.1475 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000616 | -10875.709582 | <-- min BFGS

| trial step | 1.000000 | 0.000474 | -10875.767617 | <-- min BFGS

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

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

BFGS: improving iteration 12 with line minimization (lambda= 4.346026)

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

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

| Memory Disk |

| Model and support data 141.3 MB 104.2 MB |

| Electronic energy minimisation requirements 12.8 MB 0.0 MB |

| Geometry minimisation requirements 15.8 MB 0.0 MB |

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

| Approx. total storage required per process 169.8 MB 104.2 MB |

| |

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

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

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

Unit Cell

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

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

2.8935128 -1.6705704 -0.0000000 2.1714731 0.0000000 0.0000000

-0.0000000 3.3411408 0.0000000 1.0857366 1.8805509 -0.0000000

-0.0000000 0.0000000 21.7633364 0.0000000 -0.0000000 0.2887051

Lattice parameters(A) Cell Angles

a = 3.341141 alpha = 90.000000

b = 3.341141 beta = 90.000000

c = 21.763336 gamma = 120.000000

Current cell volume = 210.399965 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.429675 x

x Se 2 0.666667 0.333333 0.587881 x

x Se 3 1.333333 0.666667 0.763008 x

x Se 4 1.333333 0.666667 0.921214 x

x Se 5 1.000000 1.000000 1.096342 x

x Se 6 1.000000 1.000000 1.254548 x

x Nb 1 0.333333 0.666667 0.505662 x

x Nb 2 0.333333 0.666667 0.347882 x

x Nb 3 1.000000 1.000000 0.838995 x

x Nb 4 1.000000 1.000000 0.681215 x

x Nb 5 0.666667 1.333333 1.172329 x

x Nb 6 0.666667 1.333333 1.014549 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08744836E+004 1237.73 <-- SCF

1 -1.08772818E+004 2.33189822E-001 1239.44 <-- SCF

2 -1.08773486E+004 5.56155753E-003 1241.92 <-- SCF

3 -1.08758991E+004 -1.20789835E-001 1244.25 <-- SCF

4 -1.08757706E+004 -1.07061136E-002 1246.62 <-- SCF

5 -1.08757655E+004 -4.26624432E-004 1249.16 <-- SCF

6 -1.08757651E+004 -3.62508118E-005 1251.61 <-- SCF

7 -1.08757648E+004 -2.67389720E-005 1254.02 <-- SCF

8 -1.08757647E+004 -1.40342874E-006 1256.20 <-- SCF

9 -1.08757647E+004 3.45970237E-007 1257.88 <-- SCF

10 -1.08757647E+004 1.22711474E-007 1259.58 <-- SCF

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

Final energy = -10875.76474758 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 -0.97043 \*

\* Se 2 -0.00000 0.00000 0.81903 \*

\* Se 3 -0.00000 -0.00000 -0.97043 \*

\* Se 4 -0.00000 0.00000 0.81903 \*

\* Se 5 -0.00000 0.00000 -0.97043 \*

\* Se 6 -0.00000 -0.00000 0.81903 \*

\* Nb 1 0.00000 -0.00000 -0.18908 \*

\* Nb 2 -0.00000 0.00000 0.34048 \*

\* Nb 3 0.00000 0.00000 -0.18908 \*

\* Nb 4 -0.00000 0.00000 0.34048 \*

\* Nb 5 0.00000 -0.00000 -0.18908 \*

\* Nb 6 -0.00000 0.00000 0.34048 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -2.219226 -0.000000 0.000000 \*

\* y -0.000000 -2.219226 -0.000000 \*

\* z 0.000000 -0.000000 -3.973858 \*

\* \*

\* Pressure: 2.8041 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000616 | -10875.709582 | <-- min BFGS

| trial step | 1.000000 | 0.000474 | -10875.767617 | <-- min BFGS

| line step | 4.346026 | -0.000562 | -10875.764723 | <-- min BFGS

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

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

BFGS: improving iteration 12 with quad minimization (lambda= 2.530909)

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

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

| Memory Disk |

| Model and support data 142.9 MB 104.2 MB |

| Electronic energy minimisation requirements 12.9 MB 0.0 MB |

| Geometry minimisation requirements 15.9 MB 0.0 MB |

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

| Approx. total storage required per process 171.6 MB 104.2 MB |

| |

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

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

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

Unit Cell

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

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

2.9090541 -1.6795432 -0.0000000 2.1598723 0.0000000 0.0000000

-0.0000000 3.3590864 0.0000000 1.0799361 1.8705042 -0.0000000

-0.0000000 0.0000000 21.7640408 0.0000000 -0.0000000 0.2886957

Lattice parameters(A) Cell Angles

a = 3.359086 alpha = 90.000000

b = 3.359086 beta = 90.000000

c = 21.764041 gamma = 120.000000

Current cell volume = 212.673073 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.429690 x

x Se 2 0.666667 0.333333 0.587977 x

x Se 3 1.333333 0.666667 0.763023 x

x Se 4 1.333333 0.666667 0.921311 x

x Se 5 1.000000 1.000000 1.096357 x

x Se 6 1.000000 1.000000 1.254644 x

x Nb 1 0.333333 0.666667 0.505819 x

x Nb 2 0.333333 0.666667 0.347614 x

x Nb 3 1.000000 1.000000 0.839152 x

x Nb 4 1.000000 1.000000 0.680947 x

x Nb 5 0.666667 1.333333 1.172486 x

x Nb 6 0.666667 1.333333 1.014281 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08753982E+004 1281.33 <-- SCF

1 -1.08762317E+004 6.94603671E-002 1282.97 <-- SCF

2 -1.08762523E+004 1.71532811E-003 1285.53 <-- SCF

3 -1.08758201E+004 -3.60160240E-002 1287.89 <-- SCF

4 -1.08757807E+004 -3.28815954E-003 1290.44 <-- SCF

5 -1.08757784E+004 -1.92466100E-004 1292.94 <-- SCF

6 -1.08757781E+004 -2.20929382E-005 1295.48 <-- SCF

7 -1.08757779E+004 -1.27892927E-005 1297.78 <-- SCF

8 -1.08757779E+004 6.63491301E-007 1299.61 <-- SCF

9 -1.08757779E+004 8.79729322E-008 1301.19 <-- SCF

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

Final energy = -10875.77794954 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 -0.91766 \*

\* Se 2 0.00000 0.00000 0.76873 \*

\* Se 3 0.00000 -0.00000 -0.91766 \*

\* Se 4 0.00000 0.00000 0.76873 \*

\* Se 5 0.00000 0.00000 -0.91766 \*

\* Se 6 0.00000 0.00000 0.76873 \*

\* Nb 1 -0.00000 0.00000 -0.28682 \*

\* Nb 2 0.00000 -0.00000 0.43574 \*

\* Nb 3 -0.00000 0.00000 -0.28682 \*

\* Nb 4 0.00000 -0.00000 0.43574 \*

\* Nb 5 -0.00000 0.00000 -0.28682 \*

\* Nb 6 0.00000 -0.00000 0.43574 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.408488 -0.000000 0.000000 \*

\* y -0.000000 -0.408488 0.000000 \*

\* z 0.000000 0.000000 -2.663049 \*

\* \*

\* Pressure: 1.1600 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000616 | -10875.709582 | <-- min BFGS

| trial step | 1.000000 | 0.000474 | -10875.767617 | <-- min BFGS

| line step | 4.346026 | -0.000562 | -10875.764723 | <-- min BFGS

| quad step | 2.530909 | 0.000015 | -10875.777988 | <-- min BFGS

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

BFGS: finished iteration 12 with enthalpy= -1.08757780E+004 eV

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

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

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

| dE/ion | 5.700507E-003 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 9.176560E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 8.137286E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 2.663049E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 13 ...

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

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

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

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

| previous | 0.000000 | 0.001002 | -10875.777988 | <-- min BFGS

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

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

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)

2.9075931 -1.6786996 -0.0000000 2.1609576 0.0000000 0.0000000

-0.0000000 3.3573993 0.0000000 1.0804788 1.8714442 -0.0000000

-0.0000000 0.0000000 21.7391116 0.0000000 -0.0000000 0.2890268

Lattice parameters(A) Cell Angles

a = 3.357399 alpha = 90.000000

b = 3.357399 beta = 90.000000

c = 21.739112 gamma = 120.000000

Current cell volume = 212.216141 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.429390 x

x Se 2 0.666667 0.333333 0.588394 x

x Se 3 1.333333 0.666667 0.762724 x

x Se 4 1.333333 0.666667 0.921727 x

x Se 5 1.000000 1.000000 1.096057 x

x Se 6 1.000000 1.000000 1.255061 x

x Nb 1 0.333333 0.666667 0.505897 x

x Nb 2 0.333333 0.666667 0.347418 x

x Nb 3 1.000000 1.000000 0.839231 x

x Nb 4 1.000000 1.000000 0.680752 x

x Nb 5 0.666667 1.333333 1.172564 x

x Nb 6 0.666667 1.333333 1.014085 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08756384E+004 1322.92 <-- SCF

1 -1.08764690E+004 6.92144468E-002 1324.61 <-- SCF

2 -1.08765050E+004 2.99739980E-003 1327.11 <-- SCF

3 -1.08762414E+004 -2.19620114E-002 1329.67 <-- SCF

4 -1.08758028E+004 -3.65481649E-002 1332.11 <-- SCF

5 -1.08758034E+004 4.23345619E-005 1334.50 <-- SCF

6 -1.08758022E+004 -9.40017112E-005 1336.84 <-- SCF

7 -1.08758022E+004 -2.12695192E-006 1339.20 <-- SCF

8 -1.08758021E+004 -1.04654803E-005 1341.30 <-- SCF

9 -1.08758021E+004 3.21349494E-007 1342.97 <-- SCF

10 -1.08758021E+004 1.41264425E-007 1344.72 <-- SCF

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

Final energy = -10875.80207713 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 -0.79933 \*

\* Se 2 0.00000 -0.00000 0.68813 \*

\* Se 3 0.00000 0.00000 -0.79933 \*

\* Se 4 0.00000 0.00000 0.68813 \*

\* Se 5 0.00000 0.00000 -0.79933 \*

\* Se 6 0.00000 0.00000 0.68813 \*

\* Nb 1 0.00000 -0.00000 -0.33884 \*

\* Nb 2 0.00000 0.00000 0.45004 \*

\* Nb 3 -0.00000 0.00000 -0.33884 \*

\* Nb 4 -0.00000 0.00000 0.45004 \*

\* Nb 5 0.00000 0.00000 -0.33884 \*

\* Nb 6 0.00000 0.00000 0.45004 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.558015 -0.000000 0.000000 \*

\* y -0.000000 -0.558015 0.000000 \*

\* z 0.000000 0.000000 -2.929950 \*

\* \*

\* Pressure: 1.3487 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.001002 | -10875.777988 | <-- min BFGS

| trial step | 1.000000 | 0.000796 | -10875.802084 | <-- min BFGS

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

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BFGS: improving iteration 13 with line minimization (lambda= 4.876901)

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Unit Cell

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

2.9019287 -1.6754293 -0.0000000 2.1651756 0.0000000 0.0000000

-0.0000000 3.3508587 0.0000000 1.0825878 1.8750971 -0.0000000

-0.0000000 0.0000000 21.6424634 0.0000000 -0.0000000 0.2903175

Lattice parameters(A) Cell Angles

a = 3.350859 alpha = 90.000000

b = 3.350859 beta = 90.000000

c = 21.642463 gamma = 120.000000

Current cell volume = 210.450297 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.428228 x

x Se 2 0.666667 0.333333 0.590009 x

x Se 3 1.333333 0.666667 0.761561 x

x Se 4 1.333333 0.666667 0.923343 x

x Se 5 1.000000 1.000000 1.094894 x

x Se 6 1.000000 1.000000 1.256676 x

x Nb 1 0.333333 0.666667 0.506202 x

x Nb 2 0.333333 0.666667 0.346661 x

x Nb 3 1.000000 1.000000 0.839535 x

x Nb 4 1.000000 1.000000 0.679994 x

x Nb 5 0.666667 1.333333 1.172869 x

x Nb 6 0.666667 1.333333 1.013328 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08733606E+004 1366.47 <-- SCF

1 -1.08859562E+004 1.04962810E+000 1368.30 <-- SCF

2 -1.08865882E+004 5.26681050E-002 1370.89 <-- SCF

3 -1.08837291E+004 -2.38262515E-001 1373.36 <-- SCF

4 -1.08758207E+004 -6.59028890E-001 1375.78 <-- SCF

5 -1.08758530E+004 2.69177598E-003 1378.11 <-- SCF

6 -1.08758248E+004 -2.35063549E-003 1380.45 <-- SCF

7 -1.08758234E+004 -1.17221048E-004 1383.03 <-- SCF

8 -1.08758206E+004 -2.32998865E-004 1385.47 <-- SCF

9 -1.08758207E+004 9.33187365E-006 1387.56 <-- SCF

10 -1.08758207E+004 2.42655860E-006 1389.30 <-- SCF

11 -1.08758207E+004 5.31522945E-007 1391.00 <-- SCF

12 -1.08758208E+004 9.13700399E-007 1392.64 <-- SCF

13 -1.08758208E+004 7.95500004E-007 1394.44 <-- SCF

14 -1.08758208E+004 8.93648224E-007 1396.20 <-- SCF

15 -1.08758208E+004 1.25390717E-006 1398.05 <-- SCF

16 -1.08758208E+004 1.04253032E-006 1399.66 <-- SCF

17 -1.08758208E+004 6.66888048E-007 1401.39 <-- SCF

18 -1.08758208E+004 7.12224667E-007 1403.11 <-- SCF

19 -1.08758208E+004 6.86889695E-007 1404.75 <-- SCF

20 -1.08758208E+004 6.95992801E-007 1406.45 <-- SCF

21 -1.08758208E+004 7.28012347E-007 1408.08 <-- SCF

22 -1.08758209E+004 7.47194067E-007 1409.72 <-- SCF

23 -1.08758209E+004 9.23891413E-007 1411.50 <-- SCF

24 -1.08758209E+004 9.28599062E-007 1413.25 <-- SCF

25 -1.08758209E+004 1.04357879E-006 1414.95 <-- SCF

26 -1.08758209E+004 1.06117763E-006 1416.70 <-- SCF

27 -1.08758209E+004 1.12706191E-006 1418.38 <-- SCF

28 -1.08758209E+004 1.17847612E-006 1420.08 <-- SCF

29 -1.08758209E+004 1.00584644E-006 1421.75 <-- SCF

30 -1.08758210E+004 1.17315065E-006 1423.41 <-- SCF

31 -1.08758210E+004 1.18427799E-006 1425.14 <-- SCF

32 -1.08758210E+004 1.17349816E-006 1426.83 <-- SCF

33 -1.08758210E+004 1.34885367E-006 1428.48 <-- SCF

34 -1.08758210E+004 1.31699009E-006 1430.22 <-- SCF

35 -1.08758210E+004 1.45271998E-006 1431.73 <-- SCF

36 -1.08758211E+004 1.45360590E-006 1433.42 <-- SCF

37 -1.08758211E+004 1.78489905E-006 1435.20 <-- SCF

38 -1.08758211E+004 1.40516578E-006 1436.83 <-- SCF

39 -1.08758211E+004 1.36473429E-006 1438.53 <-- SCF

40 -1.08758211E+004 1.38841097E-006 1440.20 <-- SCF

41 -1.08758211E+004 1.72932283E-006 1441.88 <-- SCF

42 -1.08758212E+004 1.56614879E-006 1443.50 <-- SCF

43 -1.08758212E+004 2.32902755E-006 1445.14 <-- SCF

44 -1.08758212E+004 1.61975119E-006 1446.81 <-- SCF

45 -1.08758213E+004 3.68432218E-006 1448.44 <-- SCF

46 -1.08758213E+004 3.25160213E-006 1450.11 <-- SCF

47 -1.08758213E+004 2.67000630E-006 1451.83 <-- SCF

48 -1.08758214E+004 2.53722678E-006 1453.47 <-- SCF

49 -1.08758214E+004 2.93720326E-006 1455.20 <-- SCF

50 -1.08758214E+004 3.35718254E-006 1456.98 <-- SCF

51 -1.08758215E+004 4.33800233E-006 1458.70 <-- SCF

52 -1.08758215E+004 3.54659203E-006 1460.36 <-- SCF

53 -1.08758216E+004 7.88800709E-006 1462.05 <-- SCF

54 -1.08758217E+004 5.68937533E-006 1463.69 <-- SCF

55 -1.08758217E+004 4.37133574E-006 1465.52 <-- SCF

56 -1.08758218E+004 4.03417666E-006 1467.19 <-- SCF

57 -1.08758218E+004 1.17806403E-006 1468.91 <-- SCF

58 -1.08758218E+004 3.21811404E-006 1470.61 <-- SCF

59 -1.08758219E+004 2.39381258E-006 1472.25 <-- SCF

60 -1.08758219E+004 3.12415632E-007 1474.03 <-- SCF

61 -1.08758219E+004 -3.64940176E-007 1475.80 <-- SCF

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

Final energy = -10875.82186937 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 -0.30861 \*

\* Se 2 0.00000 0.00000 0.25998 \*

\* Se 3 -0.00000 0.00000 -0.30861 \*

\* Se 4 0.00000 0.00000 0.25998 \*

\* Se 5 -0.00000 0.00000 -0.30861 \*

\* Se 6 0.00000 0.00000 0.25998 \*

\* Nb 1 0.00000 -0.00000 -0.63087 \*

\* Nb 2 -0.00000 0.00000 0.67950 \*

\* Nb 3 -0.00000 -0.00000 -0.63087 \*

\* Nb 4 0.00000 -0.00000 0.67950 \*

\* Nb 5 0.00000 -0.00000 -0.63087 \*

\* Nb 6 -0.00000 0.00000 0.67950 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.088165 -0.000000 0.000000 \*

\* y -0.000000 -0.088165 -0.000000 \*

\* z 0.000000 -0.000000 -6.367397 \*

\* \*

\* Pressure: 2.1812 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.001002 | -10875.777988 | <-- min BFGS

| trial step | 1.000000 | 0.000796 | -10875.802084 | <-- min BFGS

| line step | 4.876901 | -0.000314 | -10875.821833 | <-- min BFGS

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

BFGS: finished iteration 13 with enthalpy= -1.08758218E+004 eV

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

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

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

| dE/ion | 3.653711E-003 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 6.795024E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 4.398147E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 6.367397E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 14 ...

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

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

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

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

| previous | 0.000000 | 0.004421 | -10875.821833 | <-- min BFGS

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

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

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)

2.8755397 -1.6601936 -0.0000000 2.1850456 0.0000000 0.0000000

-0.0000000 3.3203872 0.0000000 1.0925228 1.8923050 -0.0000000

-0.0000000 0.0000000 21.8181631 0.0000000 -0.0000000 0.2879796

Lattice parameters(A) Cell Angles

a = 3.320387 alpha = 90.000000

b = 3.320387 beta = 90.000000

c = 21.818163 gamma = 120.000000

Current cell volume = 208.317751 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.427810 x

x Se 2 0.666667 0.333333 0.590216 x

x Se 3 1.333333 0.666667 0.761143 x

x Se 4 1.333333 0.666667 0.923550 x

x Se 5 1.000000 1.000000 1.094476 x

x Se 6 1.000000 1.000000 1.256883 x

x Nb 1 0.333333 0.666667 0.505810 x

x Nb 2 0.333333 0.666667 0.347264 x

x Nb 3 1.000000 1.000000 0.839144 x

x Nb 4 1.000000 1.000000 0.680597 x

x Nb 5 0.666667 1.333333 1.172477 x

x Nb 6 0.666667 1.333333 1.013930 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08743428E+004 1497.75 <-- SCF

1 -1.08779767E+004 3.02821487E-001 1499.31 <-- SCF

2 -1.08781352E+004 1.32106048E-002 1501.88 <-- SCF

3 -1.08762508E+004 -1.57032544E-001 1504.17 <-- SCF

4 -1.08759878E+004 -2.19203224E-002 1506.61 <-- SCF

5 -1.08758954E+004 -7.69713573E-003 1508.94 <-- SCF

6 -1.08758978E+004 2.05076710E-004 1511.39 <-- SCF

7 -1.08758969E+004 -7.58187966E-005 1513.73 <-- SCF

8 -1.08758972E+004 1.91910689E-005 1515.97 <-- SCF

9 -1.08758973E+004 7.40995919E-006 1517.66 <-- SCF

10 -1.08758973E+004 2.92399059E-006 1519.34 <-- SCF

11 -1.08758973E+004 1.91401591E-006 1521.08 <-- SCF

12 -1.08758973E+004 1.04084149E-006 1522.81 <-- SCF

13 -1.08758973E+004 7.16865289E-007 1524.58 <-- SCF

14 -1.08758973E+004 4.79622530E-007 1526.31 <-- SCF

15 -1.08758973E+004 3.10693026E-007 1528.09 <-- SCF

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

Final energy = -10875.89734574 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 -0.17547 \*

\* Se 2 -0.00000 0.00000 0.15246 \*

\* Se 3 -0.00000 0.00000 -0.17547 \*

\* Se 4 -0.00000 0.00000 0.15246 \*

\* Se 5 -0.00000 0.00000 -0.17547 \*

\* Se 6 -0.00000 0.00000 0.15246 \*

\* Nb 1 0.00000 -0.00000 -0.41758 \*

\* Nb 2 -0.00000 0.00000 0.44059 \*

\* Nb 3 0.00000 -0.00000 -0.41758 \*

\* Nb 4 0.00000 0.00000 0.44059 \*

\* Nb 5 0.00000 -0.00000 -0.41758 \*

\* Nb 6 -0.00000 0.00000 0.44059 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -2.487393 -0.000000 -0.000000 \*

\* y -0.000000 -2.487393 0.000000 \*

\* z -0.000000 0.000000 -5.788932 \*

\* \*

\* Pressure: 3.5879 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.004421 | -10875.821833 | <-- min BFGS

| trial step | 1.000000 | 0.001331 | -10875.897341 | <-- min BFGS

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

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BFGS: improving iteration 14 with line minimization (lambda= 1.430623)

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

| Memory Disk |

| Model and support data 143.6 MB 104.2 MB |

| Electronic energy minimisation requirements 12.7 MB 0.0 MB |

| Geometry minimisation requirements 15.6 MB 0.0 MB |

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

| Approx. total storage required per process 172.0 MB 104.2 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)

2.8641759 -1.6536328 -0.0000000 2.1937149 0.0000000 0.0000000

-0.0000000 3.3072655 0.0000000 1.0968574 1.8998128 -0.0000000

-0.0000000 0.0000000 21.8938234 0.0000000 -0.0000000 0.2869844

Lattice parameters(A) Cell Angles

a = 3.307266 alpha = 90.000000

b = 3.307266 beta = 90.000000

c = 21.893823 gamma = 120.000000

Current cell volume = 207.391219 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 0.666667 0.333333 0.427630 x

x Se 2 0.666667 0.333333 0.590306 x

x Se 3 1.333333 0.666667 0.760963 x

x Se 4 1.333333 0.666667 0.923639 x

x Se 5 1.000000 1.000000 1.094296 x

x Se 6 1.000000 1.000000 1.256972 x

x Nb 1 0.333333 0.666667 0.505642 x

x Nb 2 0.333333 0.666667 0.347523 x

x Nb 3 1.000000 1.000000 0.838975 x

x Nb 4 1.000000 1.000000 0.680857 x

x Nb 5 0.666667 1.333333 1.172308 x

x Nb 6 0.666667 1.333333 1.014190 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08756159E+004 1550.19 <-- SCF

1 -1.08763155E+004 5.83012251E-002 1551.84 <-- SCF

2 -1.08763488E+004 2.77351728E-003 1554.30 <-- SCF

3 -1.08759923E+004 -2.97090120E-002 1556.73 <-- SCF

4 -1.08759226E+004 -5.80569745E-003 1559.08 <-- SCF

5 -1.08759063E+004 -1.36001550E-003 1561.55 <-- SCF

6 -1.08759089E+004 2.11513581E-004 1563.91 <-- SCF

7 -1.08759101E+004 1.00503019E-004 1566.20 <-- SCF

8 -1.08759102E+004 1.46567933E-005 1568.23 <-- SCF

9 -1.08759103E+004 1.20067936E-006 1570.00 <-- SCF

10 -1.08759109E+004 5.72277064E-005 1571.98 <-- SCF

11 -1.08759199E+004 7.48127622E-004 1573.66 <-- SCF

12 -1.08759225E+004 2.13018978E-004 1575.52 <-- SCF

13 -1.08759243E+004 1.54070935E-004 1577.23 <-- SCF

14 -1.08759256E+004 1.02175198E-004 1579.03 <-- SCF

15 -1.08759264E+004 7.15860483E-005 1580.81 <-- SCF

16 -1.08759271E+004 5.81404950E-005 1582.47 <-- SCF

17 -1.08759276E+004 4.26513385E-005 1584.22 <-- SCF

18 -1.08759280E+004 3.38481947E-005 1585.95 <-- SCF

19 -1.08759283E+004 2.23560298E-005 1587.72 <-- SCF

20 -1.08759285E+004 1.66149200E-005 1589.44 <-- SCF

21 -1.08759287E+004 1.29019250E-005 1591.08 <-- SCF

22 -1.08759288E+004 1.07973857E-005 1592.92 <-- SCF

23 -1.08759289E+004 1.12832190E-005 1594.64 <-- SCF

24 -1.08759290E+004 7.57622706E-006 1596.44 <-- SCF

25 -1.08759291E+004 3.70249732E-006 1598.19 <-- SCF

26 -1.08759291E+004 3.14185081E-006 1599.91 <-- SCF

27 -1.08759292E+004 5.51554006E-006 1601.62 <-- SCF

28 -1.08759292E+004 -1.29558461E-007 1603.38 <-- SCF

29 -1.08759291E+004 -1.21713834E-006 1605.03 <-- SCF

30 -1.08759292E+004 5.04312298E-006 1606.84 <-- SCF

31 -1.08759294E+004 1.75495129E-005 1608.81 <-- SCF

32 -1.08759290E+004 -3.41221016E-005 1610.84 <-- SCF

33 -1.08759290E+004 9.41128820E-007 1612.62 <-- SCF

34 -1.08759290E+004 1.77512129E-006 1614.39 <-- SCF

35 -1.08759292E+004 1.17833257E-005 1616.42 <-- SCF

36 -1.08759291E+004 -9.16730776E-006 1618.30 <-- SCF

37 -1.08759292E+004 1.09244853E-005 1620.20 <-- SCF

38 -1.08759296E+004 3.74941102E-005 1622.34 <-- SCF

39 -1.08759292E+004 -3.68542589E-005 1624.52 <-- SCF

40 -1.08759284E+004 -6.34182117E-005 1626.69 <-- SCF

41 -1.08759284E+004 -7.08118589E-007 1628.97 <-- SCF

42 -1.08759282E+004 -1.53782581E-005 1630.92 <-- SCF

43 -1.08759276E+004 -5.48291346E-005 1633.28 <-- SCF

44 -1.08759306E+004 2.50973213E-004 1635.64 <-- SCF

45 -1.08759320E+004 1.13603607E-004 1638.12 <-- SCF

46 -1.08759284E+004 -2.95557738E-004 1640.42 <-- SCF

47 -1.08759279E+004 -4.49516529E-005 1642.77 <-- SCF

48 -1.08759280E+004 1.11061575E-005 1644.58 <-- SCF

49 -1.08759284E+004 3.05163060E-005 1647.02 <-- SCF

50 -1.08759285E+004 8.03315060E-006 1649.23 <-- SCF

51 -1.08759276E+004 -7.17669136E-005 1651.67 <-- SCF

52 -1.08759272E+004 -3.09932179E-005 1654.06 <-- SCF

53 -1.08759272E+004 4.15941906E-007 1656.08 <-- SCF

54 -1.08759272E+004 -1.25457126E-006 1657.88 <-- SCF

55 -1.08759272E+004 2.83534004E-008 1659.55 <-- SCF

56 -1.08759272E+004 1.41460867E-007 1661.12 <-- SCF

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

Final energy = -10875.92723501 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 -0.09882 \*

\* Se 2 0.00000 0.00000 0.10571 \*

\* Se 3 0.00000 0.00000 -0.09882 \*

\* Se 4 0.00000 -0.00000 0.10571 \*

\* Se 5 0.00000 -0.00000 -0.09882 \*

\* Se 6 0.00000 0.00000 0.10571 \*

\* Nb 1 -0.00000 0.00000 -0.23910 \*

\* Nb 2 0.00000 0.00000 0.23221 \*

\* Nb 3 -0.00000 0.00000 -0.23910 \*

\* Nb 4 0.00000 0.00000 0.23221 \*

\* Nb 5 -0.00000 0.00000 -0.23910 \*

\* Nb 6 0.00000 0.00000 0.23221 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -2.606700 -0.000000 -0.000000 \*

\* y -0.000000 -2.606700 0.000000 \*

\* z -0.000000 0.000000 -7.552350 \*

\* \*

\* Pressure: 4.2552 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.004421 | -10875.821833 | <-- min BFGS

| trial step | 1.000000 | 0.001331 | -10875.897341 | <-- min BFGS

| line step | 1.430623 | 0.001315 | -10875.927325 | <-- min BFGS

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

BFGS: finished iteration 14 with enthalpy= -1.08759273E+004 eV

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

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

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

| dE/ion | 8.791041E-003 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 2.390960E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.887985E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 7.552350E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 15 ...

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

Writing analysis data to 3R-Nb1.1Se2-7-US.castep\_bin

Writing model to 3R-Nb1.1Se2-7-US.check

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

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

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

| previous | 0.000000 | 0.007845 | -10875.927325 | <-- min BFGS

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

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

BFGS: starting iteration 15 with trial guess (lambda= 0.537512)

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

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

| Memory Disk |

| Model and support data 144.7 MB 104.2 MB |

| Electronic energy minimisation requirements 12.7 MB 0.0 MB |

| Geometry minimisation requirements 15.7 MB 0.0 MB |

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

| Approx. total storage required per process 173.2 MB 104.2 MB |

| |

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

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

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Unit Cell

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

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

2.8566613 -1.6492942 -0.0000000 2.1994856 0.0000000 0.0000000

-0.0000000 3.2985883 0.0000000 1.0997428 1.9048104 -0.0000000

-0.0000000 0.0000000 22.1584120 0.0000000 -0.0000000 0.2835576

Lattice parameters(A) Cell Angles

a = 3.298588 alpha = 90.000000

b = 3.298588 beta = 90.000000

c = 22.158412 gamma = 120.000000

Current cell volume = 208.797601 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.427646 x

x Se 2 0.666667 0.333333 0.589996 x

x Se 3 1.333333 0.666667 0.760979 x

x Se 4 1.333333 0.666667 0.923329 x

x Se 5 1.000000 1.000000 1.094313 x

x Se 6 1.000000 1.000000 1.256662 x

x Nb 1 0.333333 0.666667 0.505251 x

x Nb 2 0.333333 0.666667 0.348207 x

x Nb 3 1.000000 1.000000 0.838585 x

x Nb 4 1.000000 1.000000 0.681541 x

x Nb 5 0.666667 1.333333 1.171918 x

x Nb 6 0.666667 1.333333 1.014874 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08745416E+004 1682.83 <-- SCF

1 -1.08785487E+004 3.33928290E-001 1684.39 <-- SCF

2 -1.08786778E+004 1.07562740E-002 1687.02 <-- SCF

3 -1.08764034E+004 -1.89533987E-001 1689.47 <-- SCF

4 -1.08760980E+004 -2.54527992E-002 1691.97 <-- SCF

5 -1.08760090E+004 -7.41443330E-003 1694.28 <-- SCF

6 -1.08760077E+004 -1.10791550E-004 1696.77 <-- SCF

7 -1.08760074E+004 -2.19736578E-005 1699.09 <-- SCF

8 -1.08760074E+004 3.32471262E-006 1701.06 <-- SCF

9 -1.08760074E+004 4.85122651E-007 1702.73 <-- SCF

10 -1.08760074E+004 4.51585319E-007 1704.44 <-- SCF

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

Final energy = -10876.00744863 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 -0.14512 \*

\* Se 2 0.00000 0.00000 0.13502 \*

\* Se 3 0.00000 0.00000 -0.14512 \*

\* Se 4 -0.00000 0.00000 0.13502 \*

\* Se 5 0.00000 0.00000 -0.14512 \*

\* Se 6 -0.00000 0.00000 0.13502 \*

\* Nb 1 0.00000 0.00000 -0.01391 \*

\* Nb 2 0.00000 0.00000 0.02400 \*

\* Nb 3 0.00000 0.00000 -0.01391 \*

\* Nb 4 0.00000 0.00000 0.02400 \*

\* Nb 5 -0.00000 -0.00000 -0.01391 \*

\* Nb 6 0.00000 0.00000 0.02400 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -2.320363 -0.000000 -0.000000 \*

\* y -0.000000 -2.320363 0.000000 \*

\* z -0.000000 0.000000 -4.084243 \*

\* \*

\* Pressure: 2.9083 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.007845 | -10875.927325 | <-- min BFGS

| trial step | 0.537512 | 0.003156 | -10876.007483 | <-- min BFGS

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

BFGS: finished iteration 15 with enthalpy= -1.08760075E+004 eV

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

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

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

| dE/ion | 6.679828E-003 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.451182E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.515419E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 4.084243E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 16 ...

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

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

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

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

| previous | 0.000000 | 0.002500 | -10876.007483 | <-- min BFGS

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

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

BFGS: starting iteration 16 with trial guess (lambda= 1.000000)

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

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

| Memory Disk |

| Model and support data 146.8 MB 104.2 MB |

| Electronic energy minimisation requirements 12.8 MB 0.0 MB |

| Geometry minimisation requirements 15.8 MB 0.0 MB |

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

| Approx. total storage required per process 175.5 MB 104.2 MB |

| |

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

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

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

Unit Cell

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

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

2.8657761 -1.6545566 -0.0000000 2.1924900 0.0000000 0.0000000

-0.0000000 3.3091132 0.0000000 1.0962450 1.8987520 -0.0000000

-0.0000000 0.0000000 22.3536540 0.0000000 -0.0000000 0.2810809

Lattice parameters(A) Cell Angles

a = 3.309113 alpha = 90.000000

b = 3.309113 beta = 90.000000

c = 22.353654 gamma = 120.000000

Current cell volume = 211.983669 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.427537 x

x Se 2 0.666667 0.333333 0.590041 x

x Se 3 1.333333 0.666667 0.760871 x

x Se 4 1.333333 0.666667 0.923374 x

x Se 5 1.000000 1.000000 1.094204 x

x Se 6 1.000000 1.000000 1.256708 x

x Nb 1 0.333333 0.666667 0.505136 x

x Nb 2 0.333333 0.666667 0.348385 x

x Nb 3 1.000000 1.000000 0.838470 x

x Nb 4 1.000000 1.000000 0.681719 x

x Nb 5 0.666667 1.333333 1.171803 x

x Nb 6 0.666667 1.333333 1.015052 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08755674E+004 1726.14 <-- SCF

1 -1.08764721E+004 7.53960724E-002 1727.73 <-- SCF

2 -1.08764959E+004 1.98005518E-003 1730.39 <-- SCF

3 -1.08760834E+004 -3.43730522E-002 1732.84 <-- SCF

4 -1.08760506E+004 -2.73612390E-003 1735.41 <-- SCF

5 -1.08760481E+004 -2.04144272E-004 1738.23 <-- SCF

6 -1.08760549E+004 5.61773515E-004 1740.70 <-- SCF

7 -1.08760620E+004 5.94897841E-004 1742.84 <-- SCF

8 -1.08760705E+004 7.04966809E-004 1744.95 <-- SCF

9 -1.08760734E+004 2.44632560E-004 1747.25 <-- SCF

10 -1.08760748E+004 1.17474468E-004 1749.62 <-- SCF

11 -1.08760754E+004 4.53323417E-005 1751.44 <-- SCF

12 -1.08760755E+004 1.40265839E-005 1753.41 <-- SCF

13 -1.08760756E+004 8.54709340E-006 1755.22 <-- SCF

14 -1.08760757E+004 6.94436036E-006 1757.31 <-- SCF

15 -1.08760758E+004 4.87794380E-006 1759.08 <-- SCF

16 -1.08760758E+004 2.86762757E-006 1760.89 <-- SCF

17 -1.08760758E+004 1.74755830E-006 1762.72 <-- SCF

18 -1.08760758E+004 1.02675489E-006 1764.50 <-- SCF

19 -1.08760759E+004 8.42645075E-007 1766.20 <-- SCF

20 -1.08760759E+004 3.79884727E-007 1767.94 <-- SCF

21 -1.08760759E+004 2.11532820E-007 1769.77 <-- SCF

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

Final energy = -10876.07586519 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 -0.12523 \*

\* Se 2 0.00000 0.00000 0.04887 \*

\* Se 3 -0.00000 -0.00000 -0.12523 \*

\* Se 4 -0.00000 0.00000 0.04887 \*

\* Se 5 0.00000 -0.00000 -0.12523 \*

\* Se 6 0.00000 0.00000 0.04887 \*

\* Nb 1 0.00000 -0.00000 0.10612 \*

\* Nb 2 -0.00000 0.00000 -0.02975 \*

\* Nb 3 0.00000 -0.00000 0.10612 \*

\* Nb 4 -0.00000 0.00000 -0.02975 \*

\* Nb 5 0.00000 -0.00000 0.10612 \*

\* Nb 6 -0.00000 0.00000 -0.02975 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.264493 -0.000000 0.000000 \*

\* y -0.000000 0.264493 -0.000000 \*

\* z 0.000000 -0.000000 -1.760046 \*

\* \*

\* Pressure: 0.4104 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.002500 | -10876.007483 | <-- min BFGS

| trial step | 1.000000 | 0.000661 | -10876.075850 | <-- min BFGS

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

BFGS: finished iteration 16 with enthalpy= -1.08760758E+004 eV

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

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

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

| dE/ion | 5.697180E-003 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.252313E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.985034E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.760046E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 17 ...

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

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

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

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

| previous | 0.000000 | 0.001033 | -10876.075850 | <-- min BFGS

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

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

BFGS: starting iteration 17 with trial guess (lambda= 1.000000)

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

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

| Memory Disk |

| Model and support data 155.7 MB 104.2 MB |

| Electronic energy minimisation requirements 13.0 MB 0.0 MB |

| Geometry minimisation requirements 16.0 MB 0.0 MB |

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

| Approx. total storage required per process 184.7 MB 104.2 MB |

| |

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

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

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

Unit Cell

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

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

2.8584888 -1.6503493 -0.0000000 2.1980794 0.0000000 0.0000000

-0.0000000 3.3006985 0.0000000 1.0990397 1.9035926 -0.0000000

-0.0000000 0.0000000 22.5728231 0.0000000 -0.0000000 0.2783518

Lattice parameters(A) Cell Angles

a = 3.300699 alpha = 90.000000

b = 3.300699 beta = 90.000000

c = 22.572823 gamma = 120.000000

Current cell volume = 212.974805 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.427059 x

x Se 2 0.666667 0.333333 0.590452 x

x Se 3 1.333333 0.666667 0.760392 x

x Se 4 1.333333 0.666667 0.923785 x

x Se 5 1.000000 1.000000 1.093725 x

x Se 6 1.000000 1.000000 1.257118 x

x Nb 1 0.333333 0.666667 0.504946 x

x Nb 2 0.333333 0.666667 0.348643 x

x Nb 3 1.000000 1.000000 0.838280 x

x Nb 4 1.000000 1.000000 0.681976 x

x Nb 5 0.666667 1.333333 1.171613 x

x Nb 6 0.666667 1.333333 1.015310 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08754701E+004 1792.00 <-- SCF

1 -1.08773862E+004 1.59673913E-001 1793.83 <-- SCF

2 -1.08774604E+004 6.17989952E-003 1796.42 <-- SCF

3 -1.08769645E+004 -4.13180835E-002 1799.00 <-- SCF

4 -1.08760856E+004 -7.32489613E-002 1801.42 <-- SCF

5 -1.08760804E+004 -4.30027693E-004 1804.08 <-- SCF

6 -1.08760790E+004 -1.17734757E-004 1806.66 <-- SCF

7 -1.08760790E+004 -1.40767107E-006 1809.05 <-- SCF

8 -1.08760789E+004 -5.97234811E-006 1811.31 <-- SCF

9 -1.08760789E+004 3.72320418E-007 1813.12 <-- SCF

10 -1.08760789E+004 9.28369364E-008 1814.88 <-- SCF

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

Final energy = -10876.07889617 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.13660 \*

\* Se 2 0.00000 0.00000 -0.10580 \*

\* Se 3 0.00000 0.00000 0.13660 \*

\* Se 4 -0.00000 0.00000 -0.10580 \*

\* Se 5 0.00000 -0.00000 0.13660 \*

\* Se 6 0.00000 0.00000 -0.10580 \*

\* Nb 1 0.00000 0.00000 0.16403 \*

\* Nb 2 0.00000 0.00000 -0.19483 \*

\* Nb 3 0.00000 0.00000 0.16403 \*

\* Nb 4 0.00000 0.00000 -0.19483 \*

\* Nb 5 -0.00000 0.00000 0.16403 \*

\* Nb 6 0.00000 -0.00000 -0.19483 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.467686 -0.000000 -0.000000 \*

\* y -0.000000 0.467686 -0.000000 \*

\* z -0.000000 -0.000000 0.972495 \*

\* \*

\* Pressure: -0.6360 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.001033 | -10876.075850 | <-- min BFGS

| trial step | 1.000000 | -0.000818 | -10876.079016 | <-- min BFGS

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

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

BFGS: improving iteration 17 with line minimization (lambda= 0.558064)

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

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

| Memory Disk |

| Model and support data 157.7 MB 104.2 MB |

| Electronic energy minimisation requirements 12.9 MB 0.0 MB |

| Geometry minimisation requirements 15.9 MB 0.0 MB |

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

| Approx. total storage required per process 186.4 MB 104.2 MB |

| |

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

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

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

Unit Cell

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

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

2.8617093 -1.6522086 -0.0000000 2.1956057 0.0000000 0.0000000

-0.0000000 3.3044173 0.0000000 1.0978029 1.9014503 -0.0000000

-0.0000000 0.0000000 22.4759643 0.0000000 -0.0000000 0.2795513

Lattice parameters(A) Cell Angles

a = 3.304417 alpha = 90.000000

b = 3.304417 beta = 90.000000

c = 22.475964 gamma = 120.000000

Current cell volume = 212.539050 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.427270 x

x Se 2 0.666667 0.333333 0.590270 x

x Se 3 1.333333 0.666667 0.760604 x

x Se 4 1.333333 0.666667 0.923604 x

x Se 5 1.000000 1.000000 1.093937 x

x Se 6 1.000000 1.000000 1.256937 x

x Nb 1 0.333333 0.666667 0.505030 x

x Nb 2 0.333333 0.666667 0.348529 x

x Nb 3 1.000000 1.000000 0.838364 x

x Nb 4 1.000000 1.000000 0.681863 x

x Nb 5 0.666667 1.333333 1.171697 x

x Nb 6 0.666667 1.333333 1.015196 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08759667E+004 1836.64 <-- SCF

1 -1.08763387E+004 3.10002061E-002 1838.52 <-- SCF

2 -1.08763516E+004 1.07606462E-003 1841.14 <-- SCF

3 -1.08762578E+004 -7.81796774E-003 1843.53 <-- SCF

4 -1.08760851E+004 -1.43884887E-002 1845.91 <-- SCF

5 -1.08760844E+004 -5.71737432E-005 1848.38 <-- SCF

6 -1.08760839E+004 -4.25016710E-005 1850.69 <-- SCF

7 -1.08760839E+004 1.91158204E-006 1852.86 <-- SCF

8 -1.08760839E+004 -2.68078780E-006 1855.00 <-- SCF

9 -1.08760839E+004 1.50405298E-007 1856.72 <-- SCF

10 -1.08760839E+004 1.85730588E-008 1858.50 <-- SCF

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

Final energy = -10876.08390450 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 0.01804 \*

\* Se 2 -0.00000 -0.00000 -0.03816 \*

\* Se 3 -0.00000 0.00000 0.01804 \*

\* Se 4 0.00000 -0.00000 -0.03816 \*

\* Se 5 -0.00000 0.00000 0.01804 \*

\* Se 6 0.00000 0.00000 -0.03816 \*

\* Nb 1 -0.00000 0.00000 0.14140 \*

\* Nb 2 0.00000 0.00000 -0.12127 \*

\* Nb 3 0.00000 0.00000 0.14140 \*

\* Nb 4 -0.00000 0.00000 -0.12127 \*

\* Nb 5 0.00000 -0.00000 0.14140 \*

\* Nb 6 -0.00000 0.00000 -0.12127 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.393203 -0.000000 0.000000 \*

\* y -0.000000 0.393203 -0.000000 \*

\* z 0.000000 -0.000000 -0.236712 \*

\* \*

\* Pressure: -0.1832 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.001033 | -10876.075850 | <-- min BFGS

| trial step | 1.000000 | -0.000818 | -10876.079016 | <-- min BFGS

| line step | 0.558064 | 5.921E-006 | -10876.083901 | <-- min BFGS

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

BFGS: finished iteration 17 with enthalpy= -1.08760839E+004 eV

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

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

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

| dE/ion | 6.709907E-004 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.413957E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 6.002919E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 3.932035E-001 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 18 ...

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

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

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

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

| previous | 0.000000 | 0.000026 | -10876.083901 | <-- min BFGS

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

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

BFGS: starting iteration 18 with trial guess (lambda= 1.000000)

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Unit Cell

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

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

2.8605239 -1.6515243 -0.0000000 2.1965156 0.0000000 0.0000000

-0.0000000 3.3030485 0.0000000 1.0982578 1.9022383 -0.0000000

-0.0000000 0.0000000 22.4738777 0.0000000 -0.0000000 0.2795773

Lattice parameters(A) Cell Angles

a = 3.303049 alpha = 90.000000

b = 3.303049 beta = 90.000000

c = 22.473878 gamma = 120.000000

Current cell volume = 212.343295 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.427232 x

x Se 2 0.666667 0.333333 0.590324 x

x Se 3 1.333333 0.666667 0.760565 x

x Se 4 1.333333 0.666667 0.923657 x

x Se 5 1.000000 1.000000 1.093898 x

x Se 6 1.000000 1.000000 1.256990 x

x Nb 1 0.333333 0.666667 0.505051 x

x Nb 2 0.333333 0.666667 0.348494 x

x Nb 3 1.000000 1.000000 0.838384 x

x Nb 4 1.000000 1.000000 0.681828 x

x Nb 5 0.666667 1.333333 1.171717 x

x Nb 6 0.666667 1.333333 1.015161 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08760808E+004 1880.44 <-- SCF

1 -1.08761030E+004 1.84983670E-003 1882.23 <-- SCF

2 -1.08761040E+004 8.13582531E-005 1884.78 <-- SCF

3 -1.08760958E+004 -6.81131188E-004 1887.34 <-- SCF

4 -1.08760846E+004 -9.30603965E-004 1889.81 <-- SCF

5 -1.08760845E+004 -1.17444548E-005 1892.36 <-- SCF

6 -1.08760845E+004 -1.91726648E-006 1894.41 <-- SCF

7 -1.08760845E+004 -4.15846263E-008 1896.12 <-- SCF

8 -1.08760845E+004 4.52940821E-008 1897.83 <-- SCF

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

Final energy = -10876.08448238 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.04023 \*

\* Se 2 0.00000 0.00000 -0.04594 \*

\* Se 3 0.00000 0.00000 0.04023 \*

\* Se 4 0.00000 0.00000 -0.04594 \*

\* Se 5 0.00000 0.00000 0.04023 \*

\* Se 6 0.00000 0.00000 -0.04594 \*

\* Nb 1 -0.00000 -0.00000 0.13037 \*

\* Nb 2 0.00000 0.00000 -0.12466 \*

\* Nb 3 -0.00000 0.00000 0.13037 \*

\* Nb 4 0.00000 0.00000 -0.12466 \*

\* Nb 5 -0.00000 -0.00000 0.13037 \*

\* Nb 6 0.00000 0.00000 -0.12466 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.277139 0.000000 0.000000 \*

\* y 0.000000 0.277139 0.000000 \*

\* z 0.000000 0.000000 -0.344913 \*

\* \*

\* Pressure: -0.0698 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000026 | -10876.083901 | <-- min BFGS

| trial step | 1.000000 | 0.000017 | -10876.084485 | <-- min BFGS

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

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

BFGS: improving iteration 18 with line minimization (lambda= 2.974764)

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Unit Cell

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

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

2.8581831 -1.6501728 -0.0000000 2.1983145 0.0000000 0.0000000

-0.0000000 3.3003455 0.0000000 1.0991572 1.9037962 -0.0000000

-0.0000000 0.0000000 22.4697572 0.0000000 -0.0000000 0.2796285

Lattice parameters(A) Cell Angles

a = 3.300346 alpha = 90.000000

b = 3.300346 beta = 90.000000

c = 22.469757 gamma = 120.000000

Current cell volume = 211.957035 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.666667 0.333333 0.427155 x

x Se 2 0.666667 0.333333 0.590429 x

x Se 3 1.333333 0.666667 0.760488 x

x Se 4 1.333333 0.666667 0.923762 x

x Se 5 1.000000 1.000000 1.093822 x

x Se 6 1.000000 1.000000 1.257096 x

x Nb 1 0.333333 0.666667 0.505090 x

x Nb 2 0.333333 0.666667 0.348426 x

x Nb 3 1.000000 1.000000 0.838424 x

x Nb 4 1.000000 1.000000 0.681759 x

x Nb 5 0.666667 1.333333 1.171757 x

x Nb 6 0.666667 1.333333 1.015092 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -1.08760644E+004 1919.86 <-- SCF

1 -1.08761550E+004 7.55290686E-003 1921.67 <-- SCF

2 -1.08761588E+004 3.12428435E-004 1924.33 <-- SCF

3 -1.08761266E+004 -2.68662451E-003 1926.75 <-- SCF

4 -1.08760856E+004 -3.41465053E-003 1929.11 <-- SCF

5 -1.08760850E+004 -5.15573177E-005 1931.59 <-- SCF

6 -1.08760849E+004 -5.73199682E-006 1933.95 <-- SCF

7 -1.08760849E+004 -5.43771316E-007 1935.83 <-- SCF

8 -1.08760849E+004 5.28614854E-009 1937.53 <-- SCF

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

Final energy = -10876.08488031 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.08300 \*

\* Se 2 0.00000 0.00000 -0.06498 \*

\* Se 3 0.00000 -0.00000 0.08300 \*

\* Se 4 0.00000 0.00000 -0.06498 \*

\* Se 5 -0.00000 0.00000 0.08300 \*

\* Se 6 0.00000 0.00000 -0.06498 \*

\* Nb 1 0.00000 0.00000 0.11025 \*

\* Nb 2 -0.00000 0.00000 -0.12827 \*

\* Nb 3 0.00000 0.00000 0.11025 \*

\* Nb 4 0.00000 -0.00000 -0.12827 \*

\* Nb 5 0.00000 0.00000 0.11025 \*

\* Nb 6 0.00000 -0.00000 -0.12827 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.046998 0.000000 -0.000000 \*

\* y 0.000000 0.046998 0.000000 \*

\* z -0.000000 0.000000 -0.563085 \*

\* \*

\* Pressure: 0.1564 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000026 | -10876.083901 | <-- min BFGS

| trial step | 1.000000 | 0.000017 | -10876.084485 | <-- min BFGS

| line step | 2.974764 | -6.104E-007 | -10876.084941 | <-- min BFGS

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

BFGS: finished iteration 18 with enthalpy= -1.08760849E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 8.662641E-005 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.282741E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.569309E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 5.630852E-001 | 5.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 19 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000034 | -10876.084941 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 19 with trial guess (lambda= 1.000000)

--------------------------------------------------------------------------------

-------------------------------

Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

2.8577334 -1.6499131 -0.0000000 2.1986604 0.0000000 0.0000000

-0.0000000 3.2998263 0.0000000 1.0993302 1.9040958 -0.0000000

-0.0000000 0.0000000 22.4751746 0.0000000 -0.0000000 0.2795611

Lattice parameters(A) Cell Angles

a = 3.299826 alpha = 90.000000

b = 3.299826 beta = 90.000000

c = 22.475175 gamma = 120.000000

Current cell volume = 211.941430 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.666667 0.333333 0.427178 x

x Se 2 0.666667 0.333333 0.590409 x

x Se 3 1.333333 0.666667 0.760511 x

x Se 4 1.333333 0.666667 0.923742 x

x Se 5 1.000000 1.000000 1.093845 x

x Se 6 1.000000 1.000000 1.257076 x

x Nb 1 0.333333 0.666667 0.505120 x

x Nb 2 0.333333 0.666667 0.348393 x

x Nb 3 1.000000 1.000000 0.838453 x

x Nb 4 1.000000 1.000000 0.681726 x

x Nb 5 0.666667 1.333333 1.171787 x

x Nb 6 0.666667 1.333333 1.015060 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -1.08760841E+004 1959.58 <-- SCF

1 -1.08760941E+004 8.31061674E-004 1961.42 <-- SCF

2 -1.08760948E+004 5.70887484E-005 1963.83 <-- SCF

3 -1.08760878E+004 -5.81609785E-004 1966.36 <-- SCF

4 -1.08760861E+004 -1.44229973E-004 1968.89 <-- SCF

5 -1.08760857E+004 -2.98188615E-005 1971.36 <-- SCF

6 -1.08760857E+004 5.61787660E-007 1973.41 <-- SCF

7 -1.08760857E+004 -9.61925387E-007 1975.11 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -10876.08573021 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.06868 \*

\* Se 2 -0.00000 0.00000 -0.05550 \*

\* Se 3 0.00000 0.00000 0.06868 \*

\* Se 4 0.00000 0.00000 -0.05550 \*

\* Se 5 0.00000 0.00000 0.06868 \*

\* Se 6 -0.00000 0.00000 -0.05550 \*

\* Nb 1 -0.00000 0.00000 0.10346 \*

\* Nb 2 0.00000 0.00000 -0.11664 \*

\* Nb 3 -0.00000 0.00000 0.10346 \*

\* Nb 4 0.00000 0.00000 -0.11664 \*

\* Nb 5 -0.00000 0.00000 0.10346 \*

\* Nb 6 0.00000 0.00000 -0.11664 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x 0.037172 -0.000000 0.000000 \*

\* y -0.000000 0.037172 0.000000 \*

\* z 0.000000 0.000000 -0.521928 \*

\* \*

\* Pressure: 0.1492 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000034 | -10876.084941 | <-- min BFGS

| trial step | 1.000000 | 0.000030 | -10876.085815 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: improving iteration 19 with line minimization (lambda= 10.056674)

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-------------------------------

Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

2.8536606 -1.6475617 -0.0000000 2.2017984 0.0000000 0.0000000

-0.0000000 3.2951235 0.0000000 1.1008992 1.9068133 -0.0000000

-0.0000000 0.0000000 22.5242387 0.0000000 -0.0000000 0.2789522

Lattice parameters(A) Cell Angles

a = 3.295123 alpha = 90.000000

b = 3.295123 beta = 90.000000

c = 22.524239 gamma = 120.000000

Current cell volume = 211.799111 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.666667 0.333333 0.427386 x

x Se 2 0.666667 0.333333 0.590227 x

x Se 3 1.333333 0.666667 0.760719 x

x Se 4 1.333333 0.666667 0.923560 x

x Se 5 1.000000 1.000000 1.094053 x

x Se 6 1.000000 1.000000 1.256894 x

x Nb 1 0.333333 0.666667 0.505389 x

x Nb 2 0.333333 0.666667 0.348098 x

x Nb 3 1.000000 1.000000 0.838722 x

x Nb 4 1.000000 1.000000 0.681431 x

x Nb 5 0.666667 1.333333 1.172055 x

x Nb 6 0.666667 1.333333 1.014765 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -1.08757773E+004 1997.23 <-- SCF

1 -1.08768423E+004 8.87509430E-002 1999.00 <-- SCF

2 -1.08769091E+004 5.56689001E-003 2001.67 <-- SCF

3 -1.08763344E+004 -4.78933066E-002 2004.22 <-- SCF

4 -1.08761153E+004 -1.82609402E-002 2006.53 <-- SCF

5 -1.08760902E+004 -2.09518439E-003 2008.97 <-- SCF

6 -1.08760907E+004 4.50375980E-005 2011.39 <-- SCF

7 -1.08760897E+004 -8.15619921E-005 2013.81 <-- SCF

8 -1.08760897E+004 2.40768327E-006 2015.97 <-- SCF

9 -1.08760897E+004 2.17007934E-007 2017.69 <-- SCF

10 -1.08760897E+004 -1.14488362E-007 2019.28 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -10876.08974600 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 -0.04545 \*

\* Se 2 -0.00000 -0.00000 0.01451 \*

\* Se 3 0.00000 0.00000 -0.04545 \*

\* Se 4 -0.00000 -0.00000 0.01451 \*

\* Se 5 0.00000 0.00000 -0.04545 \*

\* Se 6 -0.00000 0.00000 0.01451 \*

\* Nb 1 0.00000 0.00000 0.04321 \*

\* Nb 2 -0.00000 -0.00000 -0.01227 \*

\* Nb 3 0.00000 0.00000 0.04321 \*

\* Nb 4 -0.00000 -0.00000 -0.01227 \*

\* Nb 5 0.00000 0.00000 0.04321 \*

\* Nb 6 -0.00000 -0.00000 -0.01227 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.077244 0.000000 0.000000 \*

\* y 0.000000 -0.077244 -0.000000 \*

\* z 0.000000 -0.000000 -0.187044 \*

\* \*

\* Pressure: 0.1138 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000034 | -10876.084941 | <-- min BFGS

| trial step | 1.000000 | 0.000030 | -10876.085815 | <-- min BFGS

| line step | 10.056674 | 1.860E-006 | -10876.089808 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 19 with enthalpy= -1.08760898E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 4.056159E-004 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 4.545447E-002 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 7.375057E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.870439E-001 | 5.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 20 ...

================================================================================

Writing analysis data to 3R-Nb1.1Se2-7-US.castep\_bin

Writing model to 3R-Nb1.1Se2-7-US.check

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000021 | -10876.089808 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

BFGS: starting iteration 20 with trial guess (lambda= 1.000000)

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Unit Cell

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Real Lattice(A) Reciprocal Lattice(1/A)

2.8528119 -1.6470717 -0.0000000 2.2024534 0.0000000 0.0000000

-0.0000000 3.2941434 0.0000000 1.1012267 1.9073806 -0.0000000

-0.0000000 0.0000000 22.5395063 0.0000000 -0.0000000 0.2787632

Lattice parameters(A) Cell Angles

a = 3.294143 alpha = 90.000000

b = 3.294143 beta = 90.000000

c = 22.539506 gamma = 120.000000

Current cell volume = 211.816622 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.666667 0.333333 0.427336 x

x Se 2 0.666667 0.333333 0.590304 x

x Se 3 1.333333 0.666667 0.760669 x

x Se 4 1.333333 0.666667 0.923637 x

x Se 5 1.000000 1.000000 1.094002 x

x Se 6 1.000000 1.000000 1.256970 x

x Nb 1 0.333333 0.666667 0.505447 x

x Nb 2 0.333333 0.666667 0.348014 x

x Nb 3 1.000000 1.000000 0.838780 x

x Nb 4 1.000000 1.000000 0.681347 x

x Nb 5 0.666667 1.333333 1.172114 x

x Nb 6 0.666667 1.333333 1.014680 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -1.08760698E+004 2041.55 <-- SCF

1 -1.08761511E+004 6.77656149E-003 2043.33 <-- SCF

2 -1.08761570E+004 4.95568551E-004 2045.91 <-- SCF

3 -1.08761179E+004 -3.26221257E-003 2048.47 <-- SCF

4 -1.08760916E+004 -2.18973415E-003 2050.84 <-- SCF

5 -1.08760901E+004 -1.25129537E-004 2053.23 <-- SCF

6 -1.08760901E+004 -6.29336801E-007 2055.62 <-- SCF

7 -1.08760901E+004 -2.23541799E-006 2057.58 <-- SCF

8 -1.08760901E+004 -1.91130168E-007 2059.41 <-- SCF

9 -1.08760901E+004 1.98557587E-007 2061.22 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -10876.09007182 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 -0.01340 \*

\* Se 2 0.00000 -0.00000 -0.00004 \*

\* Se 3 0.00000 0.00000 -0.01340 \*

\* Se 4 0.00000 -0.00000 -0.00004 \*

\* Se 5 -0.00000 -0.00000 -0.01340 \*

\* Se 6 0.00000 0.00000 -0.00004 \*

\* Nb 1 -0.00000 0.00000 0.01609 \*

\* Nb 2 0.00000 0.00000 -0.00266 \*

\* Nb 3 -0.00000 0.00000 0.01609 \*

\* Nb 4 0.00000 0.00000 -0.00266 \*

\* Nb 5 -0.00000 0.00000 0.01609 \*

\* Nb 6 0.00000 0.00000 -0.00266 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.054055 0.000000 0.000000 \*

\* y 0.000000 -0.054055 -0.000000 \*

\* z 0.000000 -0.000000 -0.023224 \*

\* \*

\* Pressure: 0.0438 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 0.000021 | -10876.089808 | <-- min BFGS

| trial step | 1.000000 | 3.758E-006 | -10876.090151 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 20 with enthalpy= -1.08760902E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.858020E-005 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.609459E-002 | 3.000000E-002 | eV/A | Yes | <-- BFGS

| |dR|max | 1.901867E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 5.405500E-002 | 5.000000E-002 | GPa | No | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

================================================================================

Starting BFGS iteration 21 ...

================================================================================

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.702E-006 | -10876.090151 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

--------------------------------------------------------------------------------

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)

2.8530678 -1.6472195 -0.0000000 2.2022558 0.0000000 0.0000000

-0.0000000 3.2944390 0.0000000 1.1011279 1.9072095 -0.0000000

-0.0000000 0.0000000 22.5401223 0.0000000 -0.0000000 0.2787556

Lattice parameters(A) Cell Angles

a = 3.294439 alpha = 90.000000

b = 3.294439 beta = 90.000000

c = 22.540122 gamma = 120.000000

Current cell volume = 211.860422 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.666667 0.333333 0.427324 x

x Se 2 0.666667 0.333333 0.590324 x

x Se 3 1.333333 0.666667 0.760658 x

x Se 4 1.333333 0.666667 0.923657 x

x Se 5 1.000000 1.000000 1.093991 x

x Se 6 1.000000 1.000000 1.256991 x

x Nb 1 0.333333 0.666667 0.505463 x

x Nb 2 0.333333 0.666667 0.347989 x

x Nb 3 1.000000 1.000000 0.838797 x

x Nb 4 1.000000 1.000000 0.681322 x

x Nb 5 0.666667 1.333333 1.172130 x

x Nb 6 0.666667 1.333333 1.014655 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

------------------------------------------------------------------------ <-- SCF

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

------------------------------------------------------------------------ <-- SCF

Initial -1.08760905E+004 2083.16 <-- SCF

1 -1.08760946E+004 3.47005947E-004 2084.92 <-- SCF

2 -1.08760950E+004 3.33364393E-005 2087.44 <-- SCF

3 -1.08760917E+004 -2.79260263E-004 2089.86 <-- SCF

4 -1.08760903E+004 -1.17823443E-004 2092.38 <-- SCF

5 -1.08760901E+004 -1.30983299E-005 2094.64 <-- SCF

6 -1.08760901E+004 3.25959181E-007 2096.70 <-- SCF

7 -1.08760901E+004 -3.71948802E-007 2098.44 <-- SCF

------------------------------------------------------------------------ <-- SCF

Final energy = -10876.09009787 eV

(energy not corrected for finite basis set)

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 -0.00587 \*

\* Se 2 -0.00000 0.00000 -0.00347 \*

\* Se 3 0.00000 -0.00000 -0.00587 \*

\* Se 4 -0.00000 0.00000 -0.00347 \*

\* Se 5 -0.00000 0.00000 -0.00587 \*

\* Se 6 -0.00000 0.00000 -0.00347 \*

\* Nb 1 0.00000 0.00000 0.00627 \*

\* Nb 2 -0.00000 0.00000 0.00307 \*

\* Nb 3 -0.00000 0.00000 0.00627 \*

\* Nb 4 -0.00000 0.00000 0.00307 \*

\* Nb 5 -0.00000 0.00000 0.00627 \*

\* Nb 6 -0.00000 0.00000 0.00307 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Stress Tensor \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.001858 -0.000000 -0.000000 \*

\* y -0.000000 -0.001858 -0.000000 \*

\* z -0.000000 -0.000000 0.012982 \*

\* \*

\* Pressure: -0.0031 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

+------------+-------------+-------------+-----------------+ <-- min BFGS

| Step | lambda | F.delta | enthalpy | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

| previous | 0.000000 | 1.702E-006 | -10876.090151 | <-- min BFGS

| trial step | 1.000000 | 5.510E-008 | -10876.090176 | <-- min BFGS

+------------+-------------+-------------+-----------------+ <-- min BFGS

BFGS: finished iteration 21 with enthalpy= -1.08760902E+004 eV

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| Parameter | value | tolerance | units | OK? | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

| dE/ion | 2.029665E-006 | 1.000000E-005 | eV | Yes | <-- BFGS

| |F|max | 6.270755E-003 | 3.000000E-002 | eV/A | Yes | <-- BFGS

| |dR|max | 5.670256E-004 | 1.000000E-003 | A | Yes | <-- BFGS

| Smax | 1.298156E-002 | 5.000000E-002 | GPa | Yes | <-- BFGS

+-----------+-----------------+-----------------+------------+-----+ <-- BFGS

BFGS: Geometry optimization completed successfully.

================================================================================

BFGS: Final Configuration:

================================================================================

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Unit Cell

-------------------------------

Real Lattice(A) Reciprocal Lattice(1/A)

2.8530678 -1.6472195 -0.0000000 2.2022558 0.0000000 0.0000000

-0.0000000 3.2944390 0.0000000 1.1011279 1.9072095 -0.0000000

-0.0000000 0.0000000 22.5401223 0.0000000 -0.0000000 0.2787556

Lattice parameters(A) Cell Angles

a = 3.294439 alpha = 90.000000

b = 3.294439 beta = 90.000000

c = 22.540122 gamma = 120.000000

Current cell volume = 211.860422 A\*\*3

-------------------------------

Cell Contents

-------------------------------

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

x----------------------------------------------------------x

x Se 1 0.666667 0.333333 0.427324 x

x Se 2 0.666667 0.333333 0.590324 x

x Se 3 1.333333 0.666667 0.760658 x

x Se 4 1.333333 0.666667 0.923657 x

x Se 5 1.000000 1.000000 1.093991 x

x Se 6 1.000000 1.000000 1.256991 x

x Nb 1 0.333333 0.666667 0.505463 x

x Nb 2 0.333333 0.666667 0.347989 x

x Nb 3 1.000000 1.000000 0.838797 x

x Nb 4 1.000000 1.000000 0.681322 x

x Nb 5 0.666667 1.333333 1.172130 x

x Nb 6 0.666667 1.333333 1.014655 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

BFGS: Final Enthalpy = -1.08760902E+004 eV

BFGS: Final <frequency> = 220.75227 cm-1

BFGS: Final bulk modulus = 266.25742 GPa

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Symmetrised Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

\* -------------------------------------------------------------------------- \*

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 -0.00587 \*

\* Se 2 -0.00000 0.00000 -0.00347 \*

\* Se 3 0.00000 -0.00000 -0.00587 \*

\* Se 4 -0.00000 0.00000 -0.00347 \*

\* Se 5 -0.00000 0.00000 -0.00587 \*

\* Se 6 -0.00000 0.00000 -0.00347 \*

\* Nb 1 0.00000 0.00000 0.00627 \*

\* Nb 2 -0.00000 0.00000 0.00307 \*

\* Nb 3 -0.00000 0.00000 0.00627 \*

\* Nb 4 -0.00000 0.00000 0.00307 \*

\* Nb 5 -0.00000 0.00000 0.00627 \*

\* Nb 6 -0.00000 0.00000 0.00307 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\*\*\*\*\*\*\*\*\*\*\* Symmetrised Stress Tensor \*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (GPa) \*

\* --------------------------------------------- \*

\* x y z \*

\* \*

\* x -0.001858 -0.000000 -0.000000 \*

\* y -0.000000 -0.001858 -0.000000 \*

\* z -0.000000 -0.000000 0.012982 \*

\* \*

\* Pressure: -0.0031 \*

\* \*

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Pseudo atomic calculation performed for Se 4s2 4p4

Converged in 18 iterations to a total energy of -256.4822 eV

Pseudo atomic calculation performed for Nb 4s2 4p6 4d4 5s1

Converged in 18 iterations to a total energy of -1541.3312 eV

Charge spilling parameter for spin component 1 = 0.24%

Atomic Populations (Mulliken)

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Species Ion s p d f Total Charge (e)

==============================================================

Se 1 1.33 4.20 0.00 0.00 5.53 0.47

Se 2 1.32 4.22 0.00 0.00 5.54 0.46

Se 3 1.33 4.20 0.00 0.00 5.53 0.47

Se 4 1.32 4.22 0.00 0.00 5.54 0.46

Se 5 1.33 4.20 0.00 0.00 5.53 0.47

Se 6 1.32 4.22 0.00 0.00 5.54 0.46

Nb 1 2.66 6.72 4.08 0.00 13.46 -0.46

Nb 2 2.65 6.72 4.10 0.00 13.47 -0.47

Nb 3 2.66 6.72 4.08 0.00 13.46 -0.46

Nb 4 2.65 6.72 4.10 0.00 13.47 -0.47

Nb 5 2.66 6.72 4.08 0.00 13.46 -0.46

Nb 6 2.65 6.72 4.10 0.00 13.47 -0.47

==============================================================

Bond Population Length (A)

============================================================

Se 3 -- Nb 3 -6.25 2.59226

Se 1 -- Nb 1 -6.25 2.59226

Se 5 -- Nb 5 -6.25 2.59226

Se 5 -- Nb 6 -6.30 2.61066

Se 3 -- Nb 4 -6.30 2.61066

Se 1 -- Nb 2 -6.30 2.61066

Se 4 -- Nb 3 -6.50 2.69749

Se 2 -- Nb 1 -6.50 2.69749

Se 6 -- Nb 5 -6.50 2.69749

Se 6 -- Nb 2 -6.24 2.79729

Se 2 -- Nb 4 -6.24 2.79729

Se 4 -- Nb 6 -6.24 2.79729

============================================================

All bands spilling parameter for spin component 1 = 0.24%

Hirshfeld Analysis

------------------

Species Ion Hirshfeld Charge (e) Spin (hbar/2)

===================================================

Se 1 -0.16 0.00

Se 2 -0.15 0.00

Se 3 -0.16 0.00

Se 4 -0.15 0.00

Se 5 -0.16 0.00

Se 6 -0.15 0.00

Nb 1 0.16 0.00

Nb 2 0.15 0.00

Nb 3 0.16 0.00

Nb 4 0.15 0.00

Nb 5 0.16 0.00

Nb 6 0.15 0.00

===================================================

Writing analysis data to 3R-Nb1.1Se2-7-US.castep\_bin

Writing model to 3R-Nb1.1Se2-7-US.check

A BibTeX formatted list of references used in this run has been written to

3R-Nb1.1Se2-7-US.bib

Initialisation time = 0.59 s

Calculation time = 2118.94 s

Finalisation time = 1.48 s

Total time = 2121.02 s

Overall parallel efficiency rating: Good (75%)

Data was distributed by:-

G-vector (2-way); efficiency rating: Very good (83%)

k-point (7-way); efficiency rating: Very good (88%)