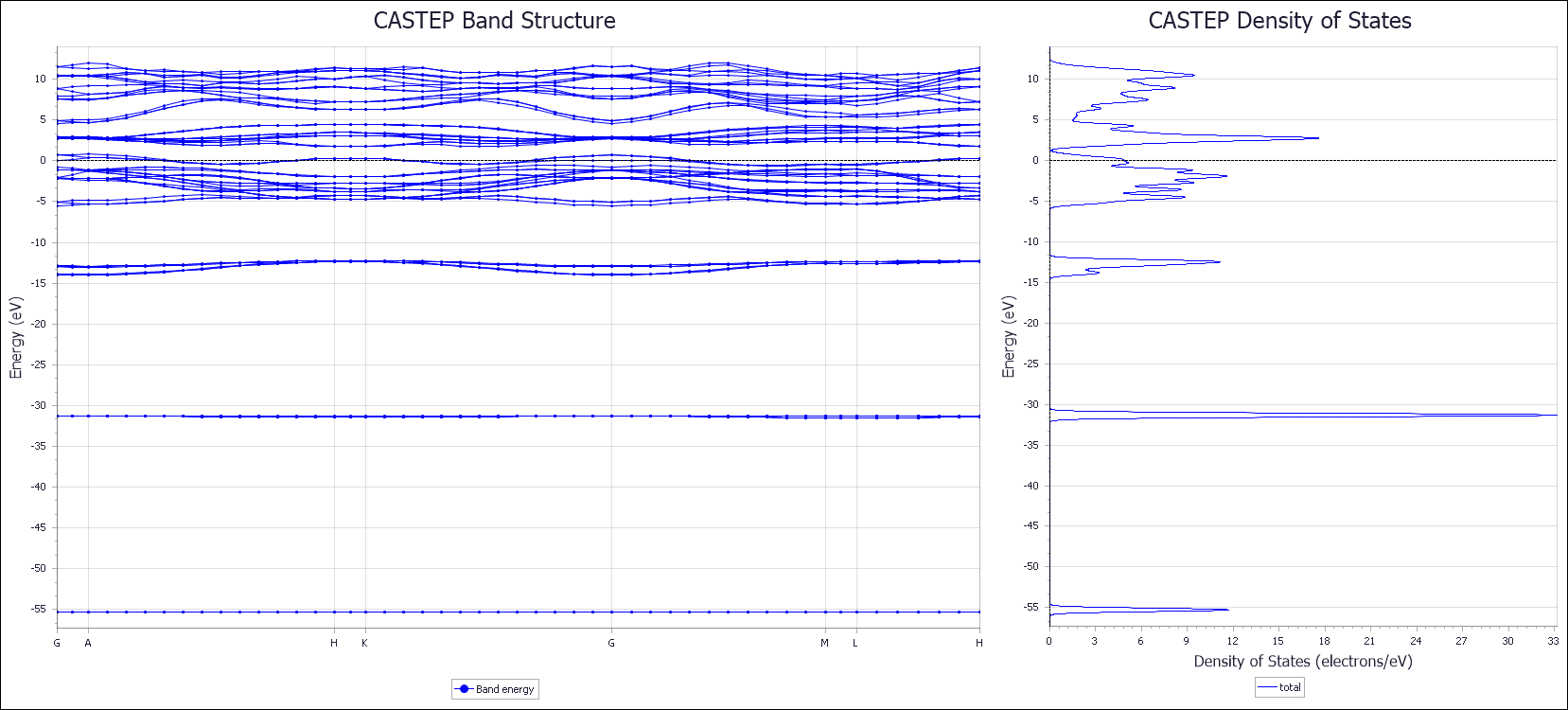
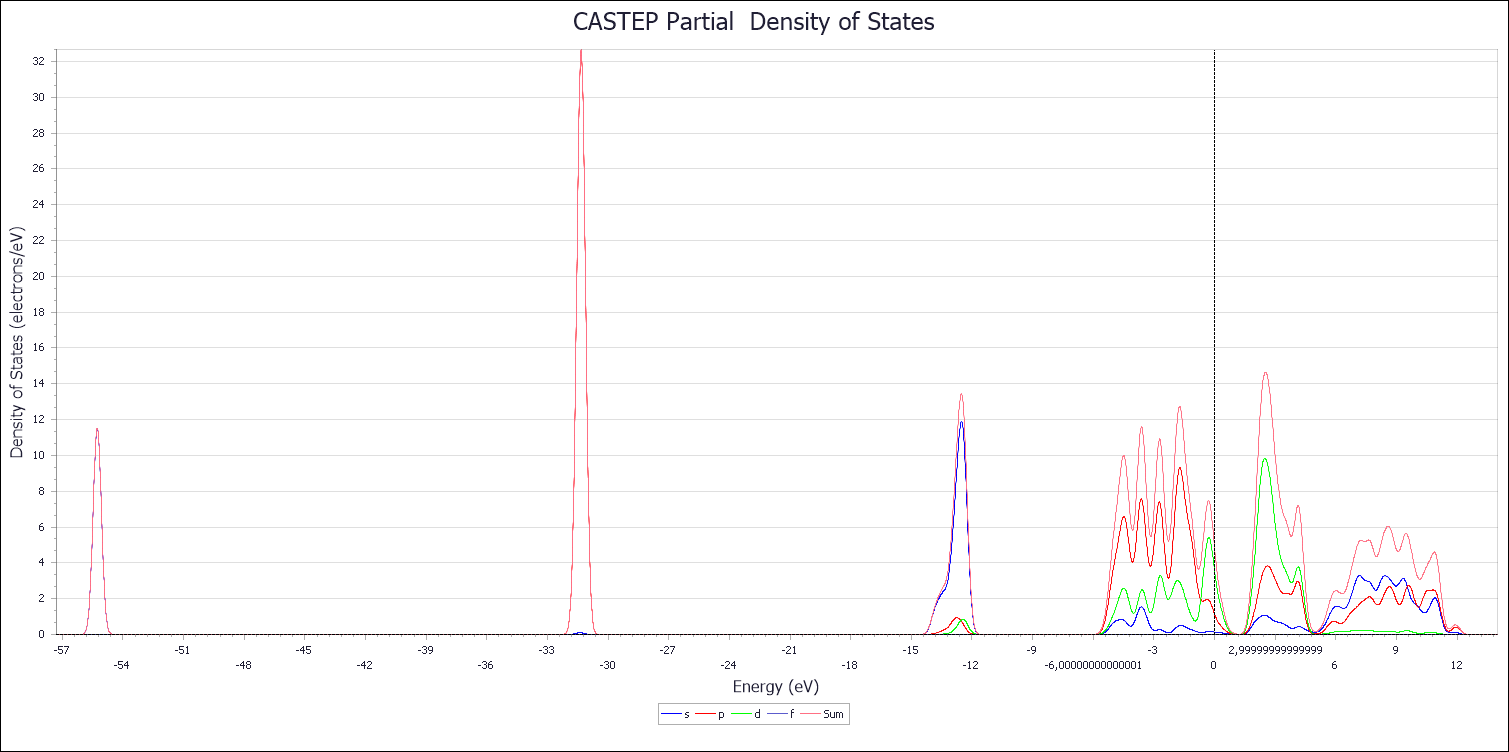
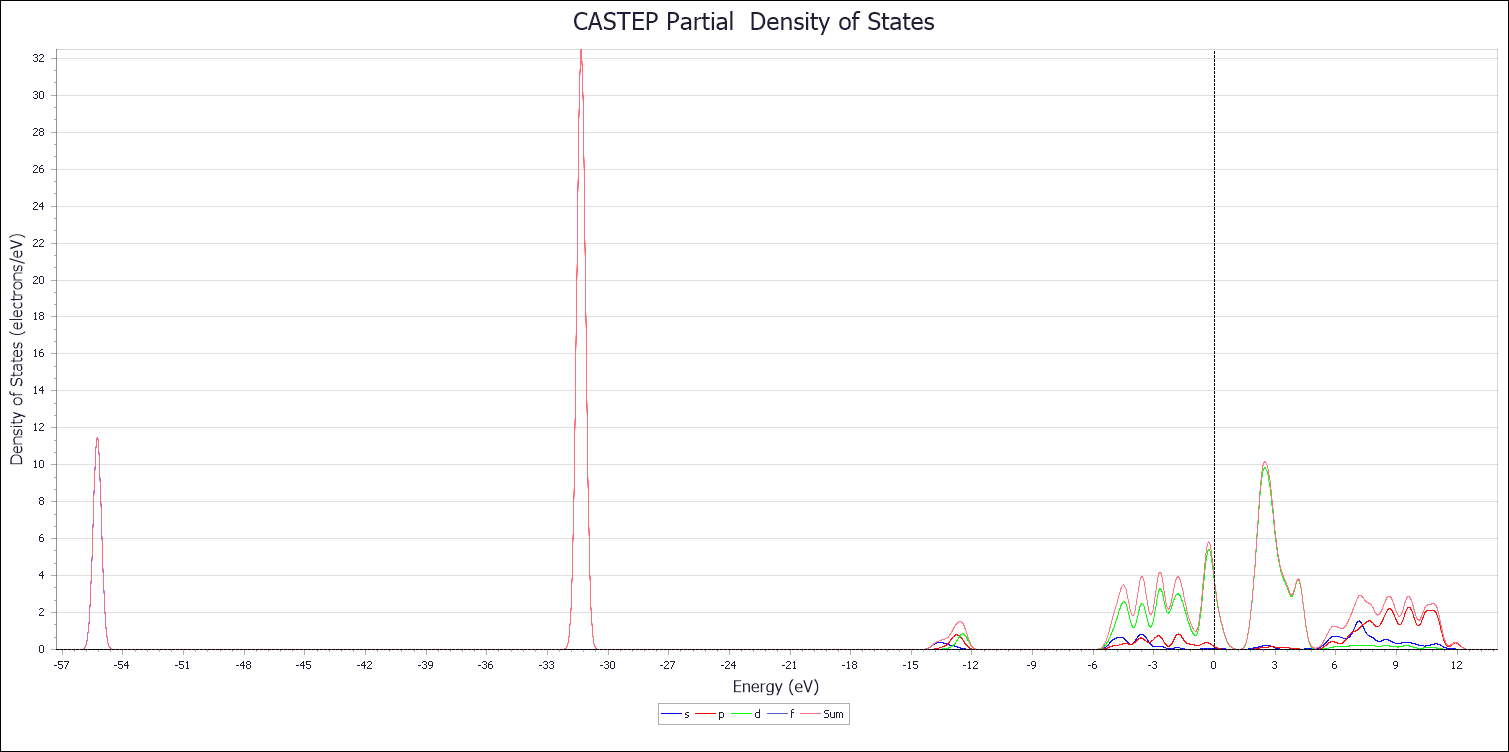
3R-NbSe2-US-7 CASTEP GeomOpt



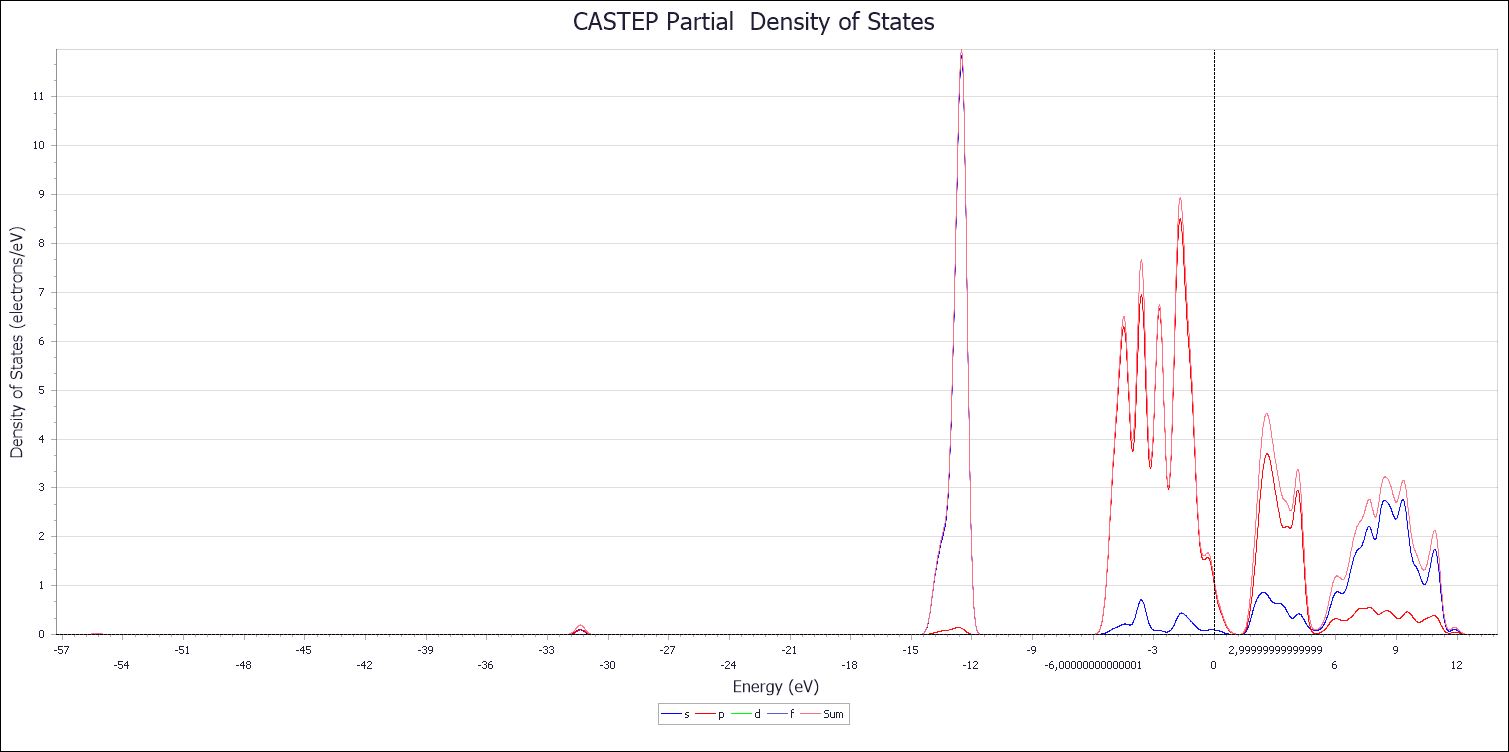
3R-NbSe2-US-7 PDOS-Total

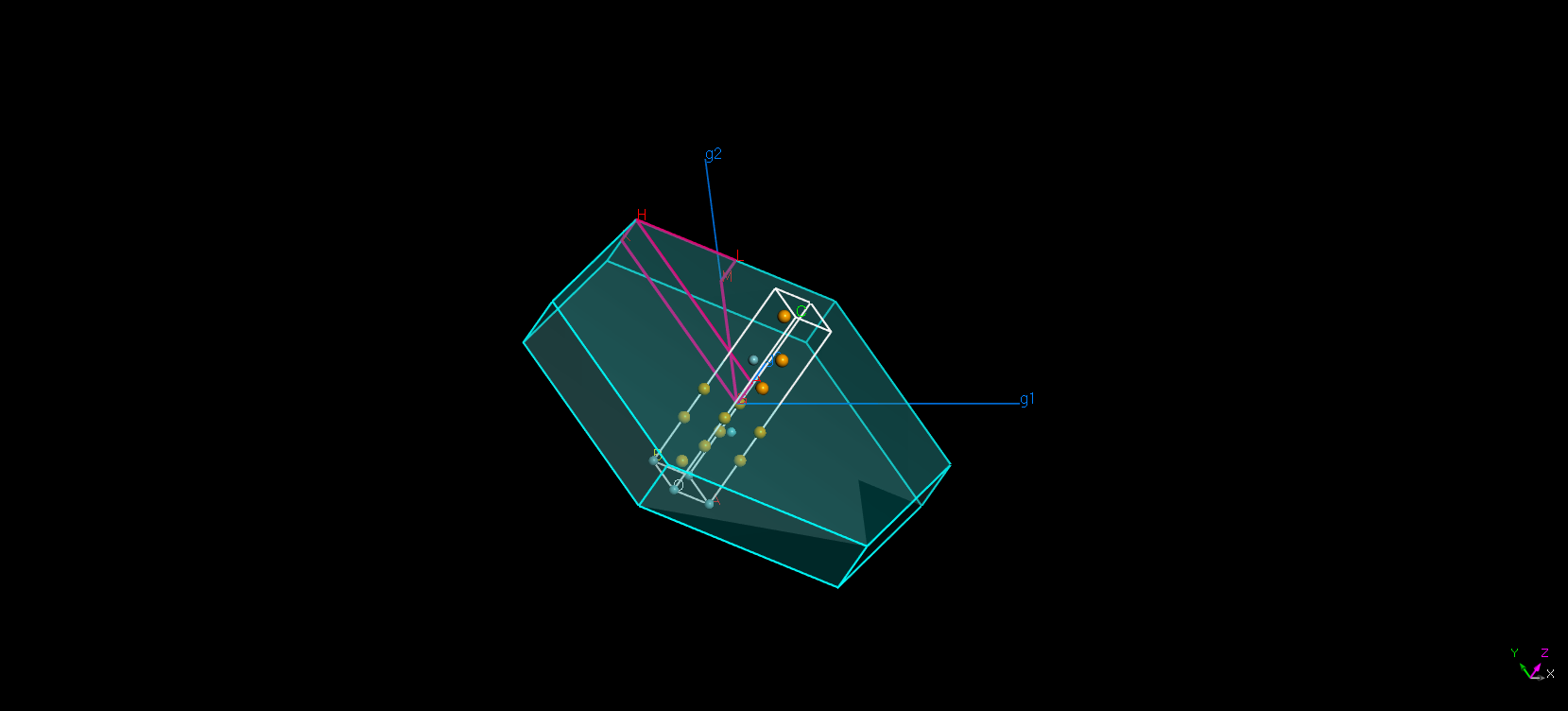


3R-NbSe2-US-7 PDOS-Nb



3R-NbSe2-US-7 PDOS-Se





Job started on host DESKTOP-UVBHK2J

at Sun Mar 8 11:21:54 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

Info: number of up-spin electrons is not equal to the

number of down-spins but spin\_polarized=false

- consider setting spin\_polarized=true.

Info: odd number of electrons detected and spin\_polarized=false

but fix\_occupancy=true

- consider setting fix\_occupancy=false

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-NbSe2-US-7.check

type of calculation : geometry optimization

stress calculation : on

density difference calculation : off

electron localisation func (ELF) calculation : off

Hirshfeld analysis : on

unlimited duration calculation

timing information : on

memory usage estimate : on

write final potential to formatted file : off

write final density to formatted file : off

write BibTeX reference list : on

checkpoint writing : both castep\_bin and check files

output length unit : A

output mass unit : amu

output time unit : ps

output charge unit : e

output spin unit : hbar/2

output energy unit : eV

output force unit : eV/A

output velocity unit : A/ps

output pressure unit : GPa

output inv\_length unit : 1/A

output frequency unit : cm-1

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

output volume unit : A\*\*3

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

output dipole unit : D

output efield unit : eV/A/e

output entropy unit : J/mol/K

wavefunctions paging : none

random number generator seed : randomised (112155596)

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 : 75.00

net charge of system : 0.000

net spin of system : 1.000

number of up spins : 38.00

number of down spins : 37.00

treating system as non-spin-polarized

number of bands : 38

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* 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 : 0.2368E-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)

2.9888269 -1.7256000 0.0000000 2.1022246 0.0000000 0.0000000

0.0000000 3.4512000 0.0000000 1.0511123 1.8205799 0.0000000

0.0000000 0.0000000 18.8270000 0.0000000 0.0000000 0.3337327

Lattice parameters(A) Cell Angles

a = 3.451200 alpha = 90.000000

b = 3.451200 beta = 90.000000

c = 18.827000 gamma = 120.000000

Current cell volume = 194.201245 A\*\*3

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Cell Contents

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

Total number of ions in cell = 9

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 0.333333 0.666667 -0.087400 x

x Se 2 0.333333 0.666667 0.089600 x

x Se 3 1.000000 1.000000 0.245933 x

x Se 4 1.000000 1.000000 0.422933 x

x Se 5 0.666667 1.333333 0.579267 x

x Se 6 0.666667 1.333333 0.756267 x

x Nb 1 0.000000 0.000000 0.001400 x

x Nb 2 0.666667 0.333333 0.334733 x

x Nb 3 0.333333 0.666667 0.668067 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 = 0.836087E-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 96.5 MB 87.0 MB |

| Electronic energy minimisation requirements 9.1 MB 0.0 MB |

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

| Approx. total storage required per process 105.6 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 -3.93791597E+003 2.20 <-- SCF

1 -6.01139389E+003 2.30386436E+002 3.41 <-- SCF

2 -6.21814124E+003 2.29719274E+001 4.28 <-- SCF

3 -6.22657224E+003 9.36777427E-001 5.12 <-- SCF

4 -6.22344858E+003 -3.47072738E-001 6.50 <-- SCF

5 -6.22309127E+003 -3.97007190E-002 8.05 <-- SCF

6 -6.22306577E+003 -2.83378353E-003 9.38 <-- SCF

7 -6.22308045E+003 1.63149938E-003 10.84 <-- SCF

8 -6.22309199E+003 1.28135856E-003 12.27 <-- SCF

9 -6.22310105E+003 1.00692608E-003 13.66 <-- SCF

10 -6.22310782E+003 7.52854912E-004 15.08 <-- SCF

11 -6.22311260E+003 5.31001001E-004 16.31 <-- SCF

12 -6.22311650E+003 4.32823108E-004 17.39 <-- SCF

13 -6.22311928E+003 3.09200241E-004 18.45 <-- SCF

14 -6.22312143E+003 2.38940972E-004 19.50 <-- SCF

15 -6.22312295E+003 1.68492011E-004 20.58 <-- SCF

16 -6.22312409E+003 1.26826679E-004 21.64 <-- SCF

17 -6.22312497E+003 9.77168946E-005 22.75 <-- SCF

18 -6.22312564E+003 7.45961489E-005 23.86 <-- SCF

19 -6.22312617E+003 5.93055563E-005 24.89 <-- SCF

20 -6.22312659E+003 4.58847247E-005 25.97 <-- SCF

21 -6.22312691E+003 3.62264785E-005 27.05 <-- SCF

22 -6.22312718E+003 2.92523317E-005 28.11 <-- SCF

23 -6.22312739E+003 2.33990566E-005 29.22 <-- SCF

24 -6.22312755E+003 1.85517405E-005 30.30 <-- SCF

25 -6.22312769E+003 1.52427610E-005 31.41 <-- SCF

26 -6.22312780E+003 1.23790183E-005 32.45 <-- SCF

27 -6.22312790E+003 1.03412233E-005 33.48 <-- SCF

28 -6.22312797E+003 8.28964344E-006 34.55 <-- SCF

29 -6.22312803E+003 6.82691609E-006 35.56 <-- SCF

30 -6.22312809E+003 5.95117980E-006 36.61 <-- SCF

31 -6.22312813E+003 5.32933100E-006 37.67 <-- SCF

32 -6.22312817E+003 4.02720906E-006 38.73 <-- SCF

33 -6.22312819E+003 2.55732334E-006 39.72 <-- SCF

34 -6.22312821E+003 2.47884112E-006 40.78 <-- SCF

35 -6.22312824E+003 2.44576245E-006 41.91 <-- SCF

36 -6.22312826E+003 2.08290373E-006 42.97 <-- SCF

37 -6.22312828E+003 2.55860950E-006 44.00 <-- SCF

38 -6.22312830E+003 2.39202084E-006 45.06 <-- SCF

39 -6.22312831E+003 1.26847886E-006 46.05 <-- SCF

40 -6.22312832E+003 9.02602108E-007 47.09 <-- SCF

41 -6.22312833E+003 1.57320962E-006 48.17 <-- SCF

42 -6.22312833E+003 -9.40854952E-007 49.05 <-- SCF

43 -6.22312835E+003 2.21558774E-006 50.12 <-- SCF

44 -6.22312836E+003 1.24453613E-006 51.19 <-- SCF

45 -6.22312836E+003 4.79845053E-007 52.20 <-- SCF

46 -6.22312835E+003 -1.05660884E-006 53.28 <-- SCF

47 -6.22312835E+003 2.40530715E-008 54.33 <-- SCF

48 -6.22312835E+003 2.03539706E-007 55.39 <-- SCF

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

Final energy = -6223.128353371 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 -6.22312970E+003 56.61 <-- SCF

1 -6.22312984E+003 1.44895976E-005 57.53 <-- SCF

2 -6.22312984E+003 5.10493028E-007 58.55 <-- SCF

3 -6.22312983E+003 -1.49155364E-006 59.58 <-- SCF

4 -6.22312983E+003 -7.04193356E-008 60.67 <-- SCF

5 -6.22312983E+003 1.02891231E-007 61.69 <-- SCF

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

Final energy = -6223.129826472 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 -6.22313120E+003 63.03 <-- SCF

1 -6.22313118E+003 -2.85619195E-006 63.91 <-- SCF

2 -6.22313118E+003 3.00825377E-008 64.94 <-- SCF

3 -6.22313118E+003 4.87193586E-008 66.11 <-- SCF

4 -6.22313118E+003 1.63107952E-008 67.08 <-- SCF

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

Final energy = -6223.131176878 eV

(energy not corrected for finite basis set)

For future reference: finite basis dEtot/dlog(Ecut) = -0.136033eV

Total energy corrected for finite basis set = -6223.131121 eV

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

| Memory Disk |

| Model and support data 96.5 MB 87.0 MB |

| Electronic energy minimisation requirements 9.1 MB 0.0 MB |

| Geometry minimisation requirements 11.0 MB 0.0 MB |

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

| Approx. total storage required per process 116.7 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 0.21415 \*

\* Se 2 0.00000 0.00000 -0.04787 \*

\* Se 3 -0.00000 0.00000 0.21415 \*

\* Se 4 0.00000 0.00000 -0.04787 \*

\* Se 5 0.00000 0.00000 0.21415 \*

\* Se 6 0.00000 0.00000 -0.04787 \*

\* Nb 1 0.00000 0.00000 -0.16628 \*

\* Nb 2 0.00000 0.00000 -0.16628 \*

\* Nb 3 0.00000 0.00000 -0.16628 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.168728 -0.000000 0.000000 \*

\* y -0.000000 -0.168728 0.000000 \*

\* z 0.000000 0.000000 -1.839913 \*

\* \*

\* Pressure: 0.7258 \*

\* \*

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

BFGS: finished iteration 0 with enthalpy= -6.22313112E+003 eV

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

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

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

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

| |F|max | 2.141505E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

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

| Smax | 1.839913E+000 | 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 | 0.000112 | -6223.131121 | <-- min BFGS

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

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

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

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

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

| Memory Disk |

| Model and support data 96.5 MB 87.0 MB |

| Electronic energy minimisation requirements 9.1 MB 0.0 MB |

| Geometry minimisation requirements 11.1 MB 0.0 MB |

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

| Approx. total storage required per process 116.7 MB 87.0 MB |

| |

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

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

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

Unit Cell

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

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

2.9891631 -1.7257941 0.0000000 2.1019881 -0.0000000 0.0000000

0.0000000 3.4515882 0.0000000 1.0509941 1.8203751 0.0000000

0.0000000 0.0000000 18.8500934 0.0000000 0.0000000 0.3333238

Lattice parameters(A) Cell Angles

a = 3.451588 alpha = 90.000000

b = 3.451588 beta = 90.000000

c = 18.850093 gamma = 120.000000

Current cell volume = 194.483200 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.087387 x

x Se 2 0.333333 0.666667 0.089597 x

x Se 3 1.000000 1.000000 0.245947 x

x Se 4 1.000000 1.000000 0.422930 x

x Se 5 0.666667 1.333333 0.579280 x

x Se 6 0.666667 1.333333 0.756264 x

x Nb 1 -0.000000 0.000000 0.001390 x

x Nb 2 0.666667 0.333333 0.334723 x

x Nb 3 0.333333 0.666667 0.668056 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22313186E+003 78.12 <-- SCF

1 -6.22313665E+003 5.31914479E-004 79.14 <-- SCF

2 -6.22313687E+003 2.46585429E-005 80.80 <-- SCF

3 -6.22313453E+003 -2.59795512E-004 82.20 <-- SCF

4 -6.22313401E+003 -5.78268167E-005 84.23 <-- SCF

5 -6.22313395E+003 -6.62149394E-006 86.36 <-- SCF

6 -6.22313395E+003 -5.21903512E-009 88.02 <-- SCF

7 -6.22313395E+003 1.00501701E-007 89.25 <-- SCF

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

Final energy = -6223.133953828 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 -0.00000 0.23474 \*

\* Se 2 -0.00000 -0.00000 -0.07506 \*

\* Se 3 -0.00000 -0.00000 0.23474 \*

\* Se 4 -0.00000 -0.00000 -0.07506 \*

\* Se 5 -0.00000 -0.00000 0.23474 \*

\* Se 6 -0.00000 -0.00000 -0.07506 \*

\* Nb 1 0.00000 -0.00000 -0.15968 \*

\* Nb 2 0.00000 -0.00000 -0.15968 \*

\* Nb 3 0.00000 -0.00000 -0.15968 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.041100 0.000000 -0.000000 \*

\* y 0.000000 -0.041100 0.000000 \*

\* z -0.000000 0.000000 -1.539445 \*

\* \*

\* Pressure: 0.5405 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000112 | -6223.131121 | <-- min BFGS

| trial step | 1.000000 | 0.000095 | -6223.133933 | <-- min BFGS

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

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

BFGS: improving iteration 1 with line minimization (lambda= 6.561078)

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

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

| Memory Disk |

| Model and support data 96.6 MB 87.0 MB |

| Electronic energy minimisation requirements 9.2 MB 0.0 MB |

| Geometry minimisation requirements 11.1 MB 0.0 MB |

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

| Approx. total storage required per process 116.9 MB 87.0 MB |

| |

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

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

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

Unit Cell

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

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

2.9910327 -1.7268735 0.0000000 2.1006742 -0.0000000 0.0000000

0.0000000 3.4537471 0.0000000 1.0503371 1.8192372 0.0000000

0.0000000 0.0000000 18.9785173 0.0000000 0.0000000 0.3310683

Lattice parameters(A) Cell Angles

a = 3.453747 alpha = 90.000000

b = 3.453747 beta = 90.000000

c = 18.978517 gamma = 120.000000

Current cell volume = 196.053217 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.087313 x

x Se 2 0.333333 0.666667 0.089580 x

x Se 3 1.000000 1.000000 0.246021 x

x Se 4 1.000000 1.000000 0.422914 x

x Se 5 0.666667 1.333333 0.579354 x

x Se 6 0.666667 1.333333 0.756247 x

x Nb 1 -0.000000 0.000000 0.001332 x

x Nb 2 0.666667 0.333333 0.334666 x

x Nb 3 0.333333 0.666667 0.667999 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22303851E+003 100.16 <-- SCF

1 -6.22322974E+003 2.12487350E-002 101.64 <-- SCF

2 -6.22323712E+003 8.19456260E-004 104.06 <-- SCF

3 -6.22316332E+003 -8.19969825E-003 106.08 <-- SCF

4 -6.22314396E+003 -2.15101321E-003 107.92 <-- SCF

5 -6.22314224E+003 -1.91975014E-004 109.31 <-- SCF

6 -6.22314222E+003 -1.57451159E-006 110.61 <-- SCF

7 -6.22314224E+003 1.81259752E-006 112.05 <-- SCF

8 -6.22314224E+003 -2.96086190E-008 113.23 <-- SCF

9 -6.22314224E+003 6.33879030E-007 114.31 <-- SCF

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

Final energy = -6223.142242591 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 0.37119 \*

\* Se 2 0.00000 0.00000 -0.23912 \*

\* Se 3 0.00000 -0.00000 0.37119 \*

\* Se 4 0.00000 0.00000 -0.23912 \*

\* Se 5 0.00000 -0.00000 0.37119 \*

\* Se 6 0.00000 0.00000 -0.23912 \*

\* Nb 1 0.00000 -0.00000 -0.13207 \*

\* Nb 2 0.00000 -0.00000 -0.13207 \*

\* Nb 3 -0.00000 -0.00000 -0.13207 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.462128 0.000000 0.000000 \*

\* y 0.000000 0.462128 -0.000000 \*

\* z 0.000000 -0.000000 -0.127892 \*

\* \*

\* Pressure: -0.2655 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000112 | -6223.131121 | <-- min BFGS

| trial step | 1.000000 | 0.000095 | -6223.133933 | <-- min BFGS

| line step | 6.561078 | 0.000017 | -6223.142165 | <-- min BFGS

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

BFGS: finished iteration 1 with enthalpy= -6.22314217E+003 eV

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

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

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

| dE/ion | 1.227111E-003 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 3.711924E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.656097E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 4.621278E-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 | 0.000074 | -6223.142165 | <-- min BFGS

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

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

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

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

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

| Memory Disk |

| Model and support data 97.4 MB 87.0 MB |

| Electronic energy minimisation requirements 9.2 MB 0.0 MB |

| Geometry minimisation requirements 11.2 MB 0.0 MB |

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

| Approx. total storage required per process 117.7 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)

2.9904333 -1.7265275 -0.0000000 2.1010953 -0.0000000 0.0000000

0.0000000 3.4530550 0.0000000 1.0505476 1.8196019 -0.0000000

-0.0000000 0.0000000 19.0144647 0.0000000 -0.0000000 0.3304424

Lattice parameters(A) Cell Angles

a = 3.453055 alpha = 90.000000

b = 3.453055 beta = 90.000000

c = 19.014465 gamma = 120.000000

Current cell volume = 196.345848 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.087266 x

x Se 2 0.333333 0.666667 0.089558 x

x Se 3 1.000000 1.000000 0.246068 x

x Se 4 1.000000 1.000000 0.422892 x

x Se 5 0.666667 1.333333 0.579401 x

x Se 6 0.666667 1.333333 0.756225 x

x Nb 1 -0.000000 0.000000 0.001307 x

x Nb 2 0.666667 0.333333 0.334641 x

x Nb 3 0.333333 0.666667 0.667974 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22313665E+003 126.25 <-- SCF

1 -6.22315201E+003 1.70725112E-003 127.33 <-- SCF

2 -6.22315270E+003 7.66501505E-005 129.19 <-- SCF

3 -6.22314556E+003 -7.93813097E-004 130.64 <-- SCF

4 -6.22314410E+003 -1.62295567E-004 132.33 <-- SCF

5 -6.22314386E+003 -2.67492989E-005 133.70 <-- SCF

6 -6.22314386E+003 2.00549678E-007 134.86 <-- SCF

7 -6.22314386E+003 3.87753754E-007 135.88 <-- SCF

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

Final energy = -6223.143860651 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.39844 \*

\* Se 2 0.00000 0.00000 -0.28110 \*

\* Se 3 0.00000 0.00000 0.39844 \*

\* Se 4 0.00000 0.00000 -0.28110 \*

\* Se 5 0.00000 0.00000 0.39844 \*

\* Se 6 0.00000 0.00000 -0.28110 \*

\* Nb 1 -0.00000 0.00000 -0.11734 \*

\* Nb 2 -0.00000 0.00000 -0.11734 \*

\* Nb 3 0.00000 0.00000 -0.11734 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.557446 0.000000 0.000000 \*

\* y 0.000000 0.557446 0.000000 \*

\* z 0.000000 0.000000 0.231299 \*

\* \*

\* Pressure: -0.4487 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000074 | -6223.142165 | <-- min BFGS

| trial step | 1.000000 | 0.000049 | -6223.143783 | <-- min BFGS

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

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

BFGS: improving iteration 2 with line minimization (lambda= 2.958509)

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

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

| Memory Disk |

| Model and support data 97.4 MB 87.0 MB |

| Electronic energy minimisation requirements 9.2 MB 0.0 MB |

| Geometry minimisation requirements 11.2 MB 0.0 MB |

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

| Approx. total storage required per process 117.8 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)

2.9892594 -1.7258497 -0.0000000 2.1019204 -0.0000000 0.0000000

0.0000000 3.4516995 0.0000000 1.0509602 1.8203164 -0.0000000

-0.0000000 0.0000000 19.0848680 0.0000000 -0.0000000 0.3292234

Lattice parameters(A) Cell Angles

a = 3.451699 alpha = 90.000000

b = 3.451699 beta = 90.000000

c = 19.084868 gamma = 120.000000

Current cell volume = 196.918152 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.087174 x

x Se 2 0.333333 0.666667 0.089515 x

x Se 3 1.000000 1.000000 0.246160 x

x Se 4 1.000000 1.000000 0.422849 x

x Se 5 0.666667 1.333333 0.579493 x

x Se 6 0.666667 1.333333 0.756182 x

x Nb 1 -0.000000 0.000000 0.001258 x

x Nb 2 0.666667 0.333333 0.334592 x

x Nb 3 0.333333 0.666667 0.667925 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22311355E+003 147.73 <-- SCF

1 -6.22317927E+003 7.30271303E-003 149.22 <-- SCF

2 -6.22318213E+003 3.16962320E-004 150.94 <-- SCF

3 -6.22315271E+003 -3.26878150E-003 152.62 <-- SCF

4 -6.22314621E+003 -7.21614828E-004 154.19 <-- SCF

5 -6.22314528E+003 -1.03976194E-004 155.66 <-- SCF

6 -6.22314529E+003 1.54751773E-006 157.50 <-- SCF

7 -6.22314530E+003 7.73394081E-007 158.69 <-- SCF

8 -6.22314530E+003 4.57033881E-007 159.69 <-- SCF

9 -6.22314530E+003 1.72150132E-007 160.78 <-- SCF

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

Final energy = -6223.145303128 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.44755 \*

\* Se 2 0.00000 -0.00000 -0.35003 \*

\* Se 3 0.00000 0.00000 0.44755 \*

\* Se 4 0.00000 -0.00000 -0.35003 \*

\* Se 5 0.00000 0.00000 0.44755 \*

\* Se 6 0.00000 -0.00000 -0.35003 \*

\* Nb 1 -0.00000 0.00000 -0.09753 \*

\* Nb 2 -0.00000 0.00000 -0.09753 \*

\* Nb 3 0.00000 0.00000 -0.09753 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.635283 0.000000 0.000000 \*

\* y 0.000000 0.635283 -0.000000 \*

\* z 0.000000 -0.000000 0.811836 \*

\* \*

\* Pressure: -0.6941 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000074 | -6223.142165 | <-- min BFGS

| trial step | 1.000000 | 0.000049 | -6223.143783 | <-- min BFGS

| line step | 2.958509 | 8.057E-006 | -6223.145297 | <-- min BFGS

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

BFGS: finished iteration 2 with enthalpy= -6.22314530E+003 eV

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

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

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

| dE/ion | 3.480077E-004 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 4.475527E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.654192E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 8.118361E-001 | 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 | 0.000158 | -6223.145297 | <-- 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 97.8 MB 87.0 MB |

| Electronic energy minimisation requirements 9.2 MB 0.0 MB |

| Geometry minimisation requirements 11.1 MB 0.0 MB |

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

| Approx. total storage required per process 118.1 MB 87.0 MB |

| |

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

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

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

Unit Cell

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

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

2.9861983 -1.7240824 -0.0000000 2.1040751 0.0000000 0.0000000

-0.0000000 3.4481648 0.0000000 1.0520375 1.8221824 -0.0000000

-0.0000000 0.0000000 19.1164820 0.0000000 -0.0000000 0.3286790

Lattice parameters(A) Cell Angles

a = 3.448165 alpha = 90.000000

b = 3.448165 beta = 90.000000

c = 19.116482 gamma = 120.000000

Current cell volume = 196.840574 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.087065 x

x Se 2 0.333333 0.666667 0.089450 x

x Se 3 1.000000 1.000000 0.246269 x

x Se 4 1.000000 1.000000 0.422784 x

x Se 5 0.666667 1.333333 0.579602 x

x Se 6 0.666667 1.333333 0.756117 x

x Nb 1 -0.000000 0.000000 0.001214 x

x Nb 2 0.666667 0.333333 0.334548 x

x Nb 3 0.333333 0.666667 0.667881 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22313501E+003 172.08 <-- SCF

1 -6.22316812E+003 3.67885325E-003 173.08 <-- SCF

2 -6.22316982E+003 1.87987445E-004 174.78 <-- SCF

3 -6.22315270E+003 -1.90153289E-003 176.28 <-- SCF

4 -6.22314997E+003 -3.03202235E-004 177.77 <-- SCF

5 -6.22314925E+003 -8.02833815E-005 179.19 <-- SCF

6 -6.22314927E+003 2.31562781E-006 180.47 <-- SCF

7 -6.22314927E+003 -4.75980489E-007 181.59 <-- SCF

8 -6.22314927E+003 4.50314461E-007 182.55 <-- SCF

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

Final energy = -6223.149271070 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 -0.00000 0.42885 \*

\* Se 2 -0.00000 -0.00000 -0.35615 \*

\* Se 3 -0.00000 -0.00000 0.42885 \*

\* Se 4 -0.00000 -0.00000 -0.35615 \*

\* Se 5 -0.00000 -0.00000 0.42885 \*

\* Se 6 -0.00000 0.00000 -0.35615 \*

\* Nb 1 0.00000 -0.00000 -0.07270 \*

\* Nb 2 0.00000 -0.00000 -0.07270 \*

\* Nb 3 0.00000 -0.00000 -0.07270 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.428547 -0.000000 -0.000000 \*

\* y -0.000000 0.428547 -0.000000 \*

\* z -0.000000 -0.000000 0.830135 \*

\* \*

\* Pressure: -0.5624 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000158 | -6223.145297 | <-- min BFGS

| trial step | 1.000000 | 0.000132 | -6223.149247 | <-- min BFGS

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

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

BFGS: improving iteration 3 with line minimization (lambda= 6.104570)

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

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

| Memory Disk |

| Model and support data 103.3 MB 87.0 MB |

| Electronic energy minimisation requirements 9.2 MB 0.0 MB |

| Geometry minimisation requirements 11.1 MB 0.0 MB |

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

| Approx. total storage required per process 123.6 MB 87.0 MB |

| |

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

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

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

Unit Cell

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

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

2.9705724 -1.7150607 -0.0000000 2.1151430 0.0000000 0.0000000

-0.0000000 3.4301215 0.0000000 1.0575715 1.8317676 -0.0000000

-0.0000000 0.0000000 19.2778574 0.0000000 -0.0000000 0.3259276

Lattice parameters(A) Cell Angles

a = 3.430121 alpha = 90.000000

b = 3.430121 beta = 90.000000

c = 19.277857 gamma = 120.000000

Current cell volume = 196.430265 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.086508 x

x Se 2 0.333333 0.666667 0.089118 x

x Se 3 1.000000 1.000000 0.246826 x

x Se 4 1.000000 1.000000 0.422451 x

x Se 5 0.666667 1.333333 0.580159 x

x Se 6 0.666667 1.333333 0.755784 x

x Nb 1 -0.000000 0.000000 0.000990 x

x Nb 2 0.666667 0.333333 0.334323 x

x Nb 3 0.333333 0.666667 0.667657 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22274920E+003 193.72 <-- SCF

1 -6.22366150E+003 1.01366531E-001 194.62 <-- SCF

2 -6.22371199E+003 5.61024179E-003 196.34 <-- SCF

3 -6.22325413E+003 -5.08734604E-002 197.80 <-- SCF

4 -6.22317495E+003 -8.79762190E-003 199.27 <-- SCF

5 -6.22315547E+003 -2.16453134E-003 200.67 <-- SCF

6 -6.22315568E+003 2.27192705E-005 202.23 <-- SCF

7 -6.22315568E+003 -3.86634309E-008 203.75 <-- SCF

8 -6.22315574E+003 6.53575461E-006 205.77 <-- SCF

9 -6.22315577E+003 3.29213090E-006 207.53 <-- SCF

10 -6.22315577E+003 1.06264089E-007 208.84 <-- SCF

11 -6.22315577E+003 1.19053879E-007 210.05 <-- SCF

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

Final energy = -6223.155767300 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.25299 \*

\* Se 2 0.00000 -0.00000 -0.35967 \*

\* Se 3 0.00000 -0.00000 0.25299 \*

\* Se 4 0.00000 -0.00000 -0.35967 \*

\* Se 5 0.00000 0.00000 0.25299 \*

\* Se 6 0.00000 -0.00000 -0.35967 \*

\* Nb 1 -0.00000 -0.00000 0.10668 \*

\* Nb 2 -0.00000 -0.00000 0.10668 \*

\* Nb 3 -0.00000 -0.00000 0.10668 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.564383 0.000000 0.000000 \*

\* y 0.000000 -0.564383 0.000000 \*

\* z 0.000000 0.000000 1.162939 \*

\* \*

\* Pressure: -0.0114 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000158 | -6223.145297 | <-- min BFGS

| trial step | 1.000000 | 0.000132 | -6223.149247 | <-- min BFGS

| line step | 6.104570 | -0.000040 | -6223.155767 | <-- min BFGS

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

BFGS: finished iteration 3 with enthalpy= -6.22315577E+003 eV

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

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

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

| dE/ion | 1.163332E-003 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 3.596661E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.283723E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.162939E+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 | 0.000221 | -6223.155767 | <-- 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 104.6 MB 87.0 MB |

| Electronic energy minimisation requirements 9.1 MB 0.0 MB |

| Geometry minimisation requirements 11.1 MB 0.0 MB |

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

| Approx. total storage required per process 124.8 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)

2.9732782 -1.7166229 -0.0000000 2.1132181 0.0000000 0.0000000

-0.0000000 3.4332459 0.0000000 1.0566091 1.8301006 -0.0000000

-0.0000000 0.0000000 19.1855907 0.0000000 -0.0000000 0.3274950

Lattice parameters(A) Cell Angles

a = 3.433246 alpha = 90.000000

b = 3.433246 beta = 90.000000

c = 19.185591 gamma = 120.000000

Current cell volume = 195.846414 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 0.333333 0.666667 -0.086617 x

x Se 2 0.333333 0.666667 0.089161 x

x Se 3 1.000000 1.000000 0.246716 x

x Se 4 1.000000 1.000000 0.422494 x

x Se 5 0.666667 1.333333 0.580050 x

x Se 6 0.666667 1.333333 0.755827 x

x Nb 1 -0.000000 -0.000000 0.001056 x

x Nb 2 0.666667 0.333333 0.334390 x

x Nb 3 0.333333 0.666667 0.667723 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22310614E+003 223.02 <-- SCF

1 -6.22320872E+003 1.13973494E-002 223.97 <-- SCF

2 -6.22321283E+003 4.56904741E-004 225.66 <-- SCF

3 -6.22316920E+003 -4.84832956E-003 227.25 <-- SCF

4 -6.22316114E+003 -8.95551804E-004 228.69 <-- SCF

5 -6.22315963E+003 -1.67717311E-004 230.06 <-- SCF

6 -6.22315966E+003 3.78317479E-006 231.41 <-- SCF

7 -6.22315967E+003 7.02971479E-007 232.42 <-- SCF

8 -6.22315967E+003 7.14420290E-007 233.39 <-- SCF

9 -6.22315968E+003 2.56019392E-007 234.33 <-- SCF

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

Final energy = -6223.159676418 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.22236 \*

\* Se 2 0.00000 0.00000 -0.28664 \*

\* Se 3 0.00000 0.00000 0.22236 \*

\* Se 4 -0.00000 0.00000 -0.28664 \*

\* Se 5 0.00000 0.00000 0.22236 \*

\* Se 6 0.00000 0.00000 -0.28664 \*

\* Nb 1 0.00000 0.00000 0.06428 \*

\* Nb 2 -0.00000 0.00000 0.06428 \*

\* Nb 3 0.00000 -0.00000 0.06428 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.583080 0.000000 0.000000 \*

\* y 0.000000 -0.583080 -0.000000 \*

\* z 0.000000 -0.000000 0.392305 \*

\* \*

\* Pressure: 0.2580 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000221 | -6223.155767 | <-- min BFGS

| trial step | 1.000000 | 0.000064 | -6223.159634 | <-- min BFGS

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

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

BFGS: improving iteration 4 with line minimization (lambda= 1.409726)

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Unit Cell

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

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

2.9743868 -1.7172630 -0.0000000 2.1124305 0.0000000 0.0000000

-0.0000000 3.4345260 0.0000000 1.0562152 1.8294185 -0.0000000

-0.0000000 0.0000000 19.1477866 0.0000000 -0.0000000 0.3281416

Lattice parameters(A) Cell Angles

a = 3.434526 alpha = 90.000000

b = 3.434526 beta = 90.000000

c = 19.147787 gamma = 120.000000

Current cell volume = 195.606299 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.086662 x

x Se 2 0.333333 0.666667 0.089178 x

x Se 3 1.000000 1.000000 0.246672 x

x Se 4 1.000000 1.000000 0.422511 x

x Se 5 0.666667 1.333333 0.580005 x

x Se 6 0.666667 1.333333 0.755845 x

x Nb 1 -0.000000 -0.000000 0.001084 x

x Nb 2 0.666667 0.333333 0.334417 x

x Nb 3 0.333333 0.666667 0.667750 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22315214E+003 245.64 <-- SCF

1 -6.22316795E+003 1.75628749E-003 246.59 <-- SCF

2 -6.22316865E+003 7.77277573E-005 248.20 <-- SCF

3 -6.22316157E+003 -7.85830041E-004 249.77 <-- SCF

4 -6.22316022E+003 -1.50814628E-004 251.17 <-- SCF

5 -6.22315997E+003 -2.73749317E-005 252.44 <-- SCF

6 -6.22315997E+003 1.64251888E-007 253.61 <-- SCF

7 -6.22315997E+003 3.90817254E-007 254.62 <-- SCF

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

Final energy = -6223.159974562 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 0.21066 \*

\* Se 2 -0.00000 0.00000 -0.25436 \*

\* Se 3 -0.00000 -0.00000 0.21066 \*

\* Se 4 -0.00000 0.00000 -0.25436 \*

\* Se 5 -0.00000 0.00000 0.21066 \*

\* Se 6 -0.00000 0.00000 -0.25436 \*

\* Nb 1 0.00000 -0.00000 0.04370 \*

\* Nb 2 0.00000 0.00000 0.04370 \*

\* Nb 3 0.00000 0.00000 0.04370 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.622813 -0.000000 -0.000000 \*

\* y -0.000000 -0.622813 -0.000000 \*

\* z -0.000000 -0.000000 0.045874 \*

\* \*

\* Pressure: 0.3999 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000221 | -6223.155767 | <-- min BFGS

| trial step | 1.000000 | 0.000064 | -6223.159634 | <-- min BFGS

| line step | 1.409726 | -4.648E-006 | -6223.159956 | <-- min BFGS

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

BFGS: finished iteration 4 with enthalpy= -6.22315996E+003 eV

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

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

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

| dE/ion | 4.654524E-004 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 2.543565E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.947800E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 6.228134E-001 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 5 ...

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

Writing analysis data to 3R-NbSe2-US-7.castep\_bin

Writing model to 3R-NbSe2-US-7.check

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

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

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

| previous | 0.000000 | 0.000059 | -6223.159956 | <-- min BFGS

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

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

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

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Unit Cell

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

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

2.9742701 -1.7171956 -0.0000000 2.1125133 0.0000000 0.0000000

-0.0000000 3.4343913 0.0000000 1.0562567 1.8294902 -0.0000000

-0.0000000 0.0000000 19.1570913 0.0000000 -0.0000000 0.3279822

Lattice parameters(A) Cell Angles

a = 3.434391 alpha = 90.000000

b = 3.434391 beta = 90.000000

c = 19.157091 gamma = 120.000000

Current cell volume = 195.685997 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 0.333333 0.666667 -0.086587 x

x Se 2 0.333333 0.666667 0.089121 x

x Se 3 1.000000 1.000000 0.246746 x

x Se 4 1.000000 1.000000 0.422454 x

x Se 5 0.666667 1.333333 0.580080 x

x Se 6 0.666667 1.333333 0.755788 x

x Nb 1 -0.000000 0.000000 0.001066 x

x Nb 2 0.666667 0.333333 0.334399 x

x Nb 3 0.333333 0.666667 0.667733 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22315953E+003 265.69 <-- SCF

1 -6.22316948E+003 1.10602087E-003 266.62 <-- SCF

2 -6.22317015E+003 7.45509005E-005 268.25 <-- SCF

3 -6.22316308E+003 -7.85637295E-004 270.00 <-- SCF

4 -6.22316180E+003 -1.42671780E-004 271.58 <-- SCF

5 -6.22316154E+003 -2.82127140E-005 272.92 <-- SCF

6 -6.22316155E+003 3.88060620E-007 273.89 <-- SCF

7 -6.22316155E+003 4.04488971E-007 274.91 <-- SCF

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

Final energy = -6223.161551041 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 0.19065 \*

\* Se 2 0.00000 0.00000 -0.25676 \*

\* Se 3 0.00000 -0.00000 0.19065 \*

\* Se 4 0.00000 0.00000 -0.25676 \*

\* Se 5 0.00000 -0.00000 0.19065 \*

\* Se 6 0.00000 0.00000 -0.25676 \*

\* Nb 1 -0.00000 0.00000 0.06610 \*

\* Nb 2 -0.00000 0.00000 0.06610 \*

\* Nb 3 -0.00000 0.00000 0.06610 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.625716 -0.000000 0.000000 \*

\* y -0.000000 -0.625716 0.000000 \*

\* z 0.000000 0.000000 0.044744 \*

\* \*

\* Pressure: 0.4022 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000059 | -6223.159956 | <-- min BFGS

| trial step | 1.000000 | 0.000055 | -6223.161508 | <-- min BFGS

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

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

BFGS: improving iteration 5 with line minimization (lambda= 16.152572)

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Unit Cell

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

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

2.9725020 -1.7161748 -0.0000000 2.1137699 0.0000000 0.0000000

-0.0000000 3.4323497 0.0000000 1.0568850 1.8305784 0.0000000

-0.0000000 0.0000000 19.2980808 0.0000000 -0.0000000 0.3255860

Lattice parameters(A) Cell Angles

a = 3.432350 alpha = 90.000000

b = 3.432350 beta = 90.000000

c = 19.298081 gamma = 120.000000

Current cell volume = 196.891879 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 0.333333 0.666667 -0.085456 x

x Se 2 0.333333 0.666667 0.088257 x

x Se 3 1.000000 1.000000 0.247877 x

x Se 4 1.000000 1.000000 0.421590 x

x Se 5 0.666667 1.333333 0.581210 x

x Se 6 0.666667 1.333333 0.754924 x

x Nb 1 0.000000 0.000000 0.000799 x

x Nb 2 0.666667 0.333333 0.334133 x

x Nb 3 0.333333 0.666667 0.667466 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22240963E+003 285.73 <-- SCF

1 -6.22499989E+003 2.87807216E-001 286.70 <-- SCF

2 -6.22519286E+003 2.14405426E-002 288.48 <-- SCF

3 -6.22363807E+003 -1.72754033E-001 289.97 <-- SCF

4 -6.22324201E+003 -4.40064836E-002 291.41 <-- SCF

5 -6.22318032E+003 -6.85436618E-003 292.72 <-- SCF

6 -6.22317924E+003 -1.20967079E-004 294.14 <-- SCF

7 -6.22317948E+003 2.75999545E-005 295.48 <-- SCF

8 -6.22317961E+003 1.39009712E-005 296.83 <-- SCF

9 -6.22317967E+003 7.26076464E-006 298.06 <-- SCF

10 -6.22317968E+003 5.98375773E-007 299.08 <-- SCF

11 -6.22317968E+003 1.97796395E-007 300.17 <-- SCF

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

Final energy = -6223.179681892 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 -0.02308 \*

\* Se 2 0.00000 0.00000 -0.28764 \*

\* Se 3 0.00000 -0.00000 -0.02308 \*

\* Se 4 0.00000 0.00000 -0.28764 \*

\* Se 5 0.00000 -0.00000 -0.02308 \*

\* Se 6 0.00000 0.00000 -0.28764 \*

\* Nb 1 -0.00000 -0.00000 0.31071 \*

\* Nb 2 -0.00000 -0.00000 0.31071 \*

\* Nb 3 -0.00000 -0.00000 0.31071 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -1.021919 0.000000 0.000000 \*

\* y 0.000000 -1.021919 0.000000 \*

\* z 0.000000 0.000000 -0.539728 \*

\* \*

\* Pressure: 0.8612 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000059 | -6223.159956 | <-- min BFGS

| trial step | 1.000000 | 0.000055 | -6223.161508 | <-- min BFGS

| line step | 16.152572 | 0.000028 | -6223.179633 | <-- min BFGS

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

BFGS: finished iteration 5 with enthalpy= -6.22317963E+003 eV

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

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

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

| dE/ion | 2.186326E-003 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 3.107132E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.325839E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.021919E+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 | 0.001078 | -6223.179633 | <-- min BFGS

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

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

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

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

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

| Memory Disk |

| Model and support data 104.7 MB 87.0 MB |

| Electronic energy minimisation requirements 9.3 MB 0.0 MB |

| Geometry minimisation requirements 11.2 MB 0.0 MB |

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

| Approx. total storage required per process 125.2 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)

2.9821831 -1.7217642 -0.0000000 2.1069079 0.0000000 0.0000000

-0.0000000 3.4435284 0.0000000 1.0534540 1.8246358 0.0000000

-0.0000000 0.0000000 19.5166629 0.0000000 -0.0000000 0.3219395

Lattice parameters(A) Cell Angles

a = 3.443528 alpha = 90.000000

b = 3.443528 beta = 90.000000

c = 19.516663 gamma = 120.000000

Current cell volume = 200.421147 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 0.333333 0.666667 -0.083865 x

x Se 2 0.333333 0.666667 0.086975 x

x Se 3 1.000000 1.000000 0.249469 x

x Se 4 1.000000 1.000000 0.420308 x

x Se 5 0.666667 1.333333 0.582802 x

x Se 6 0.666667 1.333333 0.753642 x

x Nb 1 0.000000 0.000000 0.000490 x

x Nb 2 0.666667 0.333333 0.333823 x

x Nb 3 0.333333 0.666667 0.667156 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22151449E+003 311.33 <-- SCF

1 -6.22748879E+003 6.63810568E-001 312.39 <-- SCF

2 -6.22788800E+003 4.43570403E-002 314.31 <-- SCF

3 -6.22461201E+003 -3.63999078E-001 315.81 <-- SCF

4 -6.22335107E+003 -1.40104418E-001 317.34 <-- SCF

5 -6.22322515E+003 -1.39916704E-002 318.89 <-- SCF

6 -6.22320193E+003 -2.57929469E-003 320.44 <-- SCF

7 -6.22320245E+003 5.80586896E-005 321.80 <-- SCF

8 -6.22320325E+003 8.88448115E-005 323.36 <-- SCF

9 -6.22320344E+003 2.08762335E-005 324.69 <-- SCF

10 -6.22320346E+003 1.88377710E-006 325.69 <-- SCF

11 -6.22320346E+003 3.59090481E-007 326.73 <-- SCF

12 -6.22320346E+003 7.37350479E-008 327.75 <-- SCF

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

Final energy = -6223.203463296 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 -0.17809 \*

\* Se 2 0.00000 -0.00000 -0.24007 \*

\* Se 3 0.00000 -0.00000 -0.17809 \*

\* Se 4 0.00000 -0.00000 -0.24007 \*

\* Se 5 0.00000 -0.00000 -0.17809 \*

\* Se 6 0.00000 -0.00000 -0.24007 \*

\* Nb 1 -0.00000 0.00000 0.41817 \*

\* Nb 2 -0.00000 0.00000 0.41817 \*

\* Nb 3 -0.00000 0.00000 0.41817 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.502284 -0.000000 0.000000 \*

\* y -0.000000 -0.502284 0.000000 \*

\* z 0.000000 0.000000 -1.055248 \*

\* \*

\* Pressure: 0.6866 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.001078 | -6223.179633 | <-- min BFGS

| trial step | 1.000000 | 0.000467 | -6223.203463 | <-- min BFGS

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

BFGS: finished iteration 6 with enthalpy= -6.22320346E+003 eV

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

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

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

| dE/ion | 2.647782E-003 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 4.181664E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 3.106931E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.055248E+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 | 0.000673 | -6223.203463 | <-- min BFGS

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

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

BFGS: starting iteration 7 with trial guess (lambda= 0.857251)

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

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

| Memory Disk |

| Model and support data 105.6 MB 92.7 MB |

| Electronic energy minimisation requirements 9.5 MB 0.0 MB |

| Geometry minimisation requirements 11.6 MB 0.0 MB |

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

| Approx. total storage required per process 126.8 MB 92.7 MB |

| |

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

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

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Unit Cell

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

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

2.9897493 -1.7261326 -0.0000000 2.1015760 -0.0000000 0.0000000

0.0000000 3.4522651 0.0000000 1.0507880 1.8200182 0.0000000

-0.0000000 0.0000000 19.7812515 0.0000000 -0.0000000 0.3176334

Lattice parameters(A) Cell Angles

a = 3.452265 alpha = 90.000000

b = 3.452265 beta = 90.000000

c = 19.781252 gamma = 120.000000

Current cell volume = 204.170351 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.082542 x

x Se 2 0.333333 0.666667 0.085917 x

x Se 3 1.000000 1.000000 0.250791 x

x Se 4 1.000000 1.000000 0.419250 x

x Se 5 0.666667 1.333333 0.584124 x

x Se 6 0.666667 1.333333 0.752584 x

x Nb 1 0.000000 0.000000 0.000226 x

x Nb 2 0.666667 0.333333 0.333559 x

x Nb 3 0.333333 0.666667 0.666892 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22177462E+003 339.73 <-- SCF

1 -6.22661119E+003 5.37397207E-001 340.78 <-- SCF

2 -6.22693870E+003 3.63896262E-002 342.52 <-- SCF

3 -6.22433273E+003 -2.89552178E-001 344.08 <-- SCF

4 -6.22332358E+003 -1.12127413E-001 345.56 <-- SCF

5 -6.22322055E+003 -1.14481500E-002 347.03 <-- SCF

6 -6.22320249E+003 -2.00645143E-003 348.50 <-- SCF

7 -6.22320273E+003 2.66971390E-005 349.98 <-- SCF

8 -6.22320350E+003 8.50052689E-005 351.44 <-- SCF

9 -6.22320368E+003 2.00996698E-005 352.78 <-- SCF

10 -6.22320370E+003 2.50211263E-006 354.25 <-- SCF

11 -6.22320371E+003 3.49883482E-007 355.97 <-- SCF

12 -6.22320371E+003 1.39458421E-008 357.53 <-- SCF

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

Final energy = -6223.203705585 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 -0.00000 -0.25499 \*

\* Se 2 -0.00000 -0.00000 -0.27793 \*

\* Se 3 -0.00000 -0.00000 -0.25499 \*

\* Se 4 0.00000 -0.00000 -0.27793 \*

\* Se 5 -0.00000 -0.00000 -0.25499 \*

\* Se 6 -0.00000 -0.00000 -0.27793 \*

\* Nb 1 0.00000 -0.00000 0.53292 \*

\* Nb 2 0.00000 0.00000 0.53292 \*

\* Nb 3 -0.00000 0.00000 0.53292 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.023384 -0.000000 0.000000 \*

\* y -0.000000 -0.023384 -0.000000 \*

\* z 0.000000 -0.000000 -0.572769 \*

\* \*

\* Pressure: 0.2065 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000673 | -6223.203463 | <-- min BFGS

| trial step | 0.857251 | -0.000042 | -6223.203648 | <-- min BFGS

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

BFGS: finished iteration 7 with enthalpy= -6.22320365E+003 eV

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

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

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

| dE/ion | 2.058309E-005 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 5.329202E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.615208E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 5.727692E-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 | 0.000125 | -6223.203648 | <-- min BFGS

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

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

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

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

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

| Memory Disk |

| Model and support data 106.9 MB 92.7 MB |

| Electronic energy minimisation requirements 9.5 MB 0.0 MB |

| Geometry minimisation requirements 11.6 MB 0.0 MB |

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

| Approx. total storage required per process 128.0 MB 92.7 MB |

| |

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

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

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

Unit Cell

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

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

2.9917003 -1.7272590 -0.0000000 2.1002055 -0.0000000 0.0000000

0.0000000 3.4545179 0.0000000 1.0501027 1.8188313 0.0000000

-0.0000000 0.0000000 19.7679573 0.0000000 -0.0000000 0.3178470

Lattice parameters(A) Cell Angles

a = 3.454518 alpha = 90.000000

b = 3.454518 beta = 90.000000

c = 19.767957 gamma = 120.000000

Current cell volume = 204.299510 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.082776 x

x Se 2 0.333333 0.666667 0.086063 x

x Se 3 1.000000 1.000000 0.250558 x

x Se 4 1.000000 1.000000 0.419397 x

x Se 5 0.666667 1.333333 0.583891 x

x Se 6 0.666667 1.333333 0.752730 x

x Nb 1 0.000000 0.000000 0.000312 x

x Nb 2 0.666667 0.333333 0.333646 x

x Nb 3 0.333333 0.666667 0.666979 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22317491E+003 372.62 <-- SCF

1 -6.22327037E+003 1.06068442E-002 373.83 <-- SCF

2 -6.22327543E+003 5.62805573E-004 377.14 <-- SCF

3 -6.22321719E+003 -6.47125253E-003 378.98 <-- SCF

4 -6.22320874E+003 -9.39682494E-004 380.55 <-- SCF

5 -6.22320639E+003 -2.61170259E-004 382.03 <-- SCF

6 -6.22320644E+003 5.71718177E-006 383.61 <-- SCF

7 -6.22320643E+003 -1.04827973E-006 384.94 <-- SCF

8 -6.22320644E+003 1.65957978E-006 386.03 <-- SCF

9 -6.22320645E+003 3.86302351E-007 387.05 <-- SCF

10 -6.22320645E+003 -1.76089802E-008 388.11 <-- SCF

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

Final energy = -6223.206445299 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 -0.18619 \*

\* Se 2 0.00000 0.00000 -0.30366 \*

\* Se 3 0.00000 0.00000 -0.18619 \*

\* Se 4 -0.00000 0.00000 -0.30366 \*

\* Se 5 -0.00000 -0.00000 -0.18619 \*

\* Se 6 0.00000 0.00000 -0.30366 \*

\* Nb 1 -0.00000 0.00000 0.48984 \*

\* Nb 2 -0.00000 0.00000 0.48984 \*

\* Nb 3 -0.00000 0.00000 0.48984 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.236003 0.000000 0.000000 \*

\* y 0.000000 0.236003 0.000000 \*

\* z 0.000000 0.000000 -0.197260 \*

\* \*

\* Pressure: -0.0916 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000125 | -6223.203648 | <-- min BFGS

| trial step | 1.000000 | 0.000070 | -6223.206374 | <-- min BFGS

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

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

BFGS: improving iteration 8 with line minimization (lambda= 2.256849)

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Unit Cell

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

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

2.9941524 -1.7286747 -0.0000000 2.0984855 -0.0000000 0.0000000

0.0000000 3.4573494 0.0000000 1.0492427 1.8173417 0.0000000

-0.0000000 0.0000000 19.7512485 0.0000000 -0.0000000 0.3181159

Lattice parameters(A) Cell Angles

a = 3.457349 alpha = 90.000000

b = 3.457349 beta = 90.000000

c = 19.751248 gamma = 120.000000

Current cell volume = 204.461582 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.083069 x

x Se 2 0.333333 0.666667 0.086247 x

x Se 3 1.000000 1.000000 0.250264 x

x Se 4 1.000000 1.000000 0.419581 x

x Se 5 0.666667 1.333333 0.583598 x

x Se 6 0.666667 1.333333 0.752914 x

x Nb 1 0.000000 0.000000 0.000421 x

x Nb 2 0.666667 0.333333 0.333755 x

x Nb 3 0.333333 0.666667 0.667088 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22315726E+003 401.30 <-- SCF

1 -6.22330761E+003 1.67057224E-002 402.73 <-- SCF

2 -6.22331530E+003 8.54476194E-004 404.81 <-- SCF

3 -6.22322421E+003 -1.01214073E-002 406.47 <-- SCF

4 -6.22321099E+003 -1.46885333E-003 408.55 <-- SCF

5 -6.22320729E+003 -4.10419729E-004 410.31 <-- SCF

6 -6.22320737E+003 8.94013403E-006 412.14 <-- SCF

7 -6.22320736E+003 -1.29213501E-006 414.09 <-- SCF

8 -6.22320738E+003 2.54416911E-006 415.61 <-- SCF

9 -6.22320739E+003 4.47194933E-007 416.95 <-- SCF

10 -6.22320739E+003 6.36477548E-009 418.11 <-- SCF

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

Final energy = -6223.207387602 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 -0.08150 \*

\* Se 2 0.00000 -0.00000 -0.34569 \*

\* Se 3 0.00000 0.00000 -0.08150 \*

\* Se 4 0.00000 -0.00000 -0.34569 \*

\* Se 5 0.00000 0.00000 -0.08150 \*

\* Se 6 0.00000 -0.00000 -0.34569 \*

\* Nb 1 -0.00000 0.00000 0.42719 \*

\* Nb 2 -0.00000 0.00000 0.42719 \*

\* Nb 3 -0.00000 -0.00000 0.42719 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.540485 0.000000 0.000000 \*

\* y 0.000000 0.540485 0.000000 \*

\* z 0.000000 0.000000 0.255815 \*

\* \*

\* Pressure: -0.4456 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000125 | -6223.203648 | <-- min BFGS

| trial step | 1.000000 | 0.000070 | -6223.206374 | <-- min BFGS

| line step | 2.256849 | -0.000013 | -6223.207342 | <-- min BFGS

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

BFGS: finished iteration 8 with enthalpy= -6.22320734E+003 eV

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

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

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

| dE/ion | 4.104393E-004 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 4.271924E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.039645E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 5.404851E-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 | 0.000115 | -6223.207342 | <-- min BFGS

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

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

BFGS: starting iteration 9 with trial guess (lambda= 1.000000)

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

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

Unit Cell

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

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

2.9940665 -1.7286251 -0.0000000 2.0985457 -0.0000000 0.0000000

0.0000000 3.4572502 0.0000000 1.0492728 1.8173939 0.0000000

-0.0000000 0.0000000 19.7567063 0.0000000 -0.0000000 0.3180280

Lattice parameters(A) Cell Angles

a = 3.457250 alpha = 90.000000

b = 3.457250 beta = 90.000000

c = 19.756706 gamma = 120.000000

Current cell volume = 204.506351 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 0.333333 0.666667 -0.082988 x

x Se 2 0.333333 0.666667 0.086125 x

x Se 3 1.000000 1.000000 0.250345 x

x Se 4 1.000000 1.000000 0.419459 x

x Se 5 0.666667 1.333333 0.583678 x

x Se 6 0.666667 1.333333 0.752792 x

x Nb 1 0.000000 0.000000 0.000463 x

x Nb 2 0.666667 0.333333 0.333796 x

x Nb 3 0.333333 0.666667 0.667130 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22320322E+003 431.73 <-- SCF

1 -6.22322877E+003 2.83851237E-003 433.03 <-- SCF

2 -6.22323034E+003 1.74320851E-004 435.27 <-- SCF

3 -6.22321364E+003 -1.85492103E-003 437.00 <-- SCF

4 -6.22321098E+003 -2.96073858E-004 438.77 <-- SCF

5 -6.22321031E+003 -7.42362588E-005 440.25 <-- SCF

6 -6.22321032E+003 1.06461081E-006 441.84 <-- SCF

7 -6.22321033E+003 4.88002212E-007 443.09 <-- SCF

8 -6.22321033E+003 4.93690268E-007 444.20 <-- SCF

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

Final energy = -6223.210329666 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 -0.09880 \*

\* Se 2 0.00000 0.00000 -0.30676 \*

\* Se 3 0.00000 0.00000 -0.09880 \*

\* Se 4 0.00000 0.00000 -0.30676 \*

\* Se 5 0.00000 -0.00000 -0.09880 \*

\* Se 6 -0.00000 0.00000 -0.30676 \*

\* Nb 1 -0.00000 0.00000 0.40556 \*

\* Nb 2 -0.00000 -0.00000 0.40556 \*

\* Nb 3 -0.00000 -0.00000 0.40556 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.452612 0.000000 -0.000000 \*

\* y 0.000000 0.452612 0.000000 \*

\* z -0.000000 0.000000 0.064499 \*

\* \*

\* Pressure: -0.3232 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000115 | -6223.207342 | <-- min BFGS

| trial step | 1.000000 | 0.000102 | -6223.210288 | <-- min BFGS

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

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

BFGS: improving iteration 9 with line minimization (lambda= 8.758026)

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Unit Cell

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

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

2.9934004 -1.7282405 -0.0000000 2.0990126 -0.0000000 0.0000000

0.0000000 3.4564811 0.0000000 1.0495063 1.8177983 0.0000000

-0.0000000 0.0000000 19.7990480 0.0000000 -0.0000000 0.3173478

Lattice parameters(A) Cell Angles

a = 3.456481 alpha = 90.000000

b = 3.456481 beta = 90.000000

c = 19.799048 gamma = 120.000000

Current cell volume = 204.853461 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.082363 x

x Se 2 0.333333 0.666667 0.085177 x

x Se 3 1.000000 1.000000 0.250970 x

x Se 4 1.000000 1.000000 0.418510 x

x Se 5 0.666667 1.333333 0.584303 x

x Se 6 0.666667 1.333333 0.751844 x

x Nb 1 0.000000 0.000000 0.000786 x

x Nb 2 0.666667 0.333333 0.334120 x

x Nb 3 0.333333 0.666667 0.667453 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22273258E+003 458.39 <-- SCF

1 -6.22430565E+003 1.74786057E-001 459.64 <-- SCF

2 -6.22441432E+003 1.20739064E-002 462.06 <-- SCF

3 -6.22344077E+003 -1.08171625E-001 464.05 <-- SCF

4 -6.22326241E+003 -1.98182752E-002 465.97 <-- SCF

5 -6.22322164E+003 -4.53046219E-003 467.53 <-- SCF

6 -6.22322130E+003 -3.74620194E-005 469.34 <-- SCF

7 -6.22322165E+003 3.95556790E-005 471.03 <-- SCF

8 -6.22322186E+003 2.32414800E-005 472.70 <-- SCF

9 -6.22322191E+003 5.61166177E-006 474.02 <-- SCF

10 -6.22322192E+003 4.31820890E-007 475.36 <-- SCF

11 -6.22322192E+003 1.41143474E-007 476.52 <-- SCF

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

Final energy = -6223.221919746 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 -0.18874 \*

\* Se 2 0.00000 0.00000 -0.03779 \*

\* Se 3 0.00000 0.00000 -0.18874 \*

\* Se 4 0.00000 0.00000 -0.03779 \*

\* Se 5 0.00000 0.00000 -0.18874 \*

\* Se 6 0.00000 0.00000 -0.03779 \*

\* Nb 1 -0.00000 0.00000 0.22653 \*

\* Nb 2 -0.00000 -0.00000 0.22653 \*

\* Nb 3 -0.00000 -0.00000 0.22653 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.008523 0.000000 0.000000 \*

\* y 0.000000 0.008523 0.000000 \*

\* z 0.000000 0.000000 -1.253648 \*

\* \*

\* Pressure: 0.4122 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000115 | -6223.207342 | <-- min BFGS

| trial step | 1.000000 | 0.000102 | -6223.210288 | <-- min BFGS

| line step | 8.758026 | 0.000014 | -6223.221923 | <-- min BFGS

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

BFGS: finished iteration 9 with enthalpy= -6.22322192E+003 eV

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

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

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

| dE/ion | 1.620019E-003 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 2.265333E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.119370E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.253648E+000 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 10 ...

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

Writing analysis data to 3R-NbSe2-US-7.castep\_bin

Writing model to 3R-NbSe2-US-7.check

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

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

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

| previous | 0.000000 | 0.000471 | -6223.221923 | <-- min BFGS

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

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

BFGS: starting iteration 10 with trial guess (lambda= 1.000000)

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

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

| Memory Disk |

| Model and support data 107.0 MB 92.7 MB |

| Electronic energy minimisation requirements 9.6 MB 0.0 MB |

| Geometry minimisation requirements 11.7 MB 0.0 MB |

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

| Approx. total storage required per process 128.3 MB 92.7 MB |

| |

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

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

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

Unit Cell

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

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

2.9940308 -1.7286045 -0.0000000 2.0985707 -0.0000000 0.0000000

0.0000000 3.4572090 0.0000000 1.0492853 1.8174155 0.0000000

-0.0000000 0.0000000 19.9800439 0.0000000 -0.0000000 0.3144730

Lattice parameters(A) Cell Angles

a = 3.457209 alpha = 90.000000

b = 3.457209 beta = 90.000000

c = 19.980044 gamma = 120.000000

Current cell volume = 206.813241 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 0.333333 0.666667 -0.081771 x

x Se 2 0.333333 0.666667 0.084364 x

x Se 3 1.000000 1.000000 0.251562 x

x Se 4 1.000000 1.000000 0.417698 x

x Se 5 0.666667 1.333333 0.584895 x

x Se 6 0.666667 1.333333 0.751031 x

x Nb 1 0.000000 0.000000 0.001007 x

x Nb 2 0.666667 0.333333 0.334340 x

x Nb 3 0.333333 0.666667 0.667674 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22266760E+003 489.47 <-- SCF

1 -6.22446912E+003 2.00168570E-001 490.44 <-- SCF

2 -6.22458215E+003 1.25591515E-002 492.16 <-- SCF

3 -6.22352270E+003 -1.17717387E-001 493.62 <-- SCF

4 -6.22327678E+003 -2.73239036E-002 495.14 <-- SCF

5 -6.22323178E+003 -4.99962365E-003 496.55 <-- SCF

6 -6.22323147E+003 -3.44463953E-005 498.16 <-- SCF

7 -6.22323184E+003 4.01680134E-005 499.80 <-- SCF

8 -6.22323202E+003 2.09620138E-005 501.30 <-- SCF

9 -6.22323210E+003 8.38510141E-006 502.48 <-- SCF

10 -6.22323211E+003 6.39104596E-007 503.62 <-- SCF

11 -6.22323211E+003 2.02501983E-007 504.92 <-- SCF

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

Final energy = -6223.232107230 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 -0.13358 \*

\* Se 2 -0.00000 0.00000 0.02027 \*

\* Se 3 -0.00000 0.00000 -0.13358 \*

\* Se 4 0.00000 -0.00000 0.02027 \*

\* Se 5 0.00000 -0.00000 -0.13358 \*

\* Se 6 0.00000 -0.00000 0.02027 \*

\* Nb 1 -0.00000 0.00000 0.11331 \*

\* Nb 2 -0.00000 0.00000 0.11331 \*

\* Nb 3 0.00000 0.00000 0.11331 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.108926 0.000000 0.000000 \*

\* y 0.000000 0.108926 0.000000 \*

\* z 0.000000 0.000000 -0.951067 \*

\* \*

\* Pressure: 0.2444 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000471 | -6223.221923 | <-- min BFGS

| trial step | 1.000000 | 0.000251 | -6223.232040 | <-- min BFGS

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

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

BFGS: improving iteration 10 with line minimization (lambda= 1.461848)

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

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

| Memory Disk |

| Model and support data 108.0 MB 92.7 MB |

| Electronic energy minimisation requirements 9.8 MB 0.0 MB |

| Geometry minimisation requirements 11.8 MB 0.0 MB |

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

| Approx. total storage required per process 129.6 MB 92.7 MB |

| |

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

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

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

Unit Cell

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

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

2.9943220 -1.7287726 -0.0000000 2.0983666 -0.0000000 0.0000000

0.0000000 3.4575452 0.0000000 1.0491833 1.8172388 0.0000000

-0.0000000 0.0000000 20.0636366 0.0000000 -0.0000000 0.3131628

Lattice parameters(A) Cell Angles

a = 3.457545 alpha = 90.000000

b = 3.457545 beta = 90.000000

c = 20.063637 gamma = 120.000000

Current cell volume = 207.718901 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.081498 x

x Se 2 0.333333 0.666667 0.083989 x

x Se 3 1.000000 1.000000 0.251835 x

x Se 4 1.000000 1.000000 0.417323 x

x Se 5 0.666667 1.333333 0.585169 x

x Se 6 0.666667 1.333333 0.750656 x

x Nb 1 0.000000 0.000000 0.001109 x

x Nb 2 0.666667 0.333333 0.334442 x

x Nb 3 0.333333 0.666667 0.667776 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22311420E+003 516.72 <-- SCF

1 -6.22349836E+003 4.26844103E-002 517.84 <-- SCF

2 -6.22352247E+003 2.67856811E-003 519.78 <-- SCF

3 -6.22328891E+003 -2.59512950E-002 521.34 <-- SCF

4 -6.22324373E+003 -5.01960255E-003 522.89 <-- SCF

5 -6.22323429E+003 -1.04927751E-003 524.36 <-- SCF

6 -6.22323441E+003 1.42539066E-005 526.05 <-- SCF

7 -6.22323451E+003 1.10900819E-005 527.45 <-- SCF

8 -6.22323457E+003 5.86189858E-006 528.61 <-- SCF

9 -6.22323458E+003 2.03102266E-006 529.89 <-- SCF

10 -6.22323459E+003 6.84910064E-008 531.31 <-- SCF

11 -6.22323459E+003 2.05957422E-008 532.67 <-- SCF

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

Final energy = -6223.234585668 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 -0.10287 \*

\* Se 2 0.00000 0.00000 0.05333 \*

\* Se 3 0.00000 0.00000 -0.10287 \*

\* Se 4 -0.00000 -0.00000 0.05333 \*

\* Se 5 -0.00000 0.00000 -0.10287 \*

\* Se 6 0.00000 0.00000 0.05333 \*

\* Nb 1 0.00000 -0.00000 0.04954 \*

\* Nb 2 0.00000 -0.00000 0.04954 \*

\* Nb 3 0.00000 -0.00000 0.04954 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.117465 -0.000000 -0.000000 \*

\* y -0.000000 0.117465 -0.000000 \*

\* z -0.000000 -0.000000 -0.821028 \*

\* \*

\* Pressure: 0.1954 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000471 | -6223.221923 | <-- min BFGS

| trial step | 1.000000 | 0.000251 | -6223.232040 | <-- min BFGS

| line step | 1.461848 | 0.000144 | -6223.234502 | <-- min BFGS

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

BFGS: finished iteration 10 with enthalpy= -6.22323450E+003 eV

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

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

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

| dE/ion | 1.397662E-003 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.028700E-001 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.383177E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 8.210282E-001 | 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 | 0.000228 | -6223.234502 | <-- 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 108.5 MB 92.7 MB |

| Electronic energy minimisation requirements 9.8 MB 0.0 MB |

| Geometry minimisation requirements 11.9 MB 0.0 MB |

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

| Approx. total storage required per process 130.1 MB 92.7 MB |

| |

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

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

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

Unit Cell

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

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

2.9909840 -1.7268454 -0.0000000 2.1007084 -0.0000000 0.0000000

0.0000000 3.4536908 0.0000000 1.0503542 1.8192669 0.0000000

-0.0000000 0.0000000 20.2090526 0.0000000 -0.0000000 0.3109094

Lattice parameters(A) Cell Angles

a = 3.453691 alpha = 90.000000

b = 3.453691 beta = 90.000000

c = 20.209053 gamma = 120.000000

Current cell volume = 208.758178 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.081305 x

x Se 2 0.333333 0.666667 0.083676 x

x Se 3 1.000000 1.000000 0.252028 x

x Se 4 1.000000 1.000000 0.417010 x

x Se 5 0.666667 1.333333 0.585362 x

x Se 6 0.666667 1.333333 0.750343 x

x Nb 1 0.000000 0.000000 0.001229 x

x Nb 2 0.666667 0.333333 0.334562 x

x Nb 3 0.333333 0.666667 0.667895 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22306619E+003 547.25 <-- SCF

1 -6.22349672E+003 4.78372257E-002 548.62 <-- SCF

2 -6.22352116E+003 2.71498949E-003 550.67 <-- SCF

3 -6.22329319E+003 -2.53296487E-002 552.61 <-- SCF

4 -6.22324770E+003 -5.05392698E-003 554.34 <-- SCF

5 -6.22323802E+003 -1.07567754E-003 556.08 <-- SCF

6 -6.22323809E+003 7.38928770E-006 558.08 <-- SCF

7 -6.22323820E+003 1.17438136E-005 559.64 <-- SCF

8 -6.22323825E+003 6.27793622E-006 560.98 <-- SCF

9 -6.22323828E+003 2.74232823E-006 562.22 <-- SCF

10 -6.22323828E+003 2.11353134E-008 563.42 <-- SCF

11 -6.22323828E+003 2.24767225E-008 564.80 <-- SCF

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

Final energy = -6223.238276880 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 -0.00000 0.01910 \*

\* Se 2 0.00000 -0.00000 -0.00117 \*

\* Se 3 0.00000 -0.00000 0.01910 \*

\* Se 4 0.00000 -0.00000 -0.00117 \*

\* Se 5 -0.00000 0.00000 0.01910 \*

\* Se 6 -0.00000 -0.00000 -0.00117 \*

\* Nb 1 0.00000 0.00000 -0.01794 \*

\* Nb 2 0.00000 0.00000 -0.01794 \*

\* Nb 3 0.00000 -0.00000 -0.01794 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.105224 -0.000000 -0.000000 \*

\* y -0.000000 0.105224 -0.000000 \*

\* z -0.000000 -0.000000 -0.098552 \*

\* \*

\* Pressure: -0.0373 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000228 | -6223.234502 | <-- min BFGS

| trial step | 1.000000 | 0.000049 | -6223.238196 | <-- min BFGS

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

BFGS: finished iteration 11 with enthalpy= -6.22323820E+003 eV

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

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

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

| dE/ion | 4.105439E-004 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.910118E-002 | 3.000000E-002 | eV/A | Yes | <-- BFGS

| |dR|max | 6.323925E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.052240E-001 | 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 | 0.000070 | -6223.238196 | <-- 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 108.9 MB 92.7 MB |

| Electronic energy minimisation requirements 9.8 MB 0.0 MB |

| Geometry minimisation requirements 11.9 MB 0.0 MB |

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

| Approx. total storage required per process 130.7 MB 92.7 MB |

| |

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

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

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

Unit Cell

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

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

2.9887579 -1.7255602 -0.0000000 2.1022731 0.0000000 0.0000000

-0.0000000 3.4511204 0.0000000 1.0511365 1.8206219 0.0000000

-0.0000000 0.0000000 20.3657306 0.0000000 -0.0000000 0.3085176

Lattice parameters(A) Cell Angles

a = 3.451120 alpha = 90.000000

b = 3.451120 beta = 90.000000

c = 20.365731 gamma = 120.000000

Current cell volume = 210.063622 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.080741 x

x Se 2 0.333333 0.666667 0.083114 x

x Se 3 1.000000 1.000000 0.252592 x

x Se 4 1.000000 1.000000 0.416448 x

x Se 5 0.666667 1.333333 0.585925 x

x Se 6 0.666667 1.333333 0.749781 x

x Nb 1 0.000000 0.000000 0.001227 x

x Nb 2 0.666667 0.333333 0.334560 x

x Nb 3 0.333333 0.666667 0.667894 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22289848E+003 578.17 <-- SCF

1 -6.22399400E+003 1.21724795E-001 579.42 <-- SCF

2 -6.22407311E+003 8.78978292E-003 581.70 <-- SCF

3 -6.22341505E+003 -7.31177261E-002 583.62 <-- SCF

4 -6.22327139E+003 -1.59620183E-002 585.55 <-- SCF

5 -6.22323956E+003 -3.53642853E-003 587.53 <-- SCF

6 -6.22324074E+003 1.30626613E-004 589.56 <-- SCF

7 -6.22324038E+003 -4.00555497E-005 591.05 <-- SCF

8 -6.22324057E+003 2.14715030E-005 592.55 <-- SCF

9 -6.22324060E+003 2.84026965E-006 593.89 <-- SCF

10 -6.22324060E+003 4.37190049E-007 594.95 <-- SCF

11 -6.22324060E+003 1.65131409E-007 596.05 <-- SCF

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

Final energy = -6223.240601034 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.05979 \*

\* Se 2 0.00000 -0.00000 -0.04039 \*

\* Se 3 0.00000 0.00000 0.05979 \*

\* Se 4 0.00000 0.00000 -0.04039 \*

\* Se 5 0.00000 -0.00000 0.05979 \*

\* Se 6 0.00000 -0.00000 -0.04039 \*

\* Nb 1 -0.00000 -0.00000 -0.01940 \*

\* Nb 2 -0.00000 -0.00000 -0.01940 \*

\* Nb 3 -0.00000 -0.00000 -0.01940 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.006052 -0.000000 0.000000 \*

\* y -0.000000 0.006052 -0.000000 \*

\* z 0.000000 -0.000000 0.048168 \*

\* \*

\* Pressure: -0.0201 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000070 | -6223.238196 | <-- min BFGS

| trial step | 1.000000 | 0.000109 | -6223.240534 | <-- min BFGS

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

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

BFGS: improving iteration 12 with line minimization (lambda= -1.688742)

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

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

| Memory Disk |

| Model and support data 109.6 MB 92.7 MB |

| Electronic energy minimisation requirements 9.6 MB 0.0 MB |

| Geometry minimisation requirements 11.7 MB 0.0 MB |

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

| Approx. total storage required per process 130.9 MB 92.7 MB |

| |

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

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

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

Unit Cell

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

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

2.9947432 -1.7290158 -0.0000000 2.0980715 -0.0000000 0.0000000

0.0000000 3.4580316 0.0000000 1.0490357 1.8169832 0.0000000

-0.0000000 0.0000000 19.9444640 0.0000000 -0.0000000 0.3150341

Lattice parameters(A) Cell Angles

a = 3.458032 alpha = 90.000000

b = 3.458032 beta = 90.000000

c = 19.944464 gamma = 120.000000

Current cell volume = 206.543203 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.082257 x

x Se 2 0.333333 0.666667 0.084625 x

x Se 3 1.000000 1.000000 0.251077 x

x Se 4 1.000000 1.000000 0.417959 x

x Se 5 0.666667 1.333333 0.584410 x

x Se 6 0.666667 1.333333 0.751292 x

x Nb 1 0.000000 0.000000 0.001231 x

x Nb 2 0.666667 0.333333 0.334565 x

x Nb 3 0.333333 0.666667 0.667898 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22077910E+003 609.27 <-- SCF

1 -6.22863304E+003 8.72659481E-001 610.23 <-- SCF

2 -6.22895242E+003 3.54871063E-002 611.94 <-- SCF

3 -6.22390019E+003 -5.61359008E-001 613.42 <-- SCF

4 -6.22338939E+003 -5.67548784E-002 615.28 <-- SCF

5 -6.22322109E+003 -1.87008851E-002 617.34 <-- SCF

6 -6.22323225E+003 1.24021637E-003 619.59 <-- SCF

7 -6.22323178E+003 -5.25244232E-005 621.66 <-- SCF

8 -6.22323290E+003 1.24457950E-004 623.34 <-- SCF

9 -6.22323285E+003 -4.94488900E-006 625.30 <-- SCF

10 -6.22323287E+003 1.58890316E-006 626.77 <-- SCF

11 -6.22323287E+003 2.91948360E-007 628.52 <-- SCF

12 -6.22323287E+003 6.50831743E-008 630.41 <-- SCF

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

Final energy = -6223.232868442 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.01220 \*

\* Se 2 -0.00000 0.00000 0.00236 \*

\* Se 3 0.00000 -0.00000 0.01220 \*

\* Se 4 0.00000 0.00000 0.00236 \*

\* Se 5 0.00000 0.00000 0.01220 \*

\* Se 6 0.00000 0.00000 0.00236 \*

\* Nb 1 0.00000 0.00000 -0.01456 \*

\* Nb 2 -0.00000 0.00000 -0.01456 \*

\* Nb 3 0.00000 0.00000 -0.01456 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.328526 0.000000 -0.000000 \*

\* y 0.000000 0.328526 -0.000000 \*

\* z -0.000000 -0.000000 -0.502932 \*

\* \*

\* Pressure: -0.0514 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000070 | -6223.238196 | <-- min BFGS

| trial step | 1.000000 | 0.000109 | -6223.240534 | <-- min BFGS

| line step | -1.688742 | 0.000223 | -6223.232782 | <-- min BFGS

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

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BFGS: improving iteration 12 with quad minimization (lambda= 1.665310)

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Unit Cell

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

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

2.9872769 -1.7247051 -0.0000000 2.1033153 0.0000000 0.0000000

-0.0000000 3.4494103 0.0000000 1.0516577 1.8215245 0.0000000

-0.0000000 0.0000000 20.4699701 0.0000000 -0.0000000 0.3069465

Lattice parameters(A) Cell Angles

a = 3.449410 alpha = 90.000000

b = 3.449410 beta = 90.000000

c = 20.469970 gamma = 120.000000

Current cell volume = 210.929609 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.080366 x

x Se 2 0.333333 0.666667 0.082740 x

x Se 3 1.000000 1.000000 0.252967 x

x Se 4 1.000000 1.000000 0.416074 x

x Se 5 0.666667 1.333333 0.586300 x

x Se 6 0.666667 1.333333 0.749407 x

x Nb 1 0.000000 0.000000 0.001226 x

x Nb 2 0.666667 0.333333 0.334559 x

x Nb 3 0.333333 0.666667 0.667893 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.21938875E+003 644.81 <-- SCF

1 -6.23204441E+003 1.40618535E+000 646.80 <-- SCF

2 -6.23330199E+003 1.39730711E-001 649.95 <-- SCF

3 -6.22599507E+003 -8.11880342E-001 652.03 <-- SCF

4 -6.22326433E+003 -3.03415703E-001 654.05 <-- SCF

5 -6.22319726E+003 -7.45131489E-003 656.44 <-- SCF

6 -6.22324293E+003 5.07415494E-003 658.36 <-- SCF

7 -6.22322137E+003 -2.39532845E-003 659.83 <-- SCF

8 -6.22322345E+003 2.30426948E-004 661.56 <-- SCF

9 -6.22322492E+003 1.63984806E-004 662.92 <-- SCF

10 -6.22322498E+003 6.17594298E-006 664.50 <-- SCF

11 -6.22322498E+003 5.21976125E-007 665.84 <-- SCF

12 -6.22322499E+003 4.41748090E-007 667.17 <-- SCF

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

Final energy = -6223.224987502 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.07552 \*

\* Se 2 -0.00000 -0.00000 -0.02232 \*

\* Se 3 0.00000 0.00000 0.07552 \*

\* Se 4 -0.00000 0.00000 -0.02232 \*

\* Se 5 0.00000 0.00000 0.07552 \*

\* Se 6 0.00000 -0.00000 -0.02232 \*

\* Nb 1 0.00000 -0.00000 -0.05319 \*

\* Nb 2 0.00000 0.00000 -0.05319 \*

\* Nb 3 -0.00000 -0.00000 -0.05319 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.082514 0.000000 -0.000000 \*

\* y 0.000000 -0.082514 -0.000000 \*

\* z -0.000000 -0.000000 0.016385 \*

\* \*

\* Pressure: 0.0495 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000070 | -6223.238196 | <-- min BFGS

| trial step | 1.000000 | 0.000109 | -6223.240534 | <-- min BFGS

| line step | -1.688742 | 0.000223 | -6223.232782 | <-- min BFGS

| quad step | 1.665310 | 0.000113 | -6223.224910 | <-- min BFGS

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

BFGS: updated estimated <frequency> = 311.93470 cm-1

BFGS: updated estimated bulk modulus = 24.06518 GPa

BFGS: finished iteration 12 with enthalpy= -6.22322491E+003 eV

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

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

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

| dE/ion | 1.476282E-003 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 7.551531E-002 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 1.921428E-002 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 8.251423E-002 | 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 | 0.000043 | -6223.224910 | <-- min BFGS

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

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

BFGS: starting iteration 13 with trial guess (lambda= 1.000000)

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

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

| Memory Disk |

| Model and support data 110.7 MB 92.7 MB |

| Electronic energy minimisation requirements 9.8 MB 0.0 MB |

| Geometry minimisation requirements 11.9 MB 0.0 MB |

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

| Approx. total storage required per process 132.5 MB 92.7 MB |

| |

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

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

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

Unit Cell

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

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

2.9906947 -1.7266784 -0.0000000 2.1009116 -0.0000000 0.0000000

0.0000000 3.4533568 0.0000000 1.0504558 1.8194428 0.0000000

-0.0000000 0.0000000 20.4660403 0.0000000 -0.0000000 0.3070054

Lattice parameters(A) Cell Angles

a = 3.453357 alpha = 90.000000

b = 3.453357 beta = 90.000000

c = 20.466040 gamma = 120.000000

Current cell volume = 211.371953 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.080243 x

x Se 2 0.333333 0.666667 0.082704 x

x Se 3 1.000000 1.000000 0.253090 x

x Se 4 1.000000 1.000000 0.416037 x

x Se 5 0.666667 1.333333 0.586424 x

x Se 6 0.666667 1.333333 0.749370 x

x Nb 1 0.000000 0.000000 0.001139 x

x Nb 2 0.666667 0.333333 0.334472 x

x Nb 3 0.333333 0.666667 0.667806 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22320767E+003 679.28 <-- SCF

1 -6.22325156E+003 4.87635060E-003 680.28 <-- SCF

2 -6.22325331E+003 1.93940026E-004 682.16 <-- SCF

3 -6.22322952E+003 -2.64343310E-003 683.72 <-- SCF

4 -6.22322613E+003 -3.76433740E-004 685.36 <-- SCF

5 -6.22322544E+003 -7.59601475E-005 686.97 <-- SCF

6 -6.22322544E+003 -9.55593008E-007 688.53 <-- SCF

7 -6.22322544E+003 2.58647385E-007 689.69 <-- SCF

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

Final energy = -6223.225437352 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.02922 \*

\* Se 2 0.00000 -0.00000 -0.02686 \*

\* Se 3 0.00000 0.00000 0.02922 \*

\* Se 4 0.00000 -0.00000 -0.02686 \*

\* Se 5 0.00000 0.00000 0.02922 \*

\* Se 6 0.00000 0.00000 -0.02686 \*

\* Nb 1 -0.00000 0.00000 -0.00236 \*

\* Nb 2 -0.00000 0.00000 -0.00236 \*

\* Nb 3 -0.00000 0.00000 -0.00236 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x 0.123080 0.000000 0.000000 \*

\* y 0.000000 0.123080 -0.000000 \*

\* z 0.000000 -0.000000 -0.033039 \*

\* \*

\* Pressure: -0.0710 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000043 | -6223.224910 | <-- min BFGS

| trial step | 1.000000 | -3.143E-006 | -6223.225404 | <-- min BFGS

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

BFGS: finished iteration 13 with enthalpy= -6.22322540E+003 eV

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

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

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

| dE/ion | 5.486178E-005 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 2.922498E-002 | 3.000000E-002 | eV/A | Yes | <-- BFGS

| |dR|max | 2.523673E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.230803E-001 | 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 | 0.000023 | -6223.225404 | <-- min BFGS

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

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

BFGS: starting iteration 14 with trial guess (lambda= 1.000000)

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Unit Cell

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

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

2.9877934 -1.7250033 -0.0000000 2.1029517 0.0000000 0.0000000

-0.0000000 3.4500067 0.0000000 1.0514759 1.8212096 0.0000000

-0.0000000 0.0000000 20.4713086 0.0000000 -0.0000000 0.3069264

Lattice parameters(A) Cell Angles

a = 3.450007 alpha = 90.000000

b = 3.450007 beta = 90.000000

c = 20.471309 gamma = 120.000000

Current cell volume = 211.016353 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.080132 x

x Se 2 0.333333 0.666667 0.082643 x

x Se 3 1.000000 1.000000 0.253202 x

x Se 4 1.000000 1.000000 0.415977 x

x Se 5 0.666667 1.333333 0.586535 x

x Se 6 0.666667 1.333333 0.749310 x

x Nb 1 0.000000 0.000000 0.001088 x

x Nb 2 0.666667 0.333333 0.334422 x

x Nb 3 0.333333 0.666667 0.667755 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22321452E+003 701.47 <-- SCF

1 -6.22324139E+003 2.98554134E-003 702.50 <-- SCF

2 -6.22324253E+003 1.26848877E-004 704.41 <-- SCF

3 -6.22322788E+003 -1.62739650E-003 706.83 <-- SCF

4 -6.22322601E+003 -2.07842341E-004 709.14 <-- SCF

5 -6.22322552E+003 -5.46546542E-005 710.92 <-- SCF

6 -6.22322551E+003 -9.83248033E-007 712.83 <-- SCF

7 -6.22322551E+003 2.67829807E-008 714.62 <-- SCF

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

Final energy = -6223.225509139 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 -0.03367 \*

\* Se 2 0.00000 -0.00000 0.00202 \*

\* Se 3 0.00000 0.00000 -0.03367 \*

\* Se 4 0.00000 -0.00000 0.00202 \*

\* Se 5 -0.00000 0.00000 -0.03367 \*

\* Se 6 0.00000 -0.00000 0.00202 \*

\* Nb 1 0.00000 0.00000 0.03165 \*

\* Nb 2 0.00000 0.00000 0.03165 \*

\* Nb 3 -0.00000 -0.00000 0.03165 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.154100 -0.000000 -0.000000 \*

\* y -0.000000 -0.154100 0.000000 \*

\* z -0.000000 0.000000 -0.312467 \*

\* \*

\* Pressure: 0.2069 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000023 | -6223.225404 | <-- min BFGS

| trial step | 1.000000 | -0.000023 | -6223.225412 | <-- min BFGS

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

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

BFGS: improving iteration 14 with line minimization (lambda= 0.503572)

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Unit Cell

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

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

2.9892337 -1.7258349 -0.0000000 2.1019385 0.0000000 0.0000000

-0.0000000 3.4516698 0.0000000 1.0509692 1.8203321 0.0000000

-0.0000000 0.0000000 20.4686933 0.0000000 -0.0000000 0.3069656

Lattice parameters(A) Cell Angles

a = 3.451670 alpha = 90.000000

b = 3.451670 beta = 90.000000

c = 20.468693 gamma = 120.000000

Current cell volume = 211.192860 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.080187 x

x Se 2 0.333333 0.666667 0.082673 x

x Se 3 1.000000 1.000000 0.253146 x

x Se 4 1.000000 1.000000 0.416007 x

x Se 5 0.666667 1.333333 0.586480 x

x Se 6 0.666667 1.333333 0.749340 x

x Nb 1 0.000000 0.000000 0.001114 x

x Nb 2 0.666667 0.333333 0.334447 x

x Nb 3 0.333333 0.666667 0.667780 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22322368E+003 727.30 <-- SCF

1 -6.22322950E+003 6.47103501E-004 728.25 <-- SCF

2 -6.22322980E+003 3.29239813E-005 730.06 <-- SCF

3 -6.22322621E+003 -3.98987781E-004 731.62 <-- SCF

4 -6.22322573E+003 -5.37387002E-005 733.17 <-- SCF

5 -6.22322561E+003 -1.29016516E-005 734.66 <-- SCF

6 -6.22322560E+003 -8.16658691E-007 735.66 <-- SCF

7 -6.22322561E+003 4.23701713E-007 736.75 <-- SCF

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

Final energy = -6223.225606162 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 -0.00000 -0.00153 \*

\* Se 2 -0.00000 0.00000 -0.01384 \*

\* Se 3 0.00000 -0.00000 -0.00153 \*

\* Se 4 -0.00000 0.00000 -0.01384 \*

\* Se 5 -0.00000 -0.00000 -0.00153 \*

\* Se 6 -0.00000 -0.00000 -0.01384 \*

\* Nb 1 0.00000 0.00000 0.01536 \*

\* Nb 2 0.00000 -0.00000 0.01536 \*

\* Nb 3 0.00000 0.00000 0.01536 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.035355 -0.000000 0.000000 \*

\* y -0.000000 -0.035355 -0.000000 \*

\* z 0.000000 -0.000000 -0.198666 \*

\* \*

\* Pressure: 0.0898 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000023 | -6223.225404 | <-- min BFGS

| trial step | 1.000000 | -0.000023 | -6223.225412 | <-- min BFGS

| line step | 0.503572 | -1.095E-006 | -6223.225560 | <-- min BFGS

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

BFGS: finished iteration 14 with enthalpy= -6.22322556E+003 eV

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

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

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

| dE/ion | 1.742349E-005 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 1.536460E-002 | 3.000000E-002 | eV/A | Yes | <-- BFGS

| |dR|max | 1.146246E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 1.986665E-001 | 5.000000E-002 | GPa | No | <-- BFGS

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

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

Starting BFGS iteration 15 ...

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

Writing analysis data to 3R-NbSe2-US-7.castep\_bin

Writing model to 3R-NbSe2-US-7.check

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

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

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

| previous | 0.000000 | 0.000023 | -6223.225560 | <-- min BFGS

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

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

BFGS: starting iteration 15 with trial guess (lambda= 1.000000)

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

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

| Memory Disk |

| Model and support data 110.7 MB 92.7 MB |

| Electronic energy minimisation requirements 9.8 MB 0.0 MB |

| Geometry minimisation requirements 11.9 MB 0.0 MB |

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

| Approx. total storage required per process 132.5 MB 92.7 MB |

| |

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

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

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

Unit Cell

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

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

2.9875896 -1.7248856 -0.0000000 2.1030952 0.0000000 0.0000000

-0.0000000 3.4497713 0.0000000 1.0515476 1.8213339 -0.0000000

-0.0000000 0.0000000 20.5197372 0.0000000 -0.0000000 0.3062020

Lattice parameters(A) Cell Angles

a = 3.449771 alpha = 90.000000

b = 3.449771 beta = 90.000000

c = 20.519737 gamma = 120.000000

Current cell volume = 211.486683 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.080078 x

x Se 2 0.333333 0.666667 0.082591 x

x Se 3 1.000000 1.000000 0.253255 x

x Se 4 1.000000 1.000000 0.415924 x

x Se 5 0.666667 1.333333 0.586588 x

x Se 6 0.666667 1.333333 0.749257 x

x Nb 1 0.000000 0.000000 0.001088 x

x Nb 2 0.666667 0.333333 0.334421 x

x Nb 3 0.333333 0.666667 0.667754 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22320612E+003 748.44 <-- SCF

1 -6.22325760E+003 5.72055651E-003 749.52 <-- SCF

2 -6.22326071E+003 3.44662028E-004 751.23 <-- SCF

3 -6.22323242E+003 -3.14300503E-003 752.89 <-- SCF

4 -6.22322715E+003 -5.85363957E-004 754.33 <-- SCF

5 -6.22322581E+003 -1.49242885E-004 755.80 <-- SCF

6 -6.22322585E+003 4.36711018E-006 757.23 <-- SCF

7 -6.22322586E+003 1.04057295E-006 758.52 <-- SCF

8 -6.22322587E+003 1.02310833E-006 759.62 <-- SCF

9 -6.22322587E+003 3.10234317E-007 760.73 <-- SCF

10 -6.22322587E+003 3.58304884E-009 762.19 <-- SCF

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

Final energy = -6223.225868134 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.00485 \*

\* Se 2 0.00000 -0.00000 -0.03440 \*

\* Se 3 0.00000 -0.00000 0.00485 \*

\* Se 4 0.00000 0.00000 -0.03440 \*

\* Se 5 0.00000 -0.00000 0.00485 \*

\* Se 6 0.00000 0.00000 -0.03440 \*

\* Nb 1 -0.00000 0.00000 0.02955 \*

\* Nb 2 -0.00000 0.00000 0.02955 \*

\* Nb 3 -0.00000 -0.00000 0.02955 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.073381 0.000000 0.000000 \*

\* y 0.000000 -0.073381 -0.000000 \*

\* z 0.000000 -0.000000 0.015464 \*

\* \*

\* Pressure: 0.0438 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000023 | -6223.225560 | <-- min BFGS

| trial step | 1.000000 | 1.137E-007 | -6223.225851 | <-- min BFGS

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

BFGS: finished iteration 15 with enthalpy= -6.22322585E+003 eV

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

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

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

| dE/ion | 3.230742E-005 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 3.439540E-002 | 3.000000E-002 | eV/A | No | <-- BFGS

| |dR|max | 2.229438E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 7.338104E-002 | 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 | 0.000012 | -6223.225851 | <-- 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 110.7 MB 92.7 MB |

| Electronic energy minimisation requirements 9.9 MB 0.0 MB |

| Geometry minimisation requirements 12.0 MB 0.0 MB |

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

| Approx. total storage required per process 132.5 MB 92.7 MB |

| |

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

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

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Unit Cell

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

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

2.9882000 -1.7252381 -0.0000000 2.1026656 0.0000000 0.0000000

-0.0000000 3.4504761 0.0000000 1.0513328 1.8209618 -0.0000000

-0.0000000 0.0000000 20.5350523 0.0000000 -0.0000000 0.3059737

Lattice parameters(A) Cell Angles

a = 3.450476 alpha = 90.000000

b = 3.450476 beta = 90.000000

c = 20.535052 gamma = 120.000000

Current cell volume = 211.731024 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.080008 x

x Se 2 0.333333 0.666667 0.082487 x

x Se 3 1.000000 1.000000 0.253325 x

x Se 4 1.000000 1.000000 0.415821 x

x Se 5 0.666667 1.333333 0.586658 x

x Se 6 0.666667 1.333333 0.749154 x

x Nb 1 0.000000 0.000000 0.001121 x

x Nb 2 0.666667 0.333333 0.334454 x

x Nb 3 0.333333 0.666667 0.667788 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22321915E+003 775.88 <-- SCF

1 -6.22324439E+003 2.80416677E-003 776.92 <-- SCF

2 -6.22324594E+003 1.72214367E-004 778.66 <-- SCF

3 -6.22322953E+003 -1.82300997E-003 780.48 <-- SCF

4 -6.22322671E+003 -3.13611435E-004 782.08 <-- SCF

5 -6.22322607E+003 -7.14321976E-005 783.47 <-- SCF

6 -6.22322607E+003 5.77919242E-007 784.91 <-- SCF

7 -6.22322608E+003 1.00587815E-006 786.08 <-- SCF

8 -6.22322609E+003 6.27648482E-007 787.16 <-- SCF

9 -6.22322609E+003 1.57747816E-007 788.31 <-- SCF

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

Final energy = -6223.226088056 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 -0.00000 0.00255 \*

\* Se 2 0.00000 -0.00000 -0.01136 \*

\* Se 3 0.00000 -0.00000 0.00255 \*

\* Se 4 0.00000 -0.00000 -0.01136 \*

\* Se 5 0.00000 -0.00000 0.00255 \*

\* Se 6 0.00000 -0.00000 -0.01136 \*

\* Nb 1 -0.00000 -0.00000 0.00880 \*

\* Nb 2 -0.00000 -0.00000 0.00880 \*

\* Nb 3 -0.00000 -0.00000 0.00880 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.040817 0.000000 0.000000 \*

\* y 0.000000 -0.040817 0.000000 \*

\* z 0.000000 0.000000 -0.003714 \*

\* \*

\* Pressure: 0.0284 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000012 | -6223.225851 | <-- min BFGS

| trial step | 1.000000 | 4.668E-006 | -6223.226054 | <-- min BFGS

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

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

BFGS: improving iteration 16 with line minimization (lambda= 1.643152)

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

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

| Memory Disk |

| Model and support data 110.7 MB 92.7 MB |

| Electronic energy minimisation requirements 9.9 MB 0.0 MB |

| Geometry minimisation requirements 12.0 MB 0.0 MB |

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

| Approx. total storage required per process 132.5 MB 92.7 MB |

| |

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

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

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

Unit Cell

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

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

2.9885926 -1.7254647 -0.0000000 2.1023894 0.0000000 0.0000000

-0.0000000 3.4509295 0.0000000 1.0511947 1.8207226 -0.0000000

-0.0000000 0.0000000 20.5449023 0.0000000 -0.0000000 0.3058270

Lattice parameters(A) Cell Angles

a = 3.450929 alpha = 90.000000

b = 3.450929 beta = 90.000000

c = 20.544902 gamma = 120.000000

Current cell volume = 211.888250 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.079963 x

x Se 2 0.333333 0.666667 0.082421 x

x Se 3 1.000000 1.000000 0.253370 x

x Se 4 1.000000 1.000000 0.415754 x

x Se 5 0.666667 1.333333 0.586703 x

x Se 6 0.666667 1.333333 0.749088 x

x Nb 1 0.000000 0.000000 0.001142 x

x Nb 2 0.666667 0.333333 0.334476 x

x Nb 3 0.333333 0.666667 0.667809 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22322390E+003 800.25 <-- SCF

1 -6.22323370E+003 1.08875849E-003 801.30 <-- SCF

2 -6.22323433E+003 7.03262012E-005 802.89 <-- SCF

3 -6.22322753E+003 -7.55475876E-004 804.42 <-- SCF

4 -6.22322638E+003 -1.28240755E-004 806.05 <-- SCF

5 -6.22322611E+003 -2.95370501E-005 807.98 <-- SCF

6 -6.22322611E+003 -1.05832707E-007 809.61 <-- SCF

7 -6.22322612E+003 6.92631544E-007 811.59 <-- SCF

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

Final energy = -6223.226115630 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 0.00000 0.00000 0.00359 \*

\* Se 2 0.00000 0.00000 0.00319 \*

\* Se 3 0.00000 0.00000 0.00359 \*

\* Se 4 0.00000 0.00000 0.00319 \*

\* Se 5 0.00000 0.00000 0.00359 \*

\* Se 6 0.00000 0.00000 0.00319 \*

\* Nb 1 -0.00000 -0.00000 -0.00679 \*

\* Nb 2 -0.00000 -0.00000 -0.00679 \*

\* Nb 3 -0.00000 -0.00000 -0.00679 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.007794 -0.000000 0.000000 \*

\* y -0.000000 -0.007794 0.000000 \*

\* z 0.000000 0.000000 0.002205 \*

\* \*

\* Pressure: 0.0045 \*

\* \*

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

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

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

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

| previous | 0.000000 | 0.000012 | -6223.225851 | <-- min BFGS

| trial step | 1.000000 | 4.668E-006 | -6223.226054 | <-- min BFGS

| line step | 1.643152 | -6.166E-007 | -6223.226089 | <-- min BFGS

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

BFGS: finished iteration 16 with enthalpy= -6.22322609E+003 eV

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

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

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

| dE/ion | 2.638149E-005 | 1.000000E-005 | eV | No | <-- BFGS

| |F|max | 6.787713E-003 | 3.000000E-002 | eV/A | Yes | <-- BFGS

| |dR|max | 3.485839E-003 | 1.000000E-003 | A | No | <-- BFGS

| Smax | 7.793668E-003 | 5.000000E-002 | GPa | Yes | <-- BFGS

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

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

Starting BFGS iteration 17 ...

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

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

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

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

| previous | 0.000000 | 2.892E-007 | -6223.226089 | <-- 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 111.1 MB 92.7 MB |

| Electronic energy minimisation requirements 9.9 MB 0.0 MB |

| Geometry minimisation requirements 12.0 MB 0.0 MB |

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

| Approx. total storage required per process 133.0 MB 92.7 MB |

| |

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

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

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

Unit Cell

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

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

2.9887249 -1.7255411 -0.0000000 2.1022963 0.0000000 0.0000000

-0.0000000 3.4510823 0.0000000 1.0511481 1.8206420 -0.0000000

-0.0000000 0.0000000 20.5442257 0.0000000 -0.0000000 0.3058370

Lattice parameters(A) Cell Angles

a = 3.451082 alpha = 90.000000

b = 3.451082 beta = 90.000000

c = 20.544226 gamma = 120.000000

Current cell volume = 211.900041 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 0.333333 0.666667 -0.079958 x

x Se 2 0.333333 0.666667 0.082426 x

x Se 3 1.000000 1.000000 0.253376 x

x Se 4 1.000000 1.000000 0.415759 x

x Se 5 0.666667 1.333333 0.586709 x

x Se 6 0.666667 1.333333 0.749093 x

x Nb 1 0.000000 0.000000 0.001132 x

x Nb 2 0.666667 0.333333 0.334465 x

x Nb 3 0.333333 0.666667 0.667798 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

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

SCF loop Energy Energy gain Timer <-- SCF

per atom (sec) <-- SCF

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

Initial -6.22322707E+003 824.83 <-- SCF

1 -6.22322631E+003 -8.45237113E-005 825.86 <-- SCF

2 -6.22322632E+003 1.22743493E-006 827.08 <-- SCF

3 -6.22322614E+003 -1.97477843E-005 828.47 <-- SCF

4 -6.22322612E+003 -2.88645984E-006 829.77 <-- SCF

5 -6.22322612E+003 8.63546050E-008 830.80 <-- SCF

6 -6.22322612E+003 4.84443740E-008 831.88 <-- SCF

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

Final energy = -6223.226117402 eV

(energy not corrected for finite basis set)

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

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 0.00023 \*

\* Se 2 0.00000 0.00000 0.00112 \*

\* Se 3 0.00000 0.00000 0.00023 \*

\* Se 4 -0.00000 0.00000 0.00112 \*

\* Se 5 0.00000 0.00000 0.00023 \*

\* Se 6 0.00000 0.00000 0.00112 \*

\* Nb 1 -0.00000 0.00000 -0.00135 \*

\* Nb 2 0.00000 -0.00000 -0.00135 \*

\* Nb 3 -0.00000 0.00000 -0.00135 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.006699 0.000000 -0.000000 \*

\* y 0.000000 -0.006699 -0.000000 \*

\* z -0.000000 -0.000000 -0.014314 \*

\* \*

\* Pressure: 0.0092 \*

\* \*

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

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

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

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

| previous | 0.000000 | 2.892E-007 | -6223.226089 | <-- min BFGS

| trial step | 1.000000 | 5.512E-008 | -6223.226096 | <-- min BFGS

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

BFGS: finished iteration 17 with enthalpy= -6.22322610E+003 eV

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

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

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

| dE/ion | 7.576014E-007 | 1.000000E-005 | eV | Yes | <-- BFGS

| |F|max | 1.345079E-003 | 3.000000E-002 | eV/A | Yes | <-- BFGS

| |dR|max | 2.242847E-004 | 1.000000E-003 | A | Yes | <-- BFGS

| Smax | 1.431386E-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)

2.9887249 -1.7255411 -0.0000000 2.1022963 0.0000000 0.0000000

-0.0000000 3.4510823 0.0000000 1.0511481 1.8206420 -0.0000000

-0.0000000 0.0000000 20.5442257 0.0000000 -0.0000000 0.3058370

Lattice parameters(A) Cell Angles

a = 3.451082 alpha = 90.000000

b = 3.451082 beta = 90.000000

c = 20.544226 gamma = 120.000000

Current cell volume = 211.900041 A\*\*3

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

Cell Contents

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

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

x Element Atom Fractional coordinates of atoms x

x Number u v w x

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

x Se 1 0.333333 0.666667 -0.079958 x

x Se 2 0.333333 0.666667 0.082426 x

x Se 3 1.000000 1.000000 0.253376 x

x Se 4 1.000000 1.000000 0.415759 x

x Se 5 0.666667 1.333333 0.586709 x

x Se 6 0.666667 1.333333 0.749093 x

x Nb 1 0.000000 0.000000 0.001132 x

x Nb 2 0.666667 0.333333 0.334465 x

x Nb 3 0.333333 0.666667 0.667798 x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

BFGS: Final Enthalpy = -6.22322610E+003 eV

BFGS: Final <frequency> = 311.93470 cm-1

BFGS: Final bulk modulus = 24.06518 GPa

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Symmetrised Forces \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* \*

\* Cartesian components (eV/A) \*

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

\* x y z \*

\* \*

\* Se 1 -0.00000 0.00000 0.00023 \*

\* Se 2 0.00000 0.00000 0.00112 \*

\* Se 3 0.00000 0.00000 0.00023 \*

\* Se 4 -0.00000 0.00000 0.00112 \*

\* Se 5 0.00000 0.00000 0.00023 \*

\* Se 6 0.00000 0.00000 0.00112 \*

\* Nb 1 -0.00000 0.00000 -0.00135 \*

\* Nb 2 0.00000 -0.00000 -0.00135 \*

\* Nb 3 -0.00000 0.00000 -0.00135 \*

\* \*

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

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

\* \*

\* Cartesian components (GPa) \*

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

\* x y z \*

\* \*

\* x -0.006699 0.000000 -0.000000 \*

\* y 0.000000 -0.006699 -0.000000 \*

\* z -0.000000 -0.000000 -0.014314 \*

\* \*

\* Pressure: 0.0092 \*

\* \*

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

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 = 0.25%

Atomic Populations (Mulliken)

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

Species Ion s p d f Total Charge (e)

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

Se 1 1.66 4.15 0.00 0.00 5.82 0.18

Se 2 1.65 4.15 0.00 0.00 5.81 0.19

Se 3 1.66 4.15 0.00 0.00 5.82 0.18

Se 4 1.65 4.15 0.00 0.00 5.81 0.19

Se 5 1.66 4.15 0.00 0.00 5.82 0.18

Se 6 1.65 4.15 0.00 0.00 5.81 0.19

Nb 1 2.61 6.85 3.92 0.00 13.38 -0.38

Nb 2 2.61 6.85 3.92 0.00 13.38 -0.38

Nb 3 2.61 6.85 3.92 0.00 13.38 -0.38

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

Bond Population Length (A)

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

Se 5 -- Nb 3 0.24 2.59716

Se 3 -- Nb 2 0.24 2.59716

Se 1 -- Nb 1 0.24 2.59716

Se 4 -- Nb 2 0.29 2.59987

Se 2 -- Nb 1 0.29 2.59987

Se 6 -- Nb 3 0.29 2.59987

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

All bands spilling parameter for spin component 1 = 0.25%

Hirshfeld Analysis

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

Species Ion Hirshfeld Charge (e) Spin (hbar/2)

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

Se 1 -0.13 0.00

Se 2 -0.13 0.00

Se 3 -0.13 0.00

Se 4 -0.13 0.00

Se 5 -0.13 0.00

Se 6 -0.13 0.00

Nb 1 0.26 0.00

Nb 2 0.26 0.00

Nb 3 0.26 0.00

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

Writing analysis data to 3R-NbSe2-US-7.castep\_bin

Writing model to 3R-NbSe2-US-7.check

A BibTeX formatted list of references used in this run has been written to

3R-NbSe2-US-7.bib

Initialisation time = 0.62 s

Calculation time = 844.14 s

Finalisation time = 1.69 s

Total time = 846.45 s

Overall parallel efficiency rating: Satisfactory (69%)

Data was distributed by:-

G-vector (2-way); efficiency rating: Very good (83%)

k-point (7-way); efficiency rating: Very good (80%)