PROGRESS REPORT: Visualizing Crystal Structures

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GENERAL METHOD FOR VISUALIZING MATERIALS USING POSCAR FILE

- **Create Structure:** Start by generating a crystal structure using a POSCAR file.
- **Visualize with VESTA:** Open the POSCAR file in VESTA. Adjust lattice parameters and explore the structure visually.
- **Convert to QE Input:** Once satisfied, convert the modified structure into an input file for Quantum ESPRESSO (QE) simulations.

BASICS OF A POSCAR FILE

BASICS OF A POSCAR FILE .....

1. GeH # This line is a comment. Ideally, you write the name of your system.
2. 4.0 4.0 1.0 # Universal scaling factor[1]. If negative, it's the total volume of the cell.
3. 0.5 -0.86 0.0 # 1st lattice vector
4. 0.5 0.86 0.0 # 2nd lattice vector
5. 0.0 0.0 15.0 # 3rd lattice vector
6. Ge H # Indicate the atomic species in your system. If you omit this line, it will follow the order in POTCAR.
7. 2 2 # Indicate how many atoms per element
8. Selective dynamics # Provides control over changing the respective coordinates of an atom during ionic relaxation[2]. Optional.
9. Direct # Cartesian coordinates or Direct (fractional) coordinates
10. 0.00 0.0 0 0.00 F F F
11. 0.33 0.67 0.02 T T T
12. 0.33 0.67 0.92 T T T
13. 0.00 0.00 0.10 T T T

[1]In this example, each of the scaling factor is only applied to the values under its respective column. However, if you input only one scaling factor then all values of all the lattice vectors are multiplied to this scaling factor.

[2]The default values of the selective dynamics flags are T.

*Letters with this color means that it's case-insensitive.

*Letters in this color are the only relevant characters for the specified command/argument.

Macam, Gennevieve 2016. (NSYSU Computational Materials Laboratory)

CRYSTAL STRUCTURES

Ashcroft & Merlin, 1976, pg. xv

Face-Centered Cubic (FCC) Crystal Structure

Elements with Face-Centered Cubic (FCC) crystal structure

Table 4.1
ELEMENTS WITH THE MONATOMIC FACE-CENTERED CUBIC CRYSTAL STRUCTURE

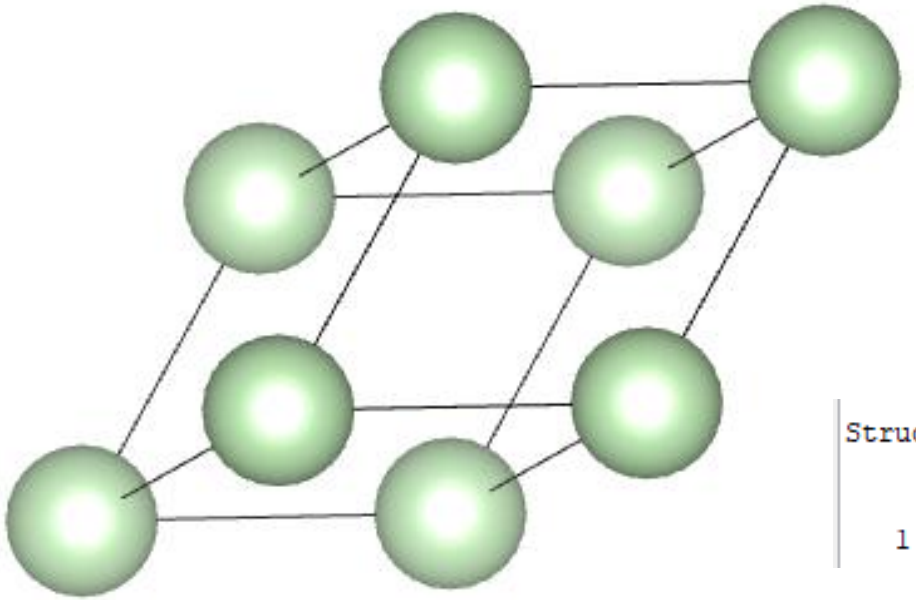
ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ar	5.26 (4.2 K)	Ir	3.84	Pt	3.92
Ag	4.09	Kr	5.72 (58 K)	δ-Pu	4.64
Al	4.05	La	5.30	Rh	3.80
Au	4.08	Ne	4.43 (4.2 K)	Sc	4.54
Ca	5.58	Ni	3.52	Sr	6.08
Ce	5.16	Pb	4.95	Th	5.08
β-Co	3.55	Pd	3.89	Xe (58 K)	6.20
Cu	3.61	Pr	5.16	Yb	5.49

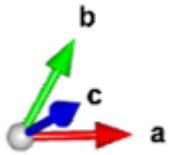
Ashcroft & Merlin, 1976, pg. 70

ARGON (Ar)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_argon_primitive
Argon FCC Primitive Crystal Structure
5.26
0.0 0.5 0.5
0.5 0.0 0.5
0.5 0.5 0.0
Ar
1
Direct
0.0 0.0 0.0
```

POSCAR file for primitive unit cell





Lattice parameters

a	b	c	alpha	beta	gamma
3.71938	3.71938	3.71938	60.0000	60.0000	60.0000

Unit-cell volume = 36.382891 Å^3

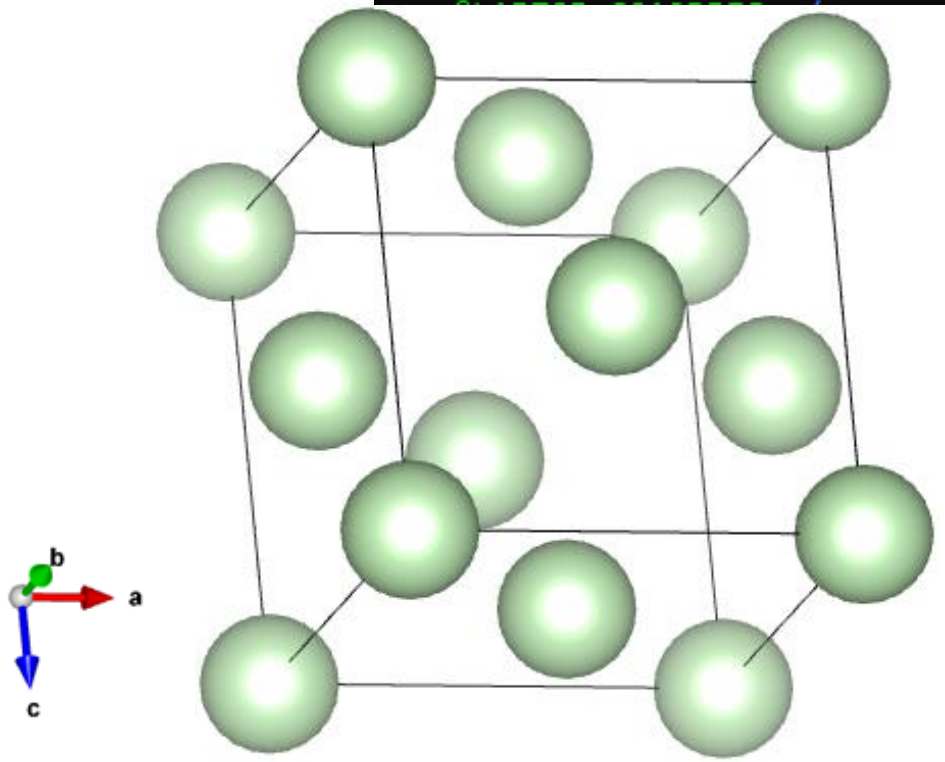
Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Ar	Ar1	0.00000	0.00000	0.00000	1.000	0.000	1a	1

ARGON (Ar)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_argon_conventional
Argon FCC Crystal Structure Conventional
5.26
1 0.0 0.0
0.0 1 0.0
0.0 0.0 1
Ar
4
Direct
0.0 0.0 0.0
0.5 0.5 0.0
0.5 0.0 0.5
0.0 0.5 0.5
```

POSCAR file for conventional unit cell



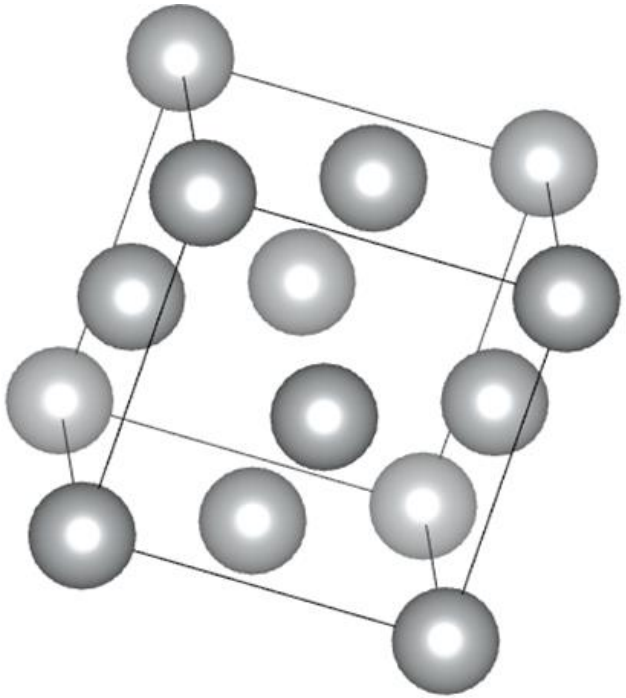

```
Lattice parameters

    a         b         c        alpha     beta      gamma
 5.26000   5.26000   5.26000   90.0000   90.0000   90.0000

Unit-cell volume = 145.531595 Å^3
```

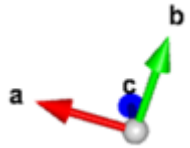
```
Structure parameters

                        x         y         z        Occ.     U     Site      Sym.
   1 Ar  Ar1         0.00000   0.00000   0.00000   1.000   0.000    1a          1
   2 Ar  Ar2         0.50000   0.50000   0.00000   1.000   0.000    1a          1
   3 Ar  Ar3         0.50000   0.00000   0.50000   1.000   0.000    1a          1
   4 Ar  Ar4         0.00000   0.50000   0.50000   1.000   0.000    1a          1
```

SILVER (Ag)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_silver_conventional
Ag FCC Conventional Crystal Structure
4.09
1 0.0 0.0
0.0 1 0.0
0.0 0.0 1
Ag
4
Direct
0.0 0.0 0.0
0.5 0.5 0.0
0.5 0.0 0.5
0.0 0.5 0.5
```

POSCAR file for conventional unit cell





Lattice parameters

a	b	c	alpha	beta	gamma
4.09000	4.09000	4.09000	90.0000	90.0000	90.0000

Unit-cell volume = 68.417937 Å^3

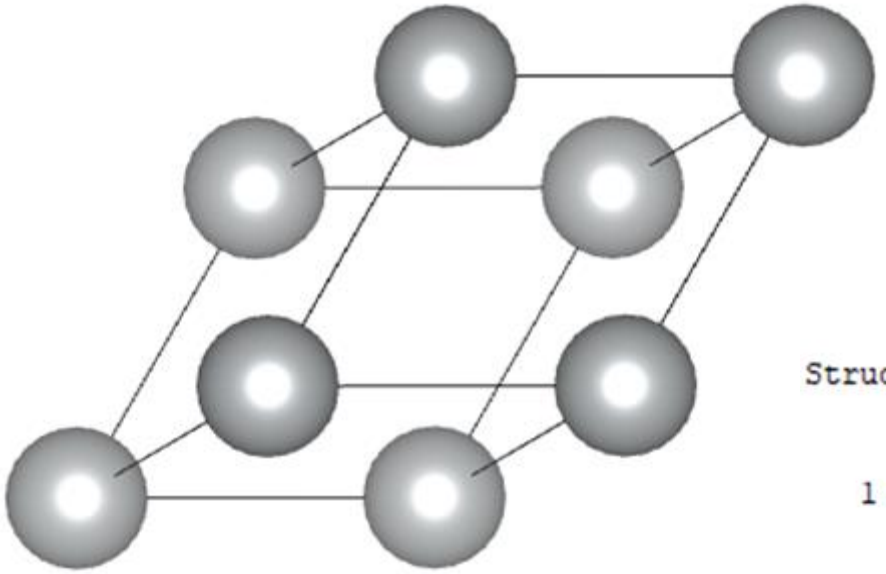
Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Ag	Ag1	0.00000	0.00000	0.00000	1.000	0.000	1a	1
2	Ag	Ag2	0.50000	0.50000	0.00000	1.000	0.000	1a	1
3	Ag	Ag3	0.50000	0.00000	0.50000	1.000	0.000	1a	1
4	Ag	Ag4	0.00000	0.50000	0.50000	1.000	0.000	1a	1

SILVER (Ag)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_silver_primitive
Silver FCC Primitive Crystal Structure
4.09
0.0 0.5 0.5
0.5 0.0 0.5
0.5 0.5 0.0
Ag
1
Direct
0.0 0.0 0.0
```

POSCAR file for primitive unit cell



Lattice parameters

a	b	c	alpha	beta	gamma
2.89207	2.89207	2.89207	60.0000	60.0000	60.0000

Unit-cell volume = 17.104488 Å^3

Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Ag	Ag1	0.00000	0.00000	0.00000	1.000	0.000	1a	1

Body-Centered Cubic (BCC) Crystal Structure

Elements with Body-Centered Cubic (BCC) crystal structure

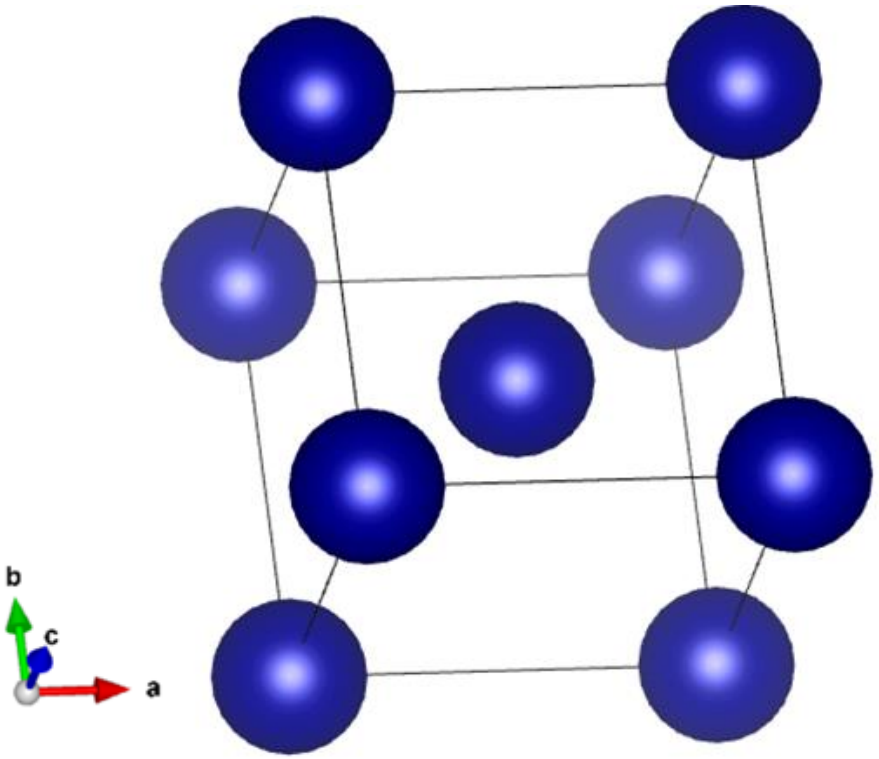
ELEMENTS WITH THE MONATOMIC BODY-CENTERED CUBIC CRYSTAL STRUCTURE

ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ba	5.02	Li	3.49 (78 K)	Ta	3.31
Cr	2.88	Mo	3.15	Tl	3.88
Cs	6.05 (78 K)	Na	4.23 (5 K)	V	3.02
Fe	2.87	Nb	3.30	W	3.16
K	5.23 (5 K)	Rb	5.59 (5 K)		

Ashcroft & Merlin, 1976, pg. 70

CHROMIUM (Cr)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Chromium_conventional
Cr BCC Conventional Crystal Structure
2.88
1 0 0
0 1 0
0 0 1
Cr
2
direct
0.0 0.0 0.0
0.5 0.5 0.5
```



POSCAR file for conventional unit cell

Lattice parameters

a	b	c	alpha	beta	gamma
2.88000	2.88000	2.88000	90.0000	90.0000	90.0000

Unit-cell volume = 23.887875 Å^3

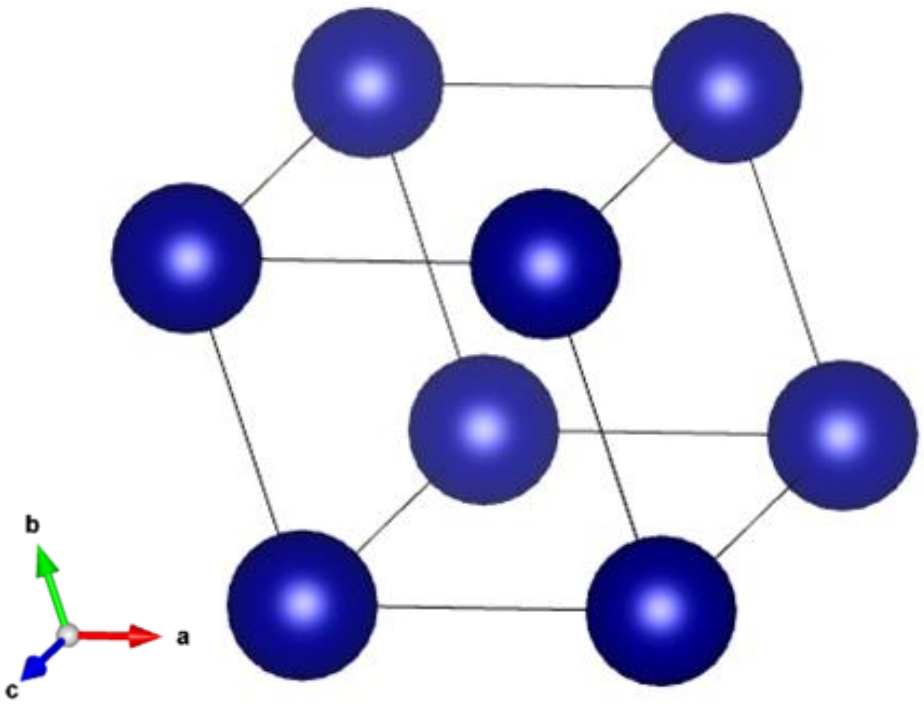
Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Cr	Cr1	0.00000	0.00000	0.00000	1.000	0.000	1a	1
2	Cr	Cr2	0.50000	0.50000	0.50000	1.000	0.000	1a	1

CHROMIUM (Cr)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Chromium_primitive
Chromium BCC Primitive Crystal Structure
2.88
0.5 0.5 -0.5
-0.5 0.5 0.5
0.5 -0.5 0.5
Cr
1
Direct
0.0 0.0 0.0
```

POSCAR file for primitive unit cell

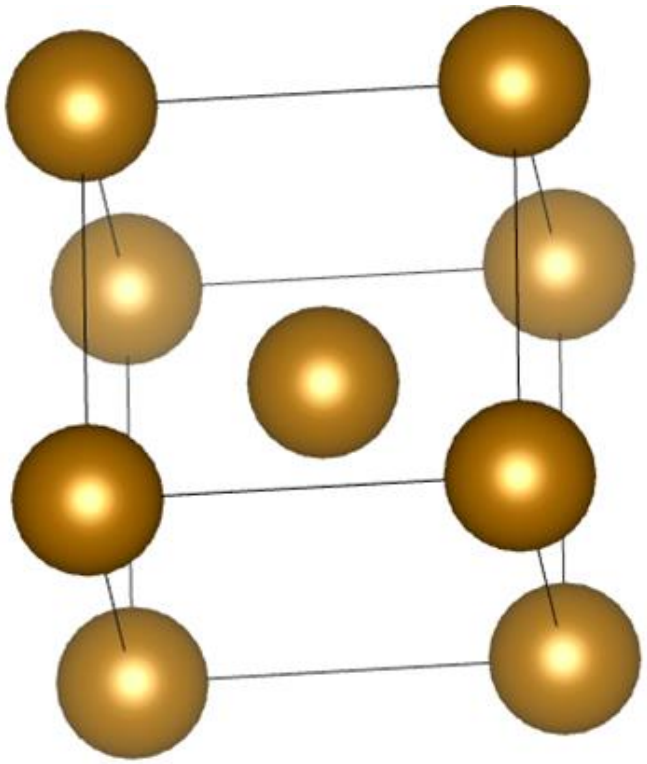



```
Lattice parameters

    a         b         c       alpha      beta       gamma
 2.49415   2.49415   2.49415 109.4712 109.4712 109.4712

Unit-cell volume = 11.943937 Å^3

Structure parameters

                        x         y         z        Occ.     U     Site       Sym.
   1 Cr  Cr1         0.00000   0.00000   0.00000   1.000    0.000    1a          1
```

IRON (Fe)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Iron_conventional
Iron BCC Conventional Crystal Structure
2.87
1 0 0
0 1 0
0 0 1
Fe
2
direct
0.0 0.0 0.0
0.5 0.5 0.5
```

POSCAR file for conventional unit cell



Lattice parameters

a	b	c	alpha	beta	gamma
2.87000	2.87000	2.87000	90.0000	90.0000	90.0000

Unit-cell volume = 23.639900 Å^3

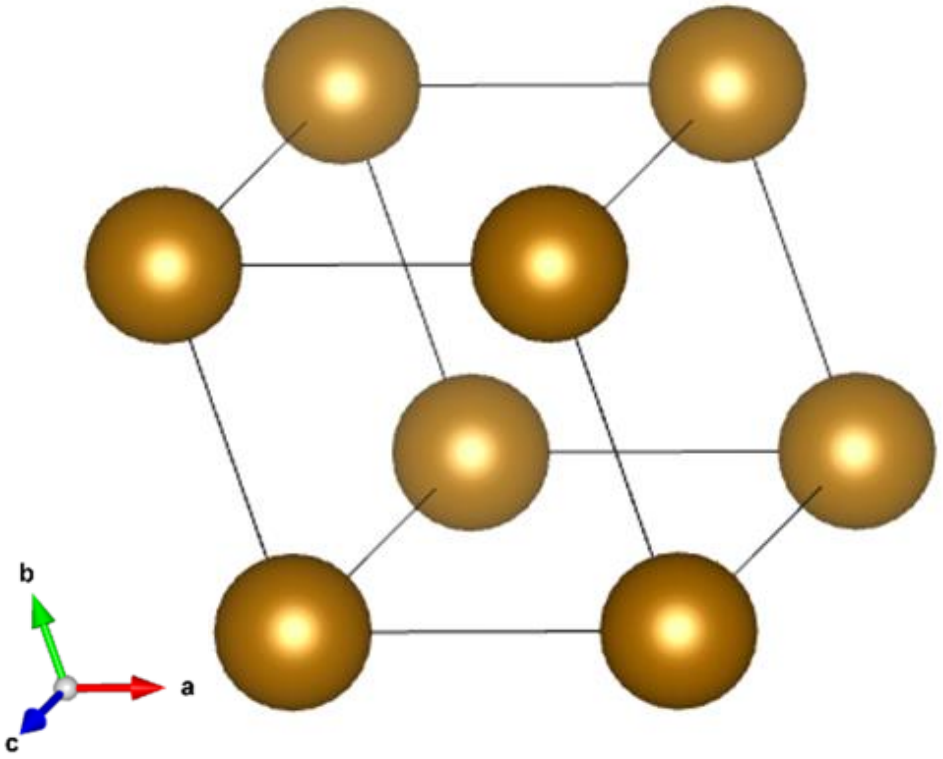
Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Fe	Fe1	0.00000	0.00000	0.00000	1.000	0.000	1a	1
2	Fe	Fe2	0.50000	0.50000	0.50000	1.000	0.000	1a	1

IRON (Fe)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Iron_primitive
Iron BCC Primitive Crystal Structure
2.87
0.5 0.5 -0.5
-0.5 0.5 0.5
0.5 -0.5 0.5
Fe
1
Direct
0.0 0.0 0.0
```

POSCAR file for primitive unit cell




```
Lattice parameters

   a        b        c        alpha    beta     gamma
 2.48549  2.48549  2.48549 109.4712 109.4712 109.4712

Unit-cell volume = 11.819948 Å^3
```

```
Structure parameters

                        x          y          z          Occ.     U     Site       Sym.
 1 Fe  Fe1          0.00000    0.00000    0.00000    1.000    0.000    1a           1
```

Tetragonal Crystal Structure

Elements with Tetragonal crystal structure

Table 7.6
ELEMENTS WITH TETRAGONAL BRAVAIS LATTICES[a]

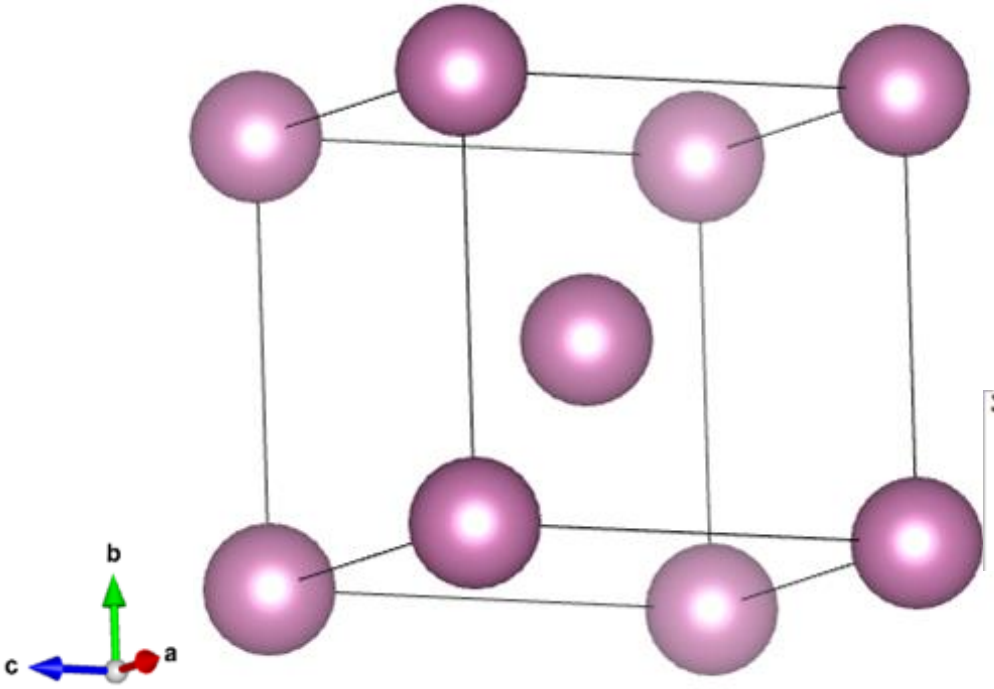
ELEMENT	a (Å)	c (Å)	BASIS
In	4.59	4.94	At face-centered positions of the conventional cell
Sn (white)	5.82	3.17	At 000, $0\,\frac{1}{2}\,\frac{1}{4}$, $\frac{1}{2}\,0\,\frac{3}{4}$, $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$, with respect to the axes of the conventional cell

Ashcroft & Merlin, 1976, pg. 127

INDIUM (In)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Indium_conventional
Indium Tetragonal Conventional Crystal Structure
4.59
1 0.0 0.0
0.0 1 0.0
0.0 0.0 1.08
In
2
Direct
0.0 0.0 0.0
0.5 0.5 0.5
```

POSCAR file for conventional unit cell



Lattice parameters

a	b	c	alpha	beta	gamma
4.59000	4.59000	4.95720	90.0000	90.0000	90.0000

Unit-cell volume = 104.438793 Å^3

Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	In	In1	0.00000	0.00000	0.00000	1.000	0.000	1a	1
2	In	In2	0.50000	0.50000	0.50000	1.000	0.000	1a	1

Hexagonal close-packed Crystal Structure

Elements with Hexagonal close-packed crystal structure

Table 4.4
ELEMENTS WITH THE HEXAGONAL CLOSE-PACKED CRYSTAL STRUCTURE

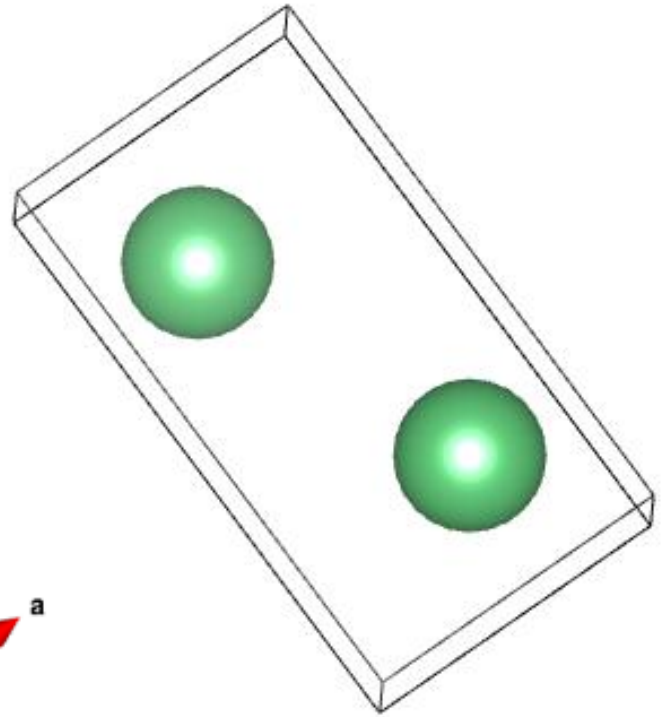
ELEMENT	a (Å)	c	c/a	ELEMENT	a (Å)	c	c/a
Be	2.29	3.58	1.56	Os	2.74	4.32	1.58
Cd	2.98	5.62	1.89	Pr	3.67	5.92	1.61
Ce	3.65	5.96	1.63	Re	2.76	4.46	1.62
α-Co	2.51	4.07	1.62	Ru	2.70	4.28	1.59
Dy	3.59	5.65	1.57	Sc	3.31	5.27	1.59
Er	3.56	5.59	1.57	Tb	3.60	5.69	1.58
Gd	3.64	5.78	1.59	Ti	2.95	4.69	1.59
He (2 K)	3.57	5.83	1.63	Tl	3.46	5.53	1.60
Hf	3.20	5.06	1.58	Tm	3.54	5.55	1.57
Ho	3.58	5.62	1.57	Y	3.65	5.73	1.57
La	3.75	6.07	1.62	Zn	2.66	4.95	1.86
Lu	3.50	5.55	1.59	Zr	3.23	5.15	1.59
Mg	3.21	5.21	1.62		—	—	
Nd	3.66	5.90	1.61	"Ideal"			1.63

Ashcroft & Merlin, 1976, pg. 77

BERYLLIUM (Be)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Beryllium_conventional
Beryllium close-packed hexagonal conventional crystal structure
2.29
1.00000000 0.00000000 0.00000000
-0.50000000 0.86602540 0.00000000
0.00000000 0.00000000 1.56000000
Be
2
Direct
0.33333333 0.66666667 0.75000000
0.66666667 0.33333333 0.25000000
```

POSCAR file for conventional unit cell



Lattice parameters

a	b	c	alpha	beta	gamma
2.29000	2.29000	3.57240	90.0000	90.0000	120.0000

Unit-cell volume = 16.224138 Å^3

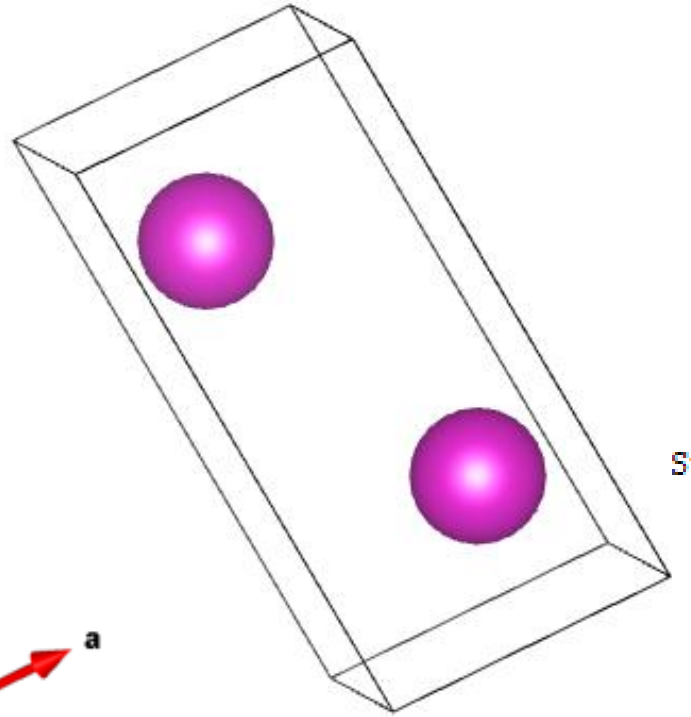
Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Be	Be1	0.33333	0.66667	0.75000	1.000	0.000	1a	1
2	Be	Be2	0.66667	0.33333	0.25000	1.000	0.000	1a	1

CADMIUM (Cd)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Cadmium_conventional
Cadmium close-packed hexagonal conventional crystal structure
2.98
1.00000000 0.00000000 0.00000000
-0.5000000 0.86600254 0.00000000
0.00000000 0.00000000 1.89000000
Cd
2
Direct
0.33333333 0.66666667 0.75000000
0.66666667 0.33333333 0.25000000
```

POSCAR file for conventional unit cell



Lattice parameters

a	b	c	alpha	beta	gamma
2.98000	2.97994	5.63220	90.0000	90.0000	120.0007

Unit-cell volume = 43.314150 Å^3

Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Cd	Cd1	0.33333	0.66667	0.75000	1.000	0.000	1a	1
2	Cd	Cd2	0.66667	0.33333	0.25000	1.000	0.000	1a	1

Diamond Crystal Structure

Elements with Diamond crystal structure

ELEMENTS WITH THE DIAMOND CRYSTAL STRUCTURE

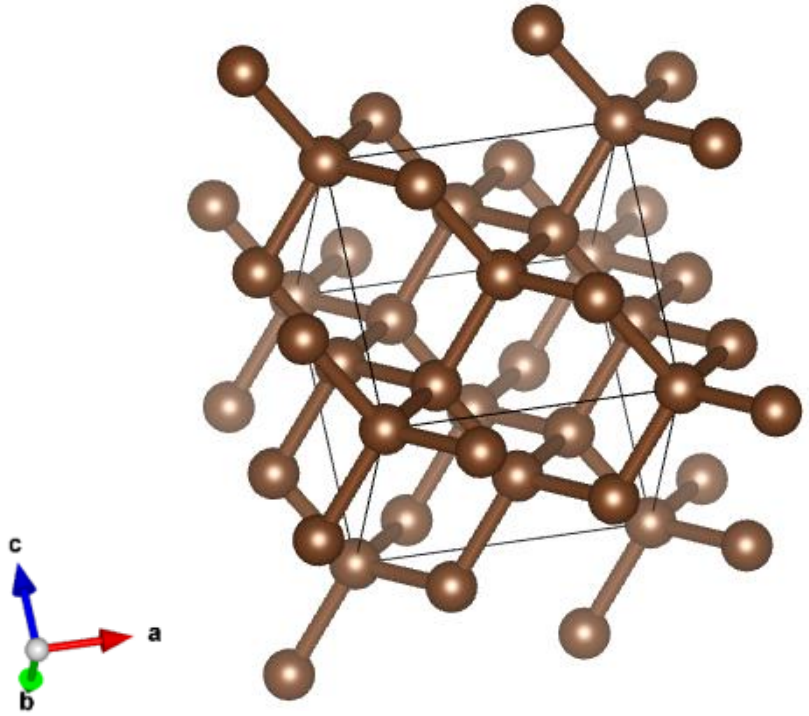
ELEMENT	CUBE SIDE a (Å)
C (diamond)	3.57
Si	5.43
Ge	5.66
α-Sn (grey)	6.49

Ashcroft & Merlin, 1976, pg. 76

CARBON (C)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Carbon_Conventional
Carbon Diamond crystal structure
3.57
1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0
C
8
Direct
0.000 0.000 0.000
0.000 0.500 0.500
0.500 0.000 0.500
0.500 0.500 0.000
0.250 0.250 0.250
0.250 0.750 0.750
0.750 0.250 0.750
0.750 0.750 0.250
```

POSCAR file for conventional unit cell



Lattice parameters

a	b	c	alpha	beta	gamma
3.57000	3.57000	3.57000	90.0000	90.0000	90.0000

Unit-cell volume = 45.499290 Å^3

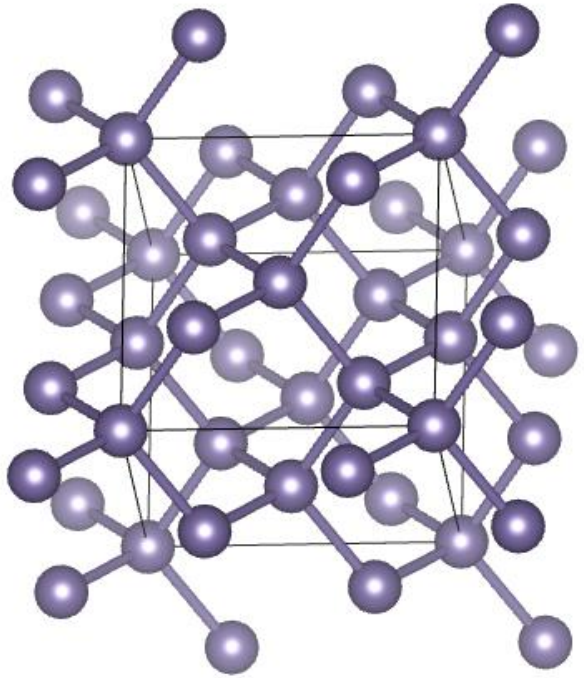
Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	C	C1	0.00000	0.00000	0.00000	1.000	0.000	1a	1
2	C	C2	0.00000	0.50000	0.50000	1.000	0.000	1a	1
3	C	C3	0.50000	0.00000	0.50000	1.000	0.000	1a	1
4	C	C4	0.50000	0.50000	0.00000	1.000	0.000	1a	1
5	C	C5	0.25000	0.25000	0.25000	1.000	0.000	1a	1
6	C	C6	0.25000	0.75000	0.75000	1.000	0.000	1a	1
7	C	C7	0.75000	0.25000	0.75000	1.000	0.000	1a	1
8	C	C8	0.75000	0.75000	0.25000	1.000	0.000	1a	1

GERMANIUM (Ge)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Germanium_Conventional
Germanium diamond conventional crystal structure
5.66
1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0
Ge
8
Direct
0.000 0.000 0.000
0.000 0.500 0.500
0.500 0.000 0.500
0.500 0.500 0.000
0.250 0.250 0.250
0.250 0.750 0.750
0.750 0.250 0.750
0.750 0.750 0.250
```

POSCAR file for conventional unit cell



Lattice parameters

a	b	c	alpha	beta	gamma
5.66000	5.66000	5.66000	90.0000	90.0000	90.0000

Unit-cell volume = 181.321481 Å^3

Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Ge	Ge1	0.00000	0.00000	0.00000	1.000	0.000	1a	1
2	Ge	Ge2	0.00000	0.50000	0.50000	1.000	0.000	1a	1
3	Ge	Ge3	0.50000	0.00000	0.50000	1.000	0.000	1a	1
4	Ge	Ge4	0.50000	0.50000	0.00000	1.000	0.000	1a	1
5	Ge	Ge5	0.25000	0.25000	0.25000	1.000	0.000	1a	1
6	Ge	Ge6	0.25000	0.75000	0.75000	1.000	0.000	1a	1
7	Ge	Ge7	0.75000	0.25000	0.75000	1.000	0.000	1a	1
8	Ge	Ge8	0.75000	0.75000	0.25000	1.000	0.000	1a	1

Rhombohedral (trigonal) Crystal Structure

Elements with Rhombohedral (trigonal) crystal structure

Table 7.5
ELEMENTS WITH RHOMBOHEDRAL (TRIGONAL) BRAVAIS LATTICES[a]

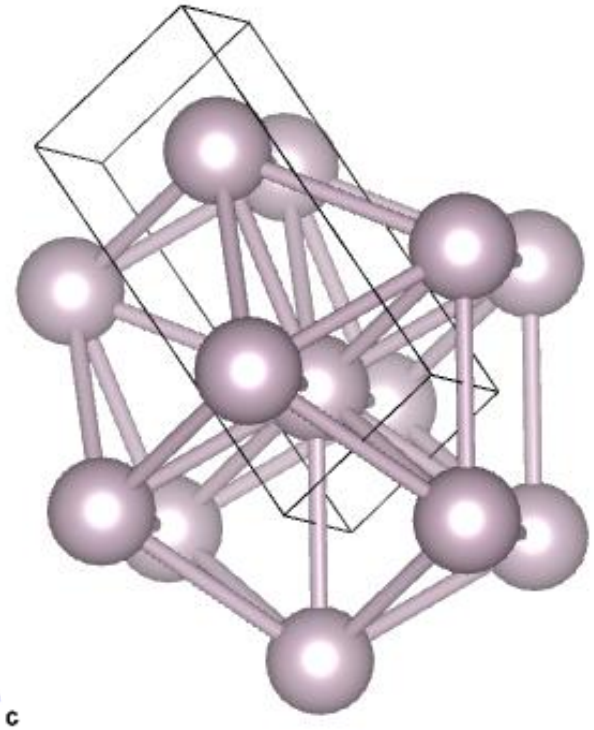
ELEMENT	a (Å)	θ	ATOMS IN PRIMITIVE CELL	BASIS
Hg (5 K)	2.99	70°45′	1	$x = 0$
As	4.13	54°10′	2	$x = \pm 0.226$
Sb	4.51	57°6′	2	$x = \pm 0.233$
Bi	4.75	57°14′	2	$x = \pm 0.237$
Sm	9.00	23°13′	3	$x = 0, \pm 0.222$

Ashcroft & Merlin, 1976, pg. 127

MERCURY (Hg)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR
Mercury Rhombohedral (Trigonal) Conventional Crystal Structure
2.99
1.0000 0.0000 0.00000
-0.5000 0.8660 0.0000
0.0000 0.0000 1.7321
Hg
2
direct
0.3333 0.6667 0.7500
0.6667 0.3333 0.2500
```

POSCAR file for conventional unit cell




```
Lattice parameters

   a         b         c        alpha     beta      gamma
 2.99000   2.98993   5.17898   90.0000   90.0000 120.0007

Unit-cell volume = 40.096312 Å^3

Structure parameters

                        x         y         z         Occ.     U     Site       Sym.
   1 Hg  Hg1         0.33330   0.66670   0.75000   1.000    0.000    1a          1
   2 Hg  Hg2         0.66670   0.33330   0.25000   1.000    0.000    1a          1
```

Sodium chloride crystal structure

Compounds with Sodium chloride crystal structure

Table 4.5
SOME COMPOUNDS WITH THE SODIUM CHLORIDE STRUCTURE

CRYSTAL	a (Å)	CRYSTAL	a (Å)	CRYSTAL	a (Å)
LiF	4.02	RbF	5.64	CaS	5.69
LiCl	5.13	RbCl	6.58	CaSe	5.91
LiBr	5.50	RbBr	6.85	CaTe	6.34
LiI	6.00	RbI	7.34	SrO	5.16
NaF	4.62	CsF	6.01	SrS	6.02
NaCl	5.64	AgF	4.92	SrSe	6.23
NaBr	5.97	AgCl	5.55	SrTe	6.47
NaI	6.47	AgBr	5.77	BaO	5.52
KF	5.35	MgO	4.21	BaS	6.39
KCl	6.29	MgS	5.20	BaSe	6.60
KBr	6.60	MgSe	5.45	BaTe	6.99
KI	7.07	CaO	4.81		

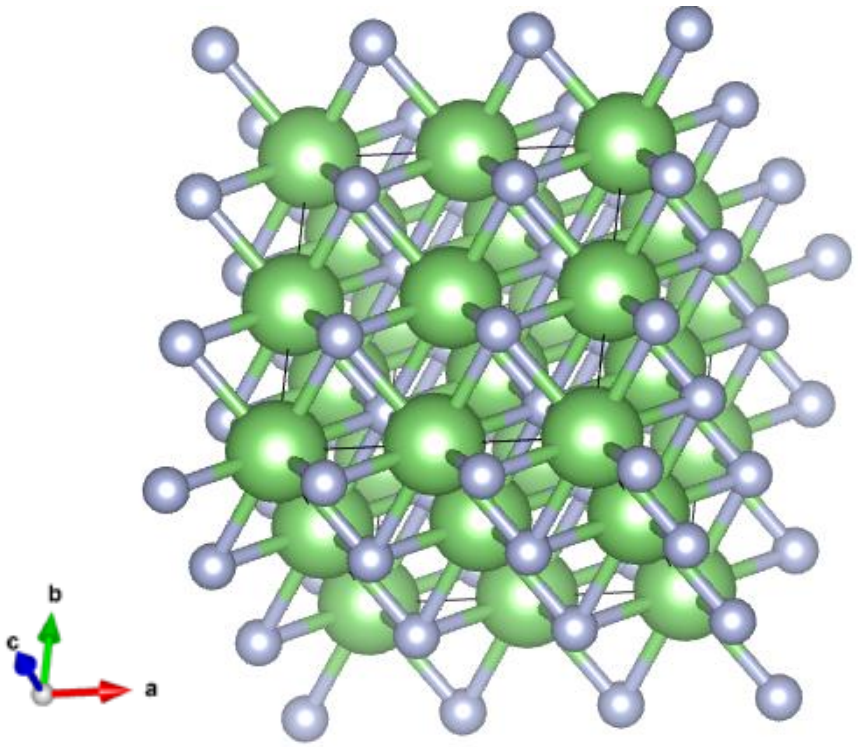
Ashcroft & Merlin, 1976, pg. 80

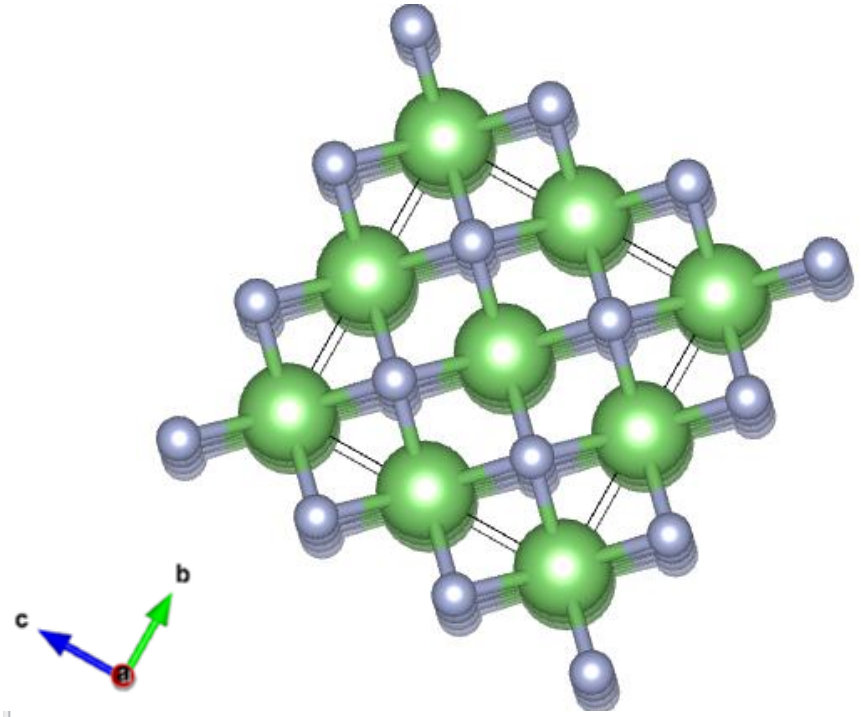
LITHIUM FLUORIDE (LiF)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Lithium_Fluoride_Conventional
Lithium fluoride sodium chloride structure
4.02
1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0
Li F
8 8
Direct
0.000 0.000 0.000
0.000 0.000 0.500
0.000 0.500 0.000
0.000 0.500 0.500
0.500 0.000 0.000
0.500 0.000 0.500
0.500 0.500 0.000
0.500 0.500 0.500
0.250 0.250 0.250
0.250 0.250 0.750
0.250 0.750 0.250
0.250 0.750 0.750
0.750 0.250 0.250
0.750 0.250 0.750
0.750 0.750 0.250
0.750 0.750 0.750
```

POSCAR file for conventional unit cell

LITHIUM FLUORIDE (LiF)





Lattice parameters

a	b	c	alpha	beta	gamma
4.02000	4.02000	4.02000	90.0000	90.0000	90.0000

Unit-cell volume = 64.964807 Å^3

Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Li	Li1	0.00000	0.00000	0.00000	1.000	0.000	1a	1
2	Li	Li2	0.00000	0.00000	0.50000	1.000	0.000	1a	1
3	Li	Li3	0.00000	0.50000	0.00000	1.000	0.000	1a	1
4	Li	Li4	0.00000	0.50000	0.50000	1.000	0.000	1a	1
5	Li	Li5	0.50000	0.00000	0.00000	1.000	0.000	1a	1
6	Li	Li6	0.50000	0.00000	0.50000	1.000	0.000	1a	1
7	Li	Li7	0.50000	0.50000	0.00000	1.000	0.000	1a	1
8	Li	Li8	0.50000	0.50000	0.50000	1.000	0.000	1a	1
9	F	F1	0.25000	0.25000	0.25000	1.000	0.000	1a	1
10	F	F2	0.25000	0.25000	0.75000	1.000	0.000	1a	1
11	F	F3	0.25000	0.75000	0.25000	1.000	0.000	1a	1
12	F	F4	0.25000	0.75000	0.75000	1.000	0.000	1a	1
13	F	F5	0.75000	0.25000	0.25000	1.000	0.000	1a	1
14	F	F6	0.75000	0.25000	0.75000	1.000	0.000	1a	1
15	F	F7	0.75000	0.75000	0.25000	1.000	0.000	1a	1
16	F	F8	0.75000	0.75000	0.75000	1.000	0.000	1a	1

Cesium chloride Crystal Structure

Compounds with Cesium chloride crystal structure

Table 4.6
SOME COMPOUNDS WITH THE CESIUM CHLORIDE STRUCTURE

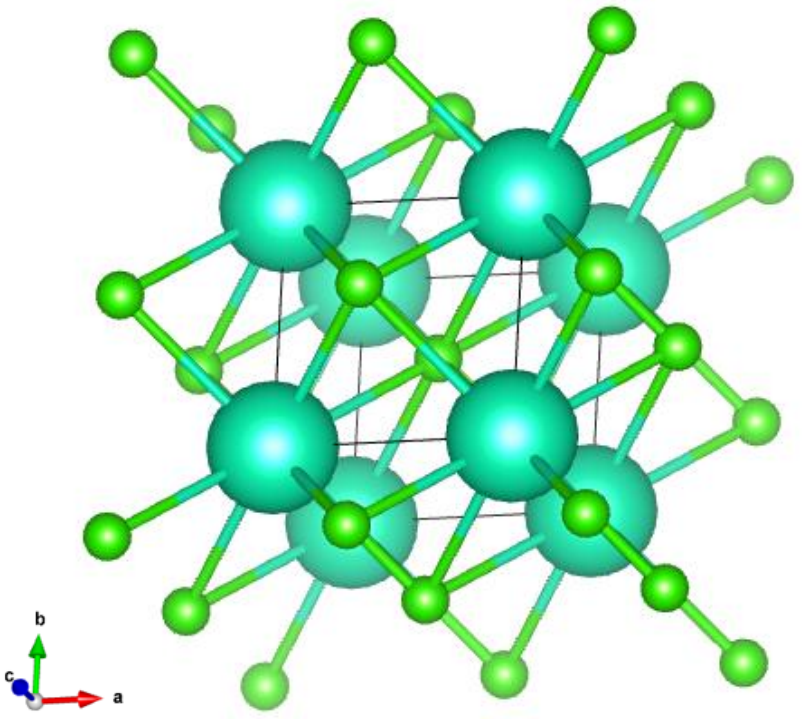
CRYSTAL	a (Å)	CRYSTAL	a (Å)
CsCl	4.12	TlCl	3.83
CsBr	4.29	TlBr	3.97
CsI	4.57	TlI	4.20

Ashcroft & Merlin, 1976, pg. 81

CESIUM CHLORIDE (CsCl)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Cesiumchloride
Cesium chloride Cesium chloride structure
4.12
1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0
Cs Cl
1 1
direct
0.0 0.0 0.0
0.5 0.5 0.5
```

POSCAR file for conventional unit cell



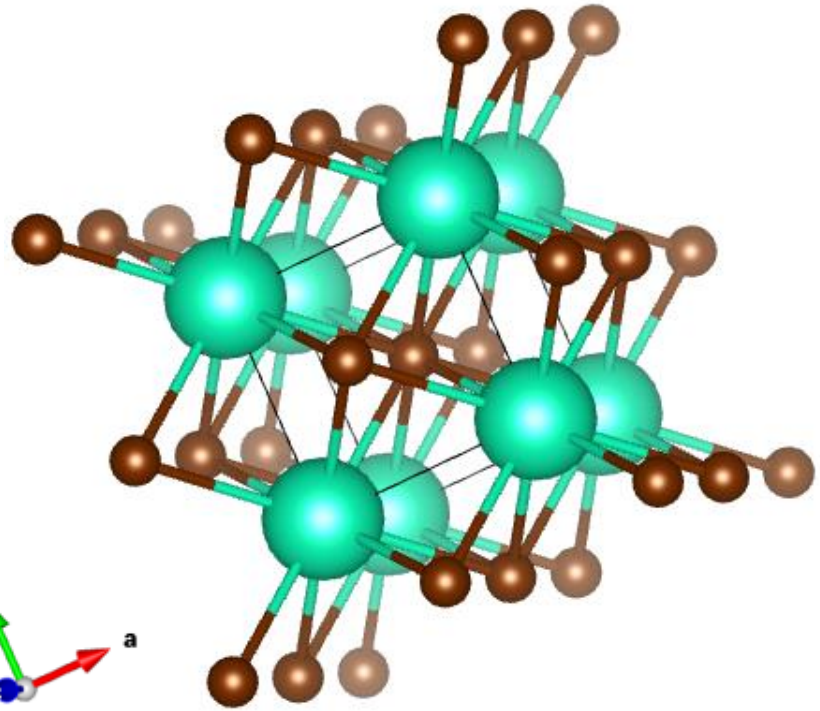

```
Lattice parameters

    a         b         c        alpha     beta      gamma
 4.12000   4.12000   4.12000   90.0000   90.0000   90.0000

Unit-cell volume = 69.934522 Å^3
```

```
Structure parameters

                        x         y         z         Occ.      U     Site       Sym.
   1 Cs  Cs1         0.00000   0.00000   0.00000   1.000     0.000    1a          1
   2 Cl  Cl1         0.50000   0.50000   0.50000   1.000     0.000    1a          1
================================================================================
```

CESIUM BROMIDE (CsBr)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Cesiumbromide
Cesium Bromide Cesium chloride structure
4.29
1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0
Cs Br
1 1
direct
0.0 0.0 0.0
0.5 0.5 0.5
```

POSCAR file for conventional unit cell




```
Lattice parameters

   a         b         c         alpha     beta      gamma
 4.29000   4.29000   4.29000   90.0000   90.0000   90.0000

Unit-cell volume = 78.953587 Å^3
```

Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Cs	Cs1	0.00000	0.00000	0.00000	1.000	0.000	1a	1
2	Br	Br1	0.50000	0.50000	0.50000	1.000	0.000	1a	1

Zincblende Crystal Structure

Compounds with Zincblende crystal structure

Table 4.7
SOME COMPOUNDS WITH THE ZINCBLENDE STRUCTURE

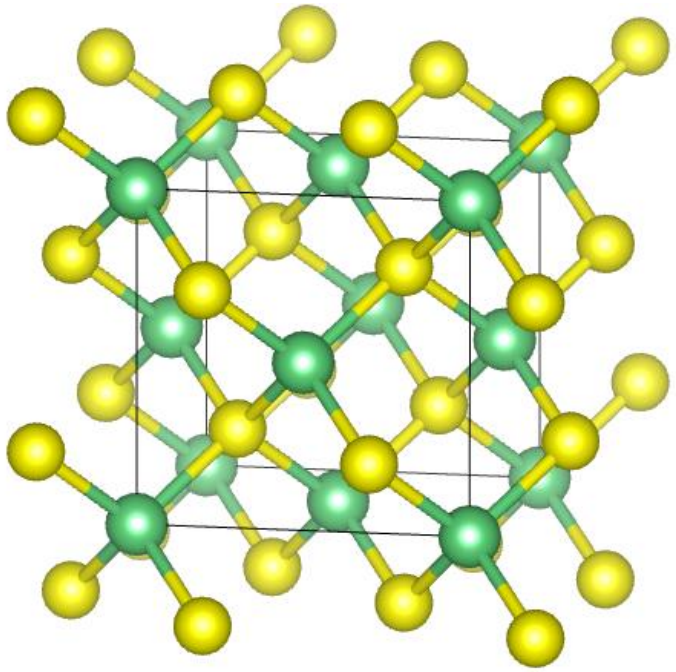
CRYSTAL	a (Å)	CRYSTAL	a (Å)	CRYSTAL	a (Å)
CuF	4.26	ZnS	5.41	AlSb	6.13
CuCl	5.41	ZnSe	5.67	GaP	5.45
CuBr	5.69	ZnTe	6.09	GaAs	5.65
CuI	6.04	CdS	5.82	GaSb	6.12
AgI	6.47	CdTe	6.48	InP	5.87
BeS	4.85	HgS	5.85	InAs	6.04
BeSe	5.07	HgSe	6.08	InSb	6.48
BeTe	5.54	HgTe	6.43	SiC	4.35
MnS (red)	5.60	AlP	5.45		
MnSe	5.82	AlAs	5.62		

Ashcroft & Merlin, 1976, pg. 81

BERYLLIUM SULFIDE (BeS)

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Berylliumsulfide
Beryllium sulfide zingblende structure
4.85
1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0
Be S
4 4
Direct
0.0000 0.0000 0.0000
0.0000 0.5000 0.5000
0.5000 0.0000 0.5000
0.5000 0.5000 0.0000
0.2500 0.2500 0.7500
0.2500 0.7500 0.2500
0.7500 0.2500 0.2500
0.7500 0.7500 0.7500
```

POSCAR file for conventional unit cell



Lattice parameters

a	b	c	alpha	beta	gamma
4.85000	4.85000	4.85000	90.0000	90.0000	90.0000

Unit-cell volume = 114.084118 Å^3

Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Be	Be1	0.00000	0.00000	0.00000	1.000	0.000	1a	1
2	Be	Be2	0.00000	0.50000	0.50000	1.000	0.000	1a	1
3	Be	Be3	0.50000	0.00000	0.50000	1.000	0.000	1a	1
4	Be	Be4	0.50000	0.50000	0.00000	1.000	0.000	1a	1
5	S	S1	0.25000	0.25000	0.75000	1.000	0.000	1a	1
6	S	S2	0.25000	0.75000	0.25000	1.000	0.000	1a	1
7	S	S3	0.75000	0.25000	0.25000	1.000	0.000	1a	1
8	S	S4	0.75000	0.75000	0.75000	1.000	0.000	1a	1

References

- Ashcroft, N. W., & Mermin, N. D. (1976). Solid state physics. Harcourt College Publishers.
- https://chem.libretexts.org/Bookshelves/Analytical_Chemistry/Physical_Methods_in_Chemistry_and_Nano_Science_%28Barron%29/07%3A_Molecular_and_Solid_State_Structure/7.01%3A_Crystal_Structure