CRYSTAL SYSTEM

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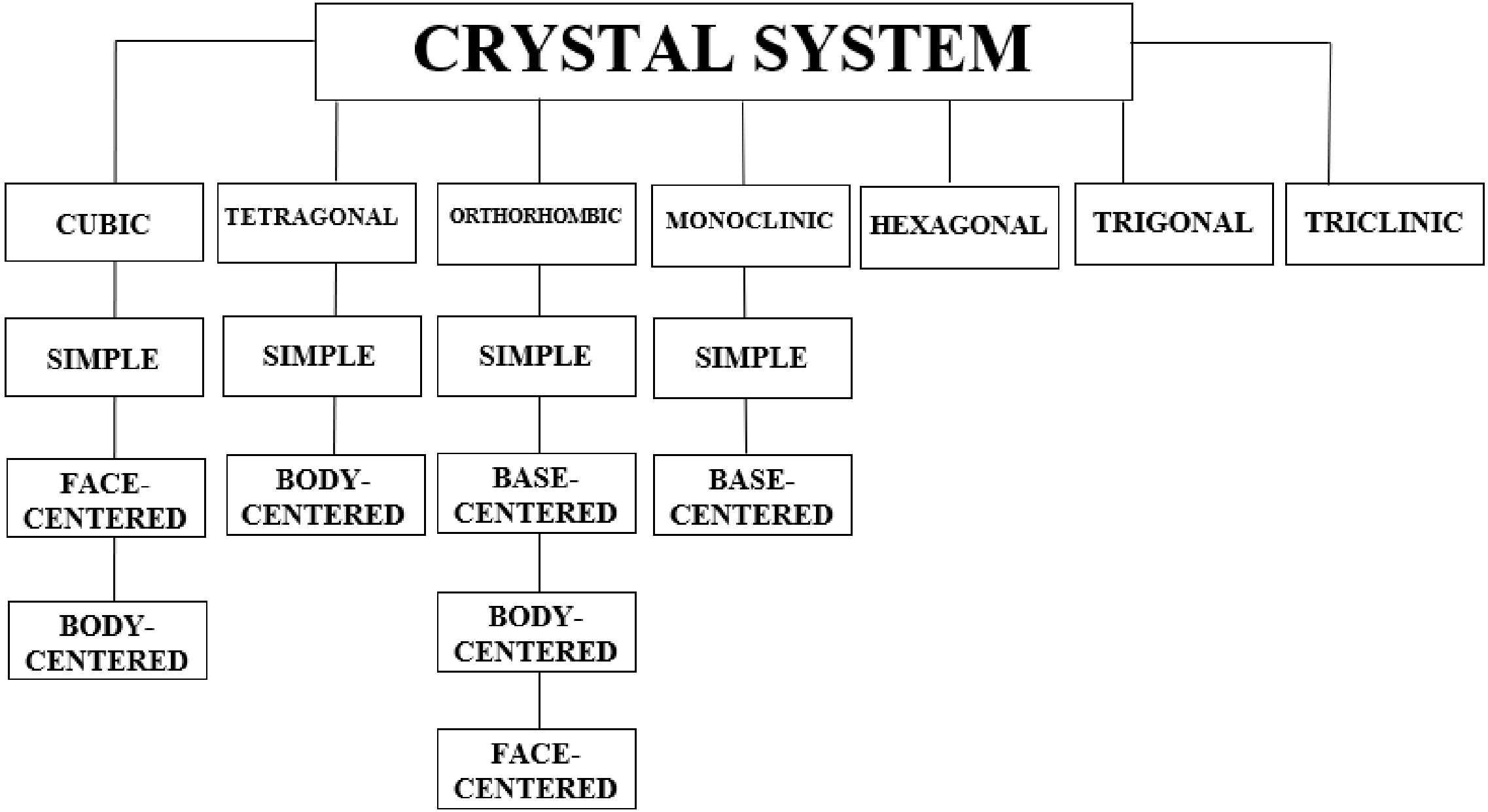
CRYSTAL SYSTEM
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BASE-CENTERED
BASE-CENTERED
BODY-CENTERED
BODY-CENTERED
FACE-CENTERED

CUBIC CRYSTAL SYSTEM

SIMPLE CUBIC	FACE-CENTERED CUBIC	BODY-CENTERED CUBIC

SIMPLE CUBIC

The simple cubic system is identical to the conventional cubic unit cell

$$\begin{aligned} \mathbf{a}_1 &= a\,\hat{\mathbf{x}} \\ \mathbf{a}_2 &= a\,\hat{\mathbf{y}} \\ \mathbf{a}_3 &= a\,\hat{\mathbf{z}}, \end{aligned}$$

with volume

$$V = a^3.$$

FACE-CENTERED CUBIC

The face-centered cubic lattice has the same periodicity as its simple cubic parent with the addition of a translation from one corner of the cube to the center of any face. Our standard face-centered cubic primitive vectors have the form

$$\begin{aligned}\mathbf{a}_1 &= \tfrac{a}{2}\,\hat{\mathbf{y}} + \tfrac{a}{2}\,\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \tfrac{a}{2}\,\hat{\mathbf{x}} + \tfrac{a}{2}\,\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \tfrac{a}{2}\,\hat{\mathbf{x}} + \tfrac{a}{2}\,\hat{\mathbf{y}},\end{aligned}$$

and the primitive cell volume is

$$V = \frac{a^3}{4}.$$

There are four face-centered cubic primitive cells in the conventional cubic cell. The face-centered cubic lattice can be considered as a rhombohedral lattice where $\alpha = 60^\circ$.

Face-centered Cubic

For Argon (Ar),

Given that $a = 5.26\ \text{Å}$, then:

$$a_1 = \frac{5.26}{2}(\hat{y} + \hat{z})$$

$$a_2 = \frac{5.26}{2}(\hat{x} + \hat{z})$$

$$a_3 = \frac{5.26}{2}(\hat{x} + \hat{y})$$

So, the primitive vectors are:

$$\begin{bmatrix} 0 & \frac{5.26}{2} & \frac{5.26}{2} \\ \frac{5.26}{2} & 0 & \frac{5.26}{2} \\ \frac{5.26}{2} & \frac{5.26}{2} & 0 \end{bmatrix}$$

Generally:

$$\begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix}$$

The primitive cell volume π:

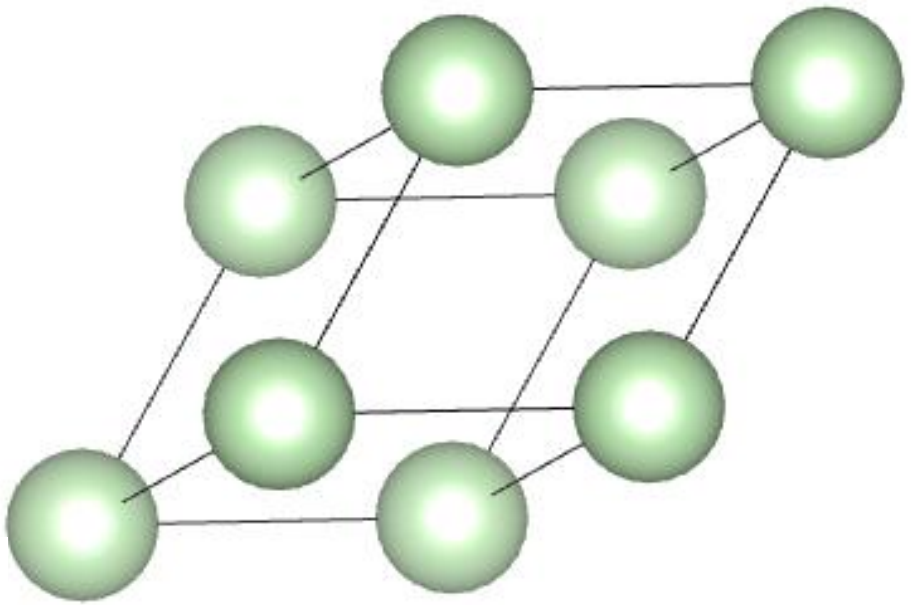
$$V = \frac{(5.26)^3}{4}$$

$$V = 36.3828\ \text{Å}^3$$

Atomic Positions

Wyckoff	Element	x	y	z
4a	Ar	0	0	0

```
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
```



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

BODY-CENTERED CUBIC

Like its predecessors in the orthorhombic and tetragonal systems, the body-centered cubic crystal has the same periodicity as its parent with the addition of a translation from one corner of the cube to its center. Our standard body-centered cubic primitive vectors have the form

$$\begin{aligned}
\mathbf{a}_1 &= -\tfrac{a}{2}\,\hat{\mathbf{x}} + \tfrac{a}{2}\,\hat{\mathbf{y}} + \tfrac{a}{2}\,\hat{\mathbf{z}} \\
\mathbf{a}_2 &= \tfrac{a}{2}\,\hat{\mathbf{x}} - \tfrac{a}{2}\,\hat{\mathbf{y}} + \tfrac{a}{2}\,\hat{\mathbf{z}} \\
\mathbf{a}_3 &= \tfrac{a}{2}\,\hat{\mathbf{x}} + \tfrac{a}{2}\,\hat{\mathbf{y}} - \tfrac{a}{2}\,\hat{\mathbf{z}},
\end{aligned}$$

and the primitive cell volume is

$$V = \frac{a^3}{2}.$$

There are two body-centered cubic primitive cells in the conventional cubic cell. The body-centered cubic lattice can be considered as a rhombohedral lattice where $\alpha = \cos^{-1}(-1/3) \approx 109.47°$.

Body-centered cubic

For Iron (Fe),

Given that $a = 2.87$,
Then:

$$a_1 = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z}) \longrightarrow \frac{-2.87}{2} \quad \frac{2.87}{2} \quad \frac{2.87}{2}$$

$$a_2 = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z}) \longrightarrow \frac{2.87}{2} \quad \frac{-2.87}{2} \quad \frac{2.87}{2}$$

$$a_3 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z}) \longrightarrow \frac{2.87}{2} \quad \frac{2.87}{2} \quad \frac{-2.87}{2}$$

So, the primitive vectors are: (generally)

$$\begin{bmatrix} -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{bmatrix}$$

The primitive cell volume of Iron is:

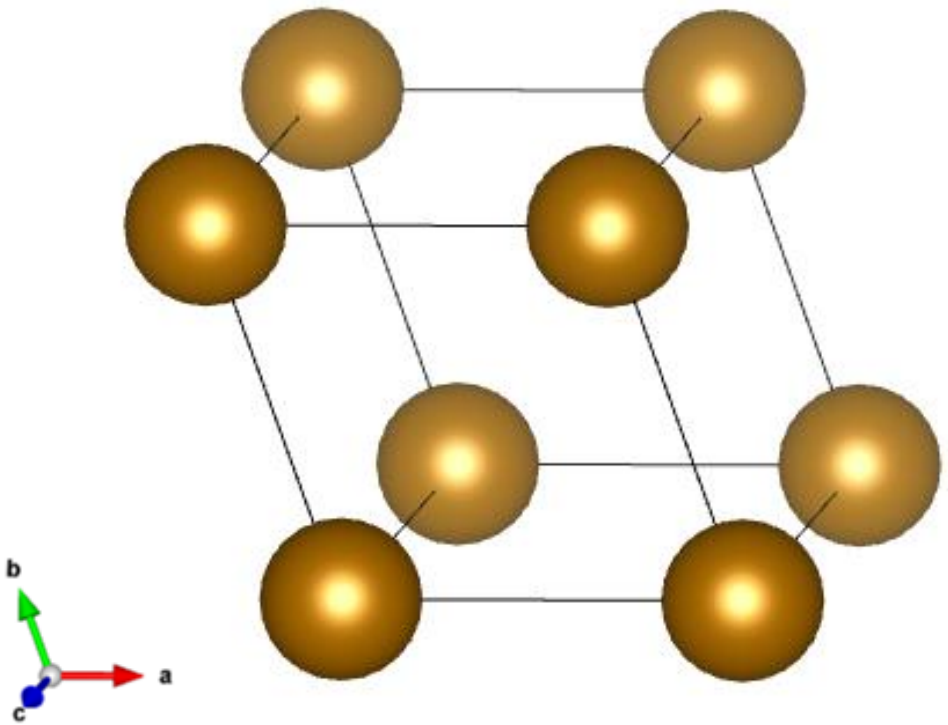
$$V = \frac{(2.87)^3}{2}$$

$$\boxed{V = 11.8199\ \text{Å}^3}$$

Atomic Positions

Wyckoff	Element	x	y	z
2a	Fe	0	0	0

```
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
```



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

TETRAGONAL CRYSTAL SYSTEM

SIMPLE TETRAGONAL	CENTERED TETRAGONAL

SIMPLE TETRAGONAL

The simple tetragonal Bravais lattice is identical to the conventional cell

$$\begin{aligned} \mathbf{a}_1 &= a\,\hat{\mathbf{x}} \\ \mathbf{a}_2 &= a\,\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\,\hat{\mathbf{z}}, \end{aligned}$$

with volume

$$V = a^2\,c.$$

CENTERED TETRAGONAL

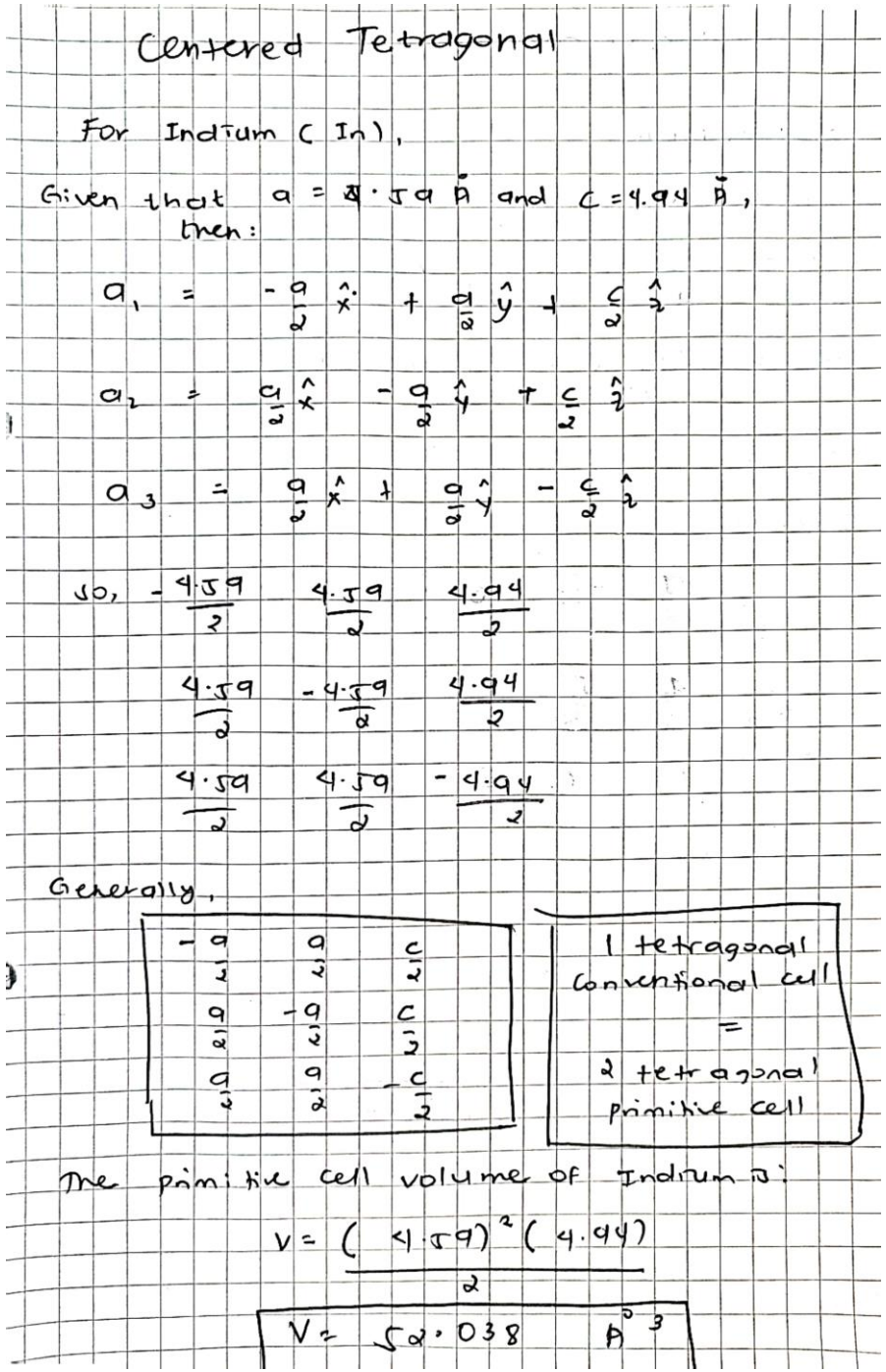
The body-centered tetragonal system has the same point group and translational symmetry as the simple tetragonal system, with the addition of a translation to the center of the parallelepiped. Our standard form of the primitive vectors is

$$\begin{aligned}
\mathbf{a}_1 &= -\tfrac{a}{2}\,\hat{\mathbf{x}} + \tfrac{a}{2}\,\hat{\mathbf{y}} + \tfrac{c}{2}\,\hat{\mathbf{z}} \\
\mathbf{a}_2 &= \tfrac{a}{2}\,\hat{\mathbf{x}} - \tfrac{a}{2}\,\hat{\mathbf{y}} + \tfrac{c}{2}\,\hat{\mathbf{z}} \\
\mathbf{a}_3 &= \tfrac{a}{2}\,\hat{\mathbf{x}} + \tfrac{a}{2}\,\hat{\mathbf{y}} - \tfrac{c}{2}\,\hat{\mathbf{z}}.
\end{aligned}$$

The volume of the primitive body-centered tetragonal unit cell is

$$V = \frac{a^2\,c}{2}.$$

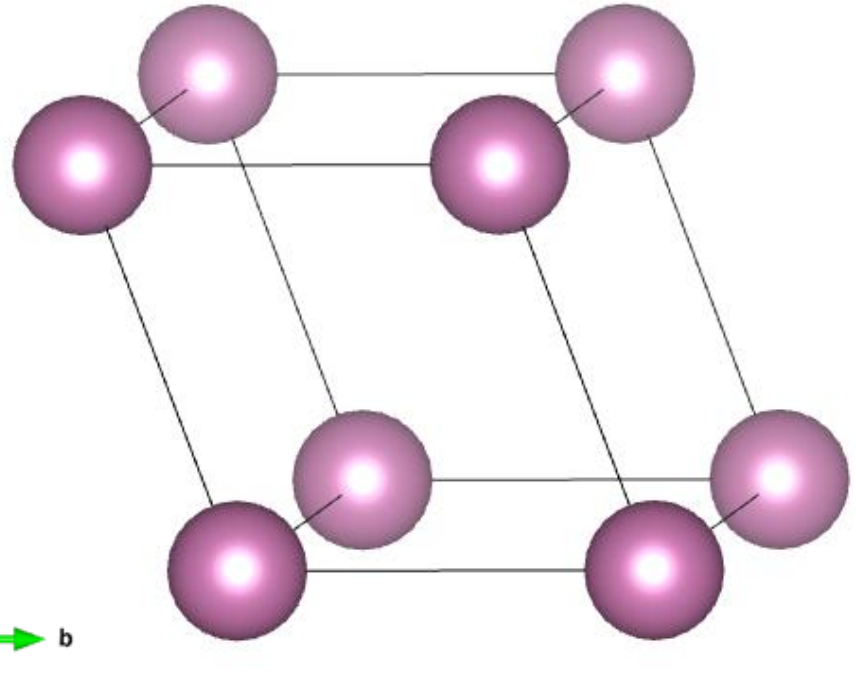
There are two primitive body-centered tetragonal unit cells in the conventional tetragonal unit cell.



Atomic Positions

Wyckoff	Element	x	y	z
2a	In	0	0	0

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Indium_primitive
Indium primitive centered tetragonal unit cell
4.59 4.59 4.94
-0.5 0.5 0.5
0.5 -0.5 0.5
0.5 0.5 -0.5
In
1
Direct
0.0 0.0 0.0
```



Lattice parameters

a	b	c	alpha	beta	gamma
3.97506	3.97506	4.27817	109.4712	109.4712	109.4712

Unit-cell volume = 52.038204 Å^3

HEXAGONAL CRYSTAL SYSTEM

HEXAGONAL

Somewhat confusingly, what might be called the simple trigonal Bravais lattice is known as the hexagonal lattice. It shares the same primitive vectors, but not point operations, as the hexagonal crystal system. The primitive vectors are identical to those of the conventional cell,

$$\begin{aligned} \mathbf{a}_1 &= \tfrac{a}{2}\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}\,a\,\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \tfrac{a}{2}\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}\,a\,\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\,\hat{\mathbf{z}}. \end{aligned}$$

The volume of the primitive cell is

$$V = \left(\frac{\sqrt{3}}{2}\right) a^2\, c.$$

Hexagonal

For Beryllium,

Given that $a = 2.29$ Å and $c = 3.58$ Å, then:

$$a_1 = \frac{2.29}{2}\hat{x} - \frac{\sqrt{3}}{2}(2.29)\hat{y}$$

$$a_2 = \frac{2.29}{2}\hat{x} + \frac{\sqrt{3}}{2}(2.29)\hat{y}$$

$$a_3 = (3.58)\hat{z}$$

Generally,

$$\begin{matrix} \frac{a}{2} & -\frac{\sqrt{3}}{2} & a & 0 \\ \frac{a}{2} & \frac{\sqrt{3}}{2} & a & 0 \\ 0 & 0 & c & \end{matrix} \longrightarrow$$

If there's 3 scaling factors:

$$\begin{matrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{matrix}$$

So, the primitive cell volume of Be is:

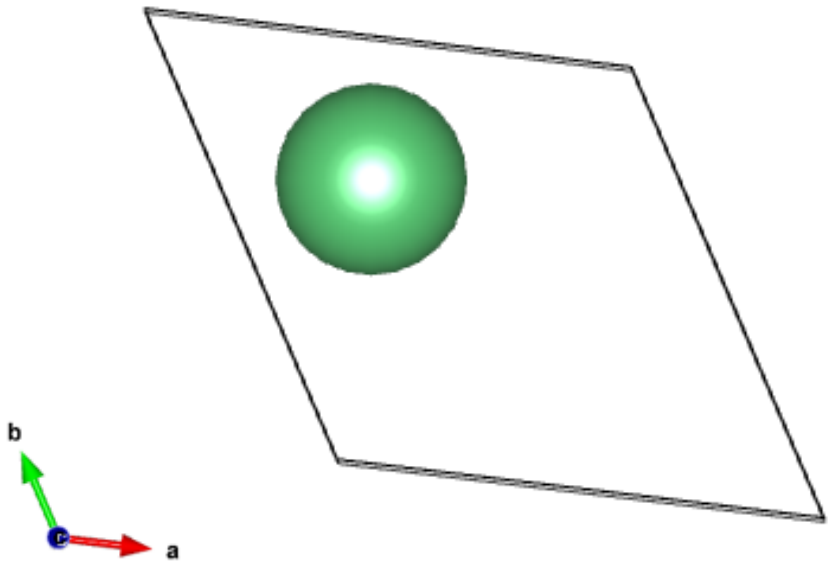
$$V = \left(\frac{\sqrt{3}}{2}\right)(2.29)^2(3.58)$$

$$V = 16.258 \text{ Å}^3$$

Atomic Positions

Wyckoff	Element	x	y	z
2d	Be	1/3	2/3	3/4

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Beryllium_primitive
Beryllium primitive hexagonal crystal structure
2.29 2.29 3.58
0.50000 -0.86603 0.00000
0.50000 0.86603 0.00000
0.00000 0.00000 1.00000
Be
1
Direct
0.33333 0.66666 0.75000
```



Lattice parameters

a	b	c	alpha	beta	gamma
2.29001	2.29001	3.58000	90.0000	90.0000	120.0003

Unit-cell volume = 16.258739 Å^3

ORTHORHOMBIC CRYSTAL SYSTEM

SIMPLE ORTHORHOMBIC	BODY-CENTERED ORTHORHOMBIC	BASE-CENTERED ORTHORHOMBIC	FACE-CENTERED ORTHORHOMBIC

SIMPLE ORTHORHOMBIC

The simple orthorhombic Bravais lattice is identical to the conventional cell

$$\begin{aligned} \mathbf{a}_1 &= a\,\hat{\mathbf{x}} \\ \mathbf{a}_2 &= b\,\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\,\hat{\mathbf{z}}, \end{aligned}$$

with volume

$$V = a\,b\,c\,.$$

BODY-CENTERED ORTHORHOMBIC

The body-centered orthorhombic lattice has the same point group and translational symmetry as the simple orthorhombic system, with the addition of a translation to the center of the parallelepiped. Our standard form of the primitive vectors is

$$\begin{aligned}
\mathbf{a}_1 &= -\frac{a}{2}\,\hat{\mathbf{x}} + \frac{b}{2}\,\hat{\mathbf{y}} + \frac{c}{2}\,\hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{a}{2}\,\hat{\mathbf{x}} - \frac{b}{2}\,\hat{\mathbf{y}} + \frac{c}{2}\,\hat{\mathbf{z}} \\
\mathbf{a}_3 &= \frac{a}{2}\,\hat{\mathbf{x}} + \frac{b}{2}\,\hat{\mathbf{y}} - \frac{c}{2}\,\hat{\mathbf{z}}.
\end{aligned}$$

The volume of the primitive body-centered orthorhombic unit cell is

$$V = \frac{a\,b\,c}{2}.$$

Body-centered Orthorhombic

In general, the primitive vectors will be:

$$\begin{matrix} -\frac{a}{2} & \frac{b}{2} & \frac{c}{2} \\ \frac{a}{2} & -\frac{b}{2} & \frac{c}{2} \\ \frac{a}{2} & \frac{b}{2} & -\frac{c}{2} \end{matrix}$$

or, in poscar file:

2nd line:	a	b	c
	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$
	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$

FACE-CENTERED ORTHORHOMBIC

While the base-centered monoclinic lattice allows translations to one base plane, the face-centered orthorhombic lattice allows translations to any of the base planes. Our standard choice for the primitive vectors of this system are given by

$$\begin{aligned}
\mathbf{a}_1 &= \frac{b}{2}\,\hat{\mathbf{y}} + \frac{c}{2}\,\hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{a}{2}\,\hat{\mathbf{x}} + \frac{c}{2}\,\hat{\mathbf{z}} \\
\mathbf{a}_3 &= \frac{a}{2}\,\hat{\mathbf{x}} + \frac{b}{2}\,\hat{\mathbf{y}}.
\end{aligned}$$

The volume of the primitive face-centered orthorhombic unit cell is

$$V = \frac{a\,b\,c}{4}\,,$$

so that there are four primitive body-centered orthorhombic unit cells in the conventional orthorhombic unit cell.

Face-centered orthorhombic

In general, the primitive vectors will be:

$$\begin{matrix} 0 & \frac{b}{2} & \frac{c}{2} \\ \frac{a}{2} & 0 & \frac{c}{2} \\ \frac{a}{2} & \frac{b}{2} & 0 \end{matrix}$$

or, in poscar file:

2nd line:

a	b	c
0	$\frac{1}{2}$	$\frac{1}{2}$
$\frac{1}{2}$	0	$\frac{1}{2}$
$\frac{1}{2}$	$\frac{1}{2}$	0

BASE-CENTERED ORTHORHOMBIC

Like the base-centered monoclinic lattice, the base-centered orthorhombic system allows a translation in one of the base planes. Unfortunately, the standard plane chosen depends on the space group, as shown in the table below. Space groups beginning with C put the translation in the $a - b$ plane, that is, the plane defined by $\mathbf{A}_1$ and $\mathbf{A}_2$. In this case the primitive vectors can be taken to be

$$\begin{aligned} \mathbf{a}_1 &= \frac{a}{2}\,\hat{\mathbf{x}} - \frac{b}{2}\,\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{a}{2}\,\hat{\mathbf{x}} + \frac{b}{2}\,\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\,\hat{\mathbf{z}}\ . \end{aligned}$$

BASE-CENTERED ORTHORHOMBIC

Space groups beginning with A put the translation in the $b - c$ plane, defined by $\mathbf{A}_2$ and $\mathbf{A}_3$. We use the primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a\,\hat{\mathbf{x}} \\ \mathbf{a}_2 &= \tfrac{b}{2}\,\hat{\mathbf{y}} - \tfrac{c}{2}\,\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \tfrac{b}{2}\,\hat{\mathbf{y}} + \tfrac{c}{2}\,\hat{\mathbf{z}}. \end{aligned}$$

The above orientation is not used by Setyawan and Curtarolo who only considered centering in the "C" plane defined by $\mathbf{a}_2$ and $\mathbf{a}_3$. A simple rotation brings the vectors into agreement. In both cases the volume of the primitive unit cell is

$$V = \frac{a\,b\,c}{2}.$$

There are two primitive base-centered orthorhombic unit cells in the conventional orthorhombic unit cell.

Base-centered Orthorhombic

For Gallium,
Given that:
$a = 4.511\ \text{Å}$ $b = 4.517\ \text{Å}$ and $c = 7.645\ \text{Å}$
Then:

$$a_1 = \frac{4.511}{2}\hat{x} - \frac{4.517}{2}\hat{y} \rightarrow \frac{4.511}{2} \quad -\frac{4.517}{2} \quad 0$$

$$a_2 = \frac{4.511}{2}\hat{x} + \frac{4.517}{2}\hat{y} \rightarrow \frac{4.511}{2} \quad \frac{4.517}{2} \quad 0$$

$$a_3 = 7.645\,\hat{z} \qquad\qquad 0 \quad 0 \quad 7.64$$

In general,

$$\frac{a}{2} \quad -\frac{b}{2} \quad 0 \qquad\qquad a \quad b \quad c$$

$$\frac{a}{2} \quad \frac{b}{2} \quad 0 \qquad \text{or} \qquad \frac{1}{2} \quad -\frac{1}{2} \quad 0$$

$$\frac{1}{2} \quad \frac{1}{2} \quad 0$$

$$0 \quad 0 \quad c \qquad\qquad 0 \quad 0 \quad 1$$

So, the primitive cell volume of Gallium is:

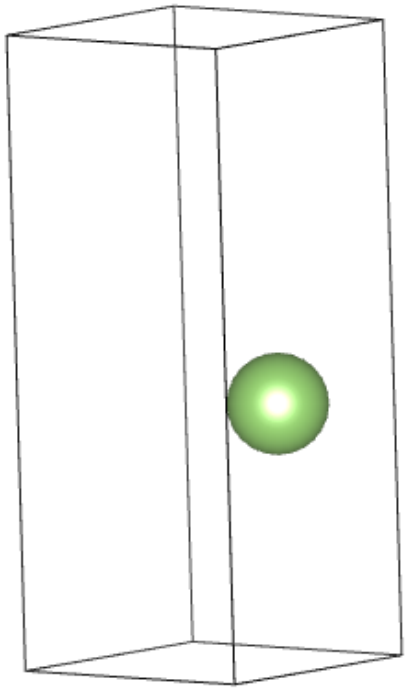
$$V = \frac{(4.511)(4.517)(7.645)}{2}$$

$$V = 77.887\ \text{Å}^3$$

Atomic Positions

Wyckoff	Element	x	y	z
	Ga	1/2	0.844304	0.415401

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Gallium_primitive
Gallium primitive base-centered orthorhombic crystal structure
4.511 4.517 7.645
0.5 -0.5 0
0.5 0.5 0
0 0 1
Ga
1
Direct
0.500000 0.844304 0.415401
```



Lattice parameters

a	b	c	alpha	beta	gamma
3.18976	3.19400	7.64500	90.0000	90.0000	90.0000

Unit-cell volume = 77.887979 Å^3

MONOCLINIC CRYSTAL SYSTEM

SIMPLE MONOCLINIC	BASE-CENTERED MONOCLINIC

SIMPLE MONOCLINIC

The simple monoclinic cell is identical to the conventional cell

$$\begin{aligned} \mathbf{a}_1 &= a\,\hat{\mathbf{x}} \\ \mathbf{a}_2 &= b\,\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\,\cos\beta\,\hat{\mathbf{x}} + c\,\sin\beta\,\hat{\mathbf{z}}, \end{aligned}$$

and the cell volume is just

$$V = a\,b\,c\,\sin\beta.$$

Simple monoclinic

For selenium,

Given that: $a = 9.45\ \text{Å}$; $b = 14.78\ \text{Å}$; $c = 15.32\ \text{Å}$ and $\alpha = \gamma = 90°$ and $\beta = 93.47°$, then:

$$a_1 = 9.45\,\hat{x}$$
$$a_2 = 14.78\,\hat{y}$$
$$a_3 = 15.32\cos(93.47°)\,\hat{x} + 15.32\sin(93.47°)\,\hat{z}$$

or

$$\begin{matrix} 9.45 & 0 & 0 \\ 0 & 14.78 & 0 \\ 15.32\cos(93.47°) & 0 & 15.32\sin(93.47°) \end{matrix}$$

In general, (POSCAR file),

2nd line:	a	b	c
	1	0	0
	0	1	0
	cos α	0	sen α

So, the primitive cell volume is:

$$V = (9.45)(14.78)(15.32)\sin(93.47°)$$

$$\boxed{V = 2135.83\ \text{Å}^3}$$

```
Selenium primitive simple monoclinic crystal structure
9.45 14.78 15.32
   1.0000000000000000    0.0000000000000000    0.0000000000000000
   0.0000000000000000    1.0000000000000000    0.0000000000000000
  -0.0605259090310000    0.0000000000000000    0.9981666265388000
Se
64
direct
   0.8341897000000000    0.8330882100000000    0.9108409300000000 Se
   0.0373695200000000    0.8590474200000000    0.1834311900000001 Se
   0.6327938399999999    0.2350761400000000    0.3116398000000001 Se
   0.1489649600000000    0.7069395500000000    0.4742580500000001 Se
   0.6479743700000000    0.9885906000000000    0.0900968400000001 Se
   0.8865077100000001    0.7208991100000000    0.0159470000000002 Se
   0.4055074400000001    0.3503817900000000    0.4715502700000002 Se
   0.5373695199999999    0.6409525800000000    0.1834311900000001 Se
   0.3865077100000001    0.7791008900000000    0.0159470000000002 Se
   0.3341897000000000    0.6669117900000000    0.9108409300000000 Se
   0.0944925599999999    0.8503817900000001    0.5284497299999998 Se
   0.7754696100000000    0.0445677100000000    0.7714163400000000 Se
   0.8672061600000001    0.7350761399999999    0.6883601999999999 Se
   0.9626304800000000    0.1409525800000000    0.8165688099999999 Se
   0.4626304800000000    0.3590474200000000    0.8165688099999999 Se
   0.3498082400000000    0.5263427700000000    0.6448188900000000 Se
   0.7331718199999999    0.5974694699999999    0.9892292600000000 Se
   0.7668281800000001    0.0974694699999999    0.0107707400000000 Se
   0.4950990000000000    0.6895654100000000    0.8027246200000000 Se
   0.0578813000000000    0.4161779000000000    0.3072897900000001 Se
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   0.4421187000000000    0.9161779000000001    0.6927102099999999 Se
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   0.7680422099999999    0.5042058100000000    0.7633873400000001 Se
   0.6134922899999999    0.2208991100000000    0.9840529999999998 Se
   0.9421187000000000    0.5838221000000000    0.6927102099999999 Se
   0.0049010000000000    0.1895654100000000    0.1972753800000000 Se
   0.1479743700000000    0.5114094000000000    0.0900968400000001 Se
   0.7589178800000000    0.5454629900000000    0.4787138599999998 Se
   0.8520256300000000    0.4885906000000000    0.9099031599999999 Se
   0.1501917600000000    0.0263427700000000    0.3551811100000000 Se
   0.8911015000000000    0.2867624700000000    0.7719323000000000 Se
   0.9895877800000000    0.6792782700000000    0.3542204800000001 Se
   0.6501917600000000    0.4736572300000000    0.3551811100000000 Se
   0.1134922899999999    0.2791008900000000    0.9840529999999998 Se
   0.3520256300000000    0.0114094000000000    0.9099031599999999 Se
   0.5578813000000000    0.0838221000000000    0.3072897900000001 Se
   0.9950990000000000    0.8104345900000000    0.8027246200000000 Se
   0.5104122200000000    0.1792782700000000    0.6457795199999999 Se
   0.6088985000000000    0.7867624700000000    0.2280677000000000 Se
   0.1327938399999999    0.2649238600000000    0.3116398000000001 Se
   0.8510350400000000    0.2930604500000000    0.5257419499999999 Se
   0.7245303900000000    0.5445677099999999    0.2285836600000000 Se
   0.7410821200000000    0.0454629900000000    0.5212861400000002 Se
   0.2680422099999999    0.9957941900000000    0.7633873400000001 Se
   0.6489649600000000    0.7930604500000000    0.4742580500000001 Se
   0.5944925599999999    0.6496182100000000    0.5284497299999998 Se
   0.2668281800000001    0.4025305300000001    0.0107707400000000 Se
   0.8498082400000000    0.9736572300000000    0.6448188900000000 Se
   0.6658103000000000    0.3330882100000000    0.0891590700000000 Se
   0.2245303900000000    0.9554322900000000    0.2285836600000000 Se
   0.2319577900000001    0.4957941900000000    0.2366126599999999 Se
   0.3911015000000000    0.2132375300000000    0.7719323000000000 Se
   0.5049010000000000    0.3104345900000000    0.1972753800000000 Se
   0.1658103000000000    0.1669117900000000    0.0891590700000000 Se
   0.3510350400000000    0.2069395500000000    0.5257419499999999 Se
   0.7319577900000001    0.0042058100000000    0.2366126599999999 Se
   0.2754696100000000    0.4554322900000000    0.7714163400000000 Se
   0.1088985000000000    0.7132375300000000    0.2280677000000000 Se
   0.2331718199999999    0.9025305300000001    0.9892292600000000 Se
   0.0104122200000000    0.3207217300000000    0.6457795199999999 Se
   0.2589178800000000    0.9545370100000001    0.4787138599999998 Se
   0.4895877800000000    0.8207217300000000    0.3542204800000001 Se
   0.3672061600000001    0.7649238600000000    0.6883601999999999 Se
```
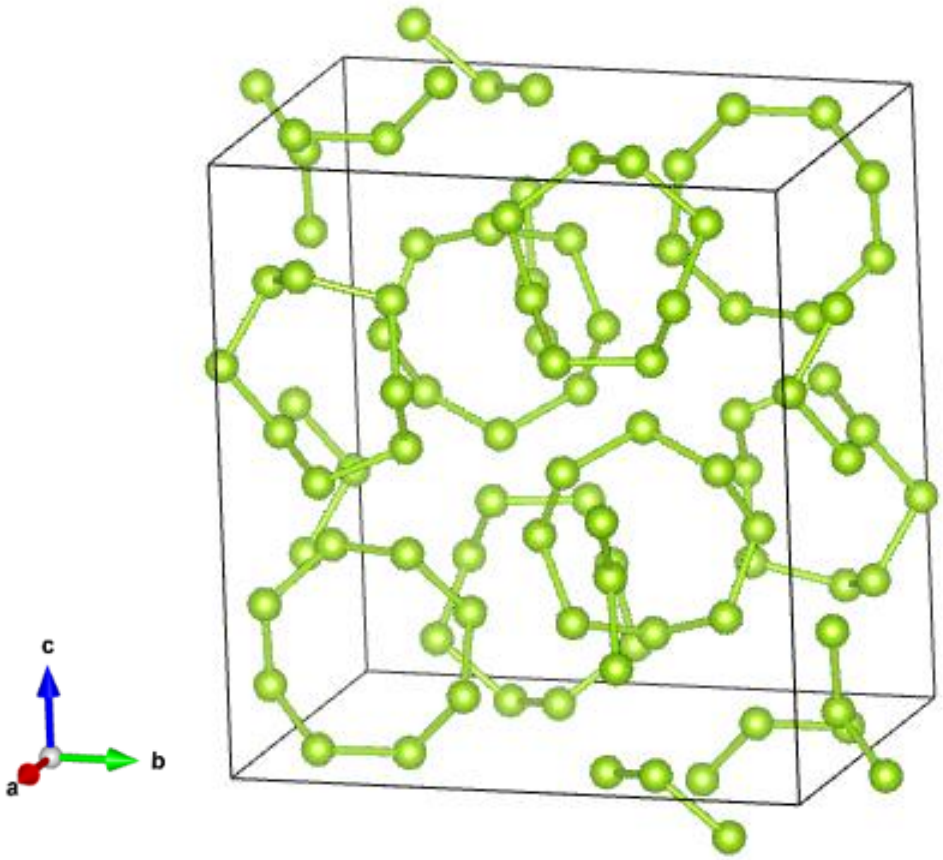



Lattice parameters

a	b	c	alpha	beta	gamma
9.45000	14.78000	15.32000	90.0000	93.4700	90.0000

Unit-cell volume = 2135.836614 Å^3

BASE-CENTERED MONOCLINIC

The base-centered monoclinic lattice is in the same crystal system as the monoclinic lattice, but its periodicity allows an additional translation in the plane defined by $\mathbf{a}_1$ and $\mathbf{a}_2$. The primitive vectors for the base-centered monoclinic lattice can be written as

$$\begin{aligned}
\mathbf{a}_1 &= \frac{a}{2}\,\hat{\mathbf{x}} - \frac{b}{2}\,\hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{a}{2}\,\hat{\mathbf{x}} + \frac{b}{2}\,\hat{\mathbf{y}} \\
\mathbf{a}_3 &= c\,\cos\beta\,\hat{\mathbf{x}} + c\,\sin\beta\,\hat{\mathbf{z}}.
\end{aligned}$$

The volume of the base-centered monoclinic unit cell is

$$V = \left(\frac{1}{2}\right) a\,b\,c\,\sin\beta,$$

Base-centered Monoclinic

The primitive vectors, in general, will be:

$$\begin{matrix} \frac{a}{2} & -\frac{b}{2} & 0 \\ \frac{a}{2} & \frac{b}{2} & 0 \\ c\cos\beta & 0 & c\sin\beta \end{matrix}$$

TRICLINIC
CRYSTAL SYSTEM

SIMPLE TRICLINIC

There are many choices for the primitive vectors in the triclinic system. We make the choice

$$\begin{aligned}
\mathbf{a}_1 &= a\,\hat{\mathbf{x}} \\
\mathbf{a}_2 &= b\,\cos\gamma\,\hat{\mathbf{x}} + b\,\sin\gamma\,\hat{\mathbf{y}} \\
\mathbf{a}_3 &= c_x\,\hat{\mathbf{x}} + c_y\,\hat{\mathbf{y}} + c_z\,\hat{\mathbf{z}},
\end{aligned}$$

where

$$\begin{aligned}
c_x &= c\,\cos\beta \\
c_y &= \frac{c\,(\cos\alpha - \cos\beta\,\cos\gamma)}{\sin\gamma}
\end{aligned}$$

and

$$c_z = \sqrt{c^2 - c_x^2 - c_y^2}.$$

The volume of the triclinic unit cell is

$$V = a\,b\,c_z\,\sin\gamma.$$

Simple Triclinic

In general, the primitive vectors will be:

$$\begin{matrix} a & 0 & 0 \\ b\cos\gamma & b\sin\gamma & 0 \\ c\cos\beta & \dfrac{c(\cos\alpha - \cos\beta\cos\gamma)}{\sin\gamma} & \sqrt{c^2 - c_x^2 - c_y^2} \end{matrix}$$

for phosphorus,

Given that:

$a = 5.67\ \text{Å}$; $b = 11.14\ \text{Å}$; and $c = 11.32\ \text{Å}$
where $\alpha = 93.47°$; $\beta = 99.49°$; and $\gamma = 100.80°$,

The primitive vectors will be:

$$\begin{matrix} 5.67 & 0 & 0 \\ -2.087427 & 10.94 & 0 \\ -1.86 & -1.05 & 11.11 \end{matrix}$$

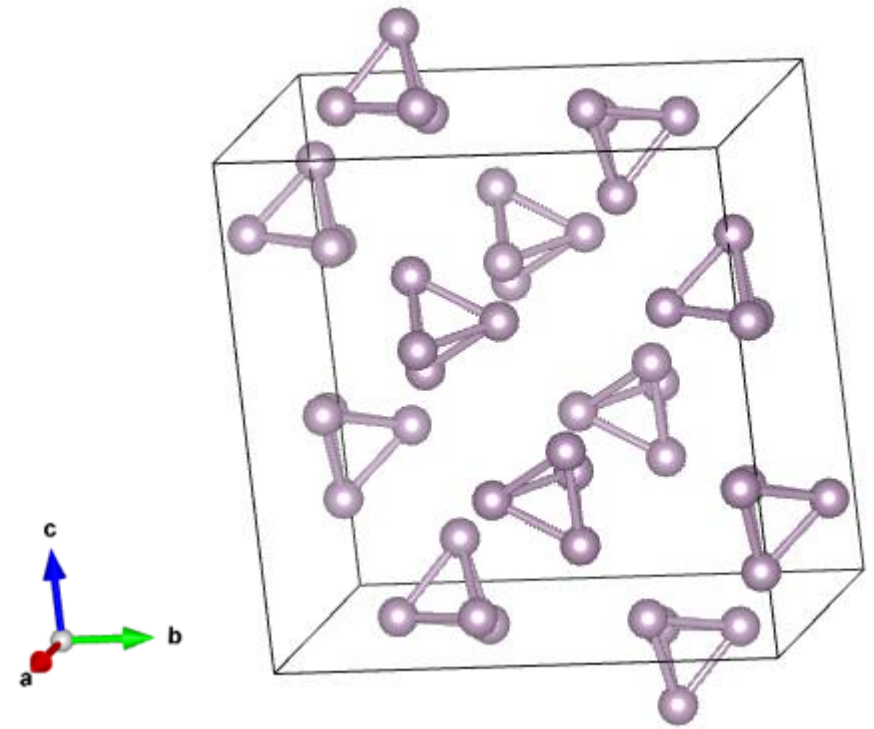
and the primitive cell volume will be:

$$V = abc_z \sin\gamma$$

$$= (5.67)(11.14)(11.11)\sin(100.80°)$$

$$\boxed{V = 689.63\ \text{Å}^3}$$

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat POSCAR_Phosphorus_primitive
Phosphorus primitive simple triclinic crystal structure
1.0
   5.6711142860363353    0.0000000000000000    0.0000000000000000
  -2.0865600265997468   10.9397556127772528    0.0000000000000000
  -1.8655915169458441   -1.0541351676492048   11.1158269508356966
P
24
direct
   0.0715771300000000    0.0012257400000000    0.1815483099999999 P
   0.9284228700000000    0.9987742600000000    0.8184516900000001 P
   0.8380791399999998    0.9474835600000000    0.3122769299999999 P
   0.1619208600000002    0.0525164400000000    0.6877230700000001 P
   0.0045006600000000    0.1402555800000000    0.3097761099999999 P
   0.9954993400000000    0.8597444200000000    0.6902238900000002 P
   0.2313722300000000    0.0105191400000000    0.3716829499999999 P
   0.7686277700000000    0.9894808600000000    0.6283170500000002 P
   0.7750221100000000    0.3731206600000000    0.0598843000000000 P
   0.2249778900000000    0.6268793400000000    0.9401157000000000 P
   0.5922482699999999    0.1805054500000000    0.0352610100000000 P
   0.4077517300000001    0.8194945499999999    0.9647389900000000 P
   0.5085773799999999    0.3058123900000000    0.1714625799999999 P
   0.4914226200000001    0.6941876100000000    0.8285374200000001 P
   0.3877889399999999    0.3214937500000000    0.9809588899999999 P
   0.6122110600000001    0.6785062500000000    0.0190411100000001 P
   0.3027542300000000    0.6871147900000000    0.4672778199999999 P
   0.6972457700000001    0.3128852100000000    0.5327221800000002 P
   0.9321813699999999    0.6270229899999999    0.3659666099999999 P
   0.0678186300000001    0.3729770100000001    0.6340333900000001 P
   0.1994915999999999    0.5102817100000000    0.3589023299999999 P
   0.8005084000000000    0.4897182900000000    0.6410976700000002 P
   0.2355383199999999    0.6805199500000000    0.2713782299999999 P
   0.7644616800000000    0.3194800500000000    0.7286217700000002 P
```



Lattice parameters

a	b	c	alpha	beta	gamma
5.67111	11.13696	11.32048	93.4739	99.4855	100.7984

Unit-cell volume = 689.632617 Å^3

TRIGONAL CRYSTAL SYSTEM

RHOMBOHEDRAL

The rhombohedral Bravais lattice has the periodicity of the conventional trigonal cell, with the addition of two translation vectors, $2/3\mathbf{A}_1 + 1/3\mathbf{A}_2 + 1/3\mathbf{A}_3$ and $1/3\mathbf{A}_1 + 2/3\mathbf{A}_2 + 2/3\mathbf{A}_3$. The primitive vectors can be taken in the form:

$$\begin{aligned}
\mathbf{a}_1 &= \frac{a}{2}\,\hat{\mathbf{x}} - \frac{a}{(2\sqrt{3})}\,\hat{\mathbf{y}} + \frac{c}{3}\,\hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{a}{\sqrt{3}}\,\hat{\mathbf{y}} + \frac{c}{3}\,\hat{\mathbf{z}} \\
\mathbf{a}_3 &= -\frac{a}{2}\,\hat{\mathbf{x}} - \frac{a}{(2\sqrt{3})}\,\hat{\mathbf{y}} + \frac{c}{3}\,\hat{\mathbf{z}},
\end{aligned}$$

and the volume of the primitive cell is one-third that of the conventional cell,

$$V = \left(\frac{2}{\sqrt{3}}\right) a^2\, c.$$

Rhombohedral

The primitive vectors, in general, will be:

$$\begin{matrix} \frac{a}{2} & \frac{-a}{(2\sqrt{3})} & \frac{c}{3} \\ 0 & \frac{a}{\sqrt{3}} & \frac{c}{3} \\ \frac{-a}{2} & \frac{-a}{(2\sqrt{3})} & \frac{c}{3} \end{matrix}$$

or, in poscar file:

2nd line:

$$\begin{matrix} a & a & c \end{matrix}$$

$$\begin{matrix} \frac{1}{2} & \frac{-1}{2\sqrt{3}} & \frac{1}{3} \\ 0 & \frac{1}{\sqrt{3}} & \frac{1}{3} \\ \frac{-1}{2} & \frac{-1}{2\sqrt{3}} & \frac{1}{3} \end{matrix}$$