Solving Solid State-Crystal Lattice problems using Jmol application

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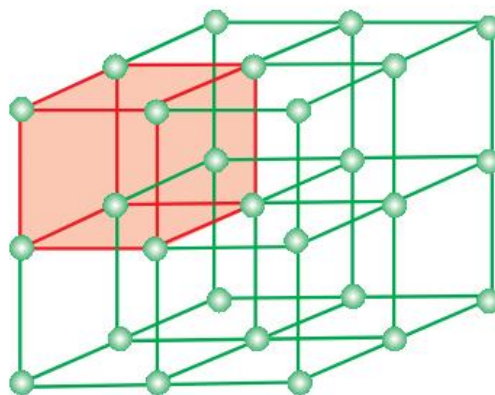*Krishnankoil, Virudhunagar-626126, Tamilnadu India.*

ABSTRACT:

This report explores crystal lattices and unit cells, fundamental to crystallography, using Jmol visualisation software. It elucidates the significance of lattices in understanding arrangement of atoms within crystals, covering primitive, body-centred, and face-centred types. Through Jmol-generated visuals, it delves into diverse unit cell structures, including simple cubic, body-centred cubic, and face-centred cubic, detailing their geometric properties and atomic arrangements. Additionally, lattice parameters' role in defining crystal symmetry is examined, using Jmol application, illustrating their relationship. By integrating theory with interactive visualisation, this report aims to provide a comprehensive understanding of crystallography principles.
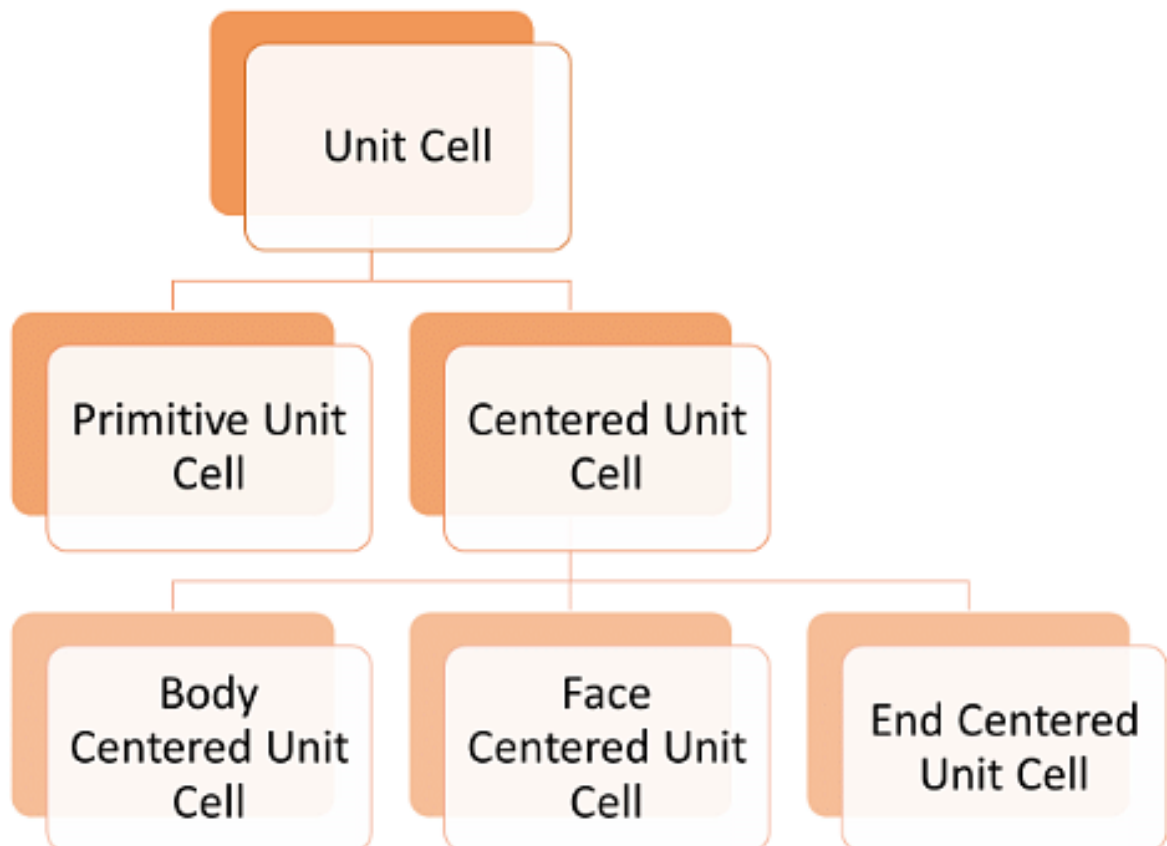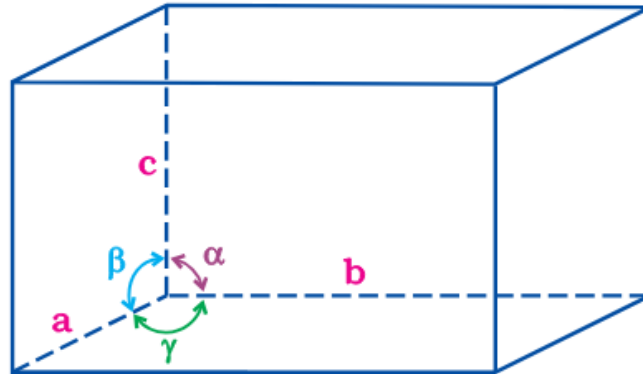
INTRODUCTION:

The main characteristic of crystalline solids is a regular and repeating pattern of constituent particles. If the three dimensional arrangement of constituent particles in a crystal is represented diagrammatically, in which each particle is depicted as a point, the arrangement is called crystal lattice. Thus, a regular three dimensional arrangement of points in space is called a crystal lattice.

- **Crystal lattice:** A regular three dimensional arrangement of particles as points in space.
- **Unit cell:** It is the smallest portion of a crystal lattice, which generates the crystal lattice.

Unit cell is the smallest portion of a crystal lattice which, when repeated in different directions, generates the entire lattice. A unit cell is characterised by:
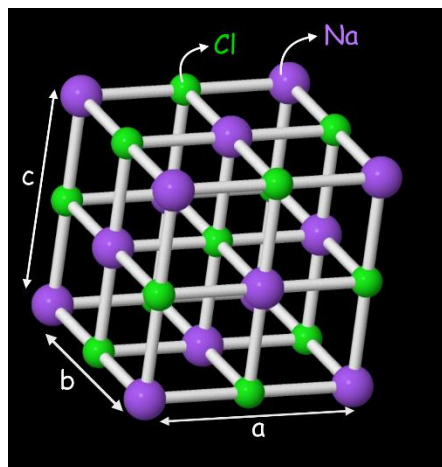
(i)   Its dimensions along the three edges, a, b and c. These edges may or may not be mutually perpendicular.

(ii)   Angles between the edges, α (between b and c) β (between a and c) and γ (between a and b). Thus, a unit cell is characterised by six parameters, a, b, c, α, β and γ

In all, there are seven types of primitive unit cells in crystals. But here we will go through the 4 major types:

- ♣ **Cubic:**
  - ✓ **Axial Distance:** a = b = c = 5.620 Å
  - ✓ **Axial angles:** α = β = γ = 90°
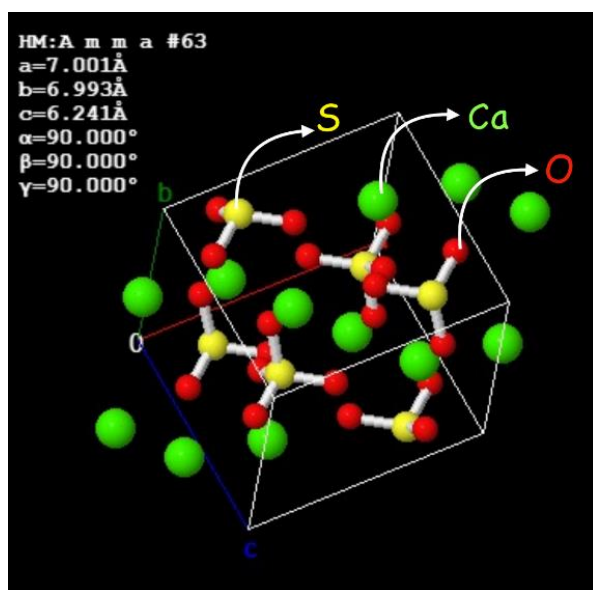 - ✓ **Examples:** NaCl


```
HM:F m -3 m #225
a=5.620Å
b=5.620Å
c=5.620Å
α=90.000°
β=90.000°
γ=90.000°
```

- ♣ **Tetragonal:**
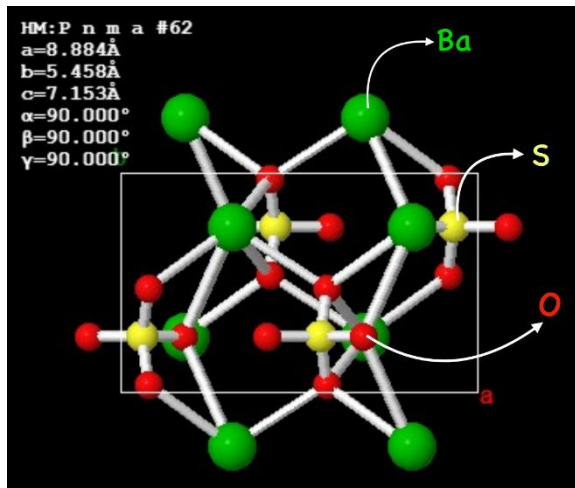 - ✓ **Axial Distance:** a = b ≠ c
  - ✓ **Axial angles:** α = β = γ = 90°
  - ✓ **Examples:** $CaSO_4$


```
HM:A m m a #63
a=7.001Å
b=6.993Å
c=6.241Å
α=90.000°
β=90.000°
γ=90.000°
```

a	7.00032 Å
b	6.99234 Å
c	6.24097 Å
α	90°
β	90°
γ	90°
Cell volume	305.487 Å³
Number of distinct elements	3
Space group number	63
Hermann-Mauguin space group symbol	A m m a
Hall space group symbol	-A 2a 2a
Has coordinates	Yes
Has disorder	No
Has F_{obs}	No

♣ **Orthorhombic:**
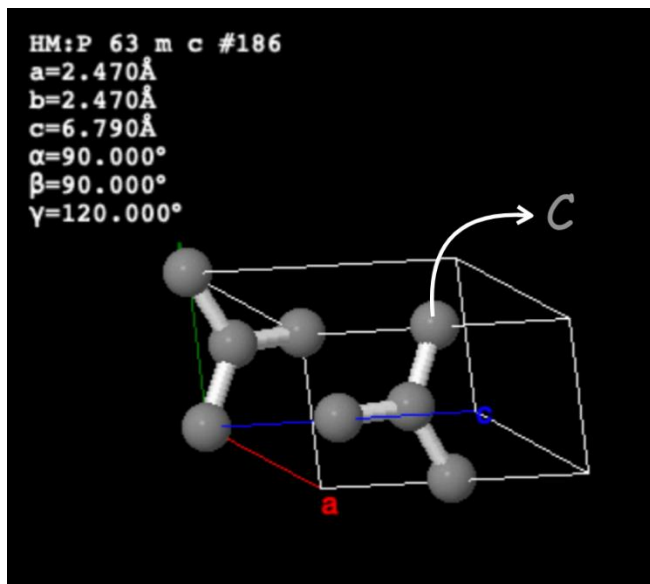
    ✓ **Axial Distance:** $a \neq b \neq c$

    ✓ **Axial angles:** $\alpha = \beta = \gamma = 90°$

    ✓ **Examples:** $BaSO_4$

a	8.884 ± 0.004 Å
b	5.458 ± 0.003 Å
c	7.153 ± 0.003 Å
α	90°
β	90°
γ	90°
Cell volume	346.8 Å³
Number of distinct elements	3
Space group number	62
Hermann-Mauguin space group symbol	P n m a
Hall space group symbol	-P 2ac 2n
Residual factor for all reflections	0.051
Has coordinates	Yes
Has disorder	No
Has F_{obs}	No

♣ **Hexagonal:**

    ✓ **Axial Distance:** $a = b \neq c$

    ✓ **Axial angles:** $\alpha = \beta = 90°$; $\gamma = 120°$

    ✓ **Examples:** Graphite

a	2.47 Å
b	2.47 Å
c	6.79 Å
α	90°
β	90°
γ	120°
Cell volume	35.9 Å³
Number of distinct elements	1
Space group number	186
Hermann-Mauguin space group symbol	P 63 m c
Hall space group symbol	P 6c -2c
Has coordinates	Yes
Has disorder	No
Has F_{obs}	No

CONCEPT OF BCC:

A body-centered cubic unit cell has an atom at each of its corners and also one atom at its body center.

Number of Atoms in BCC Cell:

Thus, in a BCC cell, we have:

- 8 corners × 1/8 per corner atom = 8 × 1/8 = 1 atom

- 1 body center atom = 1 × 1 = 1 atom

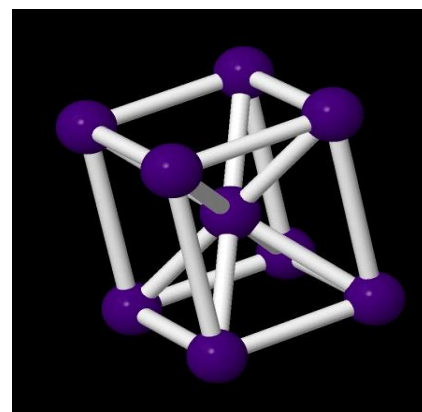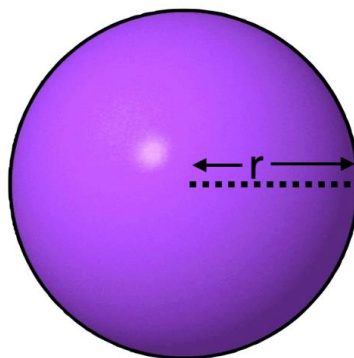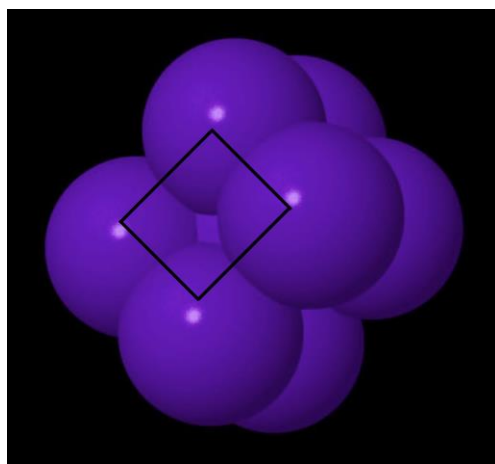Therefore, the total number of atoms present per unit cell = **2 atoms.**

PROBLEMS:

1. Sodium metal crystallizes in a body centered cubic lattice with a unit cell edge of 4.29 Å. The radius of sodium atom is approximately:

(a) 5.72 Å   **(b) 0.93 Å**   **(c) 1.86 Å**   **(d) 3.22 Å**

Solution:

For bcc, r = (√3/ 4) a

a = 4.29
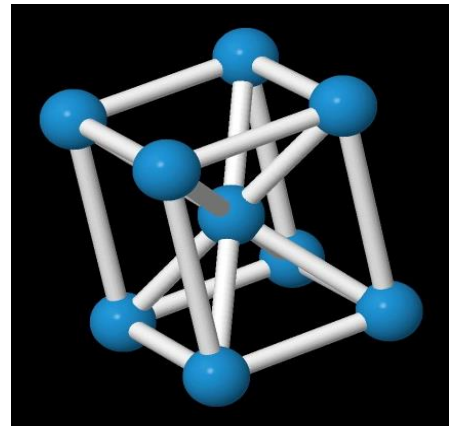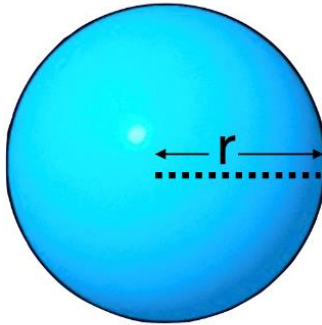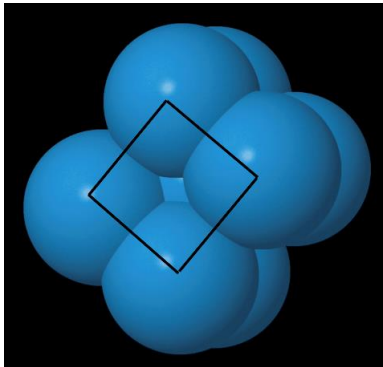
r = (√3/4) × 4.29

= 1.86

Hence option (c) is the answer.

2. Tungsten crystallizes in the body-centered cubic unit cell. If the edge of the unit cell is 316.5 pm, what is the radius of the tungsten atom?

Answer:

If a is the edge length of the bcc
unit cell, then the radius of an atom,

$r = (\sqrt{3}/ 4)\ a$

Here, a = 316.5 pm

$\therefore r = (\sqrt{3}/ 4) \times 316.5$

r = 137.04 pm

3. An element has a bcc structure having unit cells 12.08×10^{23}. Find the total number of atoms in these unit cells.

(a)24.16×10^{23}　　　　**(b)12.08×10^{23}**　　　　**(c)36.24×10^{23}**　　　　**(d)6.02×10^{23}**

Solution: Each bcc unit cell has a total of 2 atoms – one from the eight corner atoms contributing 1/8 each and one from the atom sitting at the cube center.

No. of atoms at corners $=1/8 \times 8 = 1$

No. of atoms at center $=1 \times 1 = 1$

No. of atoms per unit cell $=1+1=2$

Total number of atoms $=2 \times$Total number of unit cells

$=2 \times 12.08 \times 10^{23} =$ **24.16×10^{23}**

PROCEDURE FOR DOWNLOADING THE CIF:

[https://spoken-tutorial.org/watch/Jmol+Application/Crystal+Structure+and+Unit+Cell/English/]

1. Search and open Crystallography Open Database (COD).

2. Download CIF (Crystallographic Information File) from Crystallography Open Database (COD).

3. Open CIF files in Jmol.

4. Display unit cell and unit cell parameters on Jmol panel.

5. Display crystal structures of different crystal systems. For example Cubic (sodium chloride), Hexagonal (graphite) and Rhombohedral (calcite).