Unit Cells

1. A body centered cubic unit cell contains how many atoms? How many atoms in a primitive cubic cell? How many atoms in a body-centered cubic cell?

   Body centered unit cell: 2 atoms
   Primitive unit cell: 1 atom
   Face-centered unit cell: 4 atoms

2. An unknown metal crystallizes in a face-centered cubic arrangement with an edge length of 351 pm. The density of the unknown metal is 6.83 g/cm^3. What is the radius and atomic mass? Identify the metal.

   d = m/V $m = 6.83\frac{g}{cm^3} \times \left(351\ pm \times \frac{1 \times 10^{-10}\ cm}{1\ pm}\right)^3 = 2.95 \times 10^{-22}\ g$

   a face-centered unit cell has 4 atoms

   molar mass $= \frac{2.95 \times 10^{-22}\ g}{4\ atoms} \times \frac{6.02 \times 10^{23}\ atoms}{1\ mol} = \mathbf{44.4\ g/mol}$

   radius for fcc is $\frac{A}{\sqrt{8}} = \frac{\mathbf{351\ pm}}{\sqrt{8}} = \mathbf{124\ pm}$ **The metal could be Sc.**

3. Sodium crystallizes into a body-centered cubic unit cell. The density of sodium is 0.972 g/cm^3. What is the edge length of the unit cell? What is the radius of a sodium atom? Provide the answers in pm.

   $mass\ of\ one\ Na\ atom = \frac{22.9898\ g}{mol} \times \frac{1\ mol}{6.02 \times 10^{23} atoms} = 3.82 \times 10^{-23}\ g/atom$

   There are 2 Na atoms in each unit cell

   Mass of unit cell = 2 x (3.82 x 10^{23} g/atom) = 7.64 x 10^{-23} g

   Cell volume = unit cell mass/density $= \frac{7.64 \times 10^{-23}\ g}{0.972\ g/cm^3} = 7.86 \times 10^{-23}\ cm^3$

   Edge length = $A = \sqrt[3]{7.86 \times 10^{-23}\ cm^3} = 4.28 \times 10^{-8} cm = \mathbf{429\ pm}$

   $\boldsymbol{r = \frac{\sqrt{3}A}{4} = \frac{\sqrt{3} \times 429\ pm}{4} = 186\ pm}$

4. Barium metal has a density of 3.62 g/cm^3. It crystallizes in a cubic unit cell with an edge length of 502 pm. How many Ba atoms are in the unit cell? Which type of unit cell does Ba crystallize in?

   $mass\ of\ one\ Ba\ atom = \frac{137.327\ g}{mol} \times \frac{1\ mol}{6.02 \times 10^{23} atoms} = 2.28 \times 10^{-22}\ g/atom$

   volume of unit cell = $s^3 = \left(502\ pm \times \frac{10^{-10} cm}{1\ pm}\right)^3 = 1.265 \times 10^{-22} cm^3$

   mass of unit cell = $3.62\frac{g}{cm^3} \times (1.265 \times 10^{-22} cm^3) = 4.58 \times 10^{-22} g$

   number of Ba atoms in unit cell

   $= \frac{unit\ cell\ mass}{mass\ of\ one\ Ca\ atom} = \frac{4.58 \times 10^{-22} g}{2.28 \times 10^{-22}} = 2.01 = \mathbf{2\ atoms}$

   This would be a body-centered cubic unit cell.