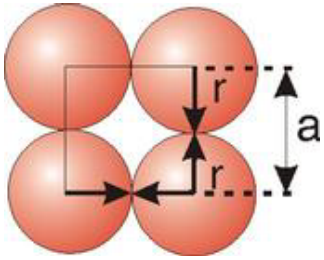
Sample problem

Polonium is the only element with a crystal structure based on the simple (primitive) cubic unit cell. Its density is 9.142 g/cm^3. Calculate the atomic radius for polonium.

- Atomic radius = r
- **PC: atoms touch along the side of the unit cell (a)**
  - **a = 2r**
- To find (a), we need the V of the Po unit cell.

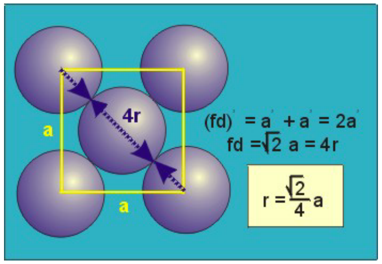


- $1\ atom\ Po \times \frac{1\ mol}{6.022\times10^{23}\ atoms\ Po} \times \frac{208.982\ g}{1\ mol} \times \frac{1\ cm^3}{9.142\ g} = 3.796\times10^{-23}\ cm^3$
- $a = \sqrt[3]{3.796\times10^{-23}\ cm^3} = 3.361\times10^{-8} cm \times \frac{1\ m}{100\ cm} \times \frac{10^{12}\ pm}{1\ m} = 336.1\ pm$
- $a = 2r \rightarrow \boldsymbol{r} = \frac{336.1\ pm}{2} = \mathbf{168.0\ pm}$

Sample problem

Silver crystallizes in a face centered cubic unit cell. Each side of the unit cell has a length of 409 pm. What is the radius of the silver atom?

- Atomic radius = r
- **FCC: atoms touch along the face diagonal**
  - One atom and two half atoms lie on face diagonal
    - **Face diagonal = 4r**
  - **Two sides of unit cell (a)** form a **right angle**
  - **Face diagonal** = **hypotenuse** of resulting right triangle

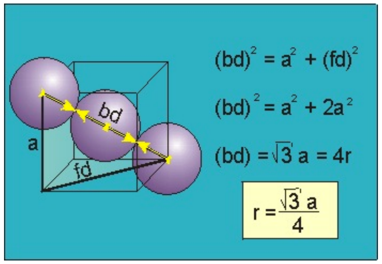


- $a^2 + a^2 = (4r)^2 \rightarrow 2a^2 = 16r^2 \rightarrow r^2 = \frac{a^2}{8}$
- $\boldsymbol{r = \frac{409\ pm}{\sqrt{8}} = 144\ pm}$

Sample problem

Tantalum has a density of 16.69 g/cm^3 and crystallizes in a BCC unit cell. What is its atomic radius in pm? (Hint: where do Ta atoms touch in a BCC cell?)

- Atomic radius = r
- **BCC: atoms touch along the body diagonal**
  - One atom and two half atoms lie on body diagonal
  - **Body diagonal = 4r**
- A **right triangle** is formed by a **side of the cell (a)**, a **face diagonal (fd)** and the **body diagonal**
  - **Body diagonal** = **hypotenuse**
  - $a^2 + a^2 = (fd)^2 \rightarrow \boldsymbol{fd = \sqrt{2a^2}}$
  - $a^2 + (\sqrt{2a^2})^2 = (4r)^2 \rightarrow a^2 + 2a^2 = 16r^2 \rightarrow \boldsymbol{r^2 = \frac{3a^2}{16}}$



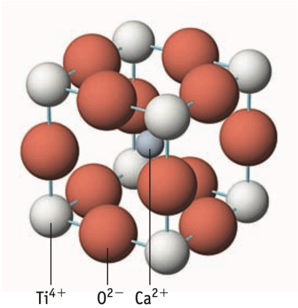
Sample problem

Tantalum has a density of 16.69 g/cm^3 and crystallizes in a BCC unit cell. What is its atomic radius in pm? (Hint: where do Ta atoms touch in a BCC cell?)

- First find (a) for Ta unit cell (from V of Ta unit cell)
  - BCC: 2 Ta atoms/unit cell
  - $2\ Ta\ atoms \times \frac{1\ mol\ Ta}{6.022\times10^{23}\ Ta\ atoms} \times \frac{180.9479\ g}{1\ mol\ Ta} \times \frac{1\ cm^3}{16.69\ g} = 3.60\times10^{-23}\ cm^3$
  - $Unit\ cell\ length\ of\ Ta\ atom\ a = \sqrt[3]{3.60\times10^{-23} cm^3} = 3.30\times10^{-8}\ cm$
- $r = \frac{(3.30\times10^{-8} cm)\sqrt{3}}{4} = 1.43\times10^{-8}\ cm \times \frac{1\ m}{100\ cm} \times \frac{10^{12}\ pm}{1\ m} = \mathbf{143\ pm}$

Sample problem

One unit cell of the common mineral perovskite is illustrated in the margin. This compound is composed of calcium and titanium cations and oxide anions. Based on the unit cell, what is the formula of perovskite?



- 1 Ca^{2+} ion in the body
- 8 Ti^{4+} ions in the corners x 1/8 = 1 Ti^{4+} ion
- 12 O^{2-} ions on the sides x ¼ = 3 O^{2-} ions
- **$CaTiO_3$**

Sample problem

If the ionic radius of Cs^{+} is 165 pm and the ionic radius of Cl^{-} is 181 pm, what is the density of CsCl? CsCl crystallizes in a BCC crystal lattice.

- BCC: Cs^{+} ion and two halves of Cl^{-} ions touch along the body diagonal (bd)
  - bd = 2(165 pm) + 2(181 pm) = 692 pm
- $a^2 + (fd)^2 = (bd)^2$ $\qquad fd = \sqrt{2a^2}$
- $a^2 + 2a^2 = (692\text{ pm})^2 \rightarrow a = 400.\text{ pm} = 4.00 \times 10^{-8}\text{ cm}$
- $V_{unit\ cell} = (4.00 \times 10^{-8}\text{ cm})^3 = 6.38 \times 10^{-23}\text{ cm}^3$
- $m_{unit\ cell} = m_{Cs\ ion} + m_{Cl\ ion}$
  - $1\ Cs\ ion \times \frac{1\ mol}{6.022\times10^{23}\ Cs\ ions} \times \frac{132.9055\ g}{1\ mol} = 2.207\times10^{-22}\ g$
  - $1\ Cl\ ion \times \frac{1\ mol}{6.022\times10^{23}\ Cs\ ions} \times \frac{35.4527\ g}{1\ mol} = 5.887\times10^{-23}\ g$
  - $m_{unit\ cell} = 2.796 \times 10^{-22}\text{ g}$
- $d = \frac{2.796\times10^{-22}\ g}{6.38\times10^{-23}\ cm^3} = \mathbf{4.38\ g/cm^3}$