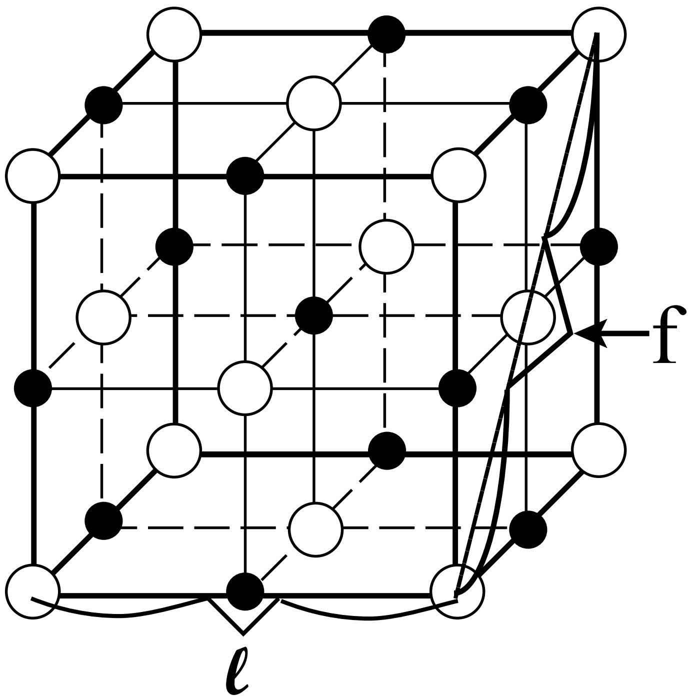
Radius Ratios for Cubic Lattices

SANTA FE COMMUNITY COLLEGE Chemistry

Coordination Number 6



In the case of coordination number of 6, each cation (●) is surrounded by 6 anions (○) and vice versa. The optimum fit is achieved when the anions just touch across the face diagonal (f) and the anions and cations just touch along the edge (ℓ).

From the diagram above one can see that... where r_- is the radius of the anion and r_+ is the radius of the cation.

$f = 4r_-$ and $\ell = 2r_- + 2r_+$ where r_- = radius of anion and r_+ = radius of cation

In a cube the length of the face diagonal (f) is equal to $\sqrt{2}$ times the length of the edge.

$$f = \sqrt{2} \cdot \ell$$

Substituting the 2 radii into the equation gives...

$$4r_- = \sqrt{2} \cdot (2r_- + 2r_+)$$

Dividing each side of the equation by 2 gives...

$$2r_- = \sqrt{2} \cdot (r_- + r_+)$$

Dividing each side by $\sqrt{2}$ gives ...

$$\frac{2r_-}{\sqrt{2}} = \sqrt{2} \cdot (r_- + r_+) \quad \text{or} \quad \sqrt{2} \cdot r_- = (r_- + r_+)$$

Subtracting r_- from each side gives...

$$(\sqrt{2} \cdot r_-) - (r_-) = r_+ \quad \text{or} \quad (\sqrt{2} - 1) \cdot (r_-) = r_+$$

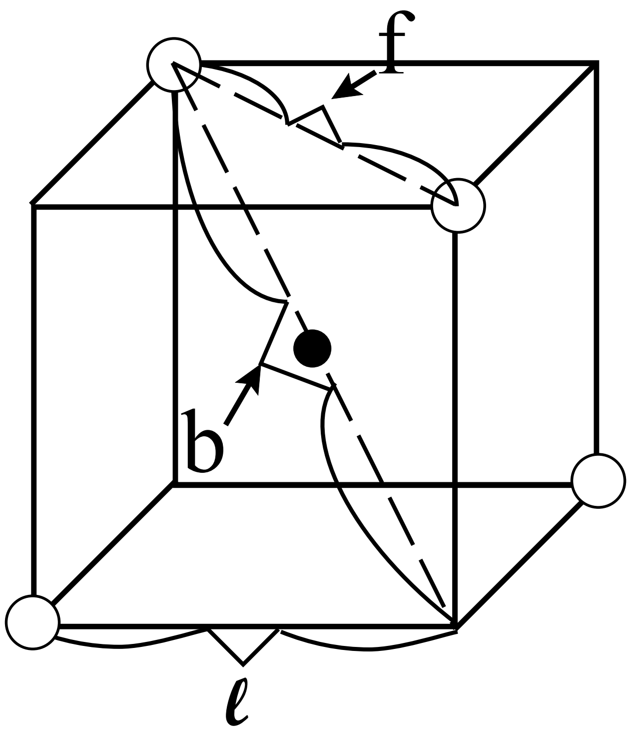
Dividing each side by r_- yields...

$$\frac{r_+}{r_-} = \sqrt{2} - 1$$

Thus the optimum fit is achieved when the cation is 0.414 times the size of the anion.

$$\frac{r_+}{r_-} = 0.414$$

Coordination Number 4



In the case of coordination number of 4, each cation (●) is surrounded by 4 anions (○) and vice versa. The optimum fit is achieved when the anions just touch across the face diagonal (f) and the anions and cations just touch along the body diagonal (b).

From the diagram above one can see that... where r_- is the radius of the anion and r_+ is the radius of the cation.

$$f = 2r_- \quad \text{and} \quad b = 2r_- + 2r_+ \quad \text{where}$$
$$r_- = \text{radius of anion} \quad \text{and} \quad r_+ = \text{radius of cation}$$

In a cube the length of the face diagonal (f) is equal to $\sqrt{2}$ times the length of the edge and body diagonal (b) is equal to $\sqrt{3}$ times the length of the edge.

$$f = \sqrt{2} \cdot \ell \quad \text{or} \quad \ell = \frac{1}{\sqrt{2}} \cdot f \quad \text{and}$$
$$b = \sqrt{3} \cdot \ell \quad \text{or} \quad \ell = \frac{1}{\sqrt{3}} \cdot b$$

Equating these two expressions for ℓ gives ...

$$\frac{1}{\sqrt{2}} \cdot f = \frac{1}{\sqrt{3}} \cdot b$$

Substituting the radii into this expression gives ...

$$\frac{1}{\sqrt{2}} \cdot (2r_-) = \frac{1}{\sqrt{3}} \cdot (2r_- + 2r_+)$$

Dividing each side of the equation by 2 gives...

$$\frac{1}{\sqrt{2}} \cdot (r_-) = \frac{1}{\sqrt{3}} \cdot (r_- + r_+)$$

Multiplying each side by $\sqrt{3}$ gives ...

$$\frac{\sqrt{3}}{\sqrt{2}} \cdot (r_-) = r_- + r_+$$

Subtracting r_- from each side gives...

$$\frac{\sqrt{3}}{\sqrt{2}} \cdot (r_-) - r_- = r_+$$

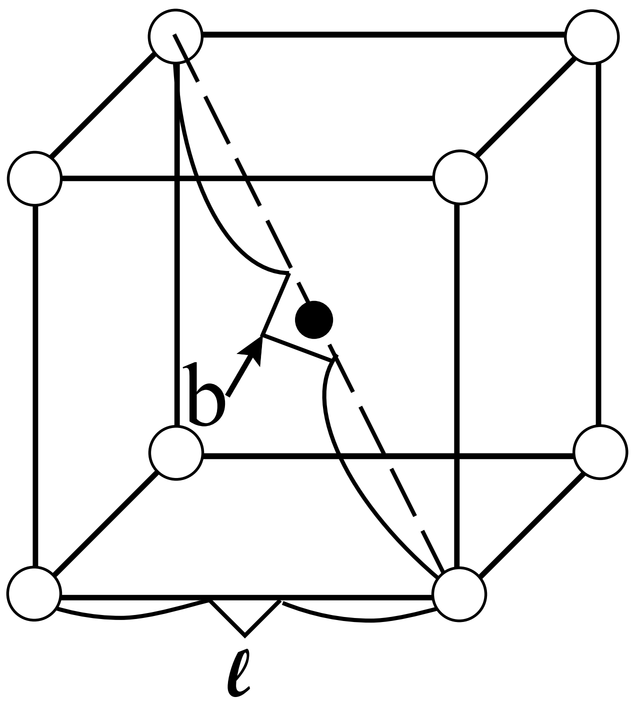
Dividing each side by r_- yields...

$$\frac{r_+}{r_-} = \frac{\sqrt{3}}{\sqrt{2}} - 1$$

Thus the optimum fit is achieved when the cation is 0.225 times the size of the anion.

$$\frac{r_+}{r_-} = 0.225$$

Coordination Number 8



In the case of coordination number of 8, each cation (●) is surrounded by 8 anions (○) and vice versa. The optimum fit is achieved when the anions just touch across the edge (ℓ) and the anions and cations just touch along the body diagonal (b).

From the diagram above one can see that... where r_- is the radius of the anion and r_+ is the radius of the cation.

$\ell = 2r_-$ and $b = 2r_- + 2r_+$ where r_- = radius of anion and r_+ = radius of cation

In a cube the length of the edge and body diagonal (b) is equal to $\sqrt{3}$ times the length of the edge.

$$b = \sqrt{3} \cdot \ell \quad \text{or} \quad \ell = \frac{1}{\sqrt{3}} \cdot b$$

Substituting the radii into this expression gives ...

$$\sqrt{3} \cdot (2r_-) = (2r_- + 2r_+)$$

Dividing each side of the equation by 2 gives...

$$\sqrt{3} \cdot (r_-) = (r_- + r_+)$$

Subtracting r_- from each side gives...

$$\sqrt{3} \cdot (r_-) - r_- = r_+$$

Dividing each side by r_- yields...

$$\frac{r_+}{r_-} = \sqrt{3} - 1$$

Thus the optimum fit is achieved when the cation is 0.732 times the size of the anion.

$$\frac{r_+}{r_-} = 0.732$$