

Crystal Structures: NaCl, CsCl, etc.

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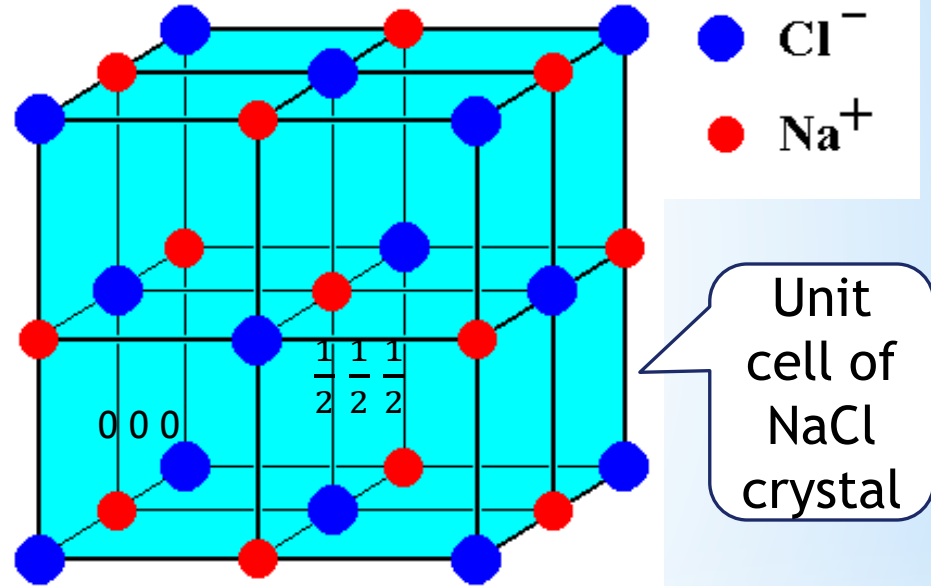
NaCl Structure

- NaCl is a cubic type of ionic crystal.
- FCC type of lattice.

$$\text{Cl}^-: 8 \times \frac{1}{8} \text{ corner} + 6 \times \frac{1}{2} \text{ faces} = 4$$

$$\text{Na}^+: 12 \times \frac{1}{4} \text{ edges} + 1 \text{ center} = 4$$

- So, total 4 NaCl molecules, each NaCl is a basis.
- Each Na^+ 6 nearest neighbor Cl^- and vice versa.
- Nearest neighbor distance = $a/2$.
- 2nd neighbor distance = $a/\sqrt{2}$
- Each Na^+ 12 2nd nearest neighbor Na^+ and vice versa.



$$\text{Cl}^-: 0\ 0\ 0, \frac{1}{2}\ \frac{1}{2}\ 0, \frac{1}{2}\ 0\ \frac{1}{2}, 0\ \frac{1}{2}\ \frac{1}{2}.$$

$$\text{Na}^+: \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}, \frac{1}{2}\ 0\ 0, 0\ \frac{1}{2}\ 0, 0\ 0\ \frac{1}{2}.$$

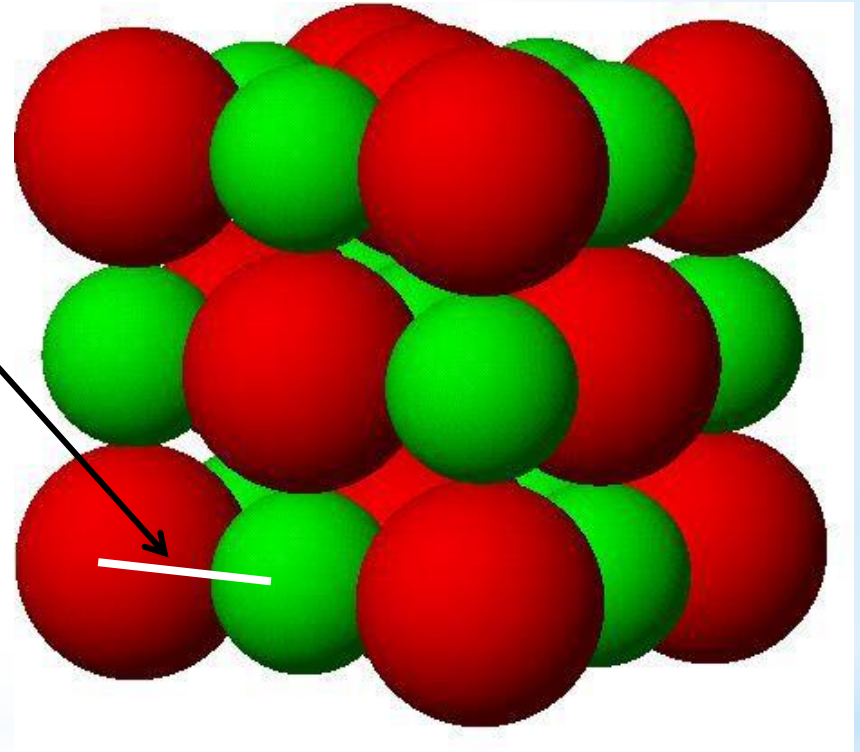
Packing Factor of NaCl structure

Closest packing along nearest neighbor distance, $a/2 = r_{\text{Na}^+} + r_{\text{Cl}^-}$

$$\text{PF} = \frac{4 \times \frac{4}{3} \pi [(r_{\text{Na}^+})^3 + (r_{\text{Cl}^-})^3]}{[2 (r_{\text{Na}^+} + r_{\text{Cl}^-})]^3}$$

$$= 0.67$$

Example: LiH, NaCl, KBr, KCl, PbS, NH_4I , AgBr, MgO, MnO, BaO, etc.



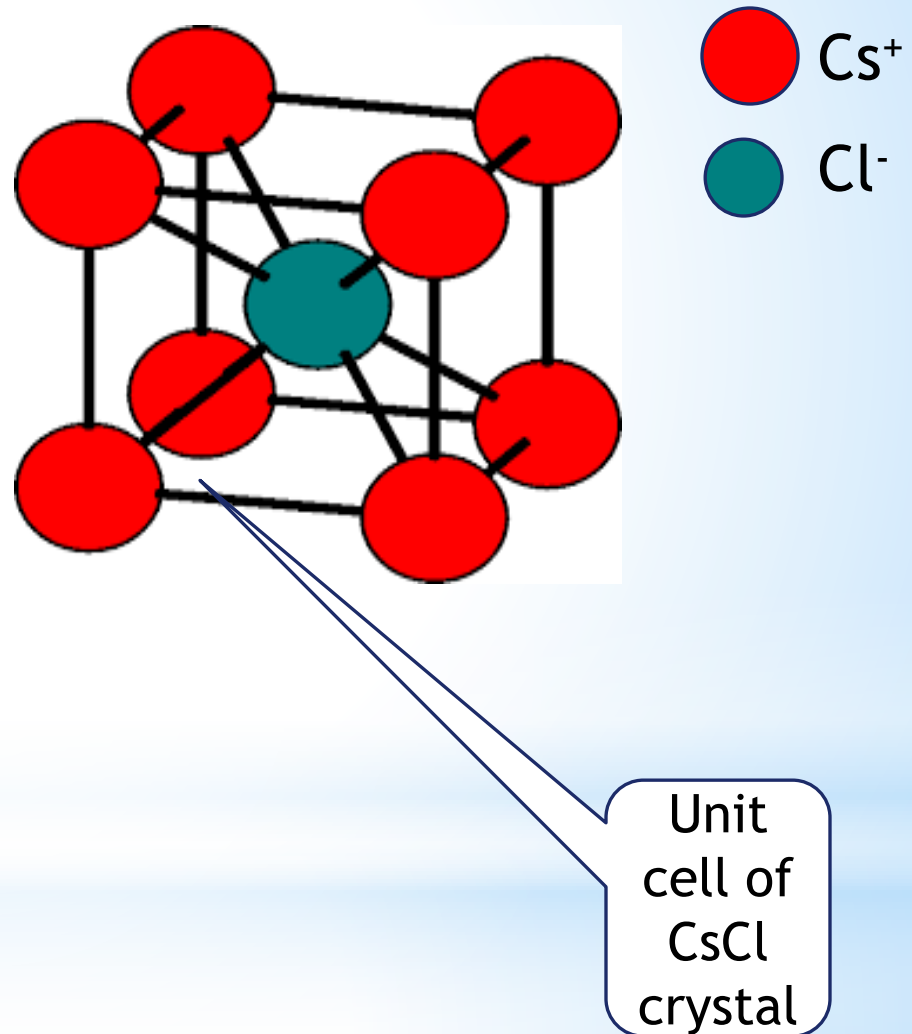
CsCl Structure

- CsCl is a simple cubic type of ionic crystal.

$$\text{Cs}^+: 8 \times \frac{1}{8} \text{ corner} = 1$$

$$\text{Cl}^-: 1 \text{ body center} = 1$$

- So, total 1 CsCl molecule (basis).
- Each Cs^+ 8 nearest neighbor Cl^- and vice versa.
- Nearest neighbor distance = $\sqrt{3}a/2$.
- 2nd neighbor distance = a
- Each Cs^+ 6 2nd nearest neighbor Cs^+ and vice versa.
- Cs^+ : 0 0 0; Cl^- : $\frac{1}{2} \frac{1}{2} \frac{1}{2}$.



Packing Factor of CsCl structure

Closest packing along nearest neighbor distance, $\sqrt{3}a/2 = r_{\text{Cs}^+} + r_{\text{Cl}^-}$

$$\text{PF} = \frac{1 \times \frac{4}{3} \pi [(r_{\text{Cs}^+})^3 + (r_{\text{Cl}^-})^3]}{[2/\sqrt{3} (r_{\text{Cs}^+} + r_{\text{Cl}^-})]^3}$$

$$= 0.684$$

Example: CsCl, CsBr, NH_4Cl , CuZn, TlI, TlBr, etc.

