E-Content

Topic: Structure of crystals

Chapter: Solid State

Physical Chemistry

B. Sc. Chemistry (H) 1st Year

By

Dr. Chandramika Bora

Department of Chemistry

Patna Science College, Patna University, Patna

STRUCTURE OF IONIC CRYSTAL

NaCl crystal

- The ionic crystal of NaCl is shown in Fig 1.
- Each sodium ion is surrounded by six chloride ions and each chloride ions is surrounded by six sodium ions.
- Thus NaCl crystal can be considered to be composed of two interpenetrating *fcc* lattices, one made up of sodium ions and the other made up of chloride ions
- A unit cell of sodium chloride can be considered to be made up of one fcc unit cell of sodium ions and one fcc unit cell of chloride ions.
- Since each such fcc unit cell has four atoms (or ions), sodium chloride crystal has four NaCl formula units per unit cell

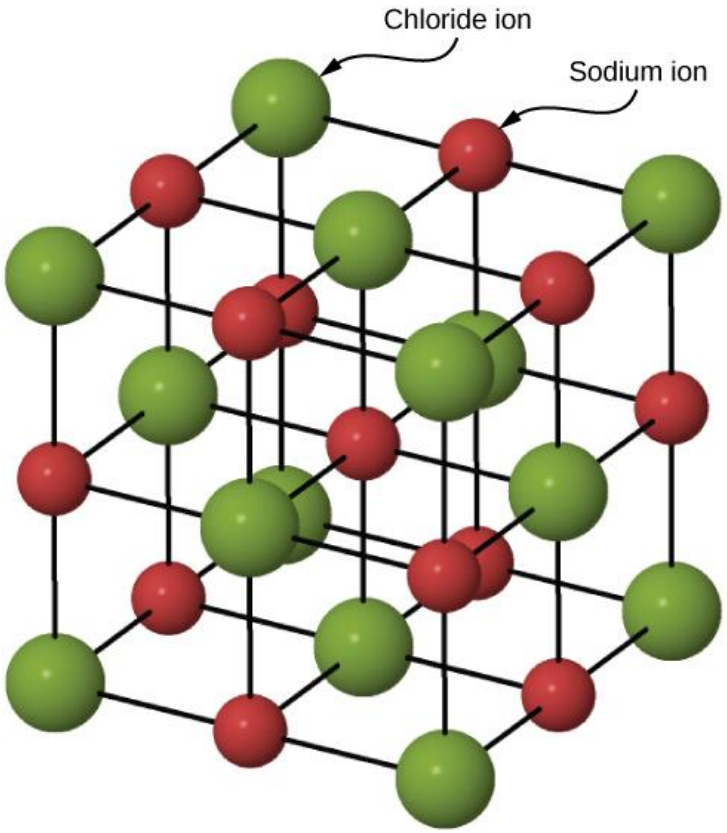


Fig 1 Structure of NaCl crystal

- For first order reflection the maximum intensity of reflection occurs at the angle of 5.9^0, 8.4^0 and 5.2^0 for 100, 110 and 111 planes, respectively as calculated.
- Since, $n\lambda = 2d\sin\theta$ so, $d \alpha 1/\sin\theta$
- If only first order reflection are considered than,

$d_{100}:d_{110}:d_{111} = 1/\sin 5.90: 1/\sin 8.40: 1/\sin 5.20$

$= 1/0.103: 1/0.146: 1/0.091$

$= 1:0.704:1.155$

- For face-centred cubic system the planes can be passed through the atom having

Miller indices 100, 110 and 111 at the relative spacing $a/2:a/2\sqrt{2}: a/\sqrt{3}$

So $d_{100}:d_{110}:d_{111} = a/2:a/2\sqrt{2}:a/\sqrt{3}$

$= 1:0.707:1.154$

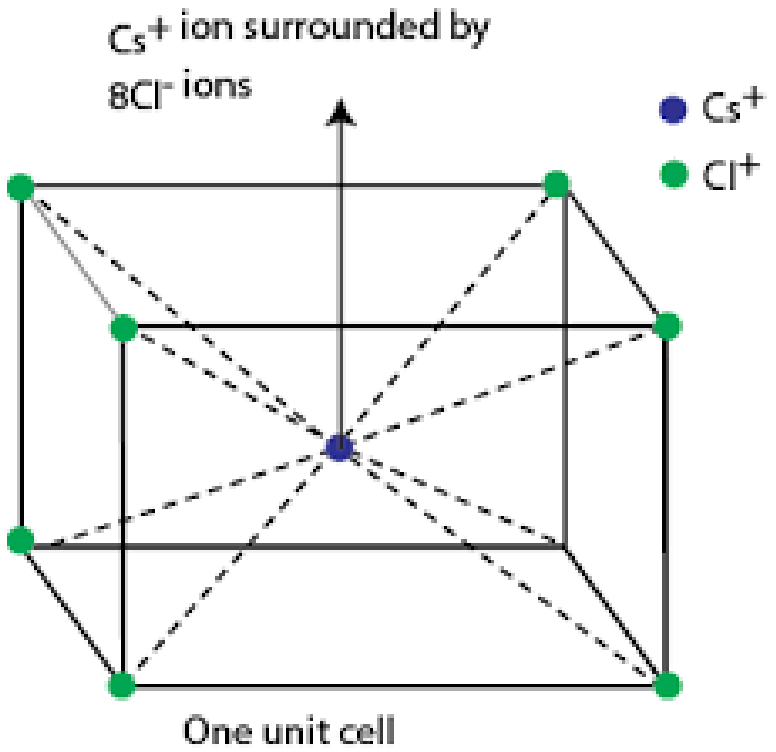
- This ratio is almost identical with the ratio from experimental observations. Hence NaCl crystal is face-centred cubic system

Structure of CsCl crystal

- Cesium chloride, CsCl, has a body centred cubic structure. In its crystal lattice, each Cs^+ ion is surrounded by 8 Cl- ions and its coordination number is 8.

- Since CsCl crystal has one Cs^+ ion at the centre and eight CI^- ions at the corners, it has one Cs^+ ion and one CI^- ion (8 X 1/8 = 1) belonging to one unit cell That is, each CsCl unit cell has one formula unit.

- The value of distance between Cs^+ ion and Cl- ion as determined by Bragg's spectrometer is 3.510^0A



Covalent Crystals:

- In covalent crystals, definite covalent bonds join all the atoms in the crystal. The structure of a covalent crystal is related to the number of valence electrons, the nature of orbitals involved in bond formation and their orientation. One of the most commonly cited example is that of **Diamond**

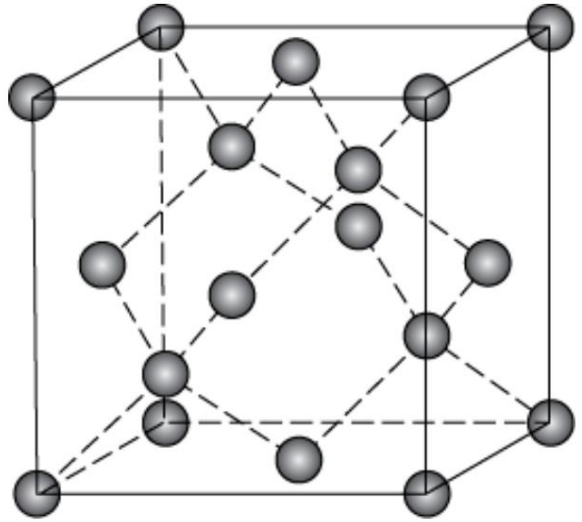


Fig. Crystal structure of diamond

- Each carbon atom in diamond is tetrahedrally bonded to four neighbouring carbon atoms. This is so since each carbon has four sp3 hybridised orbitals pointing towards the corners of a regular tetrahedron. These orbitals overlap with the similar set of orbitals on the neighbouring atoms. The C-C bond distance is 0.154 nm

- The crystal of diamond is very hard because the covalent links runs without a break throughout the whole crystal. The crystal can be cut only by breaking the covalent links. High melting point can also be explained by stating that the atoms are very firmly attached within the crystal.

Referred Books:

- P. Atkins and J. de Paula, *Physical Chemistry*, 9th Edition, W. H. Freeman, 2009
- K.L. Kapoor, *A Textbook of Physical Chemistry*, 2nd Edition, Macmillan, 2011
- G.W. Castellan, *Physical Chemistry*, 3rd Edition, Addison Wesley, 1983
- Puri, Sharma, Pathania, Principle of Physical chemistry, 44^{th} edition, 2010
- I.N. Levine, *Physical Chemistry*, 6th Edition, McGraw-Hill, 2008.