

Structure of AB Compounds

AB-structures which are based on close packings:

a) based on ccp

1. Rock salt: NaCl, LiCl, KBr, AgCl, CaO, is based on a fcc array of the anions in which the cations occupy the octahedral holes. The CN (coordination number) of each type of ions is 6.

2. Sphalerite (Zinc blende): ZnS, CuCl, CdS is based on a fcc array of the anions and the cations occupy one half of the tetrahedral holes each ions is surrounded by four neighbors.

b) based on hcp

1. Wurtzite: ZnS ZnO, BeO, MnS it is derived from hcp anion array and the cations occupy $\frac{1}{2}$ of the tetrahedral holes. The CN is 4 for both type of ions.

2. Nickel Arsenide structure: NiAs, NiS, FeS it is derived from hcp anion array and the Ni atoms occupy all octahedral holes. The cations lie at the centers of the trigonal prisms of the anions.

AB-structure which is not based on a close packing:

Cesium chloride: CeCl, CaS, CuZn the structure has cubic unit cell with each corner occupied by an anions and the cations occupy the cubic holes in the center of the cell. The CN is 8 for both types of ions.

Reference:

1. Anthony R. West, Basic Solid State Chemistry, John Wiley and Sons, LTD, 1999.
2. Shriver and Atkins, Inorganic Chemistry, Oxford University Press, 3rd edition 1999.
3. Internet.