

Structures of AB₂-compounds

AB₂ compounds have different coordination numbers for cation and anion. The most important of these compounds are the fluorite structure (CaF₂) and rutile structure (TiO₂). Four types of AB₂ structures are exemplified below:

1. Fluorite structure (CaF₂).

a. The fluorite structure can be regarded as Ca²⁺ cations forming a cubic close packed structure while the F⁻ anions occupy all the tetrahedral holes. In this description the cations are close-packed because the F⁻ anions are smaller.¹

* Li₂O is an example for a compound which crystallizes in the antifluorite structure, which is the inverse of the fluorite structure in the sense that the locations of cations and anions are reversed.

b. In the fluorite structure, the cation site (Ca²⁺) is surrounded by a cubic array of eight F anions, and the anions (F⁻) in their tetrahedral holes have four nearest neighbors. So the structure is said to have 8:4 coordination.

c. Examples of this structure are: BaCl₂, HgF₂, PbO₂, and Li₂O

2. Rutile structure (TiO₂)

a. The rutile structure can be considered an example of holes filling in a (strongly distorted!!) hcp anion arrangement, but the cations occupy only half the octahedral holes and there is considerable buckling of the close-packed anion layers.

b. Each Ti atom is surrounded by six O atoms, and each O atom is surrounded by three Ti atoms, therefore the rutile structure has 6 : 3 coordination.

c. Examples of this structure are: MnO₂, SnO₂, MgF₂, and ZnF₂

3. CdI₂

a. CdI₂ is a typical layer structure. Iodide ions are arranged in hcp.² And Cd(II) atoms fill 1/2 of alternating layers of the octahedral holes.

b. Each Cd atom is surrounded by six I atoms, and each I atom is surrounded by three Cd atoms, hence it has 6: 3 coordination.

c. Examples of this structure are MgBr₂, PbI₂, SnS₂, and Mg(OH)₂

4. CdCl₂

a. CdCl₂ is structurally related to CdI₂. The chloride ions are arranged ccp. And Cd(II) atoms are located in 1/2 of adjacent octahedral sites.

b. Each Cd atom is surrounded by six Cl atoms, and each Cl atom is surrounded by three Cd atoms, so it also has 6: 3 coordination.

c. Examples of this structure are MgCl₂, MnCl₂, FeCl₂, and CoCl₂

References:

1. Shriver & Atkins, Inorganic Chemistry, Oxford university press, Fourth edition, 2006, 86
2. R.B.Heslop/K.Jones, Inorganic Chemistry, Elsevier Scientific Publishing Company, 1976, 194