

MEF 3000/4000

Theme: Structure models

The following structure models exist:

AB: NaCl-type
NiAs-type
Zink blende-type
würtsite -type

AB₂: fluorite-type
CdI₂-type
rutile-type

ABO₃, perovskite-type

AB₂O₄, spinell-type

In addition to models of CuO and Pb₃O₄.

- Identify anions and cations in the different structures.
- Determine the coordination polyhedra around anions and cations.
- Identify dense packed layers of anion spheres for all structure types except CuO and Pb₃O₄. For the fluorite-type (CaF₂), it is the cations that form the dense packed layers. For perovskite type, the dense packed layers are formed by a combination of A and O atoms.

Consider some chosen models in larger details. Use a considerable amount of time on this since it will give a better understanding of symmetry relations, sphere packing, coordination relationships, and more.

Consider NaCl-structure

- find dense packed layers.
- describe what atoms lie on (100) and on (110) planes
- consider the Na-atoms. Describe the Bravais-lattice.

Consider NiAs- structure

- find dense packed layers.
- give the coordination polyhedra for Ni and for As
- identify 6₃ axis
- study how the octahedra holes lie along the c-axis.
- consider whether the structure has got center of symmetry

Consider zink blende (ZnS) structure

- give the coordination relationships for Zn and for S
- note Bravais-lattice by only considering the S-atoms
- do the same by considering the Zn atoms
- choose one Zn as origin. Is the structure centrosymmetric?
- What type of rotational axis runs along [100]?
- identify the octahedra holes.

Consider wurtsitt (ZnS) structure

- describe the coordination polyhedra.
- identify dense packed layers of S
- compare how the tetrahedra holes are placed along c-axis with the placement of the octahedra holes.

Consider CdI₂- structure

- compare with the NiAs-structure
- explain why the structure can be described as a layered structure.
- define the unit lattice

Consider CaF₂- structure

- identify the unit lattice
- describe the Bravais-lattice (consider first only Ca and thereafter only F)
- describe the coordination polyhedra.
- describe the dense packed layers and identify the octahedra holes.
- what type of rotational axis runs through origo (Ca) along [100] ?

Consider CuO- structure

- what type of coordination has Cu?
- identify the extra O-atoms that are needed in order to make octahedras around Cu.
- what is the reason for deformation of CuO₆-octaedera ?

Consider Pb₃O₄ structure

- are all Pb atoms identical?
- what oxidation number has Pb in Pb₃O₄ ?
- what type of coordination have the different Pb-species ?
- what is the reason that the coordination polyhedra for Pb(II) are strongly deformed?