

Lab#5: Polyhedral models

Coordination between spheres of different sizes: The crystal structure of a mineral is controlled by the size and charge of its constitutive atoms. Geometrically, closest packing is the lowest energy state, but this arrangement of atoms does not always charge balance. Most of the structures observed in crystals are compromises between charge balance and closest packing.

In silicates, oxygen is the most common anion and is usually the largest atom in the structure (O atomic radius = 1.4 angstroms versus Si atomic radius = 0.26 angstroms in tetrahedral coordination). Therefore, packing of atoms in a silicate is generally a matter of packing oxygen atoms together and fitting the cations in the voids between oxygen atoms. The size and charge of the cations determines the number of oxygen atoms that can be fit around it. The number of anions around the cation is called the coordination number (CN#). The number and arrangement of anions around a cation can be described by a polyhedron. The arrangement of these polyhedra in three dimensions determines the overall crystal structure.

Identify the coordination polyhedra and crystal system in the following minerals by examining models in the lab and/or diagrams on the attached sheets.

OXIDES

| type | mineral | anion | cation | coordination polyhedron | crystal system |
|----------------------------|---|-----------------|------------------|-------------------------|----------------|
| X_2O | ICE H ₂ O | O ²⁻ | H ⁺ | | |
| X_2O_3 Hematite Group | Perovskite CaTiO ₃ | O ²⁻ | Ca ²⁺ | | |
| | | O ²⁻ | Ti ⁴⁺ | | |
| | Corundum Al ₂ O ₃ | O ²⁻ | Al ³⁺ | | |
| XY_2O_4 Spinel Group | Magnetite Fe ₂ O ₄ | O ²⁻ | Fe ³⁺ | | |
| | | O ²⁻ | Fe ²⁺ | | |

CARBONATES

The two following minerals have the same chemical formula, but very different crystal structures (polymorphs).

| mineral | anion | cation | coordination polyhedron | crystal system |
|--------------------------------|-----------------|------------------|-------------------------|----------------|
| Calcite CaCO ₃ | O ²⁻ | C ⁴⁺ | | |
| | O ²⁻ | Ca ²⁺ | | |
| Aragonite CaCO ₃ | O ²⁻ | C ⁴⁺ | | |
| | O ²⁻ | Ca ³⁺ | | |

SILICATES

In most of the following models, rather than have a ball for each of the silica atoms and oxygen atoms, the SiO_4 element is shown as a tetrahedra. The *class* is determined by the arrangement of these tetrahedra which is a function of the number of shared oxygens on the corners of the tetrahedra.

| class | mineral | anion | cation | coordination polyhedron | crystal system |
|--|--|-----------------|--|-------------------------|----------------|
| Tectosilicates (3-d framework of SiO_4) | Quartz SiO_2 | O^{2-} | Si^{4+} | | |
| Nesosilicates (independent SiO_4) | Olivine $(\text{Mg,Fe})\text{SiO}_4$ | O^{2-} | Si^{4+} | | |
| | | O^{2-} | $\text{Fe}^{3+}, \text{Mg}^{4+}$ | | |
| | Zircon ZrSiO_4 | O^{2-} | Si^{4+} | | |
| | | O^{2-} | Zr^{4+} | | |
| | Garnet $\text{A}_3\text{B}_2\text{SiO}_4$ | O^{2-} | Si^{4+} (Or "Z") | | |
| | $\text{B}=\text{Al}, \text{Fe}^{3+}, \text{Cr}^{3+}$ | O^{2-} | "B" (Or "Y") | | |
| | $\text{A}=\text{Ca}, \text{Mg}, \text{Fe}^{2+}, \text{Mn}^{2+}$ | O^{2-} | "A" (Or "X") | | |
| Inosilicates (single or double chains of SiO_4) | Pyroxene XYZ_2O_6 $\text{Z}=\text{Si}^{4+}, \text{Al}^{3+}$ | O^{2-} | "Z" | | |
| | $\text{Y}(\text{M1 site})=\text{Mn}^{2+}, \text{Fe}^{2+}, \text{Fe}^{3+}, \text{Al}^{3+}, \text{Cr}^{3+}, \text{Ti}^{4+}$ | O^{2-} | "Y" (Or M1) | | |
| | $\text{X}(\text{M2 site})=\text{Na}^+, \text{Ca}^{2+}, \text{Mn}^{2+}, \text{Fe}^{2+}, \text{Mg}^{2+}, \text{Li}^{2+}$ | O^{2-} | "X" (Or M2) | | |
| Phyllosilicates (sheets of SiO_4) | Serpentine $\text{Mg}_3\text{Si}_2\text{O}_5(\text{OH})_4$ | O^{2-} | Si^{4+} | | |
| | | O^{2-} | Mg^{2+} | | |
| Tectosilicates (3-d framework of SiO_4) | Feldspars system between $\text{NaAlSi}_3\text{O}_8$ KAlSi_3O_8 $\text{CaAl}_2\text{Si}_2\text{O}_8$ | O^{2-} | $\text{Si}^{4+}, \text{Al}^{3+}$ | | |
| | | O^{2-} | $\text{K}^+, \text{Na}^+, \text{Ca}^{2+}$ + | | |