

GEOL.3090L – EARTH MATERIALS I
COORDINATION NUMBERS, BOND STRENGTHS, AND CRYSTAL STRUCTURES

I. Structure of Minerals

The arrangement of atoms in a crystal structure is determined by the relative size of the anions and cations. Because anions are almost always larger than cations, we usually determine how many anions can be arranged around a cation such that all the ions are touching. The larger the cation, relative to the anion, the greater the number of anions that can fit around the cation. In order to determine the coordination number (the number of anions around the cation) we need to calculate the radius ratio

$$\text{Radius ratio} = \text{Size cation} / \text{Size anion}$$

This ratio is then used to predict the coordination number (Fig. 1).

II. Bond Strength

Bond strength is a measure of the strength of the bonds that exist between an ion and its nearest neighbors. Bond strength is calculated by dividing the charge on an ion by its coordination number. For examples, in the silica tetrahedron, silica (+4) is surrounded by 4 oxygen ions. The bond strength, in e.v., is $1 (+4 \text{ charge} / 4 \text{ coordination number})$.

Types of bond strengths:

- **Isodesmic** – bond strengths are the same throughout the crystal structure.
- **Anisodesmic** – bond strengths inside of one type of polyhedral in a structure are different from that of other bonds in the structure.
- **Mesodesmic** – e.v. number is equal to $\frac{1}{2}$ the valence number of the anion.

III. Calculating coordination numbers and bond strengths

For each of the following, (a) calculate the coordination number (number of anions around the cation) and compare the calculated result with the corresponding crystal model. For these calculations use the ionic radii of Whittaker and Muntus. (b) Also calculate the bond strengths (in e.v.) for each bond. (c) Indicate the type of bond strength – isodesmic, anisodesmic, or mesodesmic.

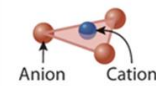
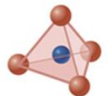
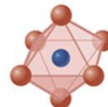
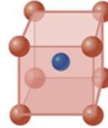
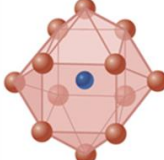
| Radius ratio R_A/R_X limits | C.N. | Geometric shape |
|----------------------------------|------|--|
| 0.155 to 0.225 | III |  <p>Anion Cation Corners of an equilateral triangle (triangular coordination)</p> |
| 0.225 to 0.414 | IV |  <p>Corners of a tetrahedron (tetrahedral coordination)</p> |
| 0.414 to 0.732 | VI |  <p>Corners of an octahedron (octahedral coordination)</p> |
| 0.732 to 1.0 | VIII |  <p>Corners of a cube (cubic coordination)</p> |
| 1.0 | XII |  <p>Corners of a cuboctahedron (close packing)</p> |

Figure 1. Coordination polyhedrons

Pyrite - FeS

Halite - NaCl

Fluorite - CaF₂

Sanidine - KAlSi₃O₈ - calculate coordination numbers for K, Al, and Si

Quartz - SiO₂

Chalcopyrite - CuFeS_2 - calculate coordination numbers for Cu and Fe

Olivine - Mg_2SiO_4 - calculate coordination number for Mg

Biotite - $\text{K}_2(\text{Mg,Fe})_2\text{AlSi}_3\text{O}_{10}(\text{OH})_2$ - calculate coordination numbers for K and Mg

Augite - $\text{CaMgSi}_2\text{O}_6$ - calculate coordination numbers for Ca and Mg

Spinel - $MgAl_2O_4$ - calculate coordination numbers for Mg and Al

IV. Basic Structures of Silicate Minerals

The major minerals in the earth's crust are the silicate minerals. The basic building block for the silicate minerals is the silica tetrahedron. The tetrahedrons can be arranged in different ways to create the various classes of silicate minerals (Fig. 2). For each of the crystal models listed below, place the model in the correct silicate structure group. Explain why you placed the structure in the particular group.

1. Olivine

2. Augite

3. Tremolite




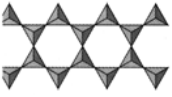
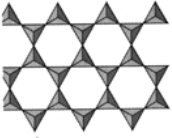

| TABLE 2.2 Major Silicate Structures | |
|--|---|
| GEOMETRY OF LINKAGE OF SiO_4 TETRAHEDRA | |
| <i>Isolated tetrahedra:</i> No sharing of oxygens between tetrahedra; individual tetrahedra linked to each other by bonding to cation between them |  |
| <i>Rings of tetrahedra:</i> Joined by shared oxygens in three-, four-, or six-membered rings |  |
| <i>Single chains:</i> Each tetrahedron linked to two others by shared oxygens; chains bonded by cations |  |
| <i>Double chains:</i> Two parallel chains joined by shared oxygens between every other pair of tetrahedra; the other pairs of tetrahedra bond to cations that lie between the chains |  |
| <i>Sheets:</i> Each tetrahedron linked to three others by shared oxygens; sheets bonded by cations |  |
| <i>Frameworks:</i> Each tetrahedron shares all its oxygens with other SiO_4 tetrahedra (in quartz) or AlO_4 tetrahedra |  |

Figure 2. Silicate structures

4. Biotite

5. Sanidine

6. Montmorillonite

7. Kaolinite