Common Structure Types

Objectives
- Structure models and CrystalMaker
- Close-packed structures
- Common structure types

Structure models
Three types of models are commonly used to illustrate a crystal structure. Space Filling models emphasize ionic radii. Polyhedron models focus on coordination between atoms or ions. Ball and stick models show the position and size of ions, chemical bonds between ions, and the lengths of the bonds.

Close-packed structures
When the coordinating and coordinated ion are the same size (radius ratio=1), the ions will be arranged in hexagonally close-packed structure (hcp) or cubic close-packed structure (ccp). These arrangements differ in the sequence of stacking. In either case, the coordination number is 12.

Most metals have close-packed structures. For instance, iron (Fe) in the Earth’s core is widely believed to have a hexagonal close-packed structure (hcp). At ambient conditions, both gold (Au) and platinum (Pt) have the cubic close-packed structure, also known as fcc, an acronym for face centered cubic. The structures of many silicates can be viewed as close-packed oxygen framework with the cations filling various structural voids (interstices).

Common structure types
Four basic common structure types will be discussed here.
NaCl type structure: face centered cubic. C.N. (coordination number) = 6, Z (number of formula units per cell) = 4. Both rock salt (NaCl) and galena (PbS) have the NaCl type structure.
CsCl type structure: simple cubic. C.N. = 8, Z = 1. CsCl (mostly synthetic) and high pressure phase of rock salt (NaCl B2 phase) have the CsCl type structure.
ZnS type structure: Zn forms a face centered cubic structure, S fills half of the tetrahedral voids. C.N. = 4, Z = 4. Both sphalerite (ZnS) and silicon carbide (SiC) have the ZnS type structure.
CaF2 type structure: Can be viewed in two ways: First, Ca forms a face centered cubic structure, F fills all the tetrahedral voids; Second, Ca forms a simple cubic structure, F fills half of the cubic voids. C.N.(Ca) = 8, C.N.(F) = 4, Z = 4. Both fluorite (CaF2) and zirconia (ZrO2) have the CaF2 type structure.