

## Structural Variations of Apatite Solid Solutions, $\text{Ca}_{10}(\text{PO}_4)_6(\text{F}, \text{Cl}, \text{OH})_2$

Kaveer S. Hazrah and Sytle M. Antao

Department of Geoscience, University of Calgary

### Summary

Apatite,  $\text{Ca}_{10}(\text{PO}_4)_6(\text{F}, \text{Cl}, \text{OH})_2$ , is the most abundant phosphate mineral in the world and has many different properties with numerous uses in geology, materials science, biology, medicine, agriculture, and dentistry. It can be found as an accessory mineral within metamorphic, igneous and sedimentary rocks. The three main natural end members are fluorapatite ( $\text{Ca}_{10}(\text{PO}_4)_6\text{F}_2$ ), chlorapatite ( $\text{Ca}_{10}(\text{PO}_4)_6\text{Cl}_2$ ) and hydroxylapatite ( $\text{Ca}_{10}(\text{PO}_4)_6\text{OH}_2$ ). Quantitative chemical compositions and backscattered electron (BSE) images on several apatite samples were obtained with an electron-probe microanalyzer (EPMA). The crystal structure of some apatite samples were studied with synchrotron high resolution powder X-ray diffraction (HRPXRD). The structure of apatite consists of a phosphate tetrahedron, a Ca1 polyhedron and a Ca2 polyhedron. The  $\text{PO}_4$  and Ca1 (9-coordinated system) structures display very little change when an anion substitution occurs, majority of the changes occur within the 6-coordinated Ca2 polyhedron due to the anion column. This anion column is where F, Cl and OH are substituted and cause major structural changes. Ca2 polyhedron has a structure known as the Ca2 triangle which consists of three Ca2 atoms and the anion column, where F, Cl and OH either lie within, above, or below it. Fluor-apatite is the most common end member, usually found in igneous rocks and has a hexagonal structure ( $P6_3/m$ ), with the F atom residing within the Ca2 triangle. Hydroxylapatite and chlorapatite are larger atoms/complexes and reside either above or below the Ca2 triangle. Depending on the anion positions, purity and solid solution content, hydroxylapatite and chlorapatite can be either monoclinic ( $P2_1/b$ ) or hexagonal ( $P6_3/m$ ). Cation substitutions, such as Mn substituting for Ca, can cause minor changes, where Mn reduces cation-oxygen bond lengths. Apatite can also occur as multiphase samples rather than in solid solution. Such is the case in one sample, where hydroxylapatite and fluor-apatite occur as two separate phases, *i.e.* OH is not substituting for F in solid solution, but rather forming as a chemically distinct zone.