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Unit-cell data and XRD compositional indicators for fluorapatite-chlorapatite crystalline solutions

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Before any mineral series can be utilized for petrologic interpretation, it should be well-understood chemically, structurally, and thermodynamically. The apatite [$Ca_5(PO_4)_3$(F,Cl,OH,CO_3)] mineral system promises to be useful in the study of both terrestrial and planetary systems. As a first step in the investigation of these minerals, Schettler, Gottschalk, and Harlov (2011, *American Mineralogist*) reported details of the synthesis and chemical characterization of a fluorapatite-chlorapatite solid solution series. Enthalpies of solution and F-Cl mixing behaviour also have been investigated for these synthetic samples (Hovis and Harlov, 2010, *American Mineralogist*). The former paper reports structures and unit-cell dimensions that were characterized at the GeoforschungZentrum-Potsdam both by Rietveld analysis of powders and single crystal XRD. In the present work, we report unit-cell results and XRD compositional indicators based on measurements at Lafayette College. For present work, XRD measurements were made on powdered samples for twenty members of the same series, employing a Scintag PAD V system, CuKα radiation, and NBS (NIST) 640a Si internal standard. Utilizing the software of Holland and Redfern (1997, *Mineralogical Magazine*), unit-cell dimensions were refined from Si-corrected machine-measured 2Θ values in conjunction with manually-identified Miller Indices. Overall, the resulting unit-cell values based on this methodology are in excellent agreement with those of Schettler et al. (2011). In cases where the Rietveld and single-crystal data of Schettler et al. (2011) produced slightly different results for the same mineral sample, present data generally agree better with the Rietveld-based results than those from the single-crystal data.

Given the different sizes of fluorapatite and chlorapatite unit cells, there are a number X-ray peaks that change positions significantly with F:Cl ratio, making these good compositional indicators. The latter include the {310}, {311}, {321}, {420}, {331}, {421}, and {502} diffraction maxima, all of which are present across the entire solid solution series and change position by more than 1° 2Θ, and in three cases by more than 1.6° 2Θ, from fluorapatite to chlorapatite. Because different peaks move at different rates with composition, any peak may be overlapped by a second peak over some portion of compositional space, but for all of the latter diffraction maxima this range is relatively restricted. The {311} peak is generally free from interference by other major peaks over the entire compositional span.

One must be cautious in the interpretation of volume behavior for this series, as Cl-rich synthetic samples contain minor amounts (mostly in the range from 4 to 8 mol%) of an oxyapatite component (Schettler et al., 2011). For oxyapatite-free samples that exist over 65% of the compositional range, volume-composition relationships imply positive volumes of mixing, whether data from Rietveld, single-crystal, or the present study are utilized. However, it will not be possible to confirm this mixing behaviour until oxyapatite-free Cl-rich samples become available.