Quantitative analysis of OH^- in fluorapatite by micro-FTIR: Determination of the molar absorption coefficient

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Introduction: Apatite [$Ca_5(PO_4)_3(F,Cl,OH^-)$] is a common mineral in igneous rocks and the only ubiquitous hydroxyl (OH^-) bearing mineral found in planetary materials [e.g., 1-3]. Consequently, apatite is an important resource for understanding the water budgets of terrestrial and planetary magmas. Fourier Transform Infrared Spectroscopy (FTIR) offers an accurate, quick, and non-destructive method for quantifying the OH^- content of apatites. Quantitative measurements of molecules from the infrared spectrum are obtained by the Beer-Lambert law, $A_i=ct\varepsilon_i$, where ε_i is the integrated molar absorption coefficient (ε_i), which must be empirically determined for each molecule/mineral. This work aims to measure this value for OH^- in apatite.

Methods: The H_2O contents of four single-crystal, gem-quality, fluorine-rich apatites were accurately measured by continuous flow mass spectrometry (CFMS). Infrared spectra were collected with a Nicolet Nexus 670 FTIR using a microscope attachment, MCT-A detector, XT-KBr beamsplitter, and Globar source. Samples were cut perpendicular to the c-axis, doubly polished to an average thickness of 60 μm, and analysed under polarized light following procedures in [4]. Peak areas were determined using OMNIC spectral analysis software, and sample thicknesses were measured using methods outlined in [5].

Results: The calculations produced ε_i = 2.52 x10^4 ± 0.26 L/mol/cm^2. This value is similar to one reported in a previous study (2.31±0.06 x 10^4) [6]; however, our reported uncertainty is higher. Our uncertainty is likely more realistic because it is based on the standard deviation of ε_i calculated from the analysis of four different apatites. It is unclear how [6] computed ε_i and associated uncertainty, but treating their data set the same way as our own, we compute ε_i = 2.02 x10^4 ± 0.46 L/mol/cm^2. Consequently, additional work is needed to better constrain ε_i for quantification of OH^- in apatite by polarized micro-FTIR.

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