

Hydroxyl ordering in igneous apatite

R. CHRIS TACKER*

North Carolina State Museum of Natural Sciences, 11 West Jones Street, Raleigh, North Carolina 27601-1029, U.S.A.

ABSTRACT

Apatites from several pegmatites and two alkaline igneous environments were analyzed by electron microprobe and by micro-FTIR spectroscopy in the region 3000–4000 cm^{-1} . Hydrogen bonding between OH and adjacent halogens shifts the OH-stretching modes and proves sensitive to the ordering of anions and cations within the apatite structure. With few exceptions, the spectrum of the stretching vibration can be modeled as a combination of peaks observed in synthetic apatites.

Relative concentrations of OH populations can be determined from unpolarized spectra of oriented specimens. Analysis of populations of OH-Cl and OH-F pairs shows that OH-Cl pairs occur at a frequency greater than expected from a random sequence. This finding confirms earlier results that Cl incorporation into the hexagonal fluorapatite structure requires a hydroxyl nearest neighbor.

Additional component bands suggest cationic ordering into the Ca2 site. Comparison of random mixing models with spectroscopic data suggests that Mn preferentially orders with OH. Limited data for the Kola apatite suggest the same for Sr and REE, in accord with previous results on the influence of OH on REE uptake. The small change in bond valence sum produced by substitution of an OH may explain the pairing of OH and Sr, but not with Mn.

Activity of HAp in apatite is proportional to the area of the peak at 3575 cm^{-1} . Activity calculated from mole fraction of HAp in the normalized microprobe analysis may overestimate the activity of water in associated exchange equilibria. Ordering of Cl-OH-F sequences produces potential complications for thermodynamic models.