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Carbonate in igneous and metamorphic fluorapatite: Two type A and two type B substitutions

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ABSTRACT

Fourier transform infrared (FTIR) microspectroscopy of igneous and metamorphic fluorapatites shows measurable carbonate in all specimens. All specimens show the presence of the type A1 and A2 (carbonate for columnar anion, Fleet et al. 2004) and the type B (carbonate for phosphate) substitutions in the carbonate ν_3 domain (1400–1600 cm^{-1}). This is the first report of the type A2 substitution in naturally occurring apatites. Spectra also show ν_3 carbonate peaks that have not been unambiguously assigned. In some spectra, two doublets can be resolved, indicating two different B-type substitutions. The presence of multiple B-type substitutions in infrared spectra is in accord with the recognition of different mechanisms of substitution of the carbonate for the phosphate tetrahedron and explains the scatter observed in published data.

Consideration of crystal structural details shows site symmetry of the carbonate group to be C_s rather than C_{2v} as has been previously assumed. Decent of C_s symmetry from D_{3h} through C_{2v} lifts degeneracy and preserves orthogonality of ν_3 doublets. Extra type B peaks are not due to lower site symmetry, and Davydov splitting can be ruled out.

Results demonstrate that carbonate contents of apatites from pegmatites and cumulate mafic magmas are well within analytical capability, opening another line of inquiry into CO_2 behavior in igneous and metamorphic rocks. The type A1 substitution shows the most promise for thermodynamic calculations that would allow extraction of CO_2 activities. Analyses show similar ratios of water to carbon dioxide activities recorded in pegmatite apatites.

Keywords: IR spectroscopy, pegmatites, analysis, chemical (mineral), thermodynamics, crystal structure