

Solid-state NMR and IR spectroscopic investigation of the role of structural water and F in carbonate-rich fluorapatite

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ABSTRACT

We have studied the substitutions in a natural well-crystallized carbonate-containing apatite-(CaF) (var. staffelite) using infrared (IR) and solid-state nuclear magnetic resonance (NMR) spectroscopic techniques. Our results show the presence of both A- and B-type carbonate plus a large amount of structural water (0.44 pfu). This sample also contains 0.21 pfu excess F, but only weak C-F dipolar coupling is observed indicating that a tetrahedral CO_3F^{3-} complex does not occur. ^{19}F NMR results indicate the presence of a second F environment in the apatite structure at a concentration similar to that of B-type carbonate but which does not differ from channel F in terms of coupling to ^{31}P or ^1H .

Keywords: Apatite-(CaF), IR spectroscopy, NMR spectroscopy