

## **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  $\text{CO}_3\text{F}^{3-}$  complex does not occur.  $^{19}\text{F}$  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  $^{31}\text{P}$  or  $^1\text{H}$ .

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