

Raman and IR studies of the effect of Fe substitution in hydroxyapatites and deuterated hydroxyapatite

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ABSTRACT

We have studied synthetic Fe-substituted hydroxyapatite $\text{Ca}_{5-x}\text{Fe}_x(\text{PO}_4)_3\text{OH}$ and the corresponding deuterated samples with varying Fe concentrations x ($0 \leq x \leq 0.3$) by Raman and IR spectroscopy at room temperature. In the IR spectra, substitution of deuterons for protons affects the OH internal mode in a way consistent with the mass difference of the substituting ions, as well as a mode attributed to vibrations of the $\text{Ca}_3\text{-(OH)}$ unit. In the Raman spectra, the frequency of all modes is not noticeably affected by the Fe substitution. Raman bands show increased width and substantial reduction in intensity with increasing amount of Fe, presumably related to disorder introduced by the substitution. We find that the disorder is smaller in the hydroxyapatites compared to the deuterated ones.

Keywords: Hydroxyapatites, Fe-substitution, Raman spectroscopy, FTIR