

Infrared spectra of carbonate apatites: Evidence for a connection between bone mineral and body fluids

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ABSTRACT

The complex asymmetric stretch (ν_3) region infrared (IR) spectrum of synthetic sodium- and carbonate-bearing hydroxylapatites (CHAP) has been interpreted using overlapped Gaussian distributions for individual carbonate ion species. There is now good agreement for the distribution of carbonate ions between phosphate (type B) and *c*-axis channel (type A) positions using three independent methods: X-ray structure site occupancies, out-of-plane bend (ν_2) band areas, and asymmetric stretch (ν_3) band areas; B/A ratios for a well-crystallized CHAP sample being 0.77, 0.78, and 0.75, respectively. The reported dominance of type B carbonate ions in bone mineral and dental enamel is attributed to the anomalous shift of type A band frequencies into the spectral region of type B, resulting from the substitution of Ca^{2+} by Na^+ in the nearest-neighbor cation shell of the channel carbonate ions. The infrared spectra show that the hydrogencarbonate (bicarbonate) ion in apatite crystals is a channel species, as are its room-temperature decomposition products, type A carbonate and labile (type L) carbonate. The research suggests that bone mineral crystals may actively communicate with body fluids through the apatite channel, pointing to a possible role for the apatite channel in mediating acid-base reactions in the body.

Keywords: Apatite structure, carbonate ion, biomineralization, biological apatite, infrared spectra, CO_2 sequestration