

Characterization of Bone Mineral Model Compounds Through Far-Infrared Spectroscopy

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Hydroxyapatite, $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$, is the primary mineral component of bone. Bone growth begins as amorphous calcium phosphate crystallizes into hydroxyapatite. As the bone matures, the size, crystallinity, and stoichiometry of the hydroxyapatite crystals change. For example, the phosphate and hydroxide sites are often substituted by other anions such as acid phosphate (HPO_4^{2-}), carbonate (CO_3^{2-}), and fluoride (F^-). The nature of the phosphate environment in bone can be characterized through analysis of a series of four phosphate bands in the far-infrared region ($500 - 650 \text{ cm}^{-1}$). The intensities and peak positions of these modes are sensitive to the hydroxyapatite crystal size, structure, and stoichiometry. Thus, we have obtained a series of bone samples from rats and rabbits of various ages. We have also grown a series of hydroxyapatite crystals, varying in (1) the initial solution concentration of calcium phosphate, (2) the initial solution concentrations of non-stoichiometric components such as carbonate and fluoride, and (3) the time of crystal growth. The far-infrared spectra of these samples were collected in the form of potassium bromide pellets. X-ray powder diffraction data has also been collected on these samples to provide a measure of average crystal size. Currently, curve-fitting and integration analysis are being applied to the infrared data to correlate the peak positions and intensities of these modes as a function of bone age and crystal size. Our results show that (1) the concentration of acid phosphate decreases as crystal size increases, (2) the peak ratio $603/563 \text{ cm}^{-1}$ increases linearly as crystal size increases, making this ratio an *in situ* measure of mineral crystallinity, (3) carbonate content is approximately constant over a wide range of crystal sizes, and (4) as crystal size increases, A-site carbonate substitution increases and B-site carbonate substitution decreases, demonstrating an evolution towards stoichiometry in maturing bone.