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Micro-Raman and FTIR Studies of Synthetic and Natural Apatites
A. ANTONAKOS, E. LIAROKAPIS, National Technical University of Athens, Greece, TH. LEVENTOURI, Florida Atlantic University, Boca Raton, FL, USA — B-type synthetic carbonate hydroxyapatite (CHAp), natural carbonate fluorapatite (CFAp) and silicon-substituted hydroxyapatite (SiHAp), have been studied by using micro-Raman and infrared (IR) spectroscopy. It was found that while B-type carbonate substitution predominates in carbonate apatites (CAps), A-type is also detected in all types of apatites. B-type carbonate substitution causes a broadening of the ν_1 P-O stretching mode that is associated with the atomic disorder within the phosphate tetrahedron. An $\sim 15 \text{ cm}^{-1}$ shift of the ν_{3c} P-O antisymmetric IR mode was observed upon heat-treatment of the CFAp to drive the carbonate off. This shift indicates that the P-O bond lengths on the mirror plane increase when carbonate leaves the apatite structure suggesting that carbonate substitutes on the mirror plane of the phosphate tetrahedra. The present results support the substitution mechanism proposed on the basis of neutron powder diffraction studies of the same samples. The intensity ratios of the ν_2 IR CO_3 and ν_1 PO_4 bands in samples with various carbonate contents provide a calibration curve for estimating the degree of carbonization of CAps.

Th. Leventouri
Florida Atlantic University

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