Structural Study of apatites containing cadmium

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The calcium apatites form an important class of natural and synthetic compounds. Fluorapatite constitute the major ore of phosphorus and hydroxyapatite makes up the mineral portion of bones and teeth in all animals. One of the main characteristics of the apatitic structure is to allow large and varied substitutions: in the cationic (Ca\textsuperscript{2+}) sites, in the anionic (PO\textsubscript{4}\textsuperscript{3-}) sites or in the channel (F\textsuperscript{-}, OH\textsuperscript{-}) sites. The knowledge of interactions of cadmium with calcium phosphate, the location of cadmium in the apatitic structure are of interest in order to investigate the relation with ores and bones. The substitution of Ca\textsuperscript{2+} with Cd\textsuperscript{2+} in apatite is of extreme biological significance since it explains the mechanisms of incorporation of cadmium into the skeletal system.

The cadmium containing apatites were prepared using a double decomposition method in a boiling aqueous medium. All the samples were characterized by X-ray diffraction, IR spectroscopy and chemical analysis.

The distribution of the calcium and cadmium ions between two non-equivalent crystallographic sites, I and II, were determined by the Rietveld method. The sites are differing in symmetry and coordination. The results of the powder-fitting structure refinements show that whatever its amount in the apatites, cadmium is located simultaneously in both cation sites with a slight preference for site II. The bond valences are in agreement with the site occupancy-factors of cations in the two sites. The interatomic distances and the bond angles were calculated and studied.

The infrared absorption spectra of apatites have been recorded over a spectral range encompassing the internal vibrations of the PO\textsubscript{4} groups. The infrared spectrum of apatites containing one cadmium per cell shows two particular bands at about 963 cm\textsuperscript{-1}. It corresponds to the splitting of the v\textsubscript{1} phosphate band.

The weak but steady variation of PO\textsubscript{4} band positions to the weak wavenumber when calcium is progressively substituted for cadmium can be attributed to the lattice volume variation and to cation oxygen interactions.

The splitting of the v\textsubscript{1} band must be correlated with the fact that the six phosphate ions, which are normally equivalent in the P6\textsubscript{3}/m symmetry, are not equivalent when a certain amount of cadmium ions substitutes for calcium ions.

Keywords: calcium apatite, cadmium substitution, Rietveld method