Structural and Microstructural Studies of Synthetic and Naturally Occurring Hydroxyapatites using Powder Diffraction

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Hydroxyapatite (HAP), the main constituent of mammalian hard tissue, is an important mineral reservoir for the metabolic activity of the organism. Structural and microstructural characterization of several naturally occurring HAP samples extracted from human tooth, goat bone, rabbit bone and synthetic HAP have been carried out using X-ray powder diffraction studies. Diffraction data were collected with a step scan mode at an interval of $0.02^{\circ}(2\theta)$ using a Bruker D8 Advance X-ray powder diffractometer equipped with a germanium crystal primary beam monochromator ($CuK\alpha_{1=}$ 1.5406 Å). Preliminary phase identification of the naturally occurring HAP samples using the ICDD data base indicated presence of small amounts of Calcite ($CaCO_3$) and Dolomite [$CaMg(CO_3)$], (2-4% each), in addition to the main HAP phase, $Ca_{10}(PO_4)_6(OH)_2$.The whole powder pattern decomposition of the naturally occurring samples indicated sharp (00l) reflections, is in agreement with the earlier reports of preferred orientation in HAP crystals along the c-axis. Rietveld analysis carried out incorporating the structural parameters of different constituents phases using the program TOPAS showed final R_{wp} values ranging between 9.9-111.5%. The average crystallize sizes in the samples vary between 500 to 400 nm. The refined P-O distances in the synthetic HAP sample differ significantly compared to these observed in the naturally occurring samples.

Keywords: hydroxyapatite, microstructure analysis, Rietveld refinement