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Rietveld refinement of the crystallographic structure of human dental enamel apatites

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ABSTRACT

Rietveld refinements using 12 sets of X-ray diffraction powder data from milligram samples of human dental enamel provide detailed information about the structure and composition of enamel apatite. The principal difference in atomic parameters between enamel apatite and Holly Springs hydroxylapatite is in O2, which is reflected in a reduction in the P-O2 bond length of 0.085 Å and PO_4 volume by 3.6%. Modeling the hexad axis scattering with a single OH^- ion gives a 0.089 Å shift of the ion further away from the mirror plane at $z = \frac{1}{4}$. The known distributed electron density along the hexad axis in enamel has been confirmed by direct comparison with synthetic hydroxylapatite. Although the CO_3^{2-} ion position could not be determined directly, evidence for partial replacement of PO_4^{3-} by CO_3^{2-} ions came from an 8% diminution of the P site occupancy compared with that in stoichiometric hydroxylapatite. The observed reduction in the P-O2 bond length and PO_4 volume in enamel is also consistent with this substitution. The loss of negative charge caused by CO_3^{2-} replacing PO_4^{3-} ions and loss of OH^- ions is compensated by loss of Ca^{2+} ions from Ca2 sites. The calculated density from the X-ray results is 3.021 g/cm^3, in agreement with deductions from previous chemical analyses.