

**W0291**

**Rietveld Structure Refinement of Precipitated Apatites with X-Ray and Neutron Diffraction Data.**

R.M. Wilson, J.C. Elliott, S.E.P. Dowker, Dental Biophysics, Queen Mary, Univ. of London, London E1 4NS, UK; R.I. Smith, ISIS, Rutherford Appleton Laboratory, OX11 0QX, UK.

Studies of a variety of synthetic precipitated apatites using both x-ray and neutron diffraction in addition to FTIR, MAS-NMR, ICP-AES and carbonate analyses have been undertaken. In particular a synthetic Na-containing  $\text{CO}_3\text{Ap}$  (12.5(7) wt %  $\text{CO}_3$ ) was studied as a simple model for biological apatites. In biological apatites, it is known that most  $\text{CO}_3^{2-}$  ions replace  $\text{PO}_4^{3-}$  ions, but their location within the  $\text{PO}_4^{3-}$  ion site remains controversial. Four structural models from the literature, with the  $\text{CO}_3^{2-}$  ion explicitly modelled using soft constraints, were fitted to the neutron diffraction data by the Rietveld method. The best model had the  $\text{CO}_3^{2-}$  ion in disorder between the mirror symmetry related faces of a vacant  $\text{PO}_4^{3-}$  sites and with the normal to the plane of the  $\text{CO}_3^{2-}$  ion at  $\sim 30^\circ$  to the  $c$ -axis. Further refinement revealed an additional (water) atom site [1]. Another synthetic apatite appears to contain formate ions [2], but the exact location of these is unclear.

R.M. Wilson, J.C. Elliott, S.E.P. Dowker, R.I. Smith. *Biomaterials* 2004; 25: 2205-2213.

R.M. Wilson, J.C. Elliott, S.E.P. Dowker. *Journal of Solid State Chemistry* 2003; 174: 132-140.

This work was supported by MRC grant No G9824467 and SBRLCF grant No RAB 03/PJ/18