RESOLVING AND UNDERSTANDING POLYMORPH CHEMISTRY IN THE CA-O-P-H SYSTEM

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The Ca-O-P-H system has been heavily studied because of its biological and commercial importance. The calcium phosphates are the basis of teeth and bones. Commercial applications include use of calcium phosphates in such diverse applications as pharmaceutical excipients, baking powder and fine china. There have been over 125 independent structural examinations within this system, by either single crystal or powder diffraction analysis, that are reference materials in the Powder Diffraction File.

A difficulty in the historical X-ray analysis of the Ca-O-P-H system has been the determination of the location and bonding of hydrogen atoms. Depending on the hydrogen bonding a system with identical chemical composition can be defined as a hydrogen phosphate, a basic phosphate or a phosphate hydrate. Indeed users of the Powder Diffraction File can easily get confused when unknowns can be adequately identified by references of identical chemical composition but different chemistry. It was a study of pharmaceutical formulas (1), many of which contained calcium phosphate excipients, that initiated this analysis.

To elucide polymorphism and chemistry in the Ca-O-P-H system ~125 diffraction and single crystal analyses from the PDF database were converted to digitized powder diffraction patterns and imported into a cluster analysis. Individual clusters were then analyzed for consistency in nomenclature, structural classification and structure type. A recent statistical quality review (2) of single crystal determinations was used to elucidate the structural chemistry within clusters and resolve literature discrepancies. The entire system consists of many clusters with each cluster defining a unique structural chemistry.

REFERENCES

[1] T. G. Fawcett, J. Faber, C. R. Hubbard, "Formulation Analysis of Off-the-Shelf Pharmaceuticals", American Pharmaceutical Review, May/June, Vol **7**, Issue 3, pp 80-83 (2004)

[2] S. Kabekkodu, "Implementation of Calculated Pattern Quality Marks in the Powder Diffraction File" presented at XXth IUCr Congress, IUCr2005, Florence, Italy and presented at the ICDD 2005 Annual Meeting, Newtown Square PA. with D. Sagnella and V. Bosnic at http://www.icdd.com/profile/march05abs/Suri_Poster-05.pdf