Powder Diffraction and Crystal Structure Prediction: A Two-Way Relationship?

Liana Vella-Zarb, James Cameron, Maryjane Tremayne, *Department of Chemistry, University of Birmingham. Edgbaston, Birmingham, UK.* E-mail: lxv495@bham.ac.uk

The most common complementary use of theoretical and experimental methods is structural rationalization from crystal structure prediction and X-ray powder diffraction techniques[1]. This aids both the rationalization of crystal structures generated in a prediction, and the characterization of solids from powder data that precludes indexing or structure solution.

Powder data from the prediction is often compared visually or purely on a fingerprinting basis with the experimental, and there are only a few cases of organic materials in which the predicted structures have been used as a starting point for Rietveld refinement[1,2]. One possible reason for this is that even though the variation in lattice parameters between the experimental and calculated structures is relatively small, the difference in the respective patterns often makes automated quantitative comparison difficult and attempts at refinement unsuccessful. As prediction calculations search for the energetically optimal packing at 0 K, use of low temperature powder data would enable a more meaningful comparison of the two profiles.

We will present our results from the study of several organic materials at low temperatures and their subsequent comparison to the predicted structures using a number of quantitative guides.

[1] Tremayne M., Grice L., Pyatt J.C., Seaton C.C., Kariuki B.M., Tsui H.H.Y., Price S.L., Cherryman J.C., *J. Am. Chem. Soc.*, 2004, **126**, 7071. [2] Payne R.S, Roberts R.I., Rowe R.C., Docherty R., *J. Comput. Chem.* , **19**, 1.

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