

## **XRPD at the heart of physical form discovery in CPOSS**

**K. Shankland<sup>1</sup>, A. J. Florence<sup>2</sup>, P. Fernandes<sup>2</sup>, A. Johnston<sup>2</sup>, N. Shankland<sup>2</sup>**

<sup>1</sup> *ISIS Facility, CCLRC Rutherford Appleton Lab, Didcot, Oxon, United Kingdom*

<sup>2</sup> *Solid State Research Group, University of Strathclyde, Glasgow, Strathclyde, United Kingdom*

The multi-centred, collaborative RCUK Basic Technology project entitled Control and Prediction of the Organic Solid-State (CPOSS)<sup>1</sup> is studying physical form diversity in organic molecular solids, with a vision of wealth creation through the rational exploitation of crystalline solids. The structure discovery and determination effort is underpinned by an automated parallel crystallisation platform, yielding ca. 30 polycrystalline samples per day from a library of ca. 70 solvents and a range of crystallisation conditions (supersaturation, temperature, agitation).<sup>2</sup> Examples, including the pharmaceuticals carbamazepine and chlorothiazide, are presented to illustrate the role of three transmission lab powder diffractometers, each utilising primary monochromated radiation and a PSD:

(a) a multi-sample foil instrument, for the identification of novel forms produced from the crystallisation search;<sup>3</sup>

(b) two capillary instruments (2 kW sealed tube and 12 kW rotating anode) used for 'routine' *DASH* structure solution and *Topas* Rietveld refinement.<sup>4</sup>

The case of 3-aza bicyclo[3.3.1]nonane-2,4-dione is also presented to illustrate the role of the *in situ* transmission powder diffraction phase survey as part of an efficient, systematic approach to discovering and determining crystal structures.

(1) [www.cposs.org.uk](http://www.cposs.org.uk).

(2) Florence et al. (2006). *J. Appl. Cryst.* 39, 922-924 & *J. Pharm. Sci.* 95, 1918-1930.

(3) Florence et al. (2003). *J. Pharm. Sci.*, 92, 1930-1938.

(4) Fernandes et al. (2007). *Acta Cryst.* E63, o202-o204 & o247-o249.