s8.m27.p8 **Gaining information at low-t with laboratory capillary x-ray powder data collection.** <u>P. Fernandes</u>,[a] A. Florence[a] and N. Shankland,[a] W.I.F. David[b] and K. Shankland,[b] *[a]Department of Pharmaceutical Sciences, University of Strathclyde, 27 Taylor Street Glasgow, G4 0NR, U.K., [b]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon., U.K. E-mail: philippe_fernandes@yahoo.com*

Keywords: X-ray powder diffraction; Differential thermal expansion; Crystal structure determination

In the context of structure solution, the challenge for experimental XRPD is to obtain the best possible estimates of diffracted intensities. The chance of achieving this is enhanced by using low-T data collections to decrease thermal vibration and so boost the intensities seen at higher diffraction angles. Further improvements to the extracted intensity information available from overlapping peaks may be gained by using multiple low-T data collections, thereby exploiting differential thermal expansion [1,2]. Just as liquid nitrogen temperatures have become the norm for laboratory single-crystal data collections, there is little doubt that the same is set to happen for XRPD structure determinations. The negligible extra cost to a data collection is vastly outweighed by the information gain. Here we present the exploitation of differential thermal expansion to retrieve an immense amount of accurate intensity data from a series of laboratory capillary X-ray powder diffraction sets collected at low-T.

[1]   W. I. F. David, K. Shankland, L. B. McCusker and Ch. Baerlocher (2002) in *Structure Determination from Powder Diffraction Data*, Ch. 1, David *et al*. (Eds), Oxford University Press, Oxford .
[2]   W. H. Zachariasen and F. H. Ellinger (1963) *Acta Crystallogr.*, **16**, 369.

s8.m27.p9 **The Set-up of the Structure Powder Diffractometer (SPODI) at the FRM-II.** <u>Hartmut Fuess</u>, Ralph Gilles, Markus Hoelzel, Michael Schlapp, Bernd Krimmer, Hans Boysen, *Darmstadt University of Technology, Materials Science, Petersenstrasse 23, Darmstadt, Germany. E-mail: hfuess@tu-darmstadt.de*

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