WWW.POWDERDATA.INFO: A RELIABLE SOURCE OF FREELY AVAILABLE, HIGH-QUALITY EXPERIMENTAL XRPD DATA

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In the last decade, structure determination from powder diffraction data (SDPD) has developed from a niche interest to a widely applied methodology. The availability of reliable, easy-to-use computer programs that implement SDPD techniques has undoubtedly been a key driver in this. However, there is currently no freely available repository of high-quality experimental XRPD data sets of known provenance with which to test out new and existing methods. Thus, it is perhaps unsurprising that a synchrotron XRPD data set of cimetidine, collected some 17 years ago[1], is still 'doing the rounds' and, in very recent work, Feng and Dong used *simulated* data when testing their *GEST* SDPD approach.[2]

At the moment, there are 35 XRPD data sets on www.powderdata.info and these are directly associated with our publication on the state of the art and challenges in solving molecular crystal structures from laboratory X-ray powder diffraction data.[3] Each individual dataset comes with two key accompanying items:

1. A metadata sheet, giving information about the compound under study and its basic crystallography.
2. An MD5 checksum, such that the authenticity of a downloaded data set can always be checked against the original file on the site.

We are making this data, and other data which will be added in the near future, available such that it can be used by anyone to gain experience in working with high-quality, previously analysed powder data - this includes testing algorithms, honing SDPD or Rietveld refinement skills and practicing indexing or Pawley / LeBail fitting.

The poster will show representative examples from www.powderdata.info and will discuss possible future improvements to the associated metadata and also the range of datasets that are made available.

1. Cernik, R. J. et al., *J. Appl. Cryst.* (1991) **24**, 222-226
2. Feng, Z. J. and Dong, C. *J. Appl. Cryst.* (2007) **40**, 583-588
3. Florence, A. J. et al., *J. Appl. Cryst.* (2005) **38**, 249-259