

at the atomic coordinates. In this contribution, we will demonstrate the use of dispersion-corrected DFT to reproduce molecular crystal structures *in silico* with unparalleled accuracy [2]. When the unit cell can be assumed to be reliable enough to be kept fixed, the computer resources required to perform an energy minimisation of all atomic coordinates are small enough for routine application, namely in the order of a couple of days on a single CPU. Because all atoms are treated independently and without reference to any user-supplied parameters or experimental data, the outcome of the dispersion-corrected DFT optimisation provides us an unbiased and independent validation criterion for the correctness of the crystal structure. Several examples will be shown.

[1] *Acta Cryst.* B63, 926.

[2] *J. Phys. Chem. B* 109, 15531.

Keywords: *ab-initio* powder structure determination, Rietveld refinement, density functional theory

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A comparison of co-crystal structure solutions through powder and single crystal techniques

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In powder diffraction, much information is lost by the collapse of the 3D space onto a 1D axis. This loss of information makes determination of the structure much more difficult. There is also some worry that this loss of information will lead to incorrect structure determination. However with single crystal techniques, the difficulty is in the preparation and growth of the single crystal. In some cases even, it is not possible to grow a single crystal. We have independently determined structures from powder and single crystal diffraction data of seven organic co crystals. The powder solutions were determined and refined with no knowledge of the single crystal solutions. We will compare the solutions given by these two techniques. This work was partially supported by Transform Pharma. Powder diffraction was performed at the National Synchrotron Light Source. The National Synchrotron Light Source at Brookhaven National Laboratory in New York, is a national user research facility funded by the U.S. Department of Energy's Office of Basic Energy Science

Keywords: powder structure determination, single-crystal structure determination, cocrystals

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The co-crystallisation and thermal behaviour of oxamic acid, nicotinamide and isonicotinamide

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In this poster, we will present our studies on a small group of molecular materials, while addressing three areas of small molecular crystallography that are of significant academic and

industrial interest: i) The systems under consideration contain both strong hydrogen bond acceptor and donor groups, making them potentially useful building units for co-crystal design and the study of supramolecular aggregation. The formation of molecular adducts of oxamic acid with both nicotinamide (vitamin B3) and isonicotinamide will be presented and the relative crystallisation and structural properties of these adducts discussed and compared to other results obtained for these isomeric amides. ii) In order to facilitate the full structural characterisation of these adducts, structure determination from X-Ray powder diffraction was required. By application of our direct space differential evolution algorithm we were able to solve the structures of these relatively complex structures from conventional laboratory data. Few molecular materials of this type have been determined from XRPD to date, but the ability to solve such structures has clear application to the emerging field of pharmaceutical co-crystals. iii) The thermal behaviour from 10 to 295K of both individual components and molecular adducts will also be presented. Such a study can be used as a valuable source of information in which to study the strength and directionality of intermolecular forces. We aim to invoke the reverse process, in which the directionality and strength of the intermolecular forces can be used to predict the thermal behaviour of a crystalline system.

References

1. McMahon, J. A., Bis, J. A., Vishweshwar, P., et al. *Z Kristallogr.* 220, 340-350

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The third structure determination by powder diffractometry round robin (SDPDRR-3)

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The maturity of a scientific technique is considered established when the method is performed successfully "on demand". While small molecule single crystal structure solution is often described as routine (most structures solve easily and quickly "on demand"), structure solution from powder diffraction (SDPD) is generally not. In consequence of some literature reporting SDPD as "routine" (e.g., [1]), a first structure solution from powder diffractometry round robin was organized in 1998 [2], and a second in 2002 [3]. Both these round robins indicated that SDPD was still difficult, the ratio (submitted correct result)/(data download) being close to 2%. With the chairman of the IUCr Commission on Powder Diffraction (<http://www.iucr-cpd.org/>) indicating it is time for a new SDPD round robin [4], the competition was announced on the 1st of February this year with a deadline at the end of April 2008, providing three months to perform two SDPDs. Powder Diffraction datasets for an organic phase, and an inorganic phases were downloadable from a webpage (<http://sdpd.univ-lemans.fr/SDPDRR3/>) with cell parameters and probable chemical formula provided. At the time of writing this abstract (half round), there were 123 data downloads and 3 successful returns. Routine appears unattained yet in spite of 200 or so SDPDs currently published per year vs ~40,000 total structures published each year solved by non-powder methods.

[1] David, W. I. F., Shankland, K., and Shankland, N., (1998). *Chem.*