

s7.m23.o2 **The 2004 Blind Test of Crystal Structure Prediction.** Graeme M Day^a and Sam Motherwell^b,
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s7.m23.o3 **Searching the CSD for Polymorphs.** Jacco van de Streek, Cambridge Crystallographic Data Centre, UK.
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Keywords: Prediction; Modelling; Blind

Two previous blind tests [1,2] have served as a evaluation of developments in computational methods of crystal structure prediction and have highlighted the merits and limitations of different approaches. As the number of researchers contributing to this field of study is rapidly increasing, a third blind test was held from October 2003 to April 2004.

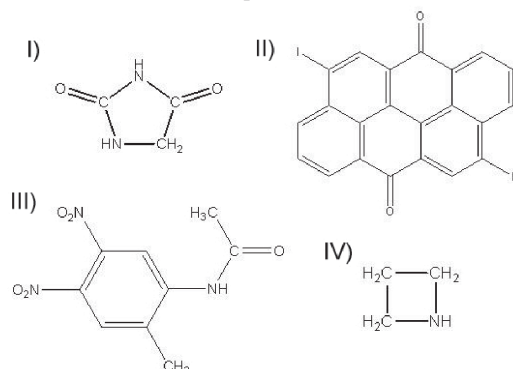


Figure 1. The four molecules included in the 2004 blind test.

Four molecules (Figure 1) were included in the test as examples of simple rigid molecules (I and IV), a molecule with more challenging atoms for lattice energy modelling (iodine in II), and a conformationally flexible molecule (III). The experimentally observed crystal structures were held by an independent referee for the duration of the exercise and only the molecular diagrams and conditions of crystallisation were provided to the participants.

Methods used and results of the test are presented and discussed in context of the previous blind tests and studies of crystal structure prediction.

- [1] J. P. M. Lommerse *et al*, *Acta Cryst* (2000), **B56**, 697-714.
 [2] W. D. S. Motherwell *et al*, *Acta Cryst* (2002), **B58**, 647-661.

Keywords: Polymorphs; CSD; Similarity

The Cambridge Structural Database (CSD, [1]) contains virtually all published crystal structures of organic and organometallic molecules, grouped by chemical compound. If two published crystal structures of the same chemical compound are different these two crystal structures are called polymorphs. Currently, polymorphs in the CSD are only flagged as such if this was explicitly mentioned in the original publication. This contribution describes how the CSD was searched for currently unflagged pairs of polymorphs based on the dissimilarity of their simulated X-ray powder diffraction (XRPD) patterns. XRPD patterns have the advantage that they are independent of the choice of origin and setting of the unit cell and, being one-dimensional, do not need to be re-oriented to find the best fit. The similarity measure used [2] is not as sensitive to peak shifts, i.e. unit-cell variations, as traditional point-by-point measures such as R-values, making comparison of crystal structures by different authors possible. The XRPD patterns were simulated using an in-house C++ library that forms the basis for e.g. the visualisation program Mercury [3]. If the similarity of the simulated XRPD patterns was "high", the two crystal structures were considered to be the same; if the similarity of the XRPD patterns was "low", the two crystal structures were inspected to see if they were true polymorphs or if the low similarity was due to an error. Details of the procedure will be described, including pitfalls and possible solutions. Time permitting, an extension to pseudo-polymorphs (polymorphs differing in solvent content) will be explained.

- [1] Allen, F. H. (2002). *Acta Cryst.* **B58**, 380-388.
 [2] De Gelder, R., Wehrens, R. & Hageman, J. A. (2001). *J. Comp. Chem.* **22**, 273-289.
 [3] Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M. K., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* **B58**, 389-397.