

M11.DD Structure Solution from Powder Data - Molecular Compounds

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Attendance: 162



A special session on Innovative Uses of the Inorganic Crystal Structure Database (ICSD) was held during the IUCr Congress in Glasgow, giving a large audience a flavour of the kind of power we can expect to find in retrieval systems for the ICSD during the next few years.

The session started with a description by Heinrich Behrens of the new management arrangements under which the ICSD is being maintained by the Fachinformationzentrum Karlsruhe (FIZ) in Germany with software being written by Vicky Karen at the National Institute for Science and Technology (NIST) in the USA. Mention was also made of the excellent work of Prof. R. Allmann in reviewing and correcting all the existing entries in the ICSD. Innovative uses of the database were described by Sidney Abrahams, who showed us how to find new ferroelectric materials by searching the ICSD for polar structures that are close to having a center of symmetry, and by Michael Berndt, standing in for Guenter Bergerhoff, who described how a derived database of standardized structures can be used to find compounds with similar structures.

Two databases related to the ICSD were described with a mouth-watering account of the kinds of searches that will be possible with their retrieval software. John Rodgers talked about the CRYSTMET file of metal structures and Michael Berndt described progress with the Pauling File which currently contains information on the structures and properties of binary compounds but which will be extended to include all inorganic and metallic compounds by 2007.

The Powder Data File (PDF) has been extended by including some 40,000 new powder patterns calculated from structures in the ICSD and John Faber showed how easy it was to search this part of the PDF for groups of compounds that shared interesting properties. Finally, Alan Hewatt gave us a glimpse into what state-of-the-art retrieval software looks like with a demonstration of his web version of the ICSD.

We all came away from the session with the feeling that, after struggling for nearly 20 years, the ICSD was about to take on a new life. With the new user-friendly software that is becoming available it will not be long before we are able to exploit the database in ways that most of us can still hardly imagine.