

## Poster Sessions

new system makes use of interactive interfaces and state-of-the-art visualization tools. To date, the project has delivered a sequence and ligand processing workflow, supported by a graphical user interface and managed by a workflow engine. The functional and interface design incorporates feedback collected from depositors and annotators.

During 2011 the project will develop the new user interface for deposition. The overall design of the system, completed modules and the prototype for the deposition interface will be presented.

The wwPDB members are: RCSB PDB (supported by NSF, NIGMS, DOE, NLM, NCI, NINDS and NIDDK), PDBe (EMBL-EBI, Wellcome Trust, BBSRC, NIGMS, and EU), PDBj (NBDC-JST) and BMRB (NLM).

**Keywords:** database, macromolecule, annotation

### MS27.P03

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#### **An overview of solvent use and solvate formation in the CSD**

László Fábrián, *School of Pharmacy, University of East Anglia, Norwich, (UK)*. E-mail: l.fabian@uea.ac.uk

As part of an ongoing investigation into solvate formation [1], [2], a database of over 90,000 solution-based crystallisation experiments has been extracted from the Cambridge Structural Database [3]. For each compound crystallised, the solvent(s) used and any solvent(s) included in the resulting crystal are listed.

Three categories of solutes were distinguished in the initial analysis of the data: organometallic compounds, organic salts and neutral organic molecules. The most frequently used solvents for organometallic compounds are hexane, dichloromethane, diethyl ether, toluene, pentane and their binary mixtures. Organic salts are most frequently crystallised from methanol, ethanol, water and acetonitrile, with the use of mixed solvents being less common for this group. Common solvents for neutral organic compounds include methanol, ethanol, hexane, dichloromethane, ethyl acetate and acetone.

The overall frequency of solvate formation is higher for organic salts and organometallic compounds than for neutral organic molecules. Surprisingly, this trend also holds for solvate formation with apolar solvents, which do not interact more strongly with ions than with neutral molecules.

The most frequently included solvent is water, which is often present in crystals grown both from water and from organic solvents. The relative frequencies of solvates with various organic solvents are similar to those found earlier by Görbitz [4]. Solvate formation propensities are obtained from these frequencies by taking into account the frequency of using each solvent for crystallisation [5]. There is a large variation in these propensities: 18% of the crystals grown from water are hydrates, but only 0.4% of the crystals obtained from ethyl acetate include solvent molecules. In fact, hydrates are more frequent than ethyl acetate solvates even among crystals grown from solutions in ethyl acetate.

Solvate formation propensities depend on whether crystals with only metal-coordinated solvent molecules are counted as solvates or not. For strongly coordinating solvents (e.g., ethanol, DMF), the difference can be more than twofold.

Data on crystallisation from mixed solvents can be used to test competition between different solvents and to make small differences between similar overall solvate formation propensities more clearly visible. Unfortunately, the exact composition of solvent mixtures is rarely reported, so these results may be biased if mixtures rich in one of the components are used more frequently than mixtures rich in other(s).

[1] L. Infantes, L. Fábrián, W. D. S. Motherwell, *CrystEngComm* **2007**, *9*, 65-

71. [2] L. Fábrián, *Acta Crystallographica* **2008**, *A64*, C93. [3] F. H. Allen, *Acta Crystallographica* **2002**, *B58*, 380-388. [4] C. H. Görbitz, H. P. Hersleth, *Acta Crystallographica* **2000**, *B56*, 526-534. [5] A. Nangia, G. R. Desiraju, *Chemical Communications* **1999**, 605-606.

**Keywords:** solvent, database, inclusion

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#### **A new interface to the cambridge structural database (CSD) in crysAlis<sup>Pro</sup>**

Fraser J. White,<sup>a</sup> Zoltán Gál,<sup>a</sup> Alexandra Griffin,<sup>a</sup> Tadeusz Skarzynski,<sup>a</sup> Mathias Meyer,<sup>a</sup> Grzegorz Prochniak,<sup>a</sup> Peter A. Wood,<sup>b</sup> Ian R. Thomas,<sup>b</sup> <sup>a</sup>*Agilent Technologies, 6 Mead Road, Yarnton, Oxfordshire, OX5 1QU, (UK)*. <sup>b</sup>*Cambridge Crystallographic Database Centre, 12 Union Road, Cambridge, CB2 1EZ, (UK)*.

Instrument time is a valuable commodity which can often be wasted with the accidental recollection of known samples. In order to avoid such mistakes cross checking unit cells with those in databases of crystal structures such as the CSD [1] prior to data collection is a useful exercise. To facilitate this we have, in conjunction with the Cambridge Crystallographic Database Centre (CCDC), developed module within CrysAlis<sup>Pro</sup> [2] which provides a simple user friendly interface to the CSD allowing fast and easy unit cell checking within our data collection software. The module and its functionality are presented herein.

[1] F.H. Allen, *Acta Cryst.* **2002**, *B58*, 380-388. [2] Agilent Technologies, CrysAlis<sup>Pro</sup> Software system, **2010**, Agilent Technologies UK Ltd.

**Keywords:** software, instrumentation, diffraction

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#### **Computer-readable database for magnetic space groups**

Harold T. Stokes, Branton J. Campbell, *Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602 (USA)*. E-mail: stokes@byu.edu

We have developed a magnetic space-group database and made it freely available over the internet. Settings for both the nuclear cell (Opechowski-Guccione setting) and magnetic cell (Belov-Neronova-Smirnova setting) are listed, as well as the transformations between them. For each space group and setting, the operators and the Wyckoff positions are given. These data are consistent with existing tables [1,2]. Both human-friendly and computer-friendly versions of the tables are available.

[1] D. Litvin, *Acta Cryst.* **2008**, *A64*, 419-424. [2] C. J. Bradley and A. P. Cracknell, *The Mathematical Theory of Symmetry in Solids* **1972** (Oxford University Press, London).

**Keywords:** magnetic space group, database

### MS28.P01

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**Boronic complexes-towards applications in functional materials**