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The predicted powder diffraction database (P2D2)

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Massive inorganic crystal structure predictions were recently performed. For millions of virtual zeolites or related materials the composition is imposed : SiO_2 or $AlPO_4$ etc. For other predicted inorganic compounds the composition was let to be free, but at least chemical elements were selected and some geometrical rules for organizing them were applied (exclusive corner sharing of polyhedra within the GRINSP software [1]). The explosion of the number of predictions justified the creation of new databases. Among them, the PCOD [2] (Predicted Crystallography Open Database) contains the crystal data of predicted titanosilicates, phosphates, vanadates, niobates, fluoroaluminates (etc). These databases open now the possibility for the identification of a newly synthesized compound by the comparison of its experimental powder pattern with predicted ones. The powder patterns calculated from the >100.000 PCOD entries were gathered into the P2D2 (Predicted Powder Diffraction Database) [3-4], allowing for identification by using any classical search-match software. To be successful, identification attempts require mainly accurate predicted cell parameters. Many improvements, by using empirical or ab initio approaches, will be needed in order to restrict the number of structure candidates to those having really a chance to exist (quite a difficult task). Prediction is obviously a large part of our future in crystallography, the P2D2 represents a small new step in that direction.
[1] A. Le Bail, J. Appl. Cryst. 38 (2005) 389-395.
[2] Predicted Crystallography Open Database - http://www.crystallography.net/pcod/
[3] A. Le Bail, Powder Diffraction (2008) in the press.
[4] Predicted Powder Diffraction Database - http://sdpd.univ-lemans.fr/cod/pcod/P2D2/

Keywords: crystal structure prediction, databases, powder diffraction

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Databases for absorption, XAFS and XANES, and future opportunities for research and investigation

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Databases for absorption include the International Union of Crystallography (IUCr) data, particularly of Creagh, Hubbell & Maslen et al.; the XCOM data of Hubbell & Scofield et al.; and the most recent FFAST (Form Factor ans Scattering Tables) of Chantler; together with experimental data using the X-ray Extended Range Technique (XERT) of Chantler. These databases typically have different purposes and uses, so that guidance and explanation is useful for a user to make informed comparisons with his experiments or medical or laboratory applications. Other databases exist, whether particularly for isolated atoms, diffraction, or condensed matter. The needs of X-ray Absorption Fine Structure (XAFS) and X-ray Absorption Near-Edge Structure (XANES) have often been somewhat different, for example needing fine spacing near absorption edges and the ability to take account of hole widths, discrete excitations, shake transitions and chemical environments to name a few. Typically, this relates to a programming environment rather than a database, and two particular examples are provided by packages by John Rehr (FEFF) and the Finite Difference Method of Yves Joly (FDMNES). This talk will discuss some key purposes and applications of these packages, and a little about how they should or should not be used.

Keywords: databases, absorption, XAFS

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Modernization of protein crystallography data formats: PDBML as a replacement for PDB?

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Recently the Worldwide Protein Data Bank (MSD-EBI in Europe, PDBj in Japan and RCSB in USA) has made available the PDB Exchange Dictionary (http://pdbml.rcsb.org/schema/pdbx.xsd), adapted from the mmCIF dictionary. The data structures provided allow better disambiguation compared to the aging PDB format, for example introducing the concept of entities - unique molecules within the record. Biological assemblies are more easily represented as well. The PDBML format is aligned with modern relational database practices - only store each piece of information once. However the problem remains that most popular software uses the PDB format for both input and output. We have looked at some of the hurdles involved in converting PDB files to PDBML format, and back again, and present a new, scalable database system, Protein SILO (PSILO) which overcomes these. The benefits of using correctly built PDBML files include more accurate interpretation of ligands and small molecules, more precise definitions of experimental conditions, categories for structure validation measures (a protein 'health check'), and far more powerful search capabilities when stored in a relational database.

Keywords: PDBML, structural databases, biomacromolecular structures

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The eCrystals Federation: Management and publication of small molecule structure data for all

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Modern data collection methods and publication processes cause a bottleneck in the dissemination of crystal structure data, which hinders the growth of databases. There is also increasing pressure from funders to make results available as widely and rapidly as possible. We have established an institutional data repository that supports, manages and disseminates metadata relating to crystal structure data. The eCrystals Federation project (http://wiki.ecrystals.