OCM04 COMMISSION ON BIOLOGICAL MACROMOLECULES
Coordinator: M. Guss

OCM04.26.1
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What is the Issue with Autodeposit?
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In macromolecular crystallographic structure solution the flow of information between stages is the key component of success. The final model is deposited in the PDB together with the information collected during the process. The dispersion of information between different formats of different programs makes the data organization and the automation of deposition a hard to achieve task. The main issue is still deciding which information is the most valuable and should be deposited. The answer depends on the view of the PDB role. The Protein Data Bank is not only the structural models repository, but it also contains a limited description of facts related to structure determination. The question is: should we enhance this information and can we achieve it using automatic tools?

The important facts missing from the PDB are: the increase in temperature factor, comments about twinning, diffuse scattering, use of multiple crystals for a single data set. Log files from numerical calculations are mostly of interest to the process of structure determination; however, it is not clear how this information would enhance the PDB deposits.

Overall, we should concentrate on how to improve the process of structure determination, which is challenging due to diversity of problems and approaches. The issue of autodeposit is subordinated to an overall improvement in crystallographic computational and database methods.
Keywords: data harvesting, data deposition, missing data

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Harvesting should be a Complete and Repeatable Record of Experiment
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The procedural and crystallographic data that are harvested and stored as a record of a crystallographic experiment should be sufficient to (1) repeat the analysis and (2) to estimate uncertainties, preferably in a completely automated fashion. It is highly likely that automated methods will be constantly developed over the next years and that there will be repeatedly be utility to a re-analysis of all structures currently in the PDB. Such analyses will be possible ony if the primary data and any associated knowledge about the experiment necessary to fully and automatically repeat the structure determination and analysis process are available. Further, even in the absence of full redeterminations of structure, re-estimates of errors and uncertainties (as in structure validation) will be done repeatedly on the entire PDB. The final structure and structure factors are not sufficient to repeat either the structure determination or the the error analysis (for example a free-R analysis is impossible if a test set is not specified; model bias can never be fully removed if an atom is placed and later removed). The data harvested from an experiment should therefore be a complete record of the process used to determine the structure, in a form that can be automatically read, repeated, and modified.
Keywords: PDB, LIMS, harvesting

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Harvesting - from Data Collection to Deposition
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The best approach to data harvesting is undoubtedly to have all relevant information regarding the experiment recorded automatically as it is determined. Provided that this is done reliably (i.e. no data are missing and all items present are also correct), this can be used in an automated pipeline requiring minimal user intervention. By far the majority of errors in the harvesting process arise from manually entered user input.

While a standard format has been developed by the IUCr for area detector image data (imgCIF and its binary equivalent, the Crystallographic Binary File or CBF), it has not been adopted widely. In the absence of a commonly used format for the image data, it is important that files written using existing commercial formats contain the essential experimental information along with the intensity data. Further, the data processing programs should record these data in a format which is readily amenable to straightforward deposition in the appropriate database.
Keywords: data collection, data processing, data harvesting

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Streamlining Data Bank Deposition and Manuscript Submission
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One of the reasons an all-electronic *Acta Crystallographica Section F* was created was to meet the increasing need for rapid publication of structural biology reports. Few have failed to notice the explosive acceleration in depositions to the Protein Data Bank (PDB) in recent years, but unrealized by many is the growing potential for depositions that have not been accompanied by a publication documenting the experiment and its results. Failure to publish means results are inaccessible to abstracting services and thus to the wider biological audience. A strategy to speed publication has emerged from collaborations between the PDB and IUCr Journals: eliminate repetition and streamline submissions by facilitating transfer of data deposited in the PDB to the journal at submission. Transfer of information for publication is through data files with content described in the PDB Exchange Data Dictionary. Deposition tools are available at each wwPDB site to assist in the preparation of these data files. Additional tools such as PDB_EXTRACT are also available to help automate the extraction of data items from popular structure determination software applications. It is hoped that a system combining publication and PDB deposition will reduce the overall effort required to perform both activities. Details and progress of this effort will be described.
Keywords: *Acta Cryst. F*, PDB, streamlining

OCM05 COMMISSION ON INORGANIC AND MINERAL STRUCTURES
Coordinator: G. Ferraris

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Modular Aspects of Inorganic and Mineral Structures
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With the increasing complexity of known inorganic and mineral structures, the importance of *moduli*, composed of a number of coordination polyhedra, became obvious for the understanding of these structures. The moduli are fragments of simpler structure types, so called *archetypes*, which have been recombined into a recombination structure according to a set of new structural principles, unit cell (chemical) twinning, crystallographic shear, non-commensurate interfaces, and coherent intergrowths. Structures built on the same principles, but with an incrementally increasing fragment size, form *accretional homologous series/polysomatic series*. The homologous approach allows distinction into *extensive* and *combinatorial* categories. *Variable-fit structures* have two (sub)lattices present in one structure. Combination of the accretional and variable-fit principle leads to new complex structures, including 'sliding series' and 'box-work structures'. *Configurational homology*

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reaches beyond the limits of the usual 'isoelemental' concept. Introduction of small but substantial changes into distinct homologous structures leads to *plesiotypes*. Structures in which one set of layers/slabs is identical (or homologous) for the entire family whereas the alternating set differs from a member to a member are *merotypes*. Besides 'proper' (*OD-* and *non-OD polytypes*), with structurally unmodified layers, '*improper' polytypes* can be recognized, with modifications of component layers, as well as *pseudopolytypes* between which pronounced changes in bonding patterns occur, and *endopolytypes* in which only, e.g., the cation component is subject to polytypy whereas the anionic framework remains (in principle) unchanged. *Non-commensurability* and *semicommensurability* can lead to polytypism.
Keywords: modular crystallography, structural series, polytypes

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OD Approach in Natural and Synthetic Inorganic Compounds: a useful Tool in Structure Solving and Structure Modeling
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The numerous researches carried on OD structures have clearly shown how that theory favours a deep insight into the various related phenomena of one-dimensional disorder, twinning (generally polysynthetic twinning), polytypism, and how it presents a comprehensive interpretation of the diverse anomalous features frequently displayed by diffraction patterns: diffraction enhancement of symmetry, diffuse spots, continuous streaking. However it is still far from constituting a 'normal' professional tool for mineralogists, inorganic chemists, material scientists. That is probably due to the erroneous assumption that the OD structures are relatively few in number and that their arrangements may be solved and described by 'normal' procedures. I shall try to clearly demonstrate its practical value and to show the various aspects in which OD approach may be extraordinarily and uniquely helpful, in particular:
a) The capability of OD approach to suggest the possible existence of new phases (new minerals in the case of natural phases) polytypically related to already known compounds, with exact indication of their crystallography and structure and its aid in overcoming serious problems during the refinement process.
b) The possibility to solve important problems where structural disorder had so far prevented the understanding of the 'real' structures. Interesting examples are presented by the C-S-H phases well known to the cement chemists, namely tobermorite, clinotobermorite, and their hydration and dehydration products.
Keywords: OD structures, polytypes, tobermorite

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Graph Theory, Symmetry and Inorganic Solids
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The Principle of Maximum Symmetry states that a structure adopts the highest symmetry consistent with the constraints acting on it.
Chemical constraints are determined by the properties of the bond graph, which for molecular compounds is the same as the bond diagram. Inorganic solids have infinite bond graphs, but a finite graph that retains all the essential nearest neighbour properties can be created by extracting one formula unit from the infinite graph. The lengths of the bonds can be predicted from this graph using the bond valence model and the principle of maximum symmetry. They necessarily have the symmetry of the graph.
Steric constraints are introduced when the bond graph is mapped into three dimensional space. The ideal space group adopted by the crystal must be a subgroup of the symmetry group of the graph, but the steric constraints may further lower the symmetry by distorting the structure along one or more of its normal coordinates.

Examples will illustrate this approach.
Keywords: bond graphs, symmetry, bond lengths

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News about the Inorganic Crystal Structure Database ICSD
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With the 2nd update 2004 82,876 entries are included in ICSD, including about 11,00 mineral structures. For about 22,000 structures a cross-reference to the Powder Diffraction File PDF is given. Inorganic structures don't contain C-H bonds together with C-C bonds in any residue. So some overlapping with organic structures is possible (e.g. with oxalate anions or tetramethylammonium cations). In addition organic residues are allowed in z*eolites and in* minerals.
For the introduction of **Structure types** the Pearson-symbols were unified as to get only one symbol per Bravais-type. The single-side centred cells were united under the letter "S". The remaining 14 symbols are: aP, mP, mS, oP, oS, oI, oF, tP, tI, hP, hR, cP, cI, cF. The number of atoms in the Pearson-symbol always refers to the standard setting, which for the rhombohedral structures is that of the rhombohedral primitive cell. The remarks of the prototype entries (one per structure type) will contain further information about the structure type in question, e.g. the "atomic environment types" of Daams & Villars [1]. The first about 100 structure types are ready to be incorporated into the first update of 2005.
Authors can easily help to complete the database ICSD! Just check your publication list against the entries in ICSD. Structures only published in a doctoral thesis or presented as a poster can be included into ICSD too.

[1] a) *J. Alloys Comp.*, 1992-97, **182**, 1-33; b) *J. Alloys Comp.*, 1992-97, **197**, 243-269; c) *J. Alloys Comp.*, 1992-97, **215**, 1-34; d) *J. Alloys Comp.*, 1992-97, **252**, 110-142
Keywords: inorganic structures, database, structure type

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Pressure Calibration Standard at high Temperature and high Pressure
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In high temperature and high pressure experiments, it is crucial to have a reliable pressure calibration standard over wide temperature and pressure ranges. At room temperature, the ruby-fluorescence pressure scale is found to accurate to within 1 % up to 55 GPa(Zha et al., 2000). However, severe discrepancies are reported between proposed pressure scales at high temperatures.
We showed previously (Matsui et al., 2000) that by combining the molecular dynamics(MD) method with quantum correction, it is possible to simulate very accurately the structural and physical properties of crystals over wide temperature and pressure ranges. Since the MD method derives thermal properties directly without any constraint on the atomic displacements, it is particularly useful and powerful for the simulation at high temperatures where anharmonic effects are important. In order to take into account the many-body forces in crystals, the breathing shell model(BSM) developed by Matsui(1998) is used for the MD simulation.
We have applied the MD method to the four cubic crystals, MgO, NaCl, Ar, and γ-Mg_2SiO_4. We show the MD simulation with BSM reproduces very accurately the observed properties of these crystals, including the volume compression data at room temperature, the volume thermal expansion data at 0 GPa, and the elastic constants and their temperature and pressure dependences. We then simulate and crosscheck the *T-P-V* equations of state of these crystals to provide them as reliable internal pressure calibration standards at high temperatures and high pressures.
Keywords: MD simulation, pressure standard, high temperature