MS.25.2

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Learning to drive a diffractometer across the World Wide Web - virtually!

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Typically the principal reason for developing of remote access services for an X-ray diffractometer system, is the potential to increase the efficiency of use, and user base, of the instrument. Remote access also facilitates the teaching of at least some of the practical aspects of crystallographic data collection. Given variable latency in the fabric of the internet, an important consideration is to the need to ensure safe operation of the remote instrument. With this in mind, we are incorporating a virtual representation of an instrument within a Web browser driven remote access service for the instrument. In addition to providing a means of training users without risking real instrument or human injury, the use of a virtual model offers a means of safely demonstrating and assessing a data collection strategy. A virtual representation also has the important benefit of providing a low-bandwidth, interactive and immediately interpretable view of the current state of the instrument, that offsets the 'dark lab' problem arising when lighting is switched off or a web-cam fails. The virtual model can be inspected from all angles and distances, and so provides flexibility not possible with a Web-cam. We are developing models for a conventional laboratory instrument, and a synchrotron beamline instrument. Web services are being used to underpin the remote access service, and a Web-cam view compliments the virtual view.

Keywords: virtual instrument, remote access, teaching

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Open repositories and web services for teaching and outreach in chemical crystallography

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The eBank-UK (http://www.ukoln.ac.uk/projects/ebank-uk) project was concerned with the problem of making publicly available the vast amount of small molecule crystal structures being generated by recent advances in crystallographic and computational instrumentation. The eCrystals repository (http://ecrystals.chem.soton.ac.uk) that arose from this project makes available all the derived and results data from a crystallographic experiment in a machine readable manner. Building on this prototype the eCrystals Federation project (http://wiki.ecrystals.chem.soton.ac.uk) will establish a network of data repositories across an international group of crystallography laboratories. Data from repositories has been harvested by CCDC and CDS and the project is also working with IUCr, RSC, Chemistry Central and Nature to integrate the system with the publication process. This process alters the traditional method of peer review and communication of structures by openly providing data where the reader or user may directly check correctness and validity by accessing all files generated during the experiment. This approach allows rapid release of crystal structure data into the public domain whilst providing a valuable educational resource and mechanisms for services to be built on the body of data for communication, further studies and reuse. Examples of communication and education services that will be presented are the use of repositories for capturing teaching laboratory experiment data and reports, Blogs for discussion of experiments and results and the potential of SecondLife for visualisation and communication. The final educational tool to be presented is the Schools eMalaria project (http://emalaria.soton.ac.uk), where children use this data in docking simulations.

Keywords: electronic publishing, crystallographic databases, computer networking

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Use of MATLAB® in teaching crystallography

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Advanced computer languages are invaluable in teaching crystallography and can be used in a variety of ways. My textbook -- Foundations of Crystallography with Computer Applications, CRC press, 2008 -- uses MATLAB®. The book displays detailed calculations on two crystal examples, hexamethylbenzene (triclinic) and anhydrous alum (trigonal). The student does corresponding calculations on a crystal—such as anthracene, benzene, diamond, rutile, or caffeine—throughout the semester. Starter programs in the book reduce the burden of coding and at the same time allow the student to progress rapidly in understanding the crystallography. The metric matrix is made the key to calculating bond distances, bond angles, unit cell volumes, interfacial crystal angles, and d-spacings. Also the metric matrix is the key to transforming between different bases, to transforming between direct and reciprocal lattices, and to comparing PDF files. Starter programs facilitate construction of multiplication tables for the point groups. Starter programs are also used to prepare graphics constructing the unit cell superimposed on the asymmetric unit, the unit cell superimposed on the reciprocal cell, and the unit cell populated with atoms. The MATLAB® graphics allow these cells to be rotated, with the result that the projections can be produced with extraordinary ease. Another computer application is the creation of parametric figures—such as spirals, seashells, and butterflies (T.H. Fay Amer. Mat. Mon. 96, 443, 1989)—which then can be combined to provide examples of point groups and space groups. The presentation will be illustrated with the author's examples and student exercises.

Keywords: crystallographic education, computer-aided instruction, symmetry

MS.25.5

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Interactive 3D Space Group Visualizer

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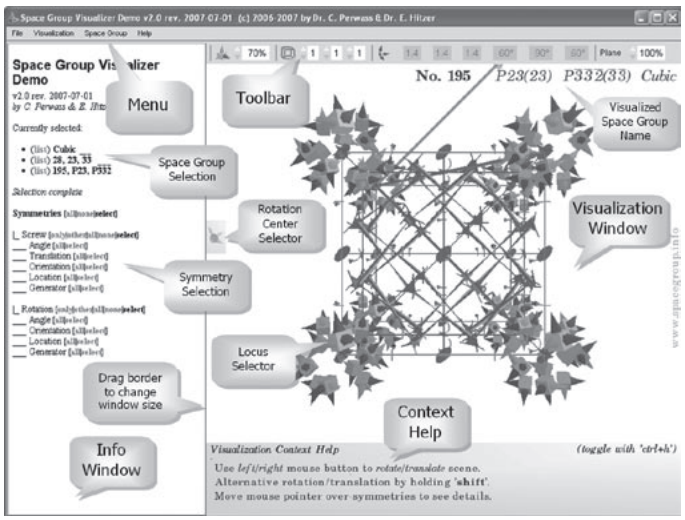
The Space Group Visualizer (SGV) for all 230 3D space groups is a standalone PC application based on the software CLUCalc. (Compare screen image of group P23 [No. 195].) Main features include:
Closely related to IT, Vol. A (2005);

Browser selection panel for 7 crystal families, crystal classes (point groups), individual space groups;
Symmetry selection menu by type, angle, translation, orientation, location, generator;
Change cell type;
Mouse control to rotate/translate visualization and interactively animate, select, and remove single symmetries;
General position (mouse) interaction: rotation/motion of general position symbols;
Vary number of cells in view, vary cell angles and lengths;
Orthographic projection, stereo colors (cinema type stereo view);
Save visualization as image file.
We will present the unique mathematical and algorithmic structure underlying the visualization software using a coordinate free approach to symmetry with Geometric Algebra. We demonstrate the powerful set of interactive visualization tools made available by the SGV. Free demo at www.spacegroup.info



Keywords: space-group symmetry, interactive computer graphics, virtual reality

MS.26.1

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In situ measurement of microorganisms metabolism under high hydrostatic pressure

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Many biotopes, e.g. deep-sea environments, subseafloor, are characterized by high hydrostatic pressure (HHP). Accordingly, most of the biosphere might live in high-pressure biotopes. Therefore, we aim at measuring microbial metabolic activities under high hydrostatic pressure, in particular to infer the contribution of microbial activity in the subsurface geochemical cycles. To avoid artifacts due to compression/decompression cycling on the behavior of microorganisms, we have developed an experimental set-up for in situ measurements at HHP in the 0-1 GPa range. This includes a low-pressure diamond anvil cell (DAC) optimized for imaging and spectroscopy, that is of interest for studying not only live microorganisms and related organic compounds, but also soft solids. A new accurate pressure gauge was also calibrated over the same pressure range. This high-pressure set-up was combined to Raman spectroscopy to investigate the alcoholic fermentation by the yeast Saccharomyces cerevisiae, as a function of pressure. Ethanol fermentation from glucose was monitored in the low-pressure DAC from ambient pressure up to 100 MPa. Our results show that below 10 MPa, fermentation proceeds three times faster than at ambient pressure and the fermentation yield is enhanced by 5 % after 24 hours. At higher pressure, the fermentation yield decreases linearly, and reaches 0 at 87(7) MPa. The respiration of selenite by a surface sediment bacterium, Shewanella oneidensis strain MR-1, could also be investigated under HHP by in situ microXANES at BM30B and ID22 beamlines of the European Synchrotron (ESRF, Grenoble) using a diamond anvil cell (ID22) or an autoclave (BM30B), to 150 MPa. We could show that Shewanella oneidensis strain MR-1 could reduce selenite into selenium to ca. 160 MPa.

Keywords: pressure, metabolism, spectroscopy

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High-pressure studies of pharmaceutical compounds

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This presentation will demonstrate how high-pressure techniques can provide a complementary method for exploring polymorphism and solvate formation in molecular solids, with a particular focus on pharmaceutical compounds. The techniques are proving useful for the identification and characterisation of new forms that do not appear in conventional polymorph screens performed under ambient conditions. This is particularly true for molecules that exhibit significant conformational flexibility. The presentation will highlight the range of strategies that have been developed for exploring polymorphism and solvate formation at high pressure, e.g. direct compression, recrystallisation from solution, effect of pressure-transmitting medium. Relationships between the effects of static compression and the effects of ball-milling will also be explored. These high-pressure methodologies are also well-suited for obtaining in a reproducible manner so-called disappearing or elusive polymorphs. Examples will be provided to demonstrate how new forms obtained at high pressure on a small scale can be recovered to ambient pressure and subsequently be used in seeding experiments under ambient conditions. The results provide insight into how the hierarchies of intermolecular interactions change with pressure and how the relative thermodynamic stabilities of different forms can change, with particular relevance to ab initio computational methods for crystal structure prediction. Furthermore, these methodologies may also have the potential to circumvent patents or enhance protection of intellectual property associated with pharmaceutical compounds.

Keywords: polymorphs, pharmaceutical compounds, high-pressure chemistry