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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

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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);