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International Tables for Crystallography, Volume F: Crystallography of Biological Macromolecules, 2001, Michael G. Rossmann & Eddy Arnold, Editors, Kluwer Academic Publishers, Dordrecht/Boston/London, 832 pp., was published in July 2001. Volume F comprises 26 chapters and a total of 72 articles written by 156 authors. More than 1300 copies of Volume F have been sold as of mid-January 2005. Further information can be found at the IUCr web site:

http://www.iucr.org/iucr-top/it/itf/itf.html

An important goal of current efforts on the ITC series is to make the volume contents electronically accessible and cross-referenced/hyperlinked so that logically connected material from different volumes can be easily linked to facilitate problem solving in research and education. Considerations for modes of electronic access to and production of a revised version of Volume F will be discussed in Florence; input from the community will be welcomed.

Keywords: International Tables, electronic access, structural biology

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Intl Tables for Crystallography Vol F1, Space-group Symmetry for Structural Biology

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A new International Tables for Crystallography (ITC) volume in preparation, *ITC Volume F1*, is intended to serve as a space-group reference for crystals containing chiral molecules such as those found in biological systems. The volume will contain the subset of *ITC Volume A* (Theo Hahn, editor) relevant to structural biology, namely 65 space groups and 24 Patterson groups. In addition, the volume will contain sections from Volume A that describe the interpretation and use of the space-group symmetry information, in a style similar to the *Brief Teaching Edition of Volume A*, also edited by Theo Hahn. Although targeted to meet the needs of structural biologists, *Volume F1* will provide a compact and relatively inexpensive compendium of space-group symmetry relevant to many fields, including organic, inorganic, and organometallic chemistry, and nanotechnology.

An important goal of current efforts on the ITC series is to make the volume contents electronically accessible and cross-referenced/hyperlinked so that logically connected material from different volumes can be easily linked to facilitate problem solving in research and education. Volume F1 will contain a summary of material in other ITC volumes relevant to crystallography of biological and other chiral molecules; the online version will provide convenient hyperlinks to enable efficient connectivity.

Keywords: International Tables, space-group symmetry, structural biology

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OCM08 COMMISSION ON HIGH PRESSURE

Coordinator: M. Kunz

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Exploring Novel Synchrotron Approaches to Structure Determination by Single-crystal XRD

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Introduction of modern area detector equipped high-pressure crystallographers in an important new tool and opened possibilities for new types of experiments. So far, however, the exploration of benefits of these detectors has been restricted only to monochromatic experiments. Polychromatic radiation has been used in high-pressure studies for almost two decades, but has never been demonstrated to be competitive with monochromatic experiments in terms of full structure determination. In this presentation it will be shown that single-crystal polychromatic diffraction (pSXD) can be successfully used for full structure determination at high pressure, and at the same time offers such advantages, as ultrashort data collection time, ability to collect diffraction data without rotating the sample and depth-resolution. By combining recent solutions developed in protein Laue crystallography, materials science, and novel detector technology, unique approaches, optimized to meet the demands of ultrahigh pressure experiments can be developed. I will describe the theory of polychromatic microdiffraction, computational and experimental methods developed to deal with its limitations, and compare pSXD to alternative methods. Special emphasis will placed on discussing aspects of working with microcrystals and multigrain aggregates (with depth-resolution), and experimental approaches to peak energy determination, and harmonic deconvolution. It will be shown that in pSDX experiments x-ray absorption near-edge spectra can be obtained at the same time as the structural data, providing additional information about the local environment of individual ions as well as their electronic state. The status of on-going development of the discussed techniques at beamline 16BMB, APS and efforts to coordinate the development of SXD techniques at other high-pressure synchrotron beamlines in the US will be presented.

Keywords: phase transitions, XAS, polychromatic diffraction

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Single Crystal Studies using the 9.8 Station at SRS Daresbury

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Synchrotron radiation offers significant advantages for high pressure single crystal studies in that significantly shorter wavelengths can be accessed than are available with conventional laboratory sources. This greatly increases the volume of reciprocal space that can be accessed and hence improves the quality of the structure refinement.

The small-molecule single-crystal beamline, 9.8, at SRS Daresbury has carried out a significant number of successful high-pressure studies. The station is equipped with a Bruker diffractometer with an Apex II CCD detector and can obtain a complete routine data set in 1.5 hours.

In this talk I will describe the procedures to index often complex diffraction patterns in the presence of significant scattering from the pressure cell materials and to proceed from indexed diffraction patterns to integrated intensities. Examples from recent work of the structures of elements including rubidium, barium, tellurium and selenium will be used to illustrate this.

Keywords: high-pressure crystallography, single-crystal structure determination, synchrotron X-ray instrumentation

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High Pressure Single Crystal Studies using Neutrons

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Over the past two decades there has been considerable progress in both the pressure range and the complexity of structures studied by high-pressure neutron diffraction. However, this development has been almost exclusively confined to powder diffraction techniques. Recently, the availability of large gem anvils has opened up the possibility of carrying out single crystal neutron diffraction studies at pressures of 10 GPa or more with samples grown in-situ in the high-pressure cell. In this talk I will describe progress to date using the new Vx Paris-Edinburgh cell on the SXD single crystal diffractometer at the ISIS pulsed neutron source.

Keywords: high-pressure crystallography, single-crystal structure determination, neutron instrumentation