possibilities for interactive consultation.
Keywords: physical properties of crystals, tensor properties, phase transitions

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International Tables for Crystallography, Volume A1
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The list of the maximal subgroups of the space groups in Volume *A* is incomplete. Volume *A*1 [1] now contains the complete data. Its Part 1 deals with group-theoretical aspects of space groups, group–subgroup relations and the underlying mathematical background. Part 2 contains complete listings of all maximal subgroups for each space group, including their general positions or their generators, their conjugacy relations and transformations to conventional settings. Part 3 lists the relations between the Wyckoff positions for every maximal subgroup of every space group, including the cell transformations and coordinate transformations. In both parts the infinitely many isomorphic subgroups have been included in a parametrized form.

The importance of listing all subgroups individually, not just their types, can be seen in the relations of the AlB_2 structure (*P*6/*mmm*) with those of ZrBeSi and $CaIn_2$ which crystallize in two *different* subgroups $P6_3/mmc$. The occupied atomic positions of AlB_2 split in different ways to the positions of the two subgroups [2].

The index of symmetry reduction to a maximal isomorphic subgroup may adopt an infinity of values, e.g. p = prime = $6n+1$ for certain isomorphic subgroups of $R\bar{3}$. Such values are actually being observed, e.g. $p = 31$ for $PtCl_3$ [3] as a hettotype of fcc packing. The necessary information for such relations is contained in Volume *A*1.

[1] *International Tables for Crystallography*, *Vol. A1*, 2004, Dordrecht: Kluwer. [2] Hoffmann R.-D., Pöttgen R., *Z. Kristallogr.* 2001, **216**, 127. [3] Müller U., *Z. Anorg. Allg. Chem.*, 2004, **630**, 1519.
Keywords: group-subgroup relations, subgroups,Wykoff positions

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Volume G: Definition and Exchange of Crystallographic Data
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Volume G[1] will be launched at this congress. The highly data-dependent nature of crystallographic studies places great importance on the need for orderly acquisition and retention of data, and for computational tools that facilitate efficient data handling. To support this data-rich environment, Volume G is dedicated to the precise definition of the most commonly used data items. Although it focuses on the Crystallographic Information File (CIF) representation of data adopted by the IUCr in 1990 for journal submissions, it also considers more recent data-language developments involving XML.

CIF data dictionaries are described for *core*, *macromolecular*, *powder*, *symmetry*, *modulated-structure* and *precision-density* studies. The underpinning dictionary languages are also detailed, as are approaches for defining and storing image (binary) data. In these dictionaries, each data item is defined in terms of attributes that characterise their allowed values and mutual relationships. These provide human-readable and machine-readable descriptions of the data. However, the main use of the definitions is in a computer-software environment, so details of computer programs and libraries used with the electronic dictionaries to validate and exchange data items are also described. A CD-ROM will accompany the volume.

[1] International Tables for Crystallography, 2005, Volume G, *Definition and exchange of crystallographic data*, edited by S.R. Hall & B. McMahon, Heidelberg: Springer.
Keywords: International Tables, CIF dictionaries, data definition

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Status of Volume A: Space-group Symmetry
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Volume A treats space groups and their applications in all fields of crystallographic research and teaching. The subject matter is presented in three parts of different length and complexity:

(i) Central core of the volume are the plane-group and space-group tabulations in Parts 6 and 7 (620 pages, two pages per group).

(ii) The first 90 pages (Parts 1 to 5) contain definitions, guides to the tables and *practical* hints for the use of the space-group data on a level corresponding to an *elementary* textbook. These parts, as well as 24 selected space-group examples, also form the "*Brief Teaching Edition of Volume A*", which is intended as a brief, inexpensive tool for class-room teaching.

(iii) The final 180 pages of text (Parts 8 to 15) are of a much higher *theoretical* level and in some places correspond to an *advanced* text book of crystallographic symmetry.

The first edition of Volume A was published in 1983, of the Teaching Edition in 1985. The fifth revised editions of both volumes appeared in 2002. These editions are based completely on electronic files, both for tables and text (*c.f. Foreword to the Fifth Edition*). A corrected reprint of the fifth edition, as well as an on-line version, of Vol. A are in preparation and scheduled for 2005.

In order to honor two deceased authors of Volume A and their contributions, two special topics will be briefly discussed: (1) P. M. de Wolff (Delft): Reduced bases and lattice characters; (2) E. F. Bertaut (Grenoble): Extended Hermann-Mauguin space-group symbols and subgroups.
Keywords: space groups, symmetry, International Tables

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Acta Cryst. (2005). A**61**, C132
Status of Volume B: Reciprocal Space – planned 3rd Edition
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The second edition of Volume B was published in 2001 and its third edition is being planned. The subdivision of the volume in five parts remains unchanged but several changes are envisaged within most parts. Among the major revisions and additions are the following:

(i) Discussions of applications of direct methods to macromolecular crystallography will be greatly expanded; (ii) Patterson and molecular-replacement techniques will be revised, also in view of their appearance in Volume F; (iii) several major changes are expected to occur in the chapter on electron diffraction and microscopy in structure determination: a new Foreword, a thorough revision of the sections on convergent-beam electron diffraction and three-dimensional reconstruction and a new section on single-particle reconstruction; (iv) the chapter on molecular modeling and computer graphics will be enriched by a section on modern graphics software for structures consisting of small and medium-sized molecules; (v) a new chapter is being written on modern extensions of the Ewald method: (a) use of FFT in efficient computation of lattice sums, and (b) departures from the usual point-charge model; (vi) a significant revision is planned of the chapter on disorder diffuse scattering of X-rays and neutrons, and (vii) the chapter on reciprocal-space images of aperiodic crystals will be revised in view of recent developments.

Details on the second edition and the above plans can be found at:
http://www.iucr.org/iucr-top/it/itb/itb.html - IUCr office
http://crystal.tau.ac.il/xtal/comit/index.html - author's office
Keywords: International Tables, reciprocal space, methodology

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Update on International Tables for Crystallography Volume F
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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

OCM07.27.10

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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