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Crystal Structures of Two Iron-containing Minerals: Sturmanite and Biraite-(Ce) (a New Mineral)
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The crystal structure of two rare iron-containing minerals will be discussed. They contain chemically different anionic groups. Iron, besides occurring in nature in two different oxidation states, has an intermediate ionic radius with respect to other cations. For this reason iron is easily allowed to enter a wide number of different structures, and it can be coupled with many other cations with larger and smaller ionic radii. In the crystal structures being described here, we will see how iron-centered polyhedra can link with cations as different in size as REE's and calcium, on one side, and carbon, on the other side.

Sturmanite, $Ca_6(Fe^{3+},Al,Mn)_2(SO_4)_2[B(OH)_4](OH)_{12}\cdot 25H_2O$, structurally, belongs to the thaumasite-ettringite group. Minerals of this group are either hexagonal (thaumasite) or trigonal (ettringite). In sturmanite, similarly to ettringite, two co-axial elements parallel to [001] can be considered as the most specific structure features. The main one is a polyhedral column formed by Fe-octahedra and Ca-polyhedra. The second structural element parallel to [001] is formed by $[SO_4]$ tetrahedra and by $B(OH)_4$ tetrahedra.

Biraite-(Ce), ideally $Ce_2Fe^{2+}(Si_2O_7)(CO_3)$, is monoclinic, space group $P2_1/c$, a 6.505(7), b 6.744(2), c 18.561(4) Å, β 108.75(2)°. It displays a new structure type, based on polyhedral sheets (001) composed by pairs of edge-sharing $[FeO_6]$ octahedra, $[Si_2O_7]$ groups, and $[CO_3]$ triangles. Ce^{3+} cations in ten-fold coordination provide the linkage between neighbour polyhedral sheets.
Keywords: crystallography of minerals, sulfates, silicates

OCM06 COMMISSION ON CHARGE, SPIN AND MOMENTUM DENSITIES
Coordinator: C. Lecomte

OCM07 COMMISSION ON INTERNATIONAL TABLES OF CRYSTALLOGRAPHY
Coordinator: H. Fuess

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International Tables. The Present and Future
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The present series of *International Tables* comprises eight volumes: a tremendous achievement realized under the chairmanship of Theo Hahn. The *Tables* present a comprehensive collection of almost all aspects of solid-state research. The basics of crystallography (space groups, subperiodic groups, symmetry relations and form-factor tables) are covered in volumes A, A1, B, C and E, and the properties of condensed matter in physics, chemistry and biology are included in the other volumes. Additional subject areas (such as materials science or powder diffraction) may need to be added. Forthcoming editions of the volumes will update and expand the subject areas already covered by the series. Further developments (such as whether large tables of numerical data, such as form factors, are needed) and the title of the series will be discussed.

The online version of the *Tables*, which will be demonstrated at the conference, may eventually lead to a completely new product.
Keywords: international tables for crystallography, publishing, fundamental crystallography

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International Tables for Crystallography Online
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The IUCr Editorial Office has been storing *International Tables for Crystallography* in various electronic formats (proprietary, SGML and LaTeX) since 1999 with a view to making the whole series of the books available online. The use of SGML conforming to our own DTD (similar to that used for the IUCr journal articles delivered through *Crystallography Journals Online*) has been central to this approach, as it allows a great deal of information about each article in *International Tables* to be captured in a highly structured way, and allows hyperlinks between articles in different volumes to be specified. The decision to make all eight volumes (a total of 6000 pages) available online was made in March 2004. The work of the IUCr Editorial Office towards the conversion of all the articles in the series to a common format (SGML/XML) and the production of PDFs and HTML versions of all articles for display online will be described. Some of the many suggestions received from the academic community for new added-value features to include in the online representation of the volumes in the series will be discussed and ways in which these ideas could be presented online will be demonstrated.
Keywords: International Tables for Crystallography, electronic publishing, internet

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International Tables: Volume E
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A list of corrections to Volume E will be given. Suggestions for additions and changes to the presentation of specific material in future editions of Volume E will be discussed. These include: additional headings in multi-column tables, reordering sequences of symmetry operations and generators, including explanations of subperiodic group symbols used by other authors, and including the explicit tables of monoclinic/inclined scanning for groups of orthorhombic and higher symmetries[1] in the web-based and/or future edition of Volume E.

[1] Litvin D.B., Kopský V., *Acta Cryst.*, 2004, A**60**, 637.
Keywords: International Tables, subperiodic groups, mathematical crystallography

OCM07.27.4
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Volume D of Int. Tables: «Physical Properties of Crystals»
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Volume D was published at the end of 2003 and 477 copies have already been sold in 2004. It is therefore off to a good start. It has 522 pages and 18 Chapters distributed in three parts: 1. Tensorial aspects of physical properties, 2. Symmetry aspects of excitations, 3. Symmetry aspects of structural phase transitions, twinning and domain structures. It is accompanied by a CDROM with two pieces of software: *Tenχar* (calculations with tensors and characters) and *G1*KoBo*-1 supporting Part 3 on structural phase transitions.

One planned Chapter didn't materialize because its potential author failed to deliver his manuscript on time, that on the "Tensorial aspects of dielectric properties". This is a very important topic in which there are new developments and new applications. If a Second Edition is considered, a new Chapter on that topic should be commissioned. Plans are already under way for such a tentative Second Edition. For instance, several Chapters bear on rapidly evolving topics, such as non-linear optics and will need updating; one Section in the Chapter on Twinning was omitted because of lack of time, that on the X-ray observations of twins and it needs to be added. When Volume D goes online, this will open up many interesting

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

OCM07.27.5
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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

OCM07.27.7
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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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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

OCM07.27.9
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Update on International Tables for Crystallography Volume F
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