

**OCM05.27.6***Acta Cryst.* (2005). **A61**, C131**Crystal Structures of Two Iron-containing Minerals: Sturmanite and Biraitite-(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<sup>3+</sup> and calcium, on one side, and carbon, on the other side.

Sturmanite,  $\text{Ca}_6(\text{Fe}^{3+}, \text{Al}, \text{Mn})_2(\text{SO}_4)_2[\text{B}(\text{OH})_4](\text{OH})_{12} \cdot 25\text{H}_2\text{O}$ , 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  $[\text{SO}_4]$  tetrahedra and by  $\text{B}(\text{OH})_4$  tetrahedra.

Biraitite-(Ce), ideally  $\text{Ce}_2\text{Fe}^{2+}(\text{Si}_2\text{O}_7)(\text{CO}_3)$ , is monoclinic, space group  $P2_1/c$ ,  $a$  6.505(7),  $b$  6.744(2),  $c$  18.561(4) Å,  $\beta$  108.75(2)°. It displays a new structure type, based on polyhedral sheets (001) composed by pairs of edge-sharing  $[\text{FeO}_6]$  octahedra,  $[\text{Si}_2\text{O}_7]$  groups, and  $[\text{CO}_3]$  triangles.  $\text{Ce}^{3+}$  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**

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**Coordinator:** H. Fuess

**OCM07.27.1***Acta Cryst.* (2005). **A61**, C131**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

**OCM07.27.2***Acta Cryst.* (2005). **A61**, C131**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

**OCM07.27.3***Acta Cryst.* (2005). **A61**, C131**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, **A60**, 637.

**Keywords:** International Tables, subperiodic groups, mathematical crystallography

**OCM07.27.4***Acta Cryst.* (2005). **A61**, C131-C132**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: *Tenxar* (calculations with tensors and characters) and *GI\*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