18-Data Bases and Communications

Definitions for CIF data items used in powder diffraction, in addition to those listed in the 1991 CIF Core Dictionary, have been proposed. It is hoped that these will be formally adopted at the XVIth IUCr Congress.

PS-18.01.12 CRYSTAL-CHEMICAL ANALYSIS OF STRUCTURES OF RARE-EARTH POLYCHALCOGENIDES. By S.A. Magarill*, N.V. Podberezskaya, N.V. Pervukhina, E.N. Ipatova and S.V. Borisov. Institute of Inorganic Chemistry, Russian Academy of Sciences, Siberian Branch, Russia.

The structures of rare-earth polychalcogenides (which contain covalently bound X_2^{2-} groups, X = S, Se, Te) were classified using the facilities of Inorganic Compounds Database (Inst. Inorg. Chem., R.A.S., S.B.) including the package for crystal-chemical computing. The studies of physico-chemical properties of rare-earth chalcogenides (imperfect chalcogen-deficient phases often represented with idealized formulae with integer coefficients) made by workers from France (Flahaut J. and Laruelle P., Prog. Sci. and Technol. Rare Earths, vol. 3, Pergamon Press, 1968, pp. 149-208), Moscow (A.A. Eliseev, G.M. Kuzmichova, Itogi nauki i tekhniki. VINITI, Ser. kristallokhimiya, 1976, v.11, p.95-131) and Siberia (I.G. Vasil'eva Doktorskaya Dissertatziya, 1992, Novosibirsk) has shown the lack of, and the poor systematization of structural data concerning polychalcogenides, these materials being rather well characterized by means of other physical methods.
Our systematization is based on the symmetry distribution of structural types. Structural data for 26 LnX_2 compounds with symmetry ranging from tetragonal to triclinic have been examined. The structures of most of the materials are close to that of Fe_2As. Close-packed cationic and anionic matrices have been revealed, their packing rules have been determined and their cationic subcells have been calculated. Structural generalizations for this class of compounds have been made using well-determined crystal-chemical characteristics including the geometry of cationic and anionic matrices and the characteristics of their mutual coordination.
Peculiarities of this class, such as frequent twinning and multiple intergrowth, the existence of several polymorphs, and the imperfection of the anionic sublattice have been pointed out.

18.02 – Journals & Crystallographic Data

OCM-18.02.01PLANS FOR *ACTA CRYSTALLOGRAPHICA*
By Charles E. Bugg, Center for Macromolecular Crystallography, University of Alabama at Birmingham, Birmingham, AL 35294-0005, U.S.A.

Acta Crystallographica now consists of four sections that cover a variety of topics of interest to the crystallographic community. The latest addition to this series, *Acta Cryst* Section D, covers the rapidly-growing field of biological crystallography, and will focus primarily on macromolecular crystallography. Each section of *Acta Cryst* will have its own Editor. These Editors will work closely with the Editor-in-Chief to develop new initiatives and policies, in collaboration with *Acta Cryst* Co-editors and the technical editing staff in Chester. Initiatives now being implemented include: broader coverage of timely topics through invited Lead Articles and reviews of selected topics; electronic submission of papers; checking and archiving of crystallographic data; and electronic handling of manuscripts.

OCM-18.02.02*ACTA CRYSTALLOGRAPHICA, SECTION D.*
By Jenny P. Glusker, The Institute for Cancer Research, 7701 Burholme Avenue, Philadelphia, PA 19111, USA.

A new section of *Acta Crystallographica*, one devoted to "Biological Crystallography" has been published. Articles considered for this section cover both structural results and the development of new methods aimed at helping to solve and interpret such crystal structures. The first issue contained papers from the conference on Direct Methods of Phasing in Macromolecular Crystallography, held in April 1992. The second issue contained a variety of macromolecular structural papers.

An account will be given of experiences of the Editors to date. The efforts of many referees and of the staff at Chester have been essential to the launching of this new section. Many articles on macromolecular structures are now in various stages of processing. All authors of macromolecular publications must submit atomic coordinates to the Protein Data Bank (Brookhaven), and provide a Brookhaven number prior to the final proof stage. A major challenge to the Editors is how to check for the validity of the reported electron density and its interpretation. It is our aim to maintain a very high quality in each article, as expected for all other sections. On the other hand, some flexibility in the requirements for information is needed at this stage, since experimental problems differ in many cases from those found for smaller molecules. Input on this subject from the crystallographic community is welcomed.

OCM-18.02.03
JOURNAL OF SYNCHROTRON RADIATION

S. S. Hasnain[1] and J. R. Helliwell[2]
1 Molecular Biophysics Group, SERC Daresbury Laboratory, Warrington WA4 4AD, U.K.
2 Department of Chemistry, University of Manchester, Manchester, M13 9PL, U.K.

In the field of Synchrotron Radiation, papers on instrumentation and methods as well as novel applications are published in a wide variety of journals. Many of these journals are not readily available to the community. Thus, a proposal for launching a new Journal, "Journal of Synchrotron Radiation" (JSR). Discussions were initiated with the IUCr in 1991.

The JSR would cover all aspects of SR, including the machine, with particular emphasis on Methods and Instrumentation. It will also provide a natural home for the novel applications of synchrotron radiation. It is clear that the provision of such a journal will not only enhance the cross-fertilisation of ideas between scientific disciplines but also allow the rapid transfer of information between communities specialising in the use of different parts of the electromagnetic spectrum.

A distinguished editorial board has been assembled covering all aspect of the SR field. The details of the proposal was provisionally approved by the Executive committee of the IUCr in August 1992,

18-Data Bases and Communications

following which it has been discussed widely at several international conferences. Also, various respective organisations and the Directors of SR laboratories have been consulted. These consultations have echoed the feeling that a Journal dedicated to SR is urgently required.

OCM-18.02.04JOURNAL OF APPLIED CRYSTALLOGRAPHY. By A.M. Glazer, Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford OX1 3PU, UK.

The Journal of Applied Crystallography is now in its 26th year, and over this time it has been continuously evolving. In recent times, a number of special features have been added to the journal, such as the incorporation of Lead Articles, where an author is invited to submit a paper on a subject of general interest to the readers. Such papers are refereed in the normal manner, but are given prominence once accepted. In addition, JAC has come to serve the crystallography community by acting as the main source of publications of computer programmes, new commercial products, and laboratory notes. From time to time, JAC also publishes Fast Communications.

Manuscripts are normally submitted to the Editor or one of the coeditors, who individually arrange for at least two referees. Each member of the team is responsible in the end for acceptance or rejection of a paper, with the Editor having the final say in case of a dispute, which, in the experience of this Editor, is very rare. The editorial team members communicate with each other regularly, principally by sending around monthly status reports to each other to ensure that everyone knows which papers have been submitted and their present position. From time to time, this procedure has picked up cases of authors submitting the same manuscript to more than one editor. The status reports are also sent to the Technical Editor in Chester who keeps an overall eye on all of the journals. Without the efficient running of the Chester offices, journals such as JAC could not successfully appear with the high quality that the crystallography community has come to expect. In this talk, present and future policy of the Journals Commission regarding JAC will be discussed.

OCM-18.02.05 CHESTER PUBLISHING OPERATIONS. By M. H. Dacombe, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The main function of the technical-editing office of the IUCr in Chester is the production of the journals *Acta Crystallographica* and *Journal of Applied Crystallography*. Over the past few years there have been considerable developments in the way in which these journals are produced.

In particular, papers intended for publication in Section C of *Acta* are now submitted direct to the Technical Editor and various checks are carried out on each structure (these checks include symmetry, geometry and previous publication) before the paper and the results of these checks are sent to a Co-editor.

Section D of *Acta* was launched in January 1993 and the possibility of starting another new journal on synchrotron radiation is under active investigation.

Machine-readable submissions to all the Union's journals is encouraged and much material is now prepared in Chester as camera-ready copy - *Fast Communications*, regular submissions, indexes and, particularly, *Regular Structural Papers* in Section C. The whole procedure for Section C has been facilitated by the use of CIFs and a by-product is that a CIF file for each structure is archived in Chester and is also available for onward transmission to the established databases. Additionally, the ninth edition of the World Directory of Crystallographers will be held in Chester as a database in CIF format. The database in Chester is accessible via email and it is intended to make it available on-line in due course. Various other publications are handled in Chester. The most important of these is the series *International Tables for Crystallography*.

OCM-18.02.06 **COMPUTERIZATION OF PUBLISHING AND RELATED DATA ARCHIVING** By B. McMahon, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England

Since the last congress of the IUCr there has been considerable investment in high-performance computing equipment in the Technical Editor's office. Six Unix-based graphics workstations and a file server reside on an Ethernet local area network; there are also network connections to IBM PC and Apple Macintosh-type machines. The network provides for data transfer between the computers and data input/output equipment: floppy disk drives supporting various formats; cartridge and open-reel tape units; CD-ROM and optical disk drives; and laser printers. There are also full network connections to the UK national academic network JANET and to the global Internet.

Structural data in papers submitted for publication to *Acta Crystallographica* are checked using a wide range of standard crystallographic software, freely donated by the community. The validated or corrected data may then be typeset without the risk of typographic errors being introduced by manual keyboarding. When these data arrive in Chester in hard-copy form, they are input to the local computer system as Crystallographic Information Files (CIFs). Authors may also submit CIFs electronically; where this is done in the case of *Regular Structural Papers* in Section C of the journal, the entire paper may be typeset automatically. The acceptance of CIF as the data transfer standard by the IUCr has ensured that these procedures can be developed for optimum efficiency.

It is the *efficiency* of the new procedures that render them cost-effective in terms of journal production. Other techniques for converting different word-processed input to the requirements of the journal are also being developed; but without exception they require more manual intervention and consequently have a less benign impact on the publishing process.

Strategies are being developed for making available to the crystallographic community the structural data stored in machine-readable form.

OCM-18.02.07
THE MACROMOLECULAR CIF DICTIONARY. By Keith D. Watenpaugh*, Upjohn Laboratories, 301 Henrietta St., Kalamazoo, MI 49007, USA; Helen M. Berman, Chemistry Department, Rutgers University, Piscataway, NJ 08855, USA; Philip E. Bourne, Department of Biochemistry and Molecular Biology, Columbia University, 630 W. 168th Street, New York, NY 10032, USA; Paula M. D. Fitzgerald, Merck Research Laboratories, P. O. Box 2000, Rahway, NJ 07065, USA.

A dictionary of Crystallographic Information File (CIF) data items to describe both the macromolecular crystallographic experiment and the structural results of the crystallographic experiment has been developed. A CIF contains crystallographic data stored in a subset of the STAR format (S. R. Hall (1991). *J. Chem. Information* **31**, 326-333). The CIF format is designed to facilitate archiving and exchange of crystallographic data in a standardized manner, with the particular goal of automating the electronic publication of crystallographic results.

The International Union of Crystallography (IUCr) has sponsored this initiative, and is actively encouraging the adoption of CIF as a standard for the field. A core dictionary of data names sufficient to describe the small molecule crystallographic experiment (S. R. Hall, F. H. Allen, and I. D. Brown (1991). *Acta Cryst.* **A47**, 655-685) was adopted by the IUCr at the 1990 International Congress in Bordeaux.