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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 XVIIIth IUCr congress.


The structures of rare-earth polychalcogenides (which contain covalently bound $X_2^+$, $X = S$, 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 polychalcogenides (imperfect chalcogen-deficient phases often realized with formulae including integer coefficients) made by workers from France (Flahaut J. and Laruelle P., Freq. Sci. and Technol. Rare Earths, vol. 3, Pergamon Press, 1968, pp. 149-208), Moscow (A.A. Eliseev, G.M. Kuz'micheva, Iogi nauki i tekhniki. VINITI, Ser. Kristallografiiya, 1976, v.11, p.95-131) and Siberia (J.G. Vanil'eva Doktorskaya Disserataziya, 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$_2$As. 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-detemined 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 polyoxides, and the imperfection of the anionic sublattice have been pointed out.

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OCM-18.02.03 ACTA CRYSTALLOGRAPHICA, SECTION D.

By Jenny P. Glazer, 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 in the field of crystallography. The first issue contained papers from the conference on Methods of Phasing in Macromolecular Crystallography, held in April 1992. The second issue contains 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 structure 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

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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), was initiated and implemented by 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 application of SR to scientific disciplines. It is clear that the provision of such a journal will not only enhance the cross-fertilization of ideas between scientific disciplines, but also allow the rapid transfer of information between communities specializing in the use of different parts of the electromagnetic spectrum.

A distinguished editorial board has been assembled covering all aspects of SR. The details of the proposal was approved by the Executive Committee of the IUCr in August 1992.
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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-18.02.04 Journal 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 editors, who individually arrange for at least two referees. Each member of the team is responsible in the end for acceptance or rejection of the 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 are being 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 we 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.

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 directly to the Technical Editor and various checks are carried out on each structure (these checks include geometry and previous publications) 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.

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 further machine on a 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: portable 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 licence holders. The validated corrected data may then be processed 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; this done in the case of Revised 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 crystallography community the structural data stored in machine-readable form.

OCM-18.02.07 The Macromolecular CIF Dictionary.
By Keith D. Watson*, 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 5000, 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, P. H. Allen, and I. D. Brown (1991), Acta Cryst. A47, 659-686) was adopted by the IUCr at the 1990 International Congress in Bordeaux.