

18-Data Bases and Communications

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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 XVth IUCr Congress.

PS-18.01.12 CRYSTAL-CHEMICAL ANALYSIS OF STRUCTURES OF RARE-EARTH POLYCHALCOGENIDES. By S.A. Magarill*, N.V. Podberezhskaya, 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 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. kristalokhimiya, 1976, v.11, p.95-131) and Siberia (I.G. Vasil'eva Doktorskaya Dissertatsiya, 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-18.02.01 PLANS 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

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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). 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,