

dimensional graphic structure display is also implemented for organic substances. All search criteria can be integrated with Boolean operators, including AND, OR and NOT, providing considerable flexibility in searches. For example, the user can search for substances containing only elements "Si" AND "O"; the user can also search for all substances containing "Si" OR "O".

The PCPDFWIN program has been developed as a Microsoft Windows 3.1 application. It runs on an Intel 386 (or above) based computer and requires at least 4 MB RAM, 6 MB hard disk space, a mouse, Microsoft Extensions and a PDF2 database on CD-ROM.

PS-18.01.09 SEQUENCE DEPENDENCE OF NON-PLANARITY OF PEPTIDES, AND EFFECT ON SECONDARY STRUCTURES. By N. Sukumar and Vasantha Pattabhi*, Department of Crystallography and Biophysics, University of Madras, Madras 600 025, India.

Non-planarity of peptides has been predicted from quantum chemical theory, and has also been observed frequently in crystal structures. A systematic study of this phenomenon is expected to give informations on the flexibility of peptide plane, and also help in model-building studies.

Class 48 of the Cambridge Crystallographic Data Base has been surveyed with this aim in mind. The analysis shows that deviations from planarity ($\Delta\omega$) range from 0° to 20° depending on the sequence. In general, deviations for Ser, Asn, Lys and His are very low in contrast with those for Phe, Pro and Leu. If Gly precedes or succeeds any residue, the deviation from planarity is significant. A linear correlation between molecular weight and torsion angle ω has been observed, indicating that deviations from planarity are involved to avoid steric interactions, and in some cases to enable hydrogen-bond formation. The analysis was extended to study the correlation between $\Delta\omega$ and the secondary structural features. The following observations have been made from the study. (i) The direction of the deviation, and the handedness of the helix seem to be correlated. (ii) In the case of peptides adopting bent conformation, the $\Delta\omega$ values are uniformly small. (iii) No such correlation was seen in the case of extended structures.

PS-18.01.10 COMPUTER-AIDED DESIGN OF NON-ISOMORPHIC HETEROCOMPOSITIONS. By A.N. Efimov, A.O. Lebedev*, Ioffe Physical-Technical Institute, St. Petersburg, Russia.

The correct choice of substrate compound and of its crystallographic orientation is of great importance for epitaxial growth of HTS. The following conditions concerning the substrate must be verified: compatibility of the substrate material with the physico-chemical conditions of growth and subsequent processing; absence of chemical interaction between substrate material and HTS; geometrical match with HTS-structure as a prerequisite for creating perfect single crystalline epitaxial layers (taking into account the temperature dependence of lattice parameters); physical properties needed for the concrete device application (for instance the small dielectric loss for HF- and UHF-range); low cost of starting materials and possibilities for industrial manufacturing of substrates. The optimal design of heterocompositions is nearly impossible without computers due to the number of compounds, and due to the number of requirements to be taken into account.

The present computer-aided design package for heterocompositions includes the following program units: an analysis of metric match

based on the coincidence site lattice concept and a modified theoretico-numerical algorithm (Santoro A., Mighell A.D., Acta Crystallogr., 1973, A29, 169-175); an analysis of structure defects connected with the symmetry aspects of genetic relations between the substrate and layer structures; computer graphics for visualization of the interfacial region.

The data base contains the following information: crystal-geometrical parameters: structure type and unit-cell constants; dependence of these parameters on temperature including the temperatures and types of phase transformations; dielectric constants; peculiarities of phase diagrams; data source.

PS-18.01.11 A UNIVERSAL FILE FORMAT FOR POWDER DIFFRACTION DATA ARCHIVE AND INTERCHANGE: THE IUCR CRYSTALLOGRAPHIC INFORMATION FILE FORMAT. By B.H. Toby, Air Products & Chemicals Inc., 7201 Hamilton Blvd, Allentown, PA 18195, USA, J.I. Langford*, School of Physics & Space Research, University of Birmingham, Birmingham B15 2TT, UK and S.R. Hall, Crystallography Centre, University of WA, Nedlands 6009, Australia.

Powder diffraction data definitions have been devised for use with the Crystallographic Information File (CIF) facility for data storage and exchange. These will permit the ready exchange of raw and processed powder data generated by diffractometers of every type - commercial sealed-tube X-ray instruments, single-wavelength synchrotron and neutron systems and energy-dispersive or time-of-flight experiments.

CIF has been developed by the IUCr for the storage of crystallographic data which range from measured intensities to structural diagrams and text in a form suitable for publication (Hall et al., Acta Cryst. A47, 655-685). CIF is composed of ASCII characters which may be edited in the normal way or transmitted via international networks (eg E-mail or FTP). A CIF is completely self-descriptive, in that data items are identified by unique tags, known as data names, which may be defined locally or globally. Global data items (ie those used outside the local environment) are carefully defined in a CIF data-name directory that is also stored electronically in a CIF-like format.

Powder diffraction data are usually measured by means of a computer-controlled diffractometer, or obtained from film by a densitometer, and are stored in a data-file format specific to the instrument used. Typically, these data are then processed by using computer programs modified to use data with the local format. If the data are to be published or archived, the diffraction pattern will often be reduced to a table of peak position and intensity values. Apart from the requirement to standardise the data-processing software, the need for a global exchange of unprocessed powder diffraction data is increasing. This need arises because of the use of total-pattern methods for

- (1) crystalline phase identification and quantification,
- (2) ab initio structure determination,
- (3) structure refinement,
- (4) studies of microstructure and
- (5) characterisation of materials with limited ordering (eg polymers and clays, where the diffraction pattern cannot adequately be represented by a set of peak parameters).

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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. Podbereskaya, 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,