correspondence with the authors. In a few cases the problems are not resolved and such entries are either flagged or omitted.

The MDF is used to check the data appearing in the Metals section of Structure Reports and also to calculate peak intensity (i.e. full profile) powder patterns for the Powder Data File (PDF) published by the Joint Committee on Powder Diffraction Standards. In addition the relevant current data on metals are sent to Crystal Data. It is planned that patterns now missing from the PDF or those requiring checking will be calculated from the structural data when they are available.

In addition to the major routines which calculate interatomic distances and powder patterns there are also routines which can display the Frank-Kasper domains, the coordination polyhedra for individual atoms or the bonds between an atom and its neighbours or combinations of these. The displays can be produced in stereo, and rotated and copied onto the line-printer. There are also search routines to find specific compounds or compounds containing various elements or combinations of elements. Indices sorted by elemental type or by structure code can be prepared and are routinely used for searching the file.

At present the file is available for private use only but a joint program is now underway to make the file publicly available through the facilities of the Canada Institute for Scientific and Technical Information (CISTI). The file in its present form will be demonstrated at the Congress.

19.X-08 THE PROTEIN DATA BANK*. By Thomas F. Koetzle, Enrique E. Abola and Frances C. Bernstein, Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973, USA

The Protein Data Bank (F. C. Bernstein, T. F. Koetzle, G. J. B. Williams, E. F. Meyer, M. D. Brice, J. R. Rodgers, O. Kennard, T. Shimanouchi, and M. Tasumi, J. Mol. Biol. (1977) 112, 535) is a computer-based archival file for structural data on biological macromolecules. The Bank presently contains atomic coordinates for more than 100 distinct molecules; RNA, DNA and polysaccharide structures are represented as well as proteins. Structure factors and phase information have been deposited for some of these studies. Bibliographic citations are included for structures when coordinates are not yet available. Data are distributed upon request from Brookhaven and centers in Cambridge, England; Osaka, Japan; and Clayton, Victoria Australia. A number of portable computer programs have been developed to enable users to extract useful information from the file.

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19.X-09 JCPDS--INTERNATIONAL CENTRE FOR DIFFRACTION DATA. By C. R. Hubbard, National Bureau of Standards, Washington, DC, USA and G. J. McCarthy, North Dakota State University, Fargo, ND, USA.

The JCPDS--International Centre for Diffraction (ICDD) is the publisher of the Powder Diffraction File (PDF). The PDF is used for identification and characterization of crystalline phases by reference to the characteristic x-ray powder diffraction pattern. The JCPDS--ICDD consists of a permanent staff based at Swarthmore, PA, and at the National Bureau of Standards, plus a voluntary organization of internationally known scientists who act as advisors. The PDF is published in a wide variety of forms and in several subsets. The primary product, a compendium of powder diffraction patterns tabulated in numerical form, is published yearly on 3" x 5" index cards in sets of approximately 2000 patterns. Today nearly 35000 cards comprise the entire PDF. The card images are also published on microfiche and in books. These card images contain (1) compound name and formula, (2) numerical pattern data, (3) a quality mark, (4) the PDF code number, (5) reference, (6) cell parameters, space group and density, (7) method of data acquisition, (8) other information characterizing the compounds, and (9) editorial comments. Along with the data cards three search manuals are published which enable a user to locate a pattern. They are the Alphabetical Index, the Hanawalt Method Search Manual and the Fink Method Search Manual.

Because of the size of the PDF, the data base has been divided into Inorganic and Organic & Organometallic subsets to assist in identification procedures and to serve the needs of specialized groups. In addition, subfiles of Minerals, Metals and Alloys, Common Phases, and NBS Patterns exist. These subfiles, except for the Common Phases, are published as card images in bound books along with appropriate search manuals. The Common Phases subfile is published only as a search manual supplement to the PDF itself.

An increasingly important method to assist in identification is computer search/match procedures. The JCPDS leases several computer readable forms of the file containing data items (1) - (4), for use with a variety of maxi and mini computer systems. The PDF can also be searched on two time sharing networks: Diffraction Data Tele Search of University Computing Co. and the Powder Diffraction Search Match (PDSM) component of the Chemical Information System (CIS). CIS provides cross linking between a large number of other data bases covering such areas as toxicology, mass spectra, Crystal Data, and Molecular Structure and Dimensions. The introduction of automated powder diffractometer systems incorporating the full file on magnetic disks is a major development in methods to assist users of the file.

Computer aided editorial evaluation is now being used to upgrade the reliability and quality of data entering the file. The principal program for this evaluation and data base building is NBS*AIDS80. The JCPDS--ICDD is extending their use of this program to evaluate all the data entering the file. Methods to reevaluate and, if necessary, correct previously published data are being explored. The evaluation of an entry entering the file includes those tests performed for a Crystal Data entry plus tests unique to indexed powder patterns. Included are checks on systematic absences, agreement between observed and calculated two-theta, calculation of M(20) and F(N) figures-of-merit, (de Wolff, J. Appl. Cryst., 1, 108, 1968; Smith and Snyder, J. Appl. Cryst., 12, 60, 1979) and a test for the presence of systematic errors as a function of two-theta (Young, Ann. Math. Stat., Vol. XII, 293, 1941).