19.X-05 THE NBS CRYSTAL DATA FILE. By Alan D. Mighell and Judith K. Stalick, Center for Materials Science, National Bureau of Standards, Washington, DC 20234.

The NBS Crystal Data File is designed for the characterization of solid-state materials. As the lattice parameters are highly diagnostic for a given compound, the file in conjunction with modern diffractometry offers an excellent way to identify unknown substances.

The file contains chemical and crystallographic data on approximately 60,000 substances of all types. It is expanding at the rate of about 5,000 compounds per year. For each compound, the following data items are included: the chemical name and formula, density, reduced cell, space group, space group number, and the literature reference. The data are obtained from the original literature by the NBS Crystal Data Center, by independent abstractors, and by the following cooperating data centers: Cambridge Crystallographic Data Centre, Inorganic Structural Data Center, Metals Data Center, and the JCPDS--International Centre for Diffraction Data.

To systematically transform and evaluate the entries for the file, a program called NBS*AIDS80 (available for distribution) has been developed. Program functions include determination of standard cells and space groups, assignment of space group numbers, determination of metric symmetry and checking of the data for consistency. In applying the program, it has been noted that full structure determinations are sometimes inadvertently carried out more than once, that symmetry (especially rhombohedral) is often missed, and that cells are sometimes not transformed correctly. Routine use of the program to analyze the data prior to publication would help to reduce such errors.

The data in the file are made available to the scientific community in several ways. The principal publication is Crystal Data Determinative Tables, in which substances are ordered by crystal system and unit cell ratios. This arrangement groups isostructural materials together. A new publication, Crystallochemical Identification Tables, is being prepared in which the data are sorted on the reduced cell parameters and like lattices are grouped together. To identify an unknown, one only needs to determine a primitive cell of the lattice, reduce this cell, and check the tables for a match. In addition to printed publications, a computer file on magnetic tape may be purchased from the NBS Office of Standard Reference Data; the file may also be searched on line through the Chemical Information System.

Projected future applications of the file include: 1) extensive use of the file in automated identification systems in which both cell determination and the file search are under computer control; 2) wider use of the file by the chemical community for the routine characterization of materials; 3) use of the file in conjunction with the powder diffraction file; 4) research projects carried out on the data within the file. Many lattice related research projects can be undertaken. One can systematically analyze such structural and lattice-related phenomena as: symmetry, coincidence-site lattices, derivative lattices, space group frequencies, and twinning. Two research projects that demonstrate the basic importance of the metric lattice in crystallography will be discussed.

19.X-06 CAMBRIDGE CRYSTALLOGRAPHIC DATABASE. Olga Kennard, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, U.K.

The Cambridge Crystallographic Database is well known to structural crystallographers and is available through Affiliated Data Centres in some 21 countries. It can be searched by a variety of program systems; a recent advance is a mini-computer version of the Cambridge system developed by R. E. Rosenfield for a PDP11/45. This opens up the possibility of direct use of the database on some of the larger diffractometer systems, which will be of importance in utilizing methods of structure solution requiring accurate molecular geometry of substructural fragments.

The past few years have seen an increasing use of the database, primarily for reviews and research projects. The database itself has been upgraded and the most recent release (January 1981) contains only 3% error-sets. There are, however, a substantial number of entries without numeric data. The question of even closer interaction with the scientific community and Journal Editors, with a view to maintaining and improving database content, will be discussed.

The major technical innovation during the past year has been the introduction of digitized chemical structural diagrams, with implications for new types of printed publications. Future plans include the creation of a new 'search' file and the views of the audience will be sought on the proposed contents of such a file, and on any new innovations which might improve database utility.

19.X-07 THE METAL DATA FILE. L.D. Calvert. Chemistry Division, National Research Council of Canada, Ottawa, Canada, K1A 0R9.

The Metal Data File (MDF) is a computer-based file in the Chemistry Division of the National Research Council of Canada. It contains the relevant data for the ~4800 intermetallic compounds with structures which have been refined in the period 1913-1979; 1980 data are being compiled and processed. In addition assigned structures amounting to a total of about 2900 have been recorded since 1975. The file is resident on a PDP-8e and is operated by programs written in Fortran. The file structure is similar to that of the Cambridge Crystallographic Database. Strong emphasis has been placed on data integrity and evaluation. Input is kept simple by using the general space group interpreting routine of A.C. Larson (Acta Cryst. (1969), A25, S1) which operates directly on the Hermann-Mauguin symbol and by using free format, numerical data input which is later formatted under program control. Data are verified by diagnostic programs which check for transcription errors and for data inconsistencies. The formula is computed from the structural parameters and compared with that given by the authors; the cell volume is compared with that expected for metallic cubic close packing; the density and volume per atom are also calculated. The major check is by interatomic distances which are selected by the criterion of Frank and Kasper (Acta Cryst. (1958) 11, 184), with appropriate allowance for atomic radii and cell volumes, and then calculated and compared with the sum of atomic radii as well as the distances given by the authors; unusual values are flagged. It has been found that up to about 25% of the original papers contain numerical errors, most of which are quite minor, but a few percent are significant. Most of these can be corrected either by an analysis of the data given or by