19.X-11 CENTRALIZED CHECKING OF MANUSCRIPTS. By M H Dacombe, International Union of Crystallography, 5 Abbey Square, Chester, England.

More than 1000 manuscripts are submitted to Acta Crystallographica and Journal of Applied Crystallography each year. It is planned that on receipt of a manuscript Co-editors will directly send one copy to the Technical Editor's office. This copy will then be checked to ensure that all the requirements of the Commission on Journals have been met. Additionally the atomic coordinates and crystal data for papers reporting structures of organic or organometallic compounds will be keyed into a word processor and transferred to the Cambridge Structural Data Centre on floppy disc where (1) bond distances will be recalculated and compared with those reported and (2) valencies will be compared with standard values. The results of both checking procedures will be sent to the Co-editor to evaluate in conjunction with the usual referees' report. This will mean that (1) the accuracy of structures reported will be checked by Cambridge before publication, (2) the need for repeated re-keying of atomic coordinates and other data both by Cambridge and the printer (who will also be able to use material keyed in Chester) will be avoided, (3) the Co-editors' often considerable workload will be reduced. Results of trials recently carried out to establish the feasibility of this planned procedure are discussed. Possible checking of inorganic structures by the Inorganic Crystal Structure Data Bank in Karlsruhe is also covered.

19.X-12 THE NEED TO STANDARDIZE STRUCTURES TO RECOGNIZE STRUCTURAL RELATIONSHIPS. By E. Parthé, Laboratoire de Cristallographie aux Rayons X, Université de Genève, 24 quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland.

Due to the lack of a standard for the description of crystal structures, the unit cells and the positional atom coordinates of two identical structures may not show any correspondence whatsoever. There are numerous examples in the literature where identical crystal structures were not recognized as such but were considered as having different structure types.

To remedy this undesirable situation a standard description of crystal structure data was proposed (Parthé, E. & Gelato, L.M., Acta Cryst., 1984, A40, 169-183 and Acta Cryst., 1985, A41, 142-151) which is based on the symmetry of the atom arrangement. To make a selection between possible structure descriptions with different origins, rotated or inverted coordinate systems, a standardization parameter is calculated. The structure description with the smallest value of the standardization parameter is taken as standardized structure description. With the completion of the STRUCTURE TIDY program (Gelato, L.M. & Parthé, E., J.Appl.Cryst., 1987, 20, xxx-xxx) the standardization is now an easy computer routine.

The most elementary use of standardized data is for the comparison of the results of different determinations of the same structure. For example, of the four 1984 data sets on $Nd_2Fe_{14}B$, without standardization it is not immediatly evident that only three are identical.

Without standardization the occupied Wyckoff positions can not be used for classification purposes. They may be different with a different choice of origin. However for standardized data a Wyckoff sequence can be stated (sequence of letters of occupied Wyckoff positions; each letter followed by a number (if > 1) which indicates how often this Wyckoff position is occupied). Two different structures with same space group and same Wyckoff sequence are isopointal. Isopointal structures with similar axial ratios, angles between the axes and values of the corresponding atomic positional parameters are isotypic.

Standardized structure data are thus useful to recognize possible isotypism, such as found with Th_6Cd_7 and $W_6(Fe,Si)_7$ having Wyckoff sequence Pbam-ih^{2}g^{2}a).

It is hoped that in the future structure data would be published in standardized form. There may be reasons not to do so but they are rare.

19.X-13 HANDLING OF CRYSTALLOGRAPHIC INFORMATION NOW AND IN THE FUTURE. by G.Bergerhoff, Institute for Inorganic Chemistry, University of Bonn, FRG.

Any scientific result has effect only if it comes to the knowledge of the scientific community. Then we all stand on the shoulders of anybody else (Paul Ewald). The classical means to distribute new results are printed journals, annual reports, handbooks, etc. David Watson collected all sources in the field of Crystallography in a CODATA Bulletin.

But progress in theory and instrumentation has increased the mass of information so much that new means have to be developed to overcome the oppressive situation. You all know the computer is the instrument which should help. But to bring it to an effective action we are forced to analyse - and to solve the problems of information handling much better than before. There are problems arising from the special structure of our science, technical problems, psychological and political problems.

The first group includes e.g. the meaning of words (structure, accuracy, inorganic), the presentation of data (unit cell dimensions, symmetry notation), the archival value of measured data (observed structure amplitudes, temperature factors).

The second group is tightly connected to the development of the computer (storage capacity, telecommunication for retrieval a n d input, CD-ROM, graphics).

Human behaviour determines the acceptibility of