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

computerized information. The user will learn to appreciate immediate and complete information, correct data, easy calculation of derived data, etc.

Because science is international all development will involve international problems (grown structure of data input, access to databases, etc.). The IUCr should be the appropriate forum to develop solutions in international cooperation.

19.2-1 TEACHING CRYSTALLOGRAPHY USING COMPUTER GRAPHICS. By T. Sakurai,K.Kobayashi*, T.Horiki*,K.Naitou**and M.Furukawa**. Faculty of Education, Shinshu University, Nagano 380 Japan;*Insti. Phys. Chem. Res., Wako, Saitama 351 Japan;**FACOM-HITAC Ltd. Chiyoda, Tokyo 102 Japan.

Acomputer graphics system for teaching crystallography was developed. The system has many features for ordinary molecular graphics. Two main functions are especially useful for teaching space group symmetry and crystal morphology. The system contains information on the spacial arrangement of the symmetry elements in the International Tables. When the lattice parameters and the name of the space group are given, the system generates three dimensional graphic image of the symmetry elements in the unit cell with the actual lattice parameters. When a symmetry element is picked up by the tablet, the symmetry related atoms are generated. The system allows self-study of symmetry operation in a three dimensional crystalline space.

The crystal habit, which depends on growth conditions can be displayed by inputting the lattice parameters, the indices of the planes, and the growth rate of each plane. The change of habit with time can be traced on the display.

The system consists of COMTEC-DS301B 3D-display backed up with FACOM M-380 Computer. The program is written in FORTRAN with Graphic software package GRIP-II.

19.2-2 TEACHING AIDS FOR CRYSTALLOGRAPHY. By Colin H.L. Kennard, Department of Chemistry, University of Queensland, Brisbane, Q. 4067, Australia.

A number of locally developed crystallographic teaching aids will be exhibited. These include an electronic blackboard software package written in Applesoft BASIC for an Apple][that illustrates the phase problem with the combination of two reflections 1 0 0 and 2 0 0, and calculates a one dimensional electron density synthesis with different combinations of phases; structure factor calculations to show systematic absences when some sort of centering occurs in a cell; the representation of two block atoms by a Fourier series. A compiled BASIC program for an IBM PC type computer allows a simple two dimensional structure determination (four atoms in an asymmetric cell, space group *Pmna*, h 0 l given) to be determined in a laboratory period. The program calculates a Patterson synthesis, and does a structure factor calculation with a subsequent electron density map.

19.2-3 SOME PROGRAMS FOR MICROCOMPUTERS. By H. Schenk, R.A.J. Driessen, B.O.Loopstra, P. Molhoek, W.J. Urban and M. Zoutberg, Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands.

In recent years our group has developed a number of crystallographic programs for micro computers, which in our opinion enrich the possibilities of crystallographic teaching. A few are in the field of crystallographic methods, others illustrate the use of crystallographic data. In this abstract two of them are presented briefly; in the Computer Lab of this conference we hope to present a few more. All programs will be available as shareware. In some cases we plan to convert the programs into tools for secondary school teaching in Holland.

Direct Methods are still of growing importance as a tool of solving crystal structures from single crystal data. However, most program systems for Direct Methods are not very transparant, if not completely black boxes. Therefore we developed a program system for micros in which the students are guided to use the symbolic addition method. The main task of the computer is to teach and to do the administration, while the students learn to take the essential decisions in a phase extension process.

Present day homscomputers such as the C64 have good graphics possibilities and therefore we converted them into molecule graphics subsystems. Our interactive graphic program PLUIT provides the following options: to display a molecule as stick, ball and stick or ball model, in mono-, or stereo-view, with or without labels. The model can be rotated, a least squares view can be calculated and also a minimum overlap view. Bond lengths and angles can be calculated and also Newman projections which give graphically all dihedral angles around a particular bond. The view matrix is that of PLUTO and can be displayed at any moment. Hard copy images of molecules and of Newman projections can be made by the normal cheap printers in graphic mode. Also real-time rotations are possible and structure data can be read from a host computer.