

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.

A computer 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 transparent, 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 homecomputers 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.