18. 3–1 ENERGY MINIMIZATION ON A CRAY-1:USE OF A VECTOR MAINFRAME. B.E. Hingerty, Health and Safety Research Division,Oak Ridge National Laboratory,P.O. Box X,Oak Ridge ,TN 37830 USA.

Semi-empirical conformational energy calculations have traditionally been carried out on either mainframe computers such as a CYBER or IBM3033 or dedicated laboratory computers such as a VAX11/780 or PDP-11/70. Because of the many trials necessary to search for the global minimum (1000 or more) exceedingly long computer time has been required. On traditional mainframes the cost has been prohibitive, while the laboratory computers can require up to 2 months to complete 1000 trials. The use of array processors to speed up computations on laboratory computers has been reported.[1] In recent years vector mainframes such as a CRAY-1 have been developed, which promise considerable savings in computer time by the use of parallel processing.
A generous grant of computer time on a CRAY-1 supercomputer has been obtained from the U.S. Dept. of Energy(DOE) in order to facilitate the computations for carcinogen-modified DNA. A sample calculation for the (+)syn adduct of benz[a]pyrene diol epoxide with dCpdG at the N2 of guanine has been used. This representative calculation took approximately 1 hr. on a PDP-11/70 under FORTRAN77 and RSX-11M-PLUS. Approximately 20 min. CPU time was required for a CYBER. Initially 108 sec. was the runtime on theCRAY-1 using unmodified code. After vectorization of the energy calculation only 13.1 sec was required. Additional improvements are expected and are in progress.

1)Pottle,C.,Pottle,M.S.,Tuttle,R.W.,Kinch,R.J.and Scheraga,H.A.,J. Comp. Chem. 1,46-58(1980)

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18. 4–1 *APPLECRYST 83, A SET OF CRYSTALLOGRAPHIC PROGRAMS FOR AN APPLE][COMPUTER.* By Colin H.L. Kennard, Department of Chemistry, University of Queensland, Brisbane, Q. 4067 Australia

This set has been written in Applesoft BASIC for the Apple][plus computer. It contains a menu which allows selection of general X-ray programs, [create/editing data file/unit cell parameters, atomic coordinates; bond distances and angles; torsion angles; mean planes through a set of atoms; and displaying a molecule in any direction on the screen or appropriate dot matrix printer]; special X-ray programs, [crystal data and percentage composition; d spacings for powder patterns; conversion of hexagonal to rhombohedral cell and vice versa; least squares refinement of cell parameters; analysis of a powder spectrum] and teaching programs, [simulations to indicate effect of centering on systematic absences, phase problem, direct methods, effect of thermal parameters and scattering factors on structure factors; and structure determination]. The set is continually being developed, but even at the present time offers a useful package for those interested in working with crystallographic data and with limited computing facilities. Disk copies (DOS 3.3) are available from the author, free with a disk and $US10 without a disk.

18. 4–2 A MICROCOMPUTER BASED CRYSTALLOGRAPHIC SYSTEM Peter S. White, Department of Chemistry, University of New Brunswick, Fredericton, New Brunswick, Canada.

The use of in-house minicomputer systems for the solution and refinement of crystal structures is now common-place. Unfortunately, most mini's have 16 bit word-lengths which result in restricted address spaces requiring extensive overlaying of programs and restricted array sizes. One alternative the VAX-type of large mini's is quite expensive, another is the current generation of micro-computers based on 16/32 bit chips such as the 68000 and the 16032. This paper will discuss the use of a 68000 based machine which is currently being used for routine crystallographic work.

The computer system is a Wicat Systems WS-150 microcomputer with 768 Kbytes of memory, a 10 Mbyte Winchester disk and a 616 Kbyte floppy disk drive, housed in a desk-top terminal which supports medium resolution graphics. In addition, there is a second terminal, a printer, a plotter and a Sky-FFP floating point processor. The operating system is similar to UNIX and supports both multiple users and multiple tasks. The programs currently in use are all written in either Fortran-77 or "C". A full set of standard crystallographic programs have been implemented including the MULTAN-80 system, SHELX-76, ORTEP-II, and PLUTO. These are all virtually the same as the main-frame versions.

The speed of a system is difficult to measure, but Sheldrick's benchmark gives a time of 130 secs, which is comparable to a number of mini-computers commonly used for such work. A better measure of performance is the fact that the system is currently supporting two active crystallographers. Details of the system will be presented, including a custom user interface and performance measurements. Methods of optimising the performance of crystallographic programs on such a system will also be discussed.

18. 4–3 INDEXING OSCILLATING-CRYSTAL PHOTOGRAPH PROCEEDED AS A DIALOGUE WITH COMPUTER. By V.I. Ivanov, V.Sh. Shekhtman, Solid State Physics Institute of the USSR Academy of Sciences, 142432 Chernogolovka, USSR.

The present paper describes the algorithm designed for solving the inverse task of the diffraction oscillating-crystal method, i.e. for determining indices of each reflection from its coordinates measured in the oscillating-crystal photograph. In the X-ray diffraction analysis, where one has to deal with the real structure of crystals undergoing phase transitions, the study and interpretation of oscillating-crystal photographs using various geometrical constructions are labour-consuming and not always single-valued. This has predetermined the design of an algorithm for analytical computation.

Let's consider the main features of the program proposed. It is assumed that the X-ray photograph is produced in the ordinary way when the crystal parameters, the indices of the direction coincident with the rotation axis [U,V,W] and the oscillation angle range are known. Then the operation of the program written as a dialogue with the computer can be conditionally divided into five stages.
1. The coordinates X_i and Y_i for each reflection are set into the computer and referred to the coordinate system of the film. Corrections are made for inaccuracy in the crystal setting. These corrections are refined by the least-squares technique (LST) with allowance for the fact that ΔX_i and ΔY_i change along the corresponding Bernal lines with H_i^{exp}. Then the identity period along the oscillation

axis is calculated by LST.
2. Search for a "reference" reflection indices. For the reflection given by an experimentor the computer will choose those indices for which $\Delta H_{\perp}^{i}$ has the least value. Considering this reflection to be situated on the Ewald sphere, we find the coordinates of the centre point of the sphere and respectively, the coordinates of spheres separated by $\pm\Delta\varphi$.
3. Indexing is carried out by comparing $H_{\perp}^{exp}$ and $H_{\perp}^{calc}$ with the criteria $\Delta H_{\perp} = min$, and the signs of indices do not contravene those of X and Y in the X-ray photograph with due regard for the position of the Ewald spheres in the reciprocal space.
4. Computations of the coordinates X_i and Y_i of the computer-simulated X-ray photograph and the discrepancy factor.
5. Results of computations can be plotted or displayed and compared with experimental ones. The lattice parameters are refined by LST. The following information can be presented on the "TV" screen in one of its quadrants or on the whole of the screen: the view of the experimental or model X-ray photograph, the reciprocal lattice net of any layer line with the Ewald sphere position and that of the reflections on the given net.

The program contains 1500 statements. The time needed for the computation of an index is 1 sec using a "SM-3" computer of the third generation (~150000 operations/sec).

18.4–4 A MINICOMPUTER PROGRAM FOR THE AUTOMATIC ANALYSIS OF PATTERSON FUNCTIONS. By T.I. Malinovsky, I.F. Burshtein, and V.S. Fundamensky, Institute of Applied Physics, Academy of Sciences MSSR, Kishinev NPO "Burevestnic", Leningrad, USSR

Nearly all crystallographic program systems for use on minicomputers include programs for structure analysis by the direct method, but lack a program to analyse the Patterson function. To eliminate this deficiency, we have written a program for automatic interpretation of the interatomic vectors, compatible with the program systems XTL (NOVA-1200) and RESTAN (SM-4 and M-6000). The program algorithm is applicable to the symmetries of Patterson functions in the triclinic, monoclinic and orthorhombic systems. Essential information about the space group symmetry, unit cell parameters, and the coordinates of the peaks in the Patterson function are read automatically from the appropriate files created by the other programs in the system. Based on this information, the present program produces the atomic coordinates and interatomic distances of a molecular fragment, which in some cases may comprise more than 50% of the structure. It is possible to proceed automatically from this stage to calculation of an electron density map. Such a program may be included in any program system for structure analysis on minicomputers. Some examples of different complexity will be demonstrated.

18.5–1 USE OF THE SERC INTERACTIVE COMPUTING FACILITY FOR MOLECULAR GRAPHICS AND MINERALOGICAL STUDIES

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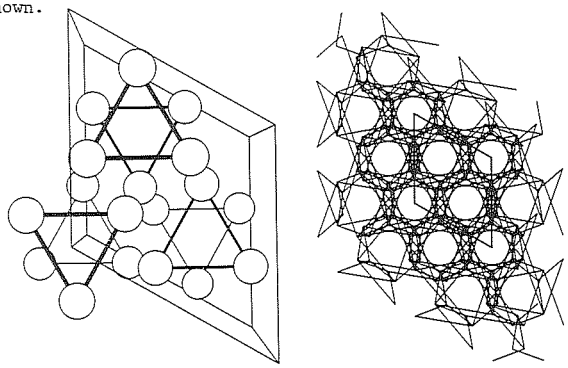
Members of the Computing Division of the Rutherford Appleton Laboratory set up and maintain a network of multi-user minicomputers for interactive working. Users of the network have access to many different types of output device, including local pen plotters and the precision III FR80 microfilm recorder. The molecular drawing program PLUTO78 has been mounted on the network, and many enhancements made in order to bring a powerful tool for molecular and mineral display to a large, geographically widely distributed research community. Several other display programs are currently being prepared, and sample output from these will be shown.



18.5–2 COMPUTER GRAPHICS OF POLYHEDRAL PACKINGS. By R. Norrestam, Chemistry Dept. B, Technical University of Denmark, DK-2800 Lyngby, Denmark.

The packing of coordination polyhedra is often used to visualize inorganic crystal structures. Frequently, pictures of such packings are simply photographs of models constructed by assembling idealized colored plastic polyhedra (see e.g. S.Andersson, Acta Cryst. (1980) B36, 2513). With the use of a high resolution raster display it is possible to obtain such pictures of comparable quality and showing the correct polyhedral geometry.
A computer program, POLY, for applying color raster graphics has been developed and some examples of the results from this program will be described. POLY is written in standard FORTRAN language, with a few supplementary color plotting routines from the UNIRAS software system.