

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. 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 super-computer 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 dCpG 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 the CRAY-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 II 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 II 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 PROCESSED 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