

**Abstract**

A highly interactive program system for carrying out crystal structure analyses on a dedicated 32-bit computer has been developed, with emphasis on suitability for inexpensive hardware. The system includes a new SHELX-compatible version of ORTEP that can be operated from an interactive graphics terminal by a menu of easily-usable commands.

**Purpose**

The experimental requirements of modern crystal structure analysis are met by commercially available automatic diffractometers. However, to perform the subsequent calculations without significant compromises demands the power of a mainframe computer. The alternative, a dedicated system, has traditionally been based on the 16-bit minicomputer (see, for example, Gabe, 1980), which is easier to use but its architectural limitations often demand complicated modifications of the mainframe algorithms.

32-bit mini- and microcomputers capable of carrying out all calculations needed by the modern structure analyst are commercially available and will soon be an economic purchase for most crystallographic laboratories. One might even foresee the time when personal computers will have the capability for this application. The purpose of our present work is to further the development of a new generation of crystallographic software to realize the full potential of the new computer hardware.

**Strategy**

The main requirement is for interactive operation of the programs. The file organization has therefore been designed to facilitate real-time running, in which instructions are typed while programs are active, so that command input is logically distinct from crystallographic data and from reflection data. At appropriate points in the run each program displays a menu that indicates user-selectable options. One advantage of this approach is that the program provides its own documentation, which is updated if the program is altered. It is thus possible to run the system without frequent reference to printed documentation. To provide for batch operation, program command files can be set up.

Crystallographic data are held in a free-format character file, which can readily be originated and manipulated by the operating system's screen editor. This is called the 'model file', since it contains all the parameters (space group, unit cell, coordinates, etc.) of the crystal model. Reflection data are in a packed binary file, for optimum disc space utilization and computational efficiency and precision. There is also a databank file containing a library of scattering factors, anomalous dispersion components, absorption coefficients, covalent and van der Waals radii for all important elements. Reference to an atom in standard chemical nomenclature in the model file, e.g. As(I), automatically forces loading of the appropriate information from the databank for (in this case) arsenic.

Hall, Stewart & Munn (1980) have given an excellent account of the possible strategies for crystallographic program systems. In the GX System independent programs communicate *via* a standard set of data files, principally the model and reflection files. Coding is simplified by avoiding the use of dynamic store allocation within programs. The total size of the system is reduced by making as much use as possible of the machine's operating system for 'housekeeping' processes such as editing the crystal model, control of the overall calculation sequence, and file management. This does not lead to problems of portability since the programs can always be installed and run in the best way to suit local conditions.

The advantages of this type of organization are: ease of installation; easy addition of new programs (routines for reading and writing the model file into and out of common storage are provided in a library); optimal use of machine resources in a multi-user environment without the need for complex virtual-memory operating systems. We have found that a configuration with 0.75 Mbyte memory and a task swapper (dynamic roll-in roll-out) facility in the operating system supports up to five interactive users with generally little deterioration of responsiveness.

**Language**

The package is written in a subset of Fortran 77 (American National Standard Programming Language FORTRAN, 1978). Compilation of the programs on microcomputers operating Microsoft Fortran (Microsoft Corporation, 1983) should be possible, although this has not yet been tried.

**Machine requirements**

The minimum hardware required to run the GX package is a central processor and memory with at least 0.5 Mbyte program address space, 10 Mbyte disc store, keyboard terminal, printer and pen plotter or other hard-copy graphics device. Some means of loading reflection data from a diffractometer will be needed, e.g. magnetic tape, data link or compatible disc. A visual display unit (VDU) with graphics capability is desirable but not essential. It may serve also as the operator terminal. A microcomputer based on a 16-bit microprocessor such as the Intel 8086 might meet
these requirements, but there is at present no experience of
GX with such hardware. The machine used for development
is a Gould SEL 32/27 minicomputer running the MPX-32
operating system (Gould Inc., 1983) with 0.75 Mbyte mem-
ory, 32 Mbyte disc, raster graphics VDUs and Tektronix
4662 multi-pen plotter. The processor is similar in power to
a VAX 11/750.

Software requirements are a single-user or multi-user
operating system (including file management and editing
facilities), and a Fortran 77 compiler. Graphics can be
implemented either via a Calcomp-compatible interface or
by direct output of ASCII characters to drive Tektronix-
compatible devices. In the first case, locally-available
Calcomp-type routines are linked to the program and the
devices are accessed according to arrangements at the local
installation. In the second case, the only requirement is a
machine-specific Fortran library routine (sometimes called
BUFFEROUT) to output characters with no embedded
carriage returns or line feeds. At the time of writing, GX has
been installed on Gould SEL 32/27 and ICL 2988
computers.

Input requirements
The initial input to GX consists of the space group and unit-
cell parameters and a list of \( h, k, l, F^2, \sigma(F^2) \). Reduction of
raw intensity data is laboratory specific, often carried out on
the diffractometer itself, and must precede input to GX.
Direction cosines defining incident and diffracted beam
directions are optional additions used in absorption and
extinction corrections.

Programs implemented
The components of the package may be grouped according
to type of calculation in the structure analysis, as follows.

(i) Operations on the reflection data and crystal model.
These include Miller index transformations, sorting on the
indices, merging equivalent reflections and removal of sys-
tematic absences, Gaussian absorption correction, empirical
absorption correction using DIFABS (Walker & Stuart,
1983), atom coordinate transformations, construction of
groups with idealized geometry, automatic addition of
atoms in theoretical positions.

(ii) Direct methods. This part of the package, known as
MITHRIL, has been described by Gilmore (1984). It pro-
vides a wide range of sophisticated multi-solution tech-
niques including the active use of higher invariants.
Although routine problems can be coped with automatic-
ally, the program can also deliver the full power of modern
direct methods to the non-specialist when required.

(iii) Fourier synthesis and peak searching. The programs in
MULTAN80 (Main et al., 1980), which use a FFT algorithm
operating on the whole unit cell, have been converted into a
general-purpose Fourier calculation package suitable for all
stages of X-ray and neutron analysis.

(iv) Structure refinement. A fast block-diagonal least-
squares program with blocks up to \( 5 \times 5 \) per isotropic atom
or up to \( 10 \times 10 \) per anisotropic atom is provided in addition
to and compatible with a general full-matrix program. The
latter incorporates flexible choice of refined parameters,
rigid-group constraints, refinement of an isotropic extinc-
tion parameter and batch scale factors, refinement of the
enantiomorph using the method of Rogers (1981), and riding
atoms. The asymmetric unit may comprise up to 200 atoms.
Run time for the full-matrix program with 1800 reflections
and 240 variables is 35 min per cycle on the Gould SEL
32/27. There are programs for analysis of weighting schemes
and publication listing of structure factors.

(v) Molecular geometry. The geometry program calculates
bond lengths, angles, contacts, torsion angles and mean
planes together with standard deviations derived from the
full normal matrix or from a diagonal error matrix. Bonds
and contacts are defined in terms of preset covalent and van
der Waals radii. Output is in publication-ready table format,
including tables of coordinates and anisotropic temperature
factors. The number of significant figures printed is deter-
mined automatically by the size of the corresponding stan-
derd error, with provision for over-riding the pre-set criteria
if required. All tables can, optionally, be screen-edited before
printing.

(vi) Crystal structure illustrations. We have developed an
interactive version of ORTEP (Johnson, 1971). An entirely
new user interface has been built into the program so that
English commands can be used. Complex operations can be
performed with a single command, such as drawing a stereo	pair or generating the contents of a unit cell. If access is
required to features of the program that do not appear in the
English subset, the original numerical instructions may be
used as well. Thus all the functions of ORTEP are retained,
while the most commonly-used instructions are available in
simple form for interactive use. When a graphics terminal is
available, the user can draw interchangeably on the terminal
and the hard-copy device, without stopping the program, by
means of device selection commands. Because Interactive
ORTEP uses the GX system's crystal model file, it is
compatible with SHELX (Sheldrick, 1976) and can, of
course, be used independently of the other GX programs.

Conclusion
Experience with GX demonstrates that its design principles
enable full-scale crystal structure analysis to be carried out
without compromise on low-cost computer systems. Copies
of the package are available from the authors.

We thank the Science and Engineering Research Council
for a grant towards the purchase of the laboratory com-
puter, the authors of programs adapted with their per-
mission, Dr D. Braga of the University of Bologna for trials
of the package, Dr D. N. J. White and other members of the
Glasgow laboratory.

References
American National Standard Programming Language
Standard Institute, New York.

R. DIAMOND, S. RAMASESHAN & K. VENKATESAN,
pp. 23.01-23.15. Bangalore: Indian Academy of Sciences.

**Crystallographers**


This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CT1 2HU, England).

Winfred O. Milligan died 18 February 1984 in Houston, Texas. Born in Coulterville, Illinois on 5 November 1908, he earned his PhD at Rice University in 1934. For the past 19 years he was Distinguished Research Professor of Chemistry and Physics at Baylor University in Waco, Texas. He was Director of Research at the Robert A. Welch Foundation, Houston from 1955, shortly after its inception, until his retirement in 1982. Professor Hugo Steinfink writes that the Foundation emerged, under his leadership, as the foremost private granting agency in the support of basic research in chemistry in the USA. Professor Milligan’s research interests were in X-ray and electron diffraction, electron microscopy, gas absorption and magnetic properties. He made fundamental contributions to the structures of lanthanide and actinide hydrous oxides and hydroxides. He was a fellow or member of, and held offices in, numerous professional societies. He was a charter member of the American Society for X-Ray and Electron Diffraction and a member of its successor society, the American Crystallographic Association.

**Book Reviews**

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS9 8JT, England) as far as practicable books will be reviewed in a country different from that of publication.


This is an interesting collection of review papers on the subject of crystalline polymers, focusing mainly on measurements of the shape of molecular chains. There are seven chapters in this volume, which are written by researchers whose approach to the subject matter is that of the experimental physicists, i.e. they are concerned with the use of experimental techniques that would discriminate between various competing theoretical models. With this rigorous approach, the conformations of the macromolecular chains are examined on the scale of a few ångströms and then increased to the level of organization that is visible in the optical microscope, i.e. morphological scale of a few micrometers.

The first chapter is written by R. D. B. Fraser, E. Suzuki & T. P. MacRae on **Computer analysis of X-ray diffraction patterns**. This paper is concerned with the use of a digital computer to interpret wide-angle X-ray scattering (WAXS) data. Using raster-scanning digital microdensitometers, the diffracted intensity can be measured at every point on a fine lattice superimposed on the photograph and the information stored in a computer. Methods of analyzing this immense amount of data with particular reference to silk fibers are discussed. This chapter is written with sufficient introductory material that those who may not be directly involved in the same area of research can benefit through its elegant style of presentation.

The second chapter is by I. H. Hall on **The determination of the structures of aromatic polyesters from their wide-angle X-ray diffraction patterns**. This contribution is concerned with the experimental WAXS study of chain conformation in polyesters such as poly(ethylene terephthalate) and poly(butylene terephthalate). A tremendous amount of unit-cell information for a series of polyesters, quite invaluable to polymer scientists, is discussed and critically reviewed. Through his clear style of writing, the author covers areas of his investigation that may involve dangers of misinterpretation and uncertainties of data that can still haunt X-ray diffraction studies.

The third chapter is by E. L. Thomas on **Transmission electron microscopy of polymers**. Electron microscopy investigations have provided much of the detailed information on polymer morphology. This chapter outlines the key techniques and the theoretical basis for interpreting images derived from either conventional TEM or scanning transmission electron microscopy (STEM). The usefulness and limitations of the various techniques are documented based on the polymer literature. The author surveys many aspects of polymer science issues, which include the 'nodule controversy in amorphous polymer glasses' and defects in polymer crystals such as screw dislocations in polyethylene. Covering 124 papers up to 1983, the reader will find it quite rewarding to go through this review, which discusses pertinent issues of polymer microscopy.

The fourth chapter is written by D. M. Sadler on **Neutron scattering by crystalline polymers: molecular conformations and their interpretation**. This manuscript attempts to answer two basic questions in polymer science, namely, what are the shapes of macromolecules inside their crystal lattice and how do the crystals form that shape? Judging from the beautiful presentation in this chapter, neutron scattering has already made remarkable progress in answering the first if not the second of these questions. Small-angle neutron scattering (SANS) data obtained from the Institut Laue–Langénin in Grenoble are discussed for materials including deuterated polyethylene, isotactic polypropylene, isotactic polystyrene and poly(ethylene oxide), even though only the work on polyethylene is discussed in detail. Also, the effects of annealing are covered only briefly and the chapter is selective in order to give special attention to the interpretation of conformations relating to the mechanisms of crystallization. Effects of orientation on the shape of the macromolecules are also covered elegantly.

The fifth chapter is by I. H. Hall & M. Toy on **The ability of small-angle X-ray scattering (SAXS) to distinguish between morphological models of crystal...**