18.4-1 RIETVELD METHOD RUNS ON IMB-AT
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For structure refinement from neutron or X-ray powder diffraction data the Rietveld method [J.Appl.Cryst.1969, 2, 65-71] is widely used. Up to now this mostly required expensive mainframe- or mini-computers of computing centers. The availability of cheap and fast (by use of floating-point coprocessors) and sufficiently accurate (32-bit single precision floating point variables in FORTRAN-77) 16-bit microprocessors together with optimizing compilers have made it promising to perform profile refinement calculations at laboratory level. Commercially available X-ray position sensitive detectors also increase the demand for decentralized, quasi on-line profile refinement. For this reason the Rietveld-version of D.B.Wiles and R.A. Young hitherto called WYRIET [J.Appl. Cryst. 1981, 14, 149-151] has been implemented on an IBM-AT microcomputer using the Ryan-McFarland FORTRAN-77 compiler.
For the convenience of the routine-user several features have been added:

1. An interactive preprocessor for the correct set up of the input-file to the main program.
2. The Pearson type VII function [M.M.Hall, et al, J.Appl.Cryst.1977, 10, 66-68] permitting continuous tuning of the profile form from Gaussian to Cauchy.
3. An interactive graphics postprocessor using the GKS-graphics system to plot the resulting spectra and to model the residual background for iterative refinement of the powder spectra by:
   -cubic spline function smoothing with user selectable dynamic weight functions
   -linear interpolation scheme with user selectable averaging range
   -cursor addressable point modelling of background polyline

Typical runtimes are 1.1 minutes per cycle for a two-phase neutron spectrum of 33 Bragg peaks measured with 1181 data points and varying 16 parameters using single precision WYRIET. A comparison with runs on a Cyber 175 60-bit computer yields identical results within several percent of standard deviation at the cost of additional refinement cycles to achieve convergence. Examples will be demonstrated. The programs are available from the author on floppy-discs.
Helpful discussions with H.Boysen and H.Schrader are acknowledged.
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18.4-2 A MICROPROCESSOR VERSION OF THE XTAL SYSTEM.
By Sydney Hall, Lutz Engelhardt and Tanya Schmah, Crystallography, University of Western Australia, Nedlands 6009.

The XTAL System is a large suite of crystallographic programs suitable for any 'laboratory' computer. It is currently implemented on computers ranging in size from the CRAY II to the Apollo DN3000. The XTAL software is written in the preprocessor language ratmac and is identical for all machines. When implemented, the source code is adapted by the preprocessor to the target computer, using a macro library containing machine-specific edit commands.

The portability and the universality of the source code, along with the versatility of file structure, are considered essential properties of the XTAL package; properties that cannot be comprimised for any particular implementation. For this reason no attempt has been made until now to adapt XTAL to smaller machines. However, the latest generation of 16-bit personal computers now provide a performance, both in speed and precision, that is comparable to existing laboratory machines, but at much lower cost.

XTAL has been implemented on an IBM PC/AT with a Definicon DSI-780 coprocessor board (Motorola 68020/68881, 17MH, 2Mb RAM). The performance of this microprocessor may be gauged from the times for a typical mixture of fortran77 calculations.

Machine:	*mVAXII*	*Sun3/110*	*DSI780*
Time(secs):	*86*	*85*	*98*

The AT/DSI configuration also has a 30Mb hard disc, a 1.2Mb floppy and Matrox PG-640 colour graphics and monitor. The problems in implementing the XTAL package arose mainly from the current limitations of the current compiler, linker and loader software supplied for the coprocessor. This required the development of pseudo overlay loading procedure. No changes to the XTAL source were needed. A similar development is also anticipated on the Commodore Amiga or MacIntosh II. Microprocessors using XTAL will be on view at the Congress microcomputing exhibit.

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18.5-1 VISUALIZATION AND FAST ENERGY CALCULATION OF PROTEIN - LIGAND INTERACTION ON 3D GRAPHIC DISPLAY.
By A. Itai, N. Tomioka and Y. Iitaka, Faculty of Pharmaceutical Sciences, University of Tokyo, Japan.

Docking simulation study on 3D graphic display between protein and ligand molecule is powerful means both for interpreting protein-ligand interactions or its biological activities, and for designing new drugs rationally, in case of protein structure is known by X-ray crystallography. We have developed a new method using three-dimensional grid points placed inside the ligand binding site of the protein. At each grid point, various physical and chemical properties, such as non-bonded interactions for various probe atoms, electorstatic potential and expected hydrogen bonding sites, are calculated and stored for the later repeated use. These tabulated data are used 1) for visualizing the spatial circumstances of ligand binding site, 2) for realtime estimation of protein-ligand interaction energy throughout the docking process. The former facilitates to find the appropreate initial location of a new ligand molecule, and the latter facilitates to find the rough energetically favorable location by local manipulation of ligand molecule.
To illustrate the usefulness of this method, we have applied the program to several enzyme systems, fitting their substrates and inhibitors.

1.Symposium on Medicinal Chemistry (1984,Tokyo)
2.Symposium on Three-Dimensional Structures and Drug Action (1986, Tokyo)
3.J. Med. Chem. 30, in press (1987)