

sists in the optimization of an appropriate function within a user-defined domain in the lattice-parameter space. Indexing up to orthorhombic; refinement up to monoclinic. New features include least-squares refinement with optional extrapolation, full interactivity, mapping option, possibility of studying nonprimitive Bravais lattices (e.g. rhombohedral), treatment of user-defined forbidden (hkl) triplets, editor for patterns and configuration.

Documentation: Computer readable (also on line) documentation is provided.

Availability: from Sinus S.C.. ul.Racławicka 33 m.40, 02-601 Warsaw, Poland.

References: Paszkowicz, W., *J. Appl. Crystallogr.* 20, 166 (1987).
Paszkowicz, W., *J. Appl. Crystallogr.* 22, 186 (1989).

Windows

For the past few months I have been immersed in trying to learn the fundamentals of the C programming language. "C" has been characterized as "sort of a hacker's language, with code sometimes readable only by its author." (Appleby, 1991, quoting Jeanne Martin). Because I generally "learn to use a language by application to a project," I am now devoting my energies to the evolution of a mechanism for the filtering of data in the Powder Diffraction File using an Organic Functional Group Index. The project specifies that the scheme must function in the environment established by WINDOWS 3.0. Thus the need for my excursion into the world of "C" and "object oriented programming".

Microsoft Windows is a graphical extension to the MS-DOS operating system. DOS is built to support a single program running at a time, while under Windows multiple programs can run concurrently. DOS has limited support for graphical output while Windows supports sophisticated, high-level graphics. DOS requires each program to provide its own user interface while Windows provides a standard set of user interface objects. Programs that run in the Windows environment are "event-driven" while application programs running under DOS have been sequence driven.

The Organic Functional Group Index project involves effort directed toward generating data structures and associated program code for the identification of entries in the PDF having specified "Organic Functional Groupings of atoms" (connectivity). The graphical attributes of the Windows environment will enhance the subsequent display of the data found for the selected entry(ies) in the PDF file on the CD-ROM.

Commercial Announcement

Powder Diffraction Pattern Simulation

POWDER, available from Scientific Services, simulates Debye-Scherrer powder diffraction patterns on either IBM PC or Macintosh computers. Useful for research and ideal for teaching, POWDER simulates patterns using crystal parameters, chemical species, and atomic locations.

The user can select from the large selection of standard crystals and modify the crystal parameters and chemical species to see how these changes affect the spacing and intensity of the pattern. Alternatively, he/she can easily construct a personal data bank.

The incident radiation can easily be modified so the user can readily see how this affects the pattern.

Features include the ability to graphically display the

The Future

We will have more to say about programming in the C language for the Windows environment. Hopefully we will be in a position to contrast the results with related programming using the recently released Pascal for Windows and/or the announced "Windows extensions for Microsoft FORTRAN".

The transition from "sequence driven" programming {where the program(mer) dictates the sequence that the user must follow to accomplish the goal} to "event driven" programming {where the user dictates the steps required to complete a given task} requires evolution of new ways of thinking. The time investment must be significant in the beginning. Old "mind sets" must be overcome and new perspectives evolved. The focus of attention can take one away from touch with other events occurring in this time of rapid expansion in the capability of personal computer hardware and the evolution of data processing methods to exploit the newly available tools.

Because of my (RG) recent ascendancy to the Executive committee of the North Dakota Academy of Science (Secretary-Treasurer to be specific) and the concomitant assignment as principal editor for the *Proceedings of The North Dakota Academy of Science*, coupled with a teaching load involving 1200 students in Foundations of Chemistry, I (RG) am not finding the time to explore the many alternative uses of computers to aid in the processing of diffraction data. Thus I (RG) am being forced to view my further association with COMPUTER COMMENTS in terms of an "event driven" mode. Both Mark and I need your help and stimulation to maintain a flow of information. We appreciate the efforts of those who have made contributions, but after six years we can count these contributions on the fingers of our two hands with no worry about not having enough sites for association.

If you do not write, I will not write.

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Roy Garvey, Department of Chemistry
North Dakota State University, Fargo, ND 58105-5516, U S A
BITNET address NU025304@NDSUVM1

to whom contributions and comments should be directed, and by:
Mark Holomany
JCPDS-International Centre for Diffraction Data
1601 Park Lane, Swarthmore, PA 19081, U S A

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atomic arrangement of the crystal planes responsible for diffraction.

The pattern along with a model of the crystal structure can be printed using a laser printer.

A license for either the Macintosh or IBM PC version of POWDER sells for \$500. Both versions are available for a fee of \$600. This gives anyone in the licensing department the right to copy and use POWDER. Universities are eligible for a 50% discount.

Orders may be placed with Scientific Software Services, 3497 School Road, Murrysville, PA 15668.

POWDER is the newest member in the family of personal computer software for research and education in crystallography and diffraction offered by Scientific Software Services. Others include CRYSTAL, for education in X-ray crystallography, STEREO PLOT, for plotting any stereogram, and DIFPAT, for simulating diffraction patterns.