Graphics And Virtual Reality

PS03.07.01 ORTEP-III: THE OAK RIDGE THERMAL ELLIPSOID PLOT PROGRAM. Michael N. Burnett, Carroll K. Johnson, Chemical Sciences Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 378316197 USA

The third revision of the Oak Ridge Thermal Ellipsoid Plot Program, ORTEP-III, is now available. The program, including source code, precompiled versions for DOS and Macintosh personal computers, the complete user manual as a downloadable Postscript file, online documentation, examples, and helper programs, is available on the World Wide Web at http://www.ornl.gov/ortep/ortep.html. The program may also be obtained via anonymous ftp from ftp.ornl.gov in the directory /pub/ortep. All inquiries, comments, questions, problems, suggestions, etc. should be sent to ortep@ornl.gov.

This update to ORTEP was undertaken to incorporate some of the advances in computing and printing technologies made since the previous release. Built into the code are drivers to produce Postscript and HPGL/2 files of the ORTEP illustrations. These files may be printed on a variety of printers and plotters and may be imported into a number of other computer applications. Also, ORTEP-III includes a screen driver built around the free graphics library PGPLOT* that permits the user to see the illustration on the screen before producing a hard copy.

Changes and new features in ORTEP-III include: number of input atoms increased from 166 to 500, number of symmetry operators increased from 48 to 96, the ability to enter symmetry operators using the format provided in the International Tables, lower case letters added for labeling, color, atom "features" to make selection of atoms more flexible, an interactive line editor for making changes to the input file without leaving the program, and the ability to produce critical net illustrations (as described elsewhere).

*Information about PGPLOT may be found on the World Wide Web at http://astro.caltech.edu/~tjp/pgplot or via e-mail to tjp@astro.caltech.edu.

Research sponsored by the Laboratory Directed Research and Development Program of the Oak Ridge National Laboratory, managed by Lockheed Martin Energy Research Corp. for the U.S. Department of Energy under Contract No. DE-AC05-96OR22464.

PS03.07.02 *TITAN*: A MOLECULAR GRAPHICS PROGRAM TO AID STRUCTURE SOLUTION AND REFINEMENT WITH THE SHELX SUITE OF PROGRAMS. Jim Simpson and Keith A. Hunter, Department of Chemistry, University of Otago, P.O. Box 56, Dunedin, NEW ZEALAND

TITAN is a Windows based molecular graphics program designed to be used exclusively in conjunction with SHELXS-86[1] for structure solution and SHELXL-93[2] and/or SHELX-76[3] for structure refinement. The program facilitates the on-screen assignment of peaks from the direct methods E-map or Patterson map to individual atom designations. Once these designations are completed, a file is written that can be input directly to the SHELXL-93 refinement program without modification. *TITAN* can also be used in the location of additional atoms in series of least-squares and difference Fourier cycles and as an aid to the inclusion of hydrogen atoms into the refinement using the HFIX and/or AFIX commands.

TITAN runs in the Windows environment and requires a 386 or better processor with a minimum of 4Mb memory. Hard-copy plots can be obtained using any Windows compatible printer. In addition, *TITAN* will generate output files that can be processed using the public-domain ray tracing software Persistence of Vision (POVRay) to produce exceptionally high quality 24-bit colour images for reproduction.

A demonstration of the operation of the *TITAN* program will be given as part of this poster presentation.

1 Sheldrick, G.M. (1986) SHELXS-86 'A program for the solution of crystal structures from diffraction data.' University of Göttingen, Federal Republic of Germany
2 Sheldrick, G.M. (1995) SHELXL-93 J. Appl. Cryst. in preparation
3. Sheldrick, G.M. (1976) SHELX-76 'Program for crystal structure determination', University of Cambridge, England

PS03.07.03 MOLDRAW: MOLECULAR GRAPHICS FOR MS-WINDOWS. D. Viterbo+, P. Ugliengo+ and G. Chiari* - +Dip. di Chimica IFM, and *Dip. di Scienze Mineralogiche e Petrologiche, Torino, Italy.

MOLDRAW [Ugliengo, Viterbo & Chiari, Z. Kristallogr., 207 (1993), 9] is a program for the graphical manipulation of molecules and crystal structures on personal computers, which can be used to analyze the conformation of molecules resulting both from diffraction techniques and from theoretical calculations, and to study the detailed structure of crystalline materials.

Recently we have undertaken the porting of the code under MS-WINDOWS, in order to take full advantage of the facilities offered by this system. The "look & feel" features of all WINDOWS applications are preserved and all operations are menu, mouse or event driven; these features make this new version of MOLDRAW very easy to learn and use.

Graphic resolution and performance are entirely determined by the WINDOWS driver. With last generation graphic boards, molecular structures may be rendered as on more costly graphic workstations. The resulting images can be printed on any WINDOWS defined printer and pasted to the clipboard or saved as bitmap files to be used by Paintbrush, Word, etc. for desktop publishing. The program may now handle very large systems such as biological macromolecules. All features present in the MS-DOS version have been improved and new facilities have been introduced. The format of the input files has been preserved.

We are currently involved in setting up a much easier interface to the crystallographic data bases, to the computational chemistry packages and to other molecular graphics systems. We are also engaged in the setting up of the following new facilities: a) simulation of powder diffraction patterns; b) representation of polyhedra; c) generation of a complete unique molecule from the given coordinates and symmetry operators; d) animation of molecular vibrations as computed by GAUSSIAN; e) input of CIF files.

The beta release of the present version, still under development, is available via anonymous ftp.