defined by the data-processing programs. In the calculated positions, it displays the logarithm of the diffraction intensity or amplitude of each reciprocal-lattice point with radius and degree of darkness according to the input values. Any planes of the reciprocal lattice can be displayed. When the index and amplitude or intensities ($h$, $k$, $l$, $F$ or $I$) of all the reflections are read, the program produces pictures very similar to real precession photographs.

**Software and hardware environment**: The program is written in Fortran77 and generates the pictures in PostScript format. In principle, it can be used on any computer that accepts the two languages. So far, it has been installed on VAX/VMS and a number of Unix computers, such as SGI, DEC-alpha, DEC-Ultrix, ESV, Sun *etc.* It can be easily installed on Unix computers.

**Documentation and availability**: The program and a detailed manual can be obtained *via* the WWW (http://gamma.mbb.ki.se/~guoguang/pattern.html) or by FTP (ftp://gamma.mbb.ki.se/pub/guoguang/pattern.tar.Z). The source code and executable codes for several types of Unix computer (SGI, DEC-alpha, ESV) are available for the whole crystallographic community.

**Note**: There are other programs which have similar functions, such as *LAYER* (by L. Barbour), *PRECESS* (by W. Furey), *HKLPLOT* (by E. Dodson) and *PLOTHKL* (by G. Pfluegl).

**Keywords**: protein crystallography; precession photography.

# Tcl/Tk-based programs. III. *CRITXPL*: graphical analysis of the *X-PLOR* refinement log files

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**The crystallographic problem**: Refinement of atomic models using *X-PLOR* (Brünger, 1992) is carried out in a number of laboratories for macromolecular crystallography. The main results of the refinement are a model and a corresponding log file that shows the process of refinement, gives crucial information on the success or failure of the process, and proposes necessary modifications, such as modifications of weights for different criteria. This log file is a long list that contains an enormous number of tables, with the criteria values as they vary during the refinement. The analysis of these tables requires a significant effort.

**Method of solution**: A program *CRITXPL* has been developed that gives a graphical representation of the variation of the minimization criteria during an *X-PLOR* refinement. The program can be run either after *X-PLOR* or in parallel with it. In the latter case, the graphics can be easily updated during the refinement. *CRITXPL* is an interactive menu-based program that continues the series of programs reported earlier (Urzhumtseva & Urzhumtsev, 1996, 1997). To start the data processing, the name of an *X-PLOR* log file is chosen through the menu. This file can contain several minimization processes. A process is defined as a sequence of *X-PLOR* refinement frames with increasing cycle number and with the same list of criteria. To identify the process to be displayed more easily, a special line of comments can be used in the *X-PLOR* script. For every process, *CRITXPL* shows, as a function of the cycle number, the plot of the gradient, of the temperature, of the $R$ and the $R_{\text{free}}$ factors, and, optionally, plots of other criteria (Fig. 1). The latest values of the criteria are displayed numerically. The full list of all criteria applied in the process analysed is given by a set of buttons that can be used to remove, to replace or to show a plot of a chosen criterion. Up to eight criteria can be shown simultaneously. Any combination of them can be chosen and changed at any moment. The processes can be displayed either one by one or together. The latter is useful for molecular dynamics; in this case, the criteria values in both the first and the last points of the chosen processes are displayed. The plots can be updated during an *X-PLOR* run and can be shown on a larger scale, and the point coordinates (the cycle number and the criterion value) can be obtained using a mouse.

**Software and hardware environment**: The computational part is written in Fortran77, and the interactive graphics part is written in Tcl/Tk (Osterhaut, 1993). The program *CRITXPL* can be run on an SGI computer and on a DEC Alpha station with the Tcl/Tk libraries installed. The program can be also run on an IBM PC or Macintosh with an X-terminal emulator, such as *exodus*, *xwin etc. CRITXPL* accepts log files produced by the 3.1x, 3.8x *X-PLOR* versions, as well as by *CNS* (Brünger *et al.*, 1998).

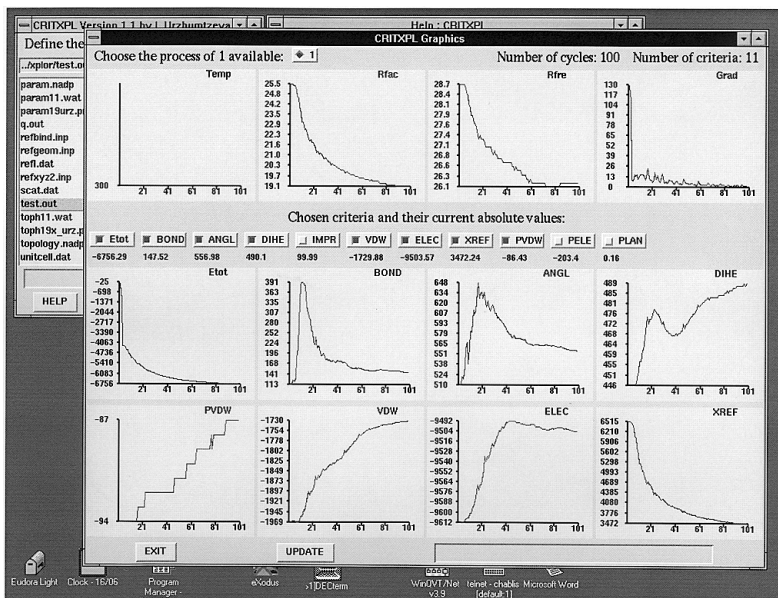**Documentation**: No special documentation is necessary, due to the



Fig. 1. View during a *CRITXPL* session.

menu-based character of the program. On-line help is available.

**Availability**: The program is available from the authors on request.

**Keywords**: *X-PLOR*; refinement; interactive graphics; Tcl/Tk.

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# TOPOS3.1 – program package for multipurpose geometrical and topological analysis of crystal structures

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**The crystallographic problem**: The program package *TOPOS* is intended for the automation of crystal–chemical analysis of both individual substances and a large set of crystal structures.

**Method of solution**: The version *TOPOS*3.1 includes the following programs.

(i) *DBMS* (database management system) allows one to edit, search and retrieve crystal structure information. All the other programs of the package (except *StatPack*) are integrated into *DBMS*.

(ii) *Dirichlet* is used for the construction of Voronoi–Dirichlet polyhedra (VDP) of atoms in crystal lattices and for the determination of geometrical and topological characteristics of atomic domains.

(iii) *AutoCN* calculates an adjacent matrix of crystal structure, including atomic coordination numbers (CN).

(iv) *ADS* (automatic description of structure) tests crystal structures for isomorphism; it determines coordination types of ligands, and the topology of complex groups and their orientations.

(v) *DiAn* performs the standard calculations of interatomic distances and bond angles.

(vi) *IsoCryst* builds, scales and rotates an image of a crystal structure and makes various standard geometrical calculations.

(vii) *StatPack* provides a statistical analysis of calculation results.

*DBMS* supports the unique binary *TOPOS* format of database files, which provides fast access to databases. *Dirichlet* applies a very fast 'gift wrapping' algorithm (Preparata & Shamos, 1985) to construct VDPs. *AutoCN* uses VDPs and an 'intersecting spheres' algorithm (Serezhkin *et al.*, 1997) to build an adjacent matrix of crystal structure. *ADS* takes this adjacent matrix, represents crystal structure as an infinite graph, then rolls it up into a finite graph and analyses its topology according to the algorithm of Blatov & Serezhkin (1992). All the other programs use standard geometrical and statistical analysis algorithms.

**Software environment**: Operating systems: MS DOS 5.0, Windows 95 or higher. Programming language: Borland Pascal with Turbo Vision library. Overlay structure: none. Subroutine libraries: Borland Pascal files for protected mode.

**Hardware environment**: Computers and installations: all IBM PC/AT 80386/87 (or higher) compatible computers (installation is to one directory of a hard disk). Minimum number of bits per word or byte: 16 bits per word. Minimum high-speed store required to run the program: 2 MB of RAM (4 MB or more recommended); Peripherals supported: CGA/EGA/VGA videoadaptors, Epson- or HP-compatible printers and mouse.

**Program specification**: Restrictions on the complexity of the calculation: some minor facilities of the package are restricted by the number (16383) of compounds per database and of atoms per compound; however, all calculations can be made for structures of any complexity.

Unusual features: the possibility of the comprehensive crystal–chemical analysis of thousands of crystal structures in an acceptable time period.

Typical run times: one or several minutes per typical compound (up to some hundreds of atoms per unit cell). The package has been tested on databases containing more than 10 000 compounds (including peptides and polynucleotides), consisting of up to 30 000 atoms.

Number of lines of code: about 50 000 lines of the source code.

Test status: more than 25 000 crystal structures of various chemical nature (from simple compounds to peptides).

**Documentation**: A user manual is available.

**Availability**: *TOPOS* is distributed on one 1.44″ MS DOS floppy disk. A free demo version is available *via* ftp://ftp.lmcp.jussieu.fr/pub/sincris/software/structure/topdemo.zip. The *TOPOS* WWW site is located at http://www.ssu.samara.ru/Common/Structure/Chemistry/IChemistry/topos.htm.

**Keywords**: Crystal–chemical analysis; geometry; topology.

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# Crystallographers

## 1999 ICDD Crystallography Scholarship Recipients are Announced

The ICDD Crystallography Scholarship Committee has selected five winners for the 1999 Scholarship program. They are: Byron DeLaBarre, McMaster University, Hamilton, Ontario, Canada; Shannon Patrick Farrell, University of Western Ontario, London, Ontario, Canada; Cora Lind, Georgia Institute of Technology, Atlanta, Georgia; Oshrit Navon, Ben-Gurion University of the Negev, Beer Sheva, Israel; K. Scott Weil (also a 1998 recipient), Carnegie Mellon University, Pittsburgh, Pennsylvania.