invariants are estimated *via* proper representations (Giacovazzo, 1977, 1980). Trial solutions are obtained by the magic-integer approach (Main, 1978) or by random phases (Baggio, Woolfson, Declercq & Germain, 1978). The best solution, selected by proper figures of merit (FOM's), is automatically processed through a cyclic procedure integrating structure-factor calculation, least-squares refinement and $2F_o-F_c$ Fourier synthesis. Owing to reflection overlap, the observations in the least-squares routine are the total intensities of groups of reflections, while intensities of single reflections constitute single observations only when they do not overlap with any other. The final outcome is a set of refined atomic parameters (x, y, z) associated with atomic species. When neutron data are processed, parameters of atomic species with negative scattering length can also be determined. If a graphic device is available, the user can follow structure solution and refinement on the screen. In the final stage, a menu-driven interface is available in order to study molecular geometry and restart refinement. Owing to the small number of observations/number-of-parameters ratio, the residual R values must be carefully considered by the user (usually final values are between 0.06 and 0.20).

Software environment: The program has been written in standard Fortran77. A module written in C is supplied for interface with X-window or DEC-Window terminals. Besides a C compiler, an Xlib library is also needed. Two ASCII files are associated with the program: the first contains coefficients for calculating scattering factors, the second, necessary for graphics, contains on-line help.

Hardware environment: The program runs on Unix and DEC workstations, on main-frame and personal computers (at least 4 Mbytes of RAM and a VGA monitor are needed).

Program specification: The source code of the program consists of 44000 Fortran lines and 2000 C lines (including comments).

Documentation: User's instructions and a program description (about 1400 lines) are supplied as an ASCII text file.

Availability: The program is available free of charge from the teams in Bari and Perugia. A licence agreement has to be signed.

Keywords: Direct methods, powder data, automatic structure determination and refinement.

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SUPERIMPOSE – a program for the unambiguous structural superposition of spatially related molecules, including macromolecules.

By KAY DIEDERICHS, *Institut für Biophysik und Strahlenbiologie der Universität Freiburg, Albertstrasse* 23, *D*-79104 *Freiburg, Germany*

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The crystallographic problem: For the comparison of structurally related molecules, it is necessary to find a rotation matrix **A** and a vector **T** such that the atomic positions **x** of a given coordinate set are superimposed (using **Ax** + **T** = **y**) on their structurally equivalent counterparts **z** in another coordinate set with the lowest possible deviation $|\mathbf{y} - \mathbf{z}|$. A prerequisite is the identification of the equivalent set of atoms. Once this set is known, established methods (Kabsch, 1978) can be applied to find the best overlay in a least-squares sense. In the case of significant macromolecular sequence homology, an equivalent set of atoms can be obtained from a sequence alignment. However, structural homology is sometimes found even if no sequence homology can be detected (see *e.g.* Kabsch, Mannherr, Suck, Pai & Holmes, 1990). In this case, the structural alignment is often found by interactive adjustment of rotational and translational parameters on a graphics terminal. This task is time consuming and, for distantly related molecules, the result is not always unambiguous.

Method of solution: In general, a six-dimensional search in orientation and translation space would be required. As this is computationally very demanding, the program described here proceeds analogously to the molecular replacement method (Rossmann, 1990). The problem is subdivided into two steps: (1) a three-dimensional rotational search that uses the intramolecular difference vectors and (2) a three-dimensional translational search in real space. The best rotation is given by that set of Eulerian angles that gives the highest value on a finite-sized grid of a product function in difference vector space. For (2), the target that is maximized is the number of atoms that fall within a 2 Å sphere of any reference coordinate. This target is calculated as a function of translation in three-dimensional space. It is at a maximum when the equivalent set of atoms is found.

Software and hardware environments: The program is written in Fortran77 and runs under the VMS and Unix operating systems. No overlay structure and no special subroutine libraries are used. The program requires less than 1 Mbyte of data space.

Program specification: The input to the program is two coordinate sets in Brookhaven Protein Data Bank (PDB) format, the first serving as a reference. The output is the second coordinate set, rotated and translated with the best parameters found. The matrix **A** and the vector **T** are reported and a statistical summary of the rotation and translation searches is given. For small proteins (around 150 amino acid residues), a typical run time is about 1 min on an Indigo R4000 workstation.

Documentation and availability: The program can be obtained by e-mail from the author (dikay@sun1.ruf.uni-freiburg.de). Documentation is included as comments in the program source. Results of a test calculation, superposition of interleukin-2 [PDB code 3INK (McKay, 1992)] on granulocyte-macrophage colony-stimulating factor [PDB code 1GMF (Diederichs, Boone & Karplus, 1991)], are given in the documentation as an implementation check.

Keywords: Molecular replacement; comparison of related structures.

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*ORTEP*92 – an improved PC version.

By IVAN VICKOVIĆ, *Laboratory of General and Inorganic Chemistry, Faculty of Science, University of Zagreb, Ul. kralja Zvonimira* 8, 41000 *Zagreb, Croatia*

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The crystallographic problem: Different programs have been employed in graphical analysis, representing crystal and molecular structures in small-molecule crystallography. Even though *ORTEP* (Johnson, 1976) is among the oldest (the first version was published in 1961), it is very popular owing to its generality, portability and its ability to take perspective into account and to represent both isolated molecules and crystal structures. Sometimes, though, it is time consuming to select the best view and to get satisfactory labeling by *ORTEP* instructions.

Originally written for main-frame computers and off-line plotters, different versions using different graphics libraries are known. Nowadays, desk-top computers are wide-spread in crystallographic laboratories and accordingly *ORTEP* has been adapted (*e.g.* Rizzoli, Sangermano, Calestani & Andreetti, 1986; Gabe, LePage, Charland, Lée & White, 1989). In this paper, an improved PC version is described. It should: (i) ensure fast quasi-rotation of a molecule to find the best view; (ii) ensure reproducibility of any precalculated pictures on different media; (iii) ensure full control of color for any individual chemical symbol, thermal ellipsoid and/or bond stick/line; (iv) ensure full control of easy labeling and label editing of chemical symbols, titles and/or distances; (v) transfer graphics data to word-processing or drawing programs.

Method of solution and program specification: As well as the original *ORTEP* program, the *ORTEP*92 version is a batch program processing an input data file. The *CSU* program (Vicković, 1988) generates such a file from atomic data written either in *SHELX*76 (Sheldrick, 1976) or any other format and supplies parameters good enough to get satisfactory initial pictures. An interactive approach has been introduced up to certain levels to enable run-time guidance through the new options. Some new instructions are added to the original *ORTEP* input data file, all following the syntax well known to *ORTEP* users. They define rotation increment and ensure full control of colors.

The best view can be obtained by monitoring the rotation of a molecule. The program is organized in such a way that a sequence of plot files is written in *ORTEP* graphics code and displayed for a rotating molecule. For any figure, the rotational matrix is saved and any precalculated figure can be easily reproduced by media available with the *ORTEP*92 program. The atom-labeling scheme may be given in the usual *ORTEP* way, but for the final labeling corrections a plot file can be easily edited by a powerful label-editing option.

User-friendly menu guidance, run-time instruction editing, run-time editing of position, size, height, width and color of chemical symbols, titles and distances make it possible to produce a multicolored figure ready for publication/poster with minimum time and effort by using a plotter and/or laser printer. Full control of hard-copy figure size is also available.

Software environment: The original code of the *ORTEP* program as well as the additional routines are written in standard Fortran77 (about 7000 code lines including comments) and tested on IBM-compatible PC/AT under MS-DOS. The code of the original *ORTEP* program has been changed as little as possible, with new routines added for new functions. The program is compiled using a Microsoft Fortran compiler (version 5.0, Microsoft Corporation, Box 97017, Redmond, WA, USA) which supports *HALO*'88 graphics libraries (Media Cybernetics, Silver Spring, MA, USA) and devices used to monitor the calculated figures stored in the *ORTEP* graphics file. Direct plotting and laser printing as well as plot-file transfer are made possible by translating *ORTEP* graphics code to RD-GL I (Roland Digital Group's graphic language) commands equivalent to HPGL (Hewlett–Packard graphic language). The executable program is prepared with no overlay and it occupies about 320 kbyte of memory.

Hardware environment: The program was designed on a desk-top configuration consisting of an IBM PC/AT compatible with microprocessor 80386/33 MHz and a mathematical coprocessor 80387, a color Trident VGA Delta Prisma 1024 × 768 (or Hercules monochrome) graphics card, an 8 pen Roland DXY-1100 (compatible with HP7475–A) plotter and a HP LaserJet III printer (both with serial/parallel RS-232C interface). The program is not supplied with a configuration setting routine for other graphics cards, plotters or printers. However, other setting parameters are allowed in the program. For a different PC environment, it is necessary to adapt the interpreter (written in Fortran as part of the *ORTEP*92 program) in order to export the *ORTEP* graphics file to the monitor and/or hard-copy devices.

Nevertheless, *ORTEP*92 can be useful for a PC that is not connected to HP devices. Since the rotational matrix for any investigated orientation is registered during on-screen animation, the best figure can be recalculated and plotted on the user's system.

Documentation and availability: New features developed in the reported version are explained in an ASCII help file. Complete documentation including sample input, help file and both executable and source-code files are available from the author by sending a stamped self-addressed label and a 1.2 kbyte diskette or by email from vickovic@srce.hr.

Keywords: Crystallography, *ORTEP*, graphics code, view, rotation, label editing.

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PROSZKI – a system of programs for powder diffraction data analysis.

By W. ŁASOCHA and K. LEWINSKI, *Faculty of Chemistry, Jagiellonian University, ul. Ingardena* 3, 30-060 *Krakow, Poland*

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The crystallographic problem: Analysis of diffraction data routinely includes profile fitting, automatic indexing and refinement of the unit-cell parameters. Although a variety of programs for this purpose exists (Smith & Gorter, 1991) and they generally require the same parameters, each one uses a proprietary format for the data files. Apart from the difficulty in preparation of the input files, this often discourages users from trying