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References


Computer Program Abstracts


The category Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Following normal submission, a Computer Program Abstract will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given on page 189 of the June 1985 issue of the Journal (J. Appl. Cryst. (1985). 18, 189–190).

NEWMAN, program for calculating and plotting Newman projections from atomic coordinates and cell constants. By H. SCHENK, N. P. BRANDENBURG, B. VAN SANTEN, E. Y. KRAFTEN and B. O. LOOPSTRA, Laboratory for Crystallography, Nieuwe Achtergracht 166, 1018 WS Amsterdam, The Netherlands

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The crystallographic problem: Crystallographers publish cell constants and coordinates, and in most cases the redundant but more informative bond lengths and angles as well. Coordinates contain all of the structural information, but bond lengths and angles contain no stereochemical information. This information might be presented by listing the torsion angles, but these are not always easy to interpret. Newman projections are stereospecific graphical representations of the torsion angles around a particular bond. These projections are much easier to interpret than angle data. A program to give Newman projections was previously written by Brandenburg (1974).

Method of solution: The atom and cell information is either entered (microcomputer versions) or read from a binary data file (mainframe version). Orthogonal coordinates are calculated, and from the distances a bonding matrix is evaluated within predefined limits on the bond lengths. Then, for a particular bond, all connected bonds are projected in a plane perpendicular to the central bond. All angles between successive projected connected bonds are calculated and printer plotted (batch mode main frames) or shown on a video display (micros such as TRS80 and IBM-PC). Optionally, the Newman projections can be plotted.

Software environment: The main-frame version is written in Fortran IV for CDC Cyber computers under NOSBE control, but is not machine dependent. It is linked without overlay. The plot routines are local. However, since only circles, straight lines and some text are plotted, local adaptations should not be difficult. Microcomputer versions are written in Basic for the TRS80 model I and IBM-PC. Since plot routines are simple, the program can be easily transferred to other micros (for example the CBM64). The Basic microcomputer versions run under NEWDOS (TRS-80 model I) and IBM-DOS 2.0, respectively.

Hardware environment: The main-frame version runs within 32 k 60-bit words, and optionally uses a plotter. The micro versions require a disk drive and a matrix printer. For the IBM-PC a color/graphics card and a printer with dotgraphics facilities are required.

Program specifications: The program does not have any serious restrictions. Run times are a few seconds CPU (main frame). The microcomputer version is interactive. The number of lines of code is approximately 1000 (Fortran) and 500 (Basic). There is no documentation in machine-readable form. Numerous tests have been run for all programs.

Documentation: A manual containing a short description of the program and input instructions is available.

Availability: The program source and documentation are available from the authors. For the main-frame version the cost of magnetic tape, copying, postage, handling and software licence is Dfl 150. For the micro version the cost is Dfl 100 (floppy disk). For developing countries special arrangements may be possible. Users are not entitled to redistribute the program.

Keywords: Newman projection; Stereospecific projection; Plotting routines.

Reference


TYPIST – a program for the tabulation of crystallographic results. By M. TOMASSINI, Department of Earth Sciences, Piazza Universita, University of Perugia, 06100 Perugia, Italy

(Received 2 January 1985; accepted 22 March 1985)

The crystallographic problem: The preparation of tables of relevant structural information is a time-consuming and error-prone task. It is possible to automate the whole process, but standard word processing programs are not well suited to this specialized purpose, as they require input of the information beforehand. We have thus written a set of programs that automatically extracts the relevant items from the output of a cry-
stalllographic refinement and prepares the necessary tables.

Method of solution: The programs (FILTER 1, FILTER 2, TABLE 1, FILTER 3, TABLE 2) run in sequence, passing information along the chain by means of temporary files. FILTER 1 is a simple program that picks up cell parameters, atomic symbols, coordinates, displacement parameters and their standard deviations from the file output of the last refinement cycle. The present version works with the SHELX76 system (Sheldrick, 1976). It is an easy matter to provide an analogous interface for other systems. FILTER 2 orders the atom list by using a linear search and insertion in an array of dynamically allocated linked lists. TABLE 1 does the actual formatting and tabulation. Three tables are produced: atomic coordinates with e.s.d.'s, displacement parameters, both isotropic and anisotropic, with e.s.d.'s and calculated H-atom positions, if any. FILTER 3 is a small interface program. TABLE 2 produces the bond distances and angles table. It is interactive, allowing the user to specify any symmetry operation. Distances and angles are optionally displayed on the screen before being written to the output file and they can be selected, deleted and reordered at will in real time. The input for the series of programs is minimal: the original least-squares output file and a few commands specified interactively in response to the program’s prompts. All the tables are ready for publication, except for a little retouching needed for inserting some unusual characters. However, being stored as text files, they can be modified with a text editor if the need should arise.

Software environment: Operating system works with the simple program that picks up cell parameters, atomic symbols, coordinates, displacement parameters and their standard deviations from the file output of the last refinement cycle. The present version works with the SHELX76 system (Sheldrick, 1976). It is an easy matter to provide an analogous interface for other systems. FILTER 2 orders the atom list by using a linear search and insertion in an array of dynamically allocated linked lists. TABLE 1 does the actual formatting and tabulation. Three tables are produced: atomic coordinates with e.s.d.'s, displacement parameters, both isotropic and anisotropic, with e.s.d.'s and calculated H-atom positions, if any. FILTER 3 is a small interface program. TABLE 2 produces the bond distances and angles table. It is interactive, allowing the user to specify any symmetry operation. Distances and angles are optionally displayed on the screen before being written to the output file and they can be selected, deleted and reordered at will in real time. The input for the series of programs is minimal: the original least-squares output file and a few commands specified interactively in response to the program’s prompts. All the tables are ready for publication, except for a little retouching needed for inserting some unusual characters. However, being stored as text files, they can be modified with a text editor if the need should arise.

Hardware environment: Computer: Prime 550, 32-bit word, 8-bit byte. For 100 atoms, 120 distances and 180 angles, TABLE 2 requires about 12 kbyte of high-speed memory. The other programs take much less space. More memory would not improve the speed of calculation. Peripherals: disk (or floppy, on a micro) and printer.

Program specification: The number of atoms that can be treated is only limited by the core memory available, provided dimensions of arrays are set accordingly. The CPU time for running all the programs is 80s for 100 atoms. The length of the programs is about 3000 lines, including comments and spacing. The programs have been in use for one year with excellent results.

IMPORTANT: The programs have been in use for one year with excellent results.

Challenge: Software environment: Operating system works with the simple program that picks up cell parameters, atomic symbols, coordinates, displacement parameters and their standard deviations from the file output of the last refinement cycle. The present version works with the SHELX76 system (Sheldrick, 1976). It is an easy matter to provide an analogous interface for other systems. FILTER 2 orders the atom list by using a linear search and insertion in an array of dynamically allocated linked lists. TABLE 1 does the actual formatting and tabulation. Three tables are produced: atomic coordinates with e.s.d.'s, displacement parameters, both isotropic and anisotropic, with e.s.d.'s and calculated H-atom positions, if any. FILTER 3 is a small interface program. TABLE 2 produces the bond distances and angles table. It is interactive, allowing the user to specify any symmetry operation. Distances and angles are optionally displayed on the screen before being written to the output file and they can be selected, deleted and reordered at will in real time. The input for the series of programs is minimal: the original least-squares output file and a few commands specified interactively in response to the program’s prompts. All the tables are ready for publication, except for a little retouching needed for inserting some unusual characters. However, being stored as text files, they can be modified with a text editor if the need should arise.

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Labratory Notes


A lathe-like crystal grinder for grinding pre-aligned crystals into cylindrical cross section

A lathe-like crystal grinder that uses a self-feeding diamond grinding wheel to grind pre-aligned crystals into cylindrical cross section is described. The instrument has been designed to provide crystals giving uniform absorption as a function of crystal rotation when used with conventional Weissenberg equipment.

Uniform absorption at a given scattering angle is a necessary condition for the application of the empirical background correction of Welberry (1983) to diffuse scattering data obtained from Weissenberg photographs of disordered molecular crystals. Such uniformity can be realized by using either spherical or cylindrical crystals. A spherical crystal, however, must be shaped before alignment and, with the removal of all crystal faces and edges, the task of aligning the crystal about a desired rotation axis becomes a difficult one. For this reason, devices that grind crystals into cylindrical cross section after the crystal has been mounted on a goniometer head and aligned about a desired rotation axis are preferred to crystal spherizers. Barbieri & Durand (1956) have described a device that utilizes a sandblasting technique to grind aligned crystals into cylinders but, unfortunately, this requires the crystal to be mounted on a metal pin. We require the crystal to be mounted on a quartz fibre in order to minimize scattering from the support. The mechanical grinder we have designed grinds the crystal in situ in the sense that, once mounted on a quartz fibre and aligned about the desired rotation axis, the crystal is not removed from the goniometer head. No realignment has been found necessary after grinding.

A labelled photograph of the instrument is shown in Fig. 1. It consists of: a base plate (F) designed to slot onto the stage of an 'Olympus' binocular microscope; three movable support plates (C),