stallographic 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: Primos 19. All the programs are written in Pascal. No overlays.

**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.

**Documentation:** For users: documentation in machine-readable form and online in the form of interactive messages. For maintenance and modification: the clear structure of the programs makes them self-documenting, comments help clarify difficult points and a few implementation-dependent details are well insulated and pointed out.

**Availability:** Documentation and program listings may be obtained from the author. (Tapes: 1600 b.p.i., EBCDIC, 1 reel 80 fixed, block size 3200 bytes).

**Keywords:** Typist; Typecryst.

**Reference**


**Laboratory 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),

![Fig. 1. An overhead photograph of the crystal grinder.](image-url)
(J) and (K); two DC 0–10 V drive motors (D) and (I); one 24 h AC drive motor (L) with a two-way friction clutch; a diamond grinding wheel (E); a spring-loaded pivoted arm (B) held against a cam (A); and a gas nozzle (G) and needle valve (H).

Support plates (C) and (J) are held to the base plate (F) by locking clamps and they are free to slide along a common keyway whose axis is parallel to the crystal rotation axis. The position of the keyway is such that the crystal rotation axis is coincident with the equator of the field of view of the microscope. Support plate (J) holds a housing for the goniometer head and drive motor (I), which rotates the goniometer head via a belt drive – chosen to minimize transfer of motor vibration to the goniometer head and crystal. Support plate (C) holds the pivoted arm (B), which houses the direct-drive grinding-wheel drive motor (D) and support plate (K), which is keyed to translate transversely to the crystal rotation axis. Support plate (K) holds the cam (A) and its drive motor (L). The nozzle (G) and associated needle valve (H) are used to direct a stream of dry nitrogen gas at ca 10 kPa onto the grinding wheel, thereby preventing the wheel from clogging with ground material.

Automatic feeding of the grinding wheel onto the crystal is provided by the cam. As the cam is rotated by drive motor (L) it causes arm (B), and hence the grinding wheel, to move about the pivot point. The ratio of the distance from the pivot point to the cam contact point and the distance from the pivot point to the grinding-wheel axis has been set at 3 to 1. Errors incurred by the grinding-wheel axis moving along the arc of a circle rather than horizontally into the crystal are of no consequence. The cam lead is ca 2.75 mm so that with the 24 h motor and the 3 to 1 distance reduction, the grinding wheel is fed onto the crystal at ca 0.04 mm h⁻¹. Presetting of the desired cylinder diameter is accomplished by means of a setting screw that translates support plate (K) towards the pivot point.

For the organic molecular crystalline compounds we have been grinding, a grinding wheel grit size of ca 140 μm at a concentration of 0.88 mg mm⁻³ has given very satisfactory results. Larger grit sizes at the same concentration produce chipping and fragmentation of the crystal while smaller grit sizes at the same concentration produce clogging of the grinding wheel. Lowering the concentration tends to produce scoring of the crystal. With the crystal and grinding wheel moving in the same direction at the point of contact, the orbital speed of the grinding wheel relative to that of the crystal is an important consideration for successful grinding. For the types of crystal we currently use crystal and grinding-wheel rotation speeds of ca 2.5 and 100.0 mm s⁻¹, respectively, produce good results. The crystal speed varies only slightly for drive-motor voltages 0–10 V and so is not critical, but the grinding-wheel speed varies from ca 0 to 400 mm s⁻¹ through the same voltage range. Grinding-wheel speeds that are too high produce chipping and fragmentation, and speeds that are too low grind at a rate slower than the grinding-wheel feed rate, the consequence being that the crystal is severed from its mounting.

Fig. 2(a) shows an aligned crystal of 1,3-dibromo-2,6-diethyl-4,5-dimethylbenzene prior to grinding. It has been mounted about its a axis on a quartz fibre of nominal diameter 0.1 mm using slow-curing epoxy adhesive. To give the fibre greater rigidity it has been glued into a quartz sleeve so that only ca 2 mm is protruding. The quartz sleeve is glued to a brass mounting pin that is clamped into the goniometer head.

Fig. 2(b) shows the crystal after grinding and after having been polished by dipping in mild solvent. Both the cylinder diameter and the length of cylindrical cross section are ca 0.5 mm—values that are less than the optimal values for diffuse scattering studies of this type of compound, but immaterial for illustration purposes in this paper. We normally use a cylinder diameter of 0.6–0.8 mm and a cylinder length in excess of 0.8 mm. This length ensures that the length of cylindrical cross section exceeds the beam width and obviates the need to face-off the free end of the crystal. Some scoring of the crystal is evident but the grooves are less than 0.01 mm deep and of no consequence.

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Fig. 2. A crystal of 1,3-dibromo-2,6-diethyl-4,5-dimethylbenzene aligned about the a axis (a) before grinding and (b) after grinding and polishing by dipping in mild solvent. The cylinder diameter is 0.5 mm.