The algorithm used in TREOR for the triclinic symmetry is more focused on the solution of genuine triclinic patterns than the corresponding algorithms originally used by Kohlbeck & Hörl (1976) for treatment of monoclinic and triclinic lattices by the same procedure. The reason is that a truly triclinic pattern can usually be given lower index limits for the low-order lines than a monoclinic pattern rewritten as a triclinic one.

In the following, the term basis line is used for a diffraction line that is given tentative indices in order to derive a unit cell. Five basis-line sets will generally be sufficient for orthorhombic tests, whereas seven sets even will sometimes be insufficient for a monoclinic pattern. The monoclinic failures have usually been caused by unit cells having one cell axis notably shorter than the two others, thus giving rise to dominant zones. More than the five first consecutive lines of the pattern may then be indexed with a common zero index. We have therefore added a special short-axis test for the monoclinic symmetry. In this test the first three lines are tentatively indexed as a two-dimensional pattern, i.e. one index is assumed to be zero. If the following three lines can be indexed by the two-dimensional lattice parameters, then the first unindexable line(s) is/are used to derive the remaining monoclinic cell parameter(s). Depending on whether the two-dimensional lattice is rectangular, i.e. a (hk0) or (0kl) zone, or not, i.e. a (hkl) zone, the program will derive two or one more parameter(s). The trial cells derived by this procedure are then tested for fit with the remaining lines, and the best solutions are saved for later refinement. The solutions are ranked primarily according to the number of indexable lines and secondarily according to the smallest cell volume. The principle used by Taupin (1973), to reject a trial lattice if a line cannot be indexed and this line is not explicitly declared as possibly extraneous, is not used. This is avoided because of the experience that it is often difficult to identify an extraneous line a priori.

In order to improve further the indexing of monoclinic lattices we have added a fast procedure suggested by Smith & Kahara (1975) for finding the (020) reflection. The relation

\[ 2Q_{020} + Q_{010} = Q_{h30} \]

(Q = \sin^2 \theta) is used as '020 detector'. If relations of this type are found, the monoclinic b axis is directly determined and in successive trials (h = 1, 2 and 3) the a axis is defined. Thereafter, the remaining two parameters c and \( \beta \) are defined by trial indexing of two low-order lines. The solutions are tested and ranked as described above.

The short-axis tests and the 020-finding algorithm are useful only for a limited number of problems. Fortunately, however, they have been found to solve many monoclinic
indexing problems, for which the more time-consuming procedure – to include more basis-line sets than those listed in Table 1 – has been less fruitful.

Thus more than 90% of indexed monoclinic patterns have been indexed without increasing the number of basis-line sets. From this it follows also that the probability is high for the presence of a truly triclinic phase, if monoclinic and higher-symmetry tests fail.

Control parameters

Although the general principles used for trial-and-error indexing are relatively simple and straight-forward, the success of the method is a function of data quality and crystallographic decisions put into the program. An essential part of the TREOR program is therefore a standard set of parameter values. They are termed normal values and represent accumulated experience from several hundreds of indexing problems. The parameters are referred to by key-words, and they may easily be changed by the user. In order to make the program user-oriented, key-words may be used in a very free way. An arbitrary number of key-words in arbitrary order may be used, and the data are given in free format.

The normal choice of basis-line sets and their index limits are listed in Table 1. A useful basis-line set must be a function of all cell parameters and must not contain an impurity line. Therefore several sets are always used.

Although the index limits rarely have to be increased, it is sometimes necessary to use more monochinic basis-line sets than those listed in Table 1. In order to avoid unduly time-consuming tests, however, the basis-line restrictions imposed on the triclinic symmetry cannot be changed by any key-words. Usually only the first 19 lines are used in the trial phase of the calculations. Furthermore, parameters obtained from the first seven lines are automatically adjusted by higher-order lines if such lines are available in the data set.

Maximum values for the unit-cell volume and the cell axes should be given by the user. The parameters are generally not crucial for orthorhombic or higher symmetries where they may be given some standard value: \( V_{\text{max}} = 2000 \, \text{Å}^3 \) and cell-axis maximum = 25 Å. For the monoclinic symmetry, however, it has been found that a first trial should be made with \( V_{\text{max}} = 1000 \, \text{Å}^3 \), after which the limit may be increased in steps of 500 Å³. The reason for this procedure is that a correct unit cell may index fewer lines than false cells of too large dimensions. Unless the correct cell is ranked as one of the five best obtained from a monoclinic basis-line set it will not be saved for eventual least-squares refinement.

Approximations based on the symmetry and the \( d \) spacing of the 20th line have been proposed for unit-cell volumes (Kohlbeck & Hörl, 1976; Shirley, 1980). Unfortunately, they are usually unreliable for monoclinic and higher symmetries. As long as the space group is unknown, systematic absences cannot be taken into account. The triclinic space groups, however, do not exhibit any systematic absences. Thus the approximation suggested by Smith (1977), \( V = 13.39 \, d_{20}^3 \), is usually rather close to the correct cell volume and may be used with an addition of a few hundred \( \text{Å}^3 \) as \( V_{\text{max}} \).

The computing time is strongly dependent on the \( V_{\text{max}} \) parameter. It is therefore important not to allow unrealistically large cell volumes in triclinic calculations, which can be very time consuming. This is another reason for treating the triclinic case separately.

An important part of the program is an extensive comment list, containing not only default values of the parameters and test examples but also recommended strategies for using the program, and a check list for interpretation of the results.

Computing methods

The reciprocal-cell relationship may be written

\[ Q(hkl) = h^2 x_1 + k^2 x_2 + l^2 x_3 + h k x_4 + h l x_5 + k l x_6. \]

Each trial set of \( x_i \) is derived from a system of linear equations \( M X = L \), where \( M \) is a square matrix containing the Miller indices, \( X \) is the unknown parameter set \( x_i \) and \( L \) is the set of observed \( Q \) values for the basis lines used. The dimensions of the \( M \) matrix and the \( X \) and \( L \) vectors depend on the symmetry. For monoclinic and higher symmetries the parameters \( x_i \) are found by Cramer’s rule. In order to minimize the computing time, sub-matrices are saved and

### Table 1. Normal basis-line sets and hkl restrictions used by TREOR

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Basis-line sets (Line numbers)</th>
<th>Max.</th>
<th>Max.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubic</td>
<td>([1(2)])</td>
<td>444</td>
<td>6</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>([(1, 2) (1, 3) (2, 3)])</td>
<td>444</td>
<td>4</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>([(1, 2, 3) (1, 3, 4)])</td>
<td>222</td>
<td>3</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>([(1, 2, 3, 4, 5, 6)])</td>
<td>111</td>
<td>1*</td>
</tr>
<tr>
<td>Triclinic</td>
<td>([(1, 2, 3, 4, 5, 6)])</td>
<td>111</td>
<td>2</td>
</tr>
</tbody>
</table>

*The first triclinic line is always set to be 100 and the second line is only given positive indices.

### Table 2. CPU times used on a VAX 11/750 to index the powder diffraction patterns in NBS Monograph No. 25, section 17 (Morris et al., 1980)

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Min. (s)</th>
<th>Max. (s)</th>
<th>Number of indexed patterns</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubic</td>
<td>1</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>3</td>
<td>91</td>
<td>5</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>18</td>
<td>73</td>
<td>4</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>6</td>
<td>107</td>
<td>19</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>16</td>
<td>216</td>
<td>15</td>
</tr>
<tr>
<td>Triclinic</td>
<td>2</td>
<td>916</td>
<td>5</td>
</tr>
</tbody>
</table>
The monoclinic data set from sodium perchlorate hydrate, contains two cubic, five tetragonal, four hexagonal, 19 orthorhombic, 18 monoclinic and six triclinic patterns. According to our experience monoclinic and triclinic patterns cannot usually be indexed reliably on the basis of powder diffraction data alone, if the cell edges are longer than 25 and 20 Å, respectively. Therefore the monoclinic phenylhydrizine hydrochloride, \( C_6H_4N_2HCl \) with \( b = 30.641 \, \text{Å} \), and the triclinic clenpentioxol hydrate, \( C_2H_2ClNO_2 \cdot 2H_2O \) with \( b = 21.939 \, \text{Å} \), were not indexed.

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For comparison a Guinier–Hägg photograph of ammonium persulfate, \( \text{(NH}_4\text{)}_2\text{S}_2\text{O}_8 \), was taken with addition of silicon as internal standard. The exposure time was 30 min, and within 15 min from the moment the photograph was dry it was measured and correctly indexed using the Guinier film-scanner system (Johansson, Palm & Werner, 1980). The standard deviations in all parameters and the average difference between observed and calculated diffraction angles were also smaller than those published in the NBS monograph. This is in agreement with the general experience that focusing-camera data are preferable for powder indexing (Shirley, 1980; Smith & Kahara, 1975).

**Final remarks**

The main parts of the program are written in Fortran IV, but some routines, for example the short-axis tests, are written in Fortran 77. These routines can easily be converted to Fortran IV. Full loading of the program on a SORD M68 microprocessor requires a core memory of 60 000 words, i.e. 120 000 bytes. Segmentation of the program is possible. The program is available from this Institute.
The authors wish to thank Professor P. Kierkegaard for his kind interest in this work. This work has received financial support from the Swedish Natural Science Research Council.

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. KRAGTEN 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; Stereo-specific projection; Plotting routines.

Reference


TYPIST – a program for the tabulation of crystallographic results. By M. TOMASSINI, Department of Earth Sciences, Piazza Università, 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-