(19) reduces to equation (94) of Fraser & Suzuki (1976) (except for a typographical error where \( a \sigma_2 - b \sigma_3 \) should read \( a \sigma_2 - b \sigma_3 \)). For an error estimate, we use

\[
E_3 = b[(\sigma_0 - \sigma_n) + \Delta](\sigma_0 + \sigma_n)\sigma_n^2/6
+ |\sigma_n - \min(0.5, 2\sigma \sigma_n)(\sigma_1^2 + \sigma_2^2)|/6,
\]

where

\[
\Delta \equiv [2\min(c_1, c_2\sin^2\sigma)]^{-1/2},
\]

\[
s_m \equiv \sigma_m + \Delta.
\]

When \( d_2 \) is large we use the first three terms in an asymptotic expansion of \( t_3(d_2) \). Equation (19) with \( N = \infty \) then becomes

\[
H_4 = \left[ a/(a - 2bd_2) \right] \exp(-a \sigma_2 - bd_2 + z)
\times \left[ 1 - (z^2 + 4z + 2)/(2dz)^2 + (z^4 + 16z^3 + 72z^2 + 96z + 24)/(32d^2) \right],
\]

where

\[
z = d_3/(2d_2).
\]

Although \( E_1, E_2, \) and \( E_3 \) are good criteria for deciding which formula to use, to save computer time we only use them in critical regions. \textsc{Cin} decides which \( H_j \) to use with the following algorithm:

1: if \( \sigma_n < 0.01 \) then go to 6 else
2: if \( \sigma_2 > 8 \) then use \( H_1 \) else
3: if \( a \sigma_2 > 12 \) then use \( H_2 \) else
4: if \( E_2 < \min(E_1, E_3) \) then use \( H_2 \) else
5: if \( E_1 < \min(E_2, E_3) \) then use \( H_1 \) else
6: if \( d_3 < 1 \) or \( d_2 < 12 \) then use \( H_3 \) else
7: use \( H_4 \).


A molecular plotting program. By R. Radhakrishnan, Department of Crystallography and Biophysics,* University of Madras, Guindy Campus, Madras-600025, India

(Received 28 October 1980; accepted 14 September 1981)

Abstract

Computer programs to project crystal packing along any of the three crystallographic axes [Chacko & Varughese (1976). J. Appl. Cryst. 9, 508–509] and to obtain a perspective view of a single molecule [Cole & Adamson (1969). Acta Cryst. A25, 535–539] have been reported. A new computer program to obtain molecular illustrations as line diagrams or perspective views with an option for stereo pairs is presented. The program allows projection of a molecule or unit-cell contents along any desired direction. It has been written for a small(8K)-memory IBM 1130 computer system where Johnson’s [Rep. ORNL-3794. (1965).]

*Contribution No. 565.

Oak Ridge National Laboratory, Tennessee] ORTEP cannot be accommodated and can be easily adapted to any system supporting Fortran IV.

Description of the program

The coordinates of the atoms are usually fed in as fractional coordinates directly obtained from crystal-structure determination, together with unit-cell parameters. The coordinates of atoms of equivalent molecules are generated by suitable symmetries and translations. Atomic coordinates may also be read in the Cartesian system in ångströms, or generated through an algorithm by Thompson (1972) if bond lengths, bond angles and dihedral angles are given. The intramolecular bond matrix is given as pairs of bonded atoms, the atoms being internally numbered in the sequen-

References


Two separate systems are maintained - the 'body' system, which need not be an orthogonal system, and an orthogonal plotting system. The coordinates in the body system are transformed to the plotting system by a suitable transformation matrix. Rotation is performed in the plotting system for projection along any desired direction and the molecule is then scaled to a suitable size. The projection of the molecule(s) is effected onto a plane perpendicular to the viewing direction unlike in the program of Chacko & Varughese (1976) where the atoms are just transferred onto the basal plane in a direction parallel to the axis of projection.

The method of obtaining perspective is the same as that described by Cole & Adamson (1969). No facility is provided to check for 'masked' bonds and atoms, in view of the rather large CPU time involved (~10 min. for 20-30 atoms). It may be noted, however, that this causes no difficulties in stereoviewing. The present program takes only 12-15 min for plotting 200-250 atoms.

The program makes use of standard IBM 1130/1800 plotter routines (FORM C26-3755-2) SCALF, to accept and store scaling information and to define the origin position; F PLOT, to set the pen position; FCHAR, for drawing alphanumeric characters. In addition, a subroutine GEOMV, kindly provided by Professor K. Sundaram, is employed to obtain Cartesian coordinates given bond lengths, bond angles and dihedral angles.

Sample diagrams prepared by the use of this program for valinomycin (Sundaram, 1974) and 2-coumaric acid (Raghunathan & Pattabhi, 1975) are given in Figs. 1, 2 and 3.

A listing of the program in Fortran IV is available from the author on request.

The author thanks Professor K. Sundaram for his encouragement and helpful discussions and for making available the subroutine GEOMV, and Dr E. Subramanian for his interest in the work. Financial assistance from the University Grants Commission and Department of Science and Technology, New Delhi, India, is gratefully acknowledged.

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