array SS(48,3,3). The translation components are handled as integers modulo 24, the translation parts τ are stored in the integer array TS(48,3); these arrays can easily be used in further programs. If a centre of symmetry is present the program provides for a centrosymmetric setting. If the user wants the origin of International Tables for X-ray Crystallography (1952), the reference number of the shift vector is evaluated. If another origin is preferred, the program asks for the shift vector. All shifts are added and applied to the symmetry operations. The shift vector that leads from the new origin to the origin of the symbol is given in the output (see Fig. 2).

The coordinates of the general position of the space group are printed at the end of the program.

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Interactive dynamic molecular display. By CHARLES L. NIX and BYRON RUBIN,* Emory University, Department of Chemistry, Atlanta, GA 30322, USA

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Abstract

A program is described to allow the dynamic graphic manipulation of molecules on a Tektronix 4054 graphics system. The program is useful for structure examination during X-ray crystal structure solution and for visualizing the results of structure determinations.

In looking at the results of a structure determination and often in the course of solving a structure it is valuable to have a facility for visualizing molecules and molecular fragments. Several Fourier programs [for example, FOURR (Hall, Stewart, Norden, Munn & Freer, 1980)] provide lists of peak positions and peak heights. Some programs go further to provide a tabulation of distances and angles between peaks and to provide scaled line-printer point plots of these potential atomic positions which the crystallographer can then join appropriately to reveal the molecule. It would be useful to have a relatively easy way to visualize the structure in three dimensions without needing to build models or resorting to sophisticated computer graphics (Langridge, Ferrin, Kuntz & Connolly, 1981). The program MODIS, which we describe here, displays a line drawing of a molecule which can be rotated on the display in three dimensions in virtually real time. The program, which has many options including one for mono or stereo viewing, is written in an extended version of Basic which contains not only commands for regular storage graphics but also commands which utilize the continuously refreshed dynamic graphics with which the Tektronix 4054 system is equipped. The dynamic graphics capability makes it possible to implement a number of features which make the program particularly useful in the crystallography laboratory.

In using MODIS, the molecular structure data, which consists of the unit-cell parameters and atomic positions, can either be entered from the keyboard or via communication with a central site computer. Thereafter the data is stored on magnetic-tape cartridges and no further communication with the central site is required.

The fractional coordinates entered are converted to Cartesian coordinates and scaled to suit the screen size and the user. In the initialization section of the program, the user specifies the minimum and maximum bond distance from which a table of bonded atoms is created. Then one of a number of program options can be chosen by pressing the appropriate user-defined key.

The orientation of the molecule on the screen can be changed under joystick control around either the horizontal (x) or vertical (y) screen axes. The rate of rotation is controlled by the extent to which the joystick is moved from its home position. MODIS also allows for a set of pre-programmed rotations for getting an overall view of the molecule. The user must enter how many degrees around each of the x, y, and z (perpendicular to the screen) axes he wishes to rotate. The rotation is executed first around x, then y and finally z. At any point the user may stop the rotation completely or stop the rotation and go to the next axis in the rotation sequence.

A center of rotation for viewing the molecule is automatically selected, but can be reset manually, if desired. An option is also provided to allow the display image to be moved anywhere on the screen.

A structure editing feature allows bonds between atoms to be made or deleted. This is used when it is necessary to alter
the bonds created automatically from the coordinate list. For automatic determination a range of distances, say 1–1.8 Å, is input and all atoms within this distance range are placed in the connectivity table.

An option to allow the output of bond angles and lengths and the dihedral angles is also available. Hard-copy output of the molecular drawing on the screen can be produced on a plotter connected to the system. In addition to the plane projections, a stereo viewing option is available.

Allowing rotation of both images of a stereo pair makes the image more realistic. The up/down method of stereo representation is used (Feldman, 1976). In stereo mode the left-eye image is displayed above the inverted image for the right eye. The two images are displayed through polarized filters and are made to converge on a half-silvered-mirror apparatus attached to the front of the display screen. The combined images are viewed through glasses which are polarized to correspond to the polarization of the left- and right-eye images.

We also use MODIS to find an appropriate view for creating a more elaborate drawing with ORTEP (Johnson, 1965).

We will be happy to reply to any inquiry, and can furnish a listing or a copy of the program on your data cassette.

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References


