A Newman projection computer program. By N. P. BRANDENBURG, Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, Amsterdam, The Netherlands

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In this paper a FORTRAN IV computer program is described, which calculates all usual Newman projections for a given crystal structure. Each projection is represented by a printed diagram and may be plotted. In conjunction with the X-Ray 72 system of crystallographic programs the program is brought to operation by just one card, but it can also be used independently if the atomic parameters and cell constants are specified.

A Newman projection is a projection along an interatomic bond showing dihedral angles as illustrated in Fig. 1. The complete set of Newman projections provides an insight into the geometry of a molecule and allows an easy construction of molecular models. Because general geometry programs confine themselves to the computation of user-specified dihedral (torsion) angles, a program has been written which calculates all Newman projections of a molecule with only a very small amount of specific data input.

The input of the program consists primarily of the atomic parameters. These can be given on cards or can be read from a binary data file in the format of the X-Ray 72 system of crystallographic programs (Stewart, Kruger, Ammon, Dickinson & Hall, 1972).

A bonding matrix, which lists the atoms bonded to each atom is computed from the parameter list by means of a set of distance criteria, defined such that interatomic distances are recognized as bonds. For the most frequently occurring distances standard criteria are built in, which can be modified or extended if necessary. The bonding matrix may also be given on cards. The flexibility of the input system is further enlarged by means of an updating system, incorporated in the program for correcting both the atomic parameter list and the bonding matrix. Projections associated with any pair of non-bonded atoms can also be calculated.

In the output bond distances and angles, a survey of fractional and projection coordinates and the list of dihedral angles is given. In addition each Newman projection is represented by a printed diagram, as shown in Fig. 2(a). To obtain the conventional drawings a subroutine is included for use on a Calcomp plotter model 563. The result of this plot subroutine is shown in Fig. 2(b).

The Newman projection program has been written in FORTRAN IV and was tested on a CDC, CYBER 73-26 computer. It uses ca. 21000 words of central memory and consists of a deck of ca. 900 cards. The program and further information may be obtained from the author. A less sophisticated ALGOL 60 Newman projection program, written by Dr H. Schenk is also available. This program utilizes the same plotter and produces plots as given in Fig. 2(b).

Reference