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An aid for the application of the Fourier transform method to planar molecules.

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Since the fundamental work of Ewald (1935) it has been shown that the structure determination of a crystal containing planar molecules may be considerably simplified by the application of Fourier transform principles (Knott, 1940; Klug, 1950).

Lipson & Taylor (1951) and Hanson (1953) have developed for this purpose optical diffraction methods which allow the square of the Fourier transform of a structure to be obtained as its two-dimensional diffraction pattern.

An alternative method consists in calculating the Fourier transform of a single molecule and then determining the most appropriate rotation of its reference frame with respect to the reciprocal axes of the crystal. The application of this procedure to a projection requires cutting the three-dimensional transform by an equatorial section of the reciprocal lattice at an angle which depends on the orientation of the molecule in the crystal. For planar molecules, this is equivalent to projecting a normal section of the transform on the equatorial section of the reciprocal lattice appropriately oriented with respect to the plane of the transform (Lipson & Cochran, 1954). The signs of the structure factors may then be obtained by direct sampling, and a first Fourier synthesis is computed which may be refined by the normal procedure.

We have applied this last method in our laboratory to a number of structure determinations, and found it very convenient to use the simple device shown in Fig. 1 for the determination of the optimum orientation of the reciprocal-lattice section.

A plot of the transform, photographically recorded on a glass plate, is projected by means of parallel light on a circular plate, on which a weighted equatorial section of the reciprocal lattice has been drawn. By giving the plate all the degrees of freedom about its centre it is easy to obtain the setting which gives the best agreement between the values of the transform sampled at reciprocal-lattice points and the experimental structure amplitudes.

The components of the apparatus are indicated in Fig. 1. They consist of a compact-source lamp *A*, a plano-convex lens *B* of 20 cm. diameter and 50 cm. focal length, a rectangular plateholder *C*, 18×24 cm., carrying the slide of the transform, and a square frame *D* mounted on a support which allows rotations through 90° around two perpendicular directions. Angles of rotations can be read on the two goniometers *E* and *F* to about 1°. The plate held in the frame *D* is made from a Perspex sheet, at the centre of which a hole is drilled in order to fix a disc by means of a pin. The weighted reciprocal-lattice section is drawn on this disc with the origin at the centre. The disc can be rotated through 360° around its centre and the angle can be read to about 1° on a graduated circle engraved on the Perspex plate.

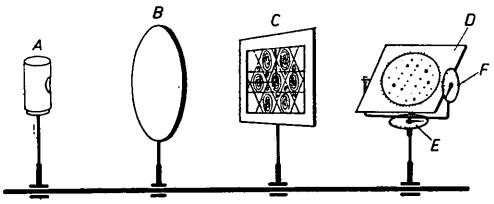

Fig. 1. Drawing of the projector used for fitting a calculated Fourier transform into a weighted reciprocal-lattice section.

A 10 cm. scale for the radius of the limiting sphere is adopted both in the drawing of the reciprocal-lattice section and in the photographic reduction of the transform.

The transform is very conveniently calculated as a double Fourier summation, using Beevers & Lipson strips. Values of the electron-density distribution of a molecular model sampled at regular intervals of an appropriate cell are used as coefficients. The time needed for this calculation (20–40 hr.) is largely compensated, in favourable cases, by the speed and simplicity by which the transform is fitted into the reciprocal lattice.

This method is simple and convenient to apply, especially when the molecules are centrosymmetrical and their centres lie at special positions of the unit cell.

Molecules lying at general positions but forming centrosymmetrical planar dimers (Lipson & Cochran, 1954) can be treated as above.

The device is also very helpful when, as in the more general case, the Fourier transform of each molecule contained in the unit cell is modulated by a 'fringe function', and the agreement between the transform and the structure amplitudes must be sought on a quasi-statistical basis (Hanson, Lipson & Taylor, 1953). It allows different possibilities to be tested in a relatively short time.

It should be mentioned, however, that this method offers no special advantages over existing techniques (Lipson & Taylor, 1951; Hanson, 1953) in the application to projections with plane symmetry *pgg*, where the projected molecules have not the same orientation. It is hoped to develop it further for this special case.

The use of the device which has been described is not limited to the application of the Fourier transform method, but may be extended to other common problems connected with X-ray structure determinations. It is, for example, currently employed in our laboratory for projecting molecular models on preliminary Fourier maps, and for making anisotropic thermal corrections.

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