*Acta Cryst.* (1952). **5**, 145

## A simplified Fly's Eye procedure.

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(*Received* 24 *August* 1951)

The Fly's Eye (Bragg, 1944; Stokes, 1946; de Vos, 1948) is now an accepted device for use in the initial stages of a crystal-structure determination, since it enables the user to decide rapidly whether or not a proposed atomic arrangement is approximately correct (Bunn, 1945; Crowfoot, Bunn, Rogers-Low & Turner-Jones, 1949). The aim of the present note is to point out that the experimental procedure can be considerably simplified by the use of the diffraction spectrometer (Taylor, Hinde & Lipson, 1951).

The Fly's Eye is a device for making diffraction gratings with a fine structure, which can be made to correspond to the projection of a crystal structure on to one face of a unit cell; the diffraction pattern obtained by illuminating this grating with a parallel beam of light should correspond to the appropriate zone of X-ray intensities. It is customary to produce diffraction gratings with several hundred elements, but this is not strictly necessary: if only four elements, corresponding to the projection of four adjacent unit cells, are used, a diffraction pattern is obtained which is crossed by two sets of parallel, equidistant fringes, which divide it into small areas corresponding to the reciprocal-lattice points.

A typical result is reproduced in Fig. 1 which shows (*a*) the diffraction pattern of a mask representing the (001) projection of a single unit cell of *p*-di-isocyanobenzene (Hulme, 1952), (*b*) a mask representing the projection of four adjacent unit cells, (*c*) the diffraction pattern of (*b*), and (*d*) the corresponding section of the reciprocal lattice weighted with the unitary structure factors (Harker & Kasper, 1948). Comparison of (*c*) and (*d*) constitutes a verification of the approximate correctness of the structure. It should be remarked, however, that the unit cell is the primitive one containing one molecule, and not the crystallographically preferable centred cell containing two molecules. The latter could be used, but it would involve making a mask with eight molecules.

The testing of a structure takes only a few minutes unless a permanent record is required; then the photographic processes take considerably longer than the rest of the operation. In addition to rapidity, however, the process has other advantages. First, it gives an undistorted representation of the reciprocal lattice, whereas the other devices quoted necessitate distortion to a square net. Secondly, it indicates which intensities are likely to be influenced by small changes in atomic position; if a reciprocal point lies in the middle of a region of zero intensity, like the point *A* in Fig. 1 (*d*), no small change will affect it appreciably, whereas if it lies on a steep gradient, like the point *B*, its intensity may be altered greatly. The disadvantage of the method—the fact that it gives diffuse areas in place of sharp spots—is likely to be of aesthetic importance only.

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*Acta Cryst.* (1952). **5**, 145

## A plea for the proper use of the Hermann–Mauguin space-group symbols.

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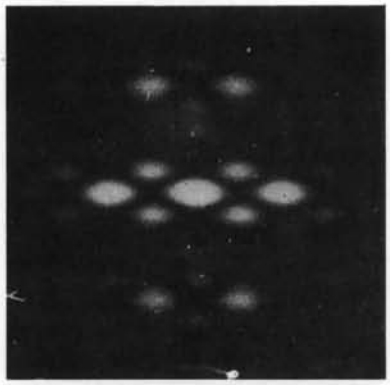
(*Received* 30 *August* 1951 *and in revised form* 27 *September* 1951)

The Hermann–Mauguin symbols for space groups are explicit about the orientation of the essential symmetry elements present in the crystal. Thus† $Pca2_1$ shows not only that there are two glide planes present, but that one is perpendicular to **a** with glide component $\frac{1}{2}$**c**, and that the other is perpendicular to **b** with glide component $\frac{1}{2}$**a**. If for reasons of convenience (or because of the accidental order in which the crystal axes were measured!) the crystal were differently oriented, it would no longer be correct to represent its space group as $Pca2_1$; it would become one of $P2_1ab$, $Pc2_1b$, $Pb2_1a$, $Pbc2_1$ and $P2_1ca$. The appropriate symbols for space groups in non-standard orientations are set out in the *Internationale Tabellen* on pp. 34–44.

Unfortunately, the power of the Hermann–Mauguin symbols to show both the orientation and the type of a symmetry element is overlooked by some workers, and this has involved the Editors of *Structure Reports* in considerable correspondence. When the absent reflexions (or tables of observed reflexions) are explicitly quoted no great harm is done, but the following examples, all

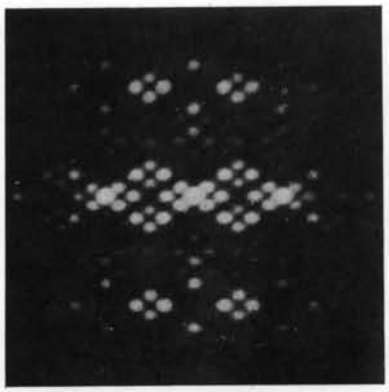
* General Editor of *Structure Reports*.

† In the new *International Tables for X-ray Crystallography* Hermann–Mauguin symbols of the type $Pca2_1$ or $P4_2/nbc$ will be printed with the nature of the axis explicitly indicated. In the *Internationale Tabellen* these were abbreviated to *Pca* and *P4/nbc*. The new usage is followed in this note, except in quoting.

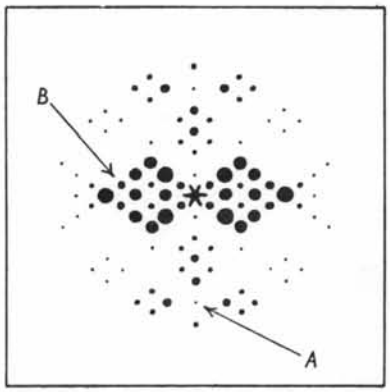


(*a*)

(*b*)



(*c*)




(*d*)

Fig. 1. (*a*) Diffraction pattern of a mask representing (001) projection of a single unit cell of *p*-di-isocyanobenzene. (*b*) Mask representing projection of four adjacent unit cells. (*c*) Diffraction pattern of (*b*). (*d*) Reciprocal lattice weighted with unitary structure factors.

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