along a plane which cuts across the chain direction, so that part of the total length of chain is taken up with corner turning, and (*c*) because the bulkier side-chains may cause the main chains to meander.

While possibility (*c*) is entirely speculative at the present stage, there are sufficient data to allow more detailed discussion of (*a*) and (*b*). The haemoglobin molecule consists of two chemically and structurally identical halves; this is shown by its dyad symmetry in the crystal, by its dissociation in dilute solution and by the fact that the molecular weight of globin is 33,000, while that of haemoglobin is 67,000. If the two halves of the molecule are related by the dyad axis, they are likely to be joined together along a plane containing that axis. Since the dyad is level with the central layer of chains, the plane joining the two halves must cut across the chain direction (Fig. 7). The total length of the molecule along *a* is about 60–70 Å (Bragg & Perutz, 1952), which means that no chain can continue along a straight line for more than about 30 Å before it is forced to turn a corner. According to Porter & Sanger (1949, p. 121) globin contains three separate chains, comprising 290 residues, which would be about 440 Å long altogether. If these are to be split up into 30 Å lengths, there must be 15 such lengths and the three chains must turn 12 corners, making 24 corners for the whole haemoglobin molecule.

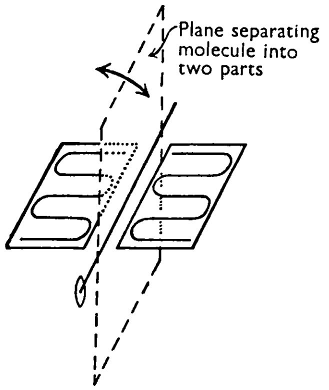

Fig. 7. The splitting of the central layer of polypeptide chains by the crystallographic dyad axis.

The fraction of chain taken up with turning corners would diminish $|F(063)|$ both by reducing the total length of straight chain and by superimposing a non-uniform background between them. No quantitative estimate of this effect is as yet possible. Further reduction may be due to possibility (*b*), i.e. lack of alinement of the chains in the two halves of the molecule. Some such lack of alinement is indicated by the weakness of $|F(006)|$ relative to $|F(063)|$. The ratio of these two amplitudes (0·62) would be compatible with a relative displacement of the two halves by about 2·5 Å in the direction normal to 001, which would reduce $|F(063)|$ by a factor of about 0·9.

For the time being it is impossible to judge whether corner turning, lack of alinement, non-uniform background and meandering from straight parallelism can account for the low absolute value of F, or whether part of the molecule is occupied by structures other than straight chains running parallel to the *a* axis.

The authors wish to thank Dr Ray Pepinsky of State College, Pennsylvania, for his kindness in calculating sixty-four alternative Fourier projections on his X RAC machine, and Mr H. E. Huxley for taking two of the precession photographs. They are grateful to the Medical Research Council for financing this research. One of them (E.R.H.) is indebted to the University of Wales for a Fellowship.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.*

Acta Cryst. (1952). **5**, 141

An illustration of the optical basis of Wilson's X-ray method for detecting centres of symmetry.

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(*Received* 27 *July* 1951)

During the development of optical methods for interpreting X-ray diffraction data (Lipson & Taylor, 1951; Taylor & Lipson, 1951), it has been necessary to prepare optical diffraction patterns of both centrosymmetrical and non-centrosymmetrical objects. The patterns given by these two types of object differ in a most striking way, as can be seen from the typical examples given in the figures. Diffraction patterns derived from centrosym-

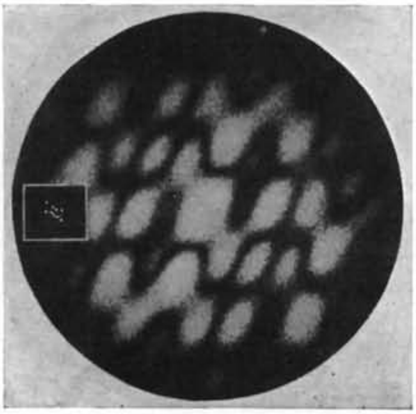

Fig. 1. Optical diffraction pattern of the centrosymmetrical arrangement of holes shown inset.

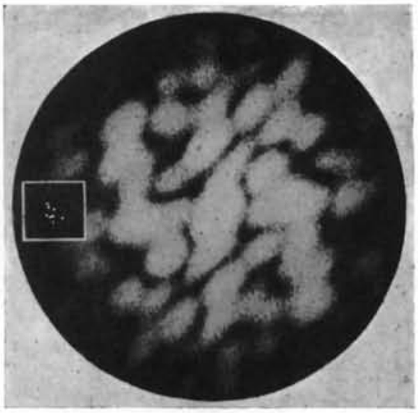

Fig. 2. Optical diffraction pattern of the non-centrosymmetrical arrangement of holes shown inset.

metrical objects consist of comparatively well-defined peaks, separated by regions of low intensity (see Fig. 1); diffraction patterns of objects without a centre of symmetry are hazier and have larger regions of medium intensity (see Fig. 2). This arises because the phase in the diffraction pattern of a centrosymmetrical object can only change in units of π and the amplitude must pass through zero at each change; continuous change of phase can occur in the diffraction pattern of a non-centrosymmetrical object without a directly related amplitude change.

This characteristic difference provides a useful visual demonstration (in two dimensions) of the optical basis of Wilson's statistical theories of the effect of a centre of symmetry on the distribution of X-ray intensities (Wilson, 1949). Optical diffraction patterns are the Fourier transforms of the two-dimensional objects from which they are derived. If, therefore, the object is made to represent the projected contents of a single unit cell of a crystal, the corresponding zone of X-ray intensities can be evaluated by sampling the optical diffraction pattern at the points of the reciprocal lattice.

Obviously the chance of obtaining a very low or very high intensity when this sampling is done on a pattern of the type represented by Fig. 1 is greater than if it is done on one of the type shown in Fig. 2, whereas the chance of a medium intensity is greater for patterns like Fig. 2. The full range of intensities cannot be recorded on a single photograph but the difference in proportion of very low intensities is very marked in the figures shown here.

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Acta Cryst (1952). **5**, 142

Sur la structure de l'indigo et de ses dérivés.

Par Hélène von Eller, *Service de Radiocristallographie du Laboratoire de Chimie C, Sorbonne, Paris, France*

(*Reçu le* 12 *juin* 1951)

La sublimation de l'indigo, du thiaindigo et du sélénoindigo, à la pression atmosphérique et à différentes températures, nous a permis d'obtenir une seule forme cristalline pour le premier composé, deux formes pour le second et au moins trois pour le troisième. Tous les cristaux se présentent en minces plaquettes allongées. Seules les formes mentionnées dans le Tableau 1 ont été retenues en vue d'une analyse structurale.

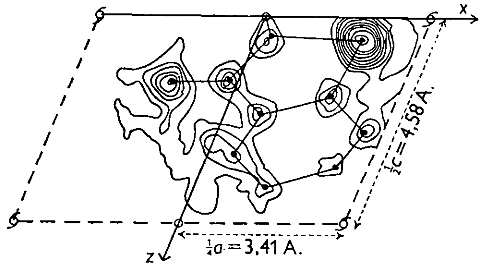

Fig. 1. Sélénoindigo extinction droite; projection de Fourier–Bragg $z0x$.

Les paramètres des mailles élémentaires de l'indigo et du sélénoindigo à extinction droite, d'une part, et ceux du thiaindigo et du sélénoindigo à extinction oblique, d'autre part, étant très voisins, nous laissent prévoir que ces cristaux sont respectivement isomorphes. Les différentes mailles élémentaires contiennent deux molécules. Ces molécules sont donc centrosymétriques et s'identifient à celles de l'isomère éthylénique *trans*. Ceci avait déjà été mis en évidence, pour l'indigo, par Reis & Schneider (1928).

Les projections de Patterson $z0x$, $x0y$ et $y0z$ du sélénoindigo à extinction droite fournissent immédiatement les coordonnées de l'atome de sélénium:

$$x = 0{,}161, \quad y = 0{,}222, \quad z = 0{,}053.$$

La méthode de l'atome lourd conduit, en particulier, à la projection de Fourier–Bragg $z0x$ (Fig. 1) sur laquelle il apparait clairement que la molécule correspond bien à l'isomère èthylénique *trans*.

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Tableau 1

	Face prépondérente	Direction d'extinction	Groupe spatial	a (Å)	b (Å)	c (Å)	β (°)	d_c	d_m	n
Indigo, extinction droite	(001)	‖ à 010	$P2_1/a$	$12{,}3_1$	$5{,}7_5$	$9{,}3_2$	116	1,48	1,48	2
Thiaindigo, extinction droite	(100)	‖ à 010	$P2_1/a$	$20{,}_2$	$3{,}9_2$	$7{,}8_2$	93	1,59	1,56	2
Thiaindigo, extinction oblique	(010)	34° de 001	$P2_1/a$	$7{,}8_2$	$20{,}_4$	$3{,}8_7$	102	1,57	1,57	2
Sélénoindigo, extinction droite	(001)	‖ à 010	$P2_1/a$	$13{,}6_6$	$5{,}9_2$	$9{,}1_7$	113	1,90	1,91	2
Sélénoindigo, extinction oblique	(010)	36° de 001	$P2_1/a$	$7{,}_8$	$21{,}_2$	4,06	109	2,04	2,15	2