them. On the basis of a monoclinic cell these spots receive the following indices:

Zero layer	060	First layer	031 and 091
Second layer	062	Third layer	033 and 093
Fourth layer	064	Fifth layer	095
Sixth layer	066		

The presumption appears strong that the five of these distinctive reflexions with $l > 2$ should have indices of similar form to those with $l \leqslant 2$.

Finally, it should be pointed out that the assumption of triclinic symmetry does not explain the low b value which corresponds to the position of the 020 reflexion. This is observed by Padurow, and has also been systematically observed by other workers. Both this effect, and also the corresponding one on the weak 040 reflexion not observed by Padurow, are accounted for by Aruja's structure. It should also be observed that the reflexion indexed by Padurow as 090 and used in calculating the b parameter is equally well indexed as 700; indeed, photometric studies show that its breadth falls in line with those of $h00$ reflexions but not with those of $0k0$ reflexions.

My thanks are due to the Directors of Ferodo Ltd. for permission to publish this communication.

References

ARUJA, E. (1943). Ph.D. Thesis, Cambridge.
PADUROW, N. N. (1950*a*). *Acta Cryst.* **3**, 204.
PADUROW, N. N. (1950*b*). *Acta Cryst.* **3**, 200.
WARREN, B. E. & BRAGG, W. L. (1930). *Z. Krystallogr.* **76**, 201.
WARREN, B. E. & HERING, K. W. (1942). *Ber. dtsch. phys. Ges.* **23**, 308.
WHITTAKER, E. J. W. (1951). *Acta Cryst.* **4**, 187.

Acta Cryst. (1952). **5**, 144

The structure of *p*-di-isocyanobenzene.

By RALPH HULME, *Chemistry Department, University College, Achimota, Gold Coast, British West Africa*

(*Received* 16 *August* 1951 *and in revised form* 24 *August* 1951)

Transparent needle-like single crystals of *p*-di-isocyanobenzene (New & Sutton, 1932) have been obtained which show a marked tendency towards chemical decomposition; this is normally complete in about three days and appears to be accelerated in X-radiation. Because of this, complete X-ray data have been obtained only about one axis (*c*), although there is a small amount of information available about the other two axes.

The X-ray photographs indicate a monoclinic unit cell,

$$a = 9{\cdot}80,\quad b = 7{\cdot}15,\quad c = 4{\cdot}72\,\text{Å},\quad \beta = 97^\circ\ 11',$$

corresponding to two molecules per unit cell. The absent reflexions correspond to one of the three space groups *C*2/*m*, *C*2, *Cm*—probably the first.

Considerations of cell size and Patterson syntheses about all three axes indicate the approximate general positions of the molecules. Trial Fourier syntheses were made for the projection along the *c* axis, the molecule being assumed to lie in the special twofold positions of the centro-symmetric space group *C*2/*m*. This led to a satisfactory electron-density map showing a plan of the molecule tilted approximately 45° about the broken line (Fig. 1). Close agreement was found between the thirty observed and calculated structure factors;

$$\Sigma(\Delta F) \div \Sigma F = 18{\cdot}5\,\%$$

(cf. Hanson & Lipson, 1952).

The resulting fractional parameters are:

	x	y	z
C_1	0·100	0	−0·21
C_2	0·050	0·167	−0·11
C_3	−0·050	0·167	0·11
N_1	0·207	0	−0·44
C_4	0·295	0	−0·62

the z parameters being less certain than the x and y parameters, since they were not directly observed. These parameters correspond to the alternative structures II or III (Fig. 1), which, in plan, differ but slightly, and only in the parameter of the terminal carbon atom. Type III seems less probable than II in view of the evidence from other physical measurements (New & Sutton, 1932; Hammick, New, Sidgwick & Sutton, 1930). Any change in the parameters towards a structure of type I is found to spoil agreement between observed and calculated structure factors very considerably.

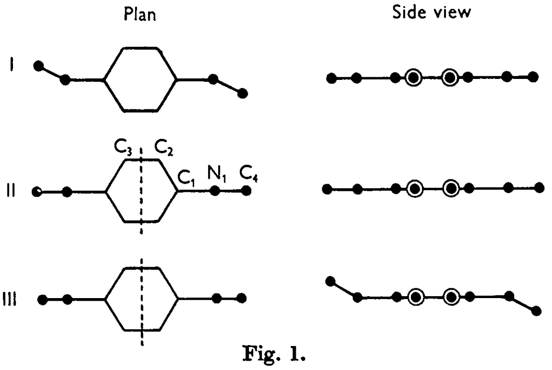

Fig. 1.

When the difficulties connected with the instability of the crystal have been more effectively surmounted, it is hoped to obtain complete data about the other axes. It will then be possible to define the atomic positions more accurately, and to decide finally between structures II and III.

My thanks for helpful discussions are due to my supervisor, Dr H. Lipson, and also to Dr A. Burawoy, both of the College of Technology, Manchester, where most of this work was carried out during the tenure of a maintenance grant from the Department of Scientific and Industrial Research.

References

HAMMICK, D. L., NEW, R. C. A., SIDGWICK, N. V. & SUTTON, L. E. (1930). *J. Chem. Soc.* p. 1876.
HANSON, A. W. & LIPSON, H. (1952). *Acta Cryst.* **5**, 145.
NEW, R. C. A. & SUTTON, L. E. (1932). *J. Chem. Soc.* p. 1415.