Crystal Structure of *Para*-bromochlorobenzene

THE structure of *p*-bromochlorobenzene has been investigated by Hendricks[1], who found the space-group to be $P2_1/a$, and the number of molecules in the unit cell to be two. In an exactly repeating crystal structure, this would make it necessary for the molecule itself to have a centre of symmetry, which is, of course, impossible. Hendricks suggested that the symmetry of the crystal might be statistical, the halogen positions in the molecules composing the structure being filled at random by bromine or chlorine, or perhaps the two possible orientations of any given molecule, differing by 180°, were equally probable.

It was decided to re-examine the crystal, in order to see if any evidence of faults or irregularities in the structure, which might give rise to diffuse spectra, could be found.

The compound crystallizes from acetone in thin plates, only the *a* faces being developed. The crystals are very volatile, and oscillation and Weissenberg photographs were taken with the specimen inside a gelatine capsule. The unit cell is monoclinic, with dimensions $a = 15{\cdot}2$ A., $b = 5{\cdot}86$ A., $c = 4{\cdot}11$ A., $\beta = 113°$, and contains two molecules. The space-group was found to be $P2_1/a$, in agreement with the results of Hendricks. Since the space-group has four general positions, only a statistical symmetry is possible, with a centre of symmetry at the centre of the average molecule. There was no sign of any diffuseness of the spectra, and the appearance of the photographs is consistent with a completely random occupation of the halogen positions by bromine or chlorine.

Two-dimensional Fourier projections were made on the *ab* and *ac* planes. For the first approximation, only the positions of the mean halogen atoms were assumed, and these were enough to fix the phases of most of the spectra. The fact that the benzene ring appeared in the preliminary projections indicates that the type of assumption made as to the nature of the structure is probably correct.

In the final projections, shown in Figs. 1 and 2, the atoms of the ring are clearly defined, although there is some false detail still at the centre of the ring, which probably has no particular significance, and may be due to the difficulty of allowing for the rather large absorption in the crystals, because of their flat shape. The height of the peaks in the *para* positions corresponds to a group with a scattering power the mean of that of chlorine and bromine.

The values of the atomic parameters are given in the following table:

	x	*y*	*z*
Br,Cl	0·169	0·173	0·466
C_1	0·081	0·356	0·482
C_2	0·095	0·533	0·666
C_3	0·013	0·676	0·678

They differ somewhat from those suggested by Hendricks, but are closely similar to those given by Bezzi and Croatto[2] for *p*-dibromobenzene, which has essentially the same structure. The sides of the benzene ring, which is regular, have a length of 1·41 A., and the carbon-halogen distance is $1{\cdot}77 \pm 0{\cdot}04$ A., a value nearly the mean of the C—Cl and C—Br distances, 1·69 A. and 1·88 A. respectively, found by de Laszlo[3] in electron diffraction work on the dichloro- and dibromo-compounds. It is also less than the C—Br of 1·84 A. given by Bezzi and Croatto.

In conclusion, I wish to express my thanks to Prof. R. W. James for his interest in this work, and to the South African Council for Scientific and Industrial Research, to which I am indebted for a grant.

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[1] Hendricks, S. B., *Z. Krist.*, **84**, 85 (1933).
[2] Bezzi and Croatto, *Gazz. Chim. Ital.*, **72**, 318 (1942); *Chem. Zentr.*, **1**, 22 (1943); *Chem. Abstracts*, 3180 (1944).
[3] de Laszlo, *Proc. Roy. Soc.*, A, **146**, 690 (1934).

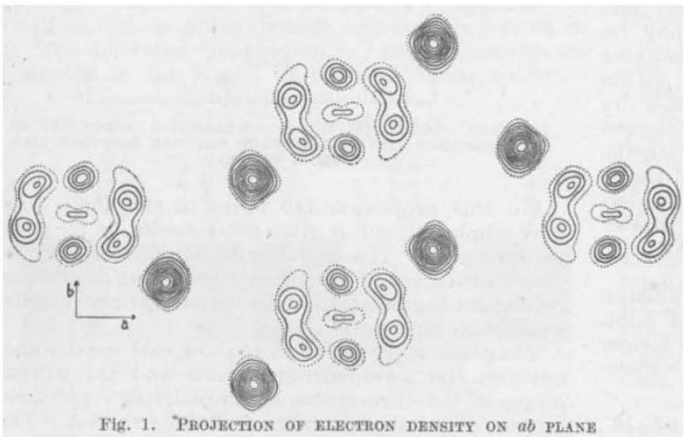

Fig. 1. PROJECTION OF ELECTRON DENSITY ON *ab* PLANE

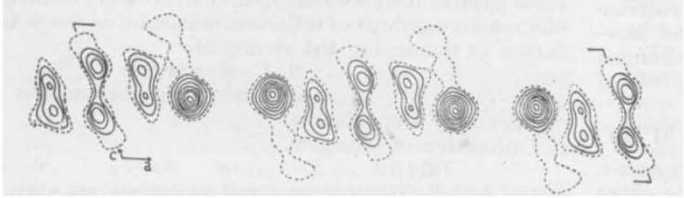

Fig. 2. PROJECTION OF ELECTRON DENSITY ON *ac* PLANE. CORNERS OF UNIT CELL ARE INDICATED

Purification of Renin by Means of Protein-Precipitating Agents

TRICHLOROACETIC acid has been used for denaturing and removing inert tissue proteins from kidney extracts containing renin[1]. It is also known that agents commonly used for removing proteins from solutions precipitate the proteins without causing denaturation in certain cases, so that the original protein may be regained. Thus trypsin and trypsinogen can be precipitated with trichloroacetic acid and the active enzymes regained[2]. In the same manner, crystalline egg albumin can be precipitated with metaphosphoric acid[3] and cathepsin by tungstic acid[4].

These investigations suggested to us the possibility of purifying renin by performing a fractional precipitation by means of such protein-precipitating agents. The blood pressure was determined by the capsular method[5].

(*A*) An extract of rabbit kidney purified by isoelectric precipitation of inactive