shows a peak electron density of 44·0 e.Å^{-3}, of which 9·6 e.Å^{-3} is due to the extrapolated portion of the f-curve, and a central curvature of 2350 e.Å^{-5}, half of which arises from the extrapolation.

Work is proceeding on the low-temperature refinement of the other two zones in the hope of obtaining final bond lengths for comparison with those derived from the three-dimensional room-temperature analysis.

We are indebted to Messrs H. Polak and A. Rathouse of I.B.M. (Israel) Ltd, Tel Aviv, and to the computing staff of the El Al Israel Airlines, Lydda, for making available to us the I.B.M. accounting machines used in the final Fourier summations.

References

HERBSTEIN, F. H. & SCHMIDT, G. M. J. (1952). *Nature, Lond.* **169**, 323.
JAMES, R. W. & BRINDLEY, G. W. (1932). *Phil. Mag.* **12**, 81.
MCWEENY, R. (1951). *Acta Cryst.* **4**, 513.

Acta Cryst. (1954). **7**, 130

A note on the crystal structure of Zeise's salt.

By J. A. WUNDERLICH and D. P. MELLOR, *The University of Sydney, Sydney, Australia*

(*Received* 20 *July* 1953)

Although Zeise's salt, $K(PtCl_3.C_2H_4)H_2O$, has been known for well over a century (Zeise, 1827), its constitution is still a matter of controversy. Each of the electronic structures proposed to account for the bond between Pt^{II} and ethylene implies some particular arrangement of the carbon atoms in relation to the $PtCl_3$ group (Chatt, 1949, 1951). An X-ray analysis of Zeise's salt has been undertaken in the hope of narrowing down the theories concerning its constitution.

Early morphological investigation by Jorgensen (1900) showed that the crystals belong to the monoclinic sphenoidal class.* Cell parameters, estimated from rotation and Weissenberg photographs, are

$$a = 10{\cdot}70,\ b = 8{\cdot}42,\ c = 4{\cdot}81\ \text{Å};\ \beta = 97°.$$

The density calculated for a cell containing two asymmetric units is 2·97 g.cm.$^{-3}$; the value found was slightly greater than 2·89 g.cm.$^{-3}$. Systematic absences of reflexions and a positive pyroelectric test are compatible with the space-group $P2_1$. The x, y and z co-ordinates of platinum, potassium and chlorine, determined from (010) and (001) Patterson and (010) electron-density projections are:

	x	y	z
Pt	0·106	0·000	0·771
Cl(2)	0·106	0·223	0·771
Cl(3)	0·106	0·777	0·771
Cl(1)	0·216	0·000	0·712
K	0·219	0·313	0·297

From these co-ordinates it follows that platinum and the three chlorine atoms are coplanar. While two of the Pt–Cl bond lengths are normal (2·32 Å), the third (Pt–Cl(1)) (Fig. 1), which is *'trans'* to the expected position of the ethylene molecule, is abnormally long (2·42 Å). Since the well known *'trans* directing' influence depends on the fact that the ethylene labilizes this chlorine atom (Cl(1)), the observed increase in bond length is of considerable interest.

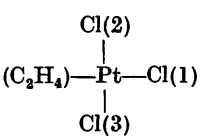

Fig. 1.

Owing to the small diffracting powers of carbon and oxygen, as compared with those of platinum, potassium and chlorine, the parameters of the former atoms are at present uncertain. However, it may be stated that it is highly improbable that there is any atom bound to platinum and collinear with it and Cl(1). Two of three minor peaks in the (010) projection may be interpreted as being due to carbon atoms forming a triangle with platinum which, when the $PtCl_3$ group is viewed side on, appears as shown in Fig. 2. (*M* represents three atoms: Pt in the plane of the paper, Cl(2) above and Cl(3) below the plane of the paper.) The C–C axis is therefore approximately at right angles to the plane of the $PtCl_3$ group. The third peak presumably represents oxygen of the water of crystallization, an assumption which appears reasonable from atomic packing considerations.

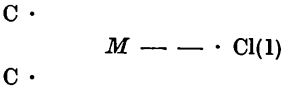

Fig. 2.

Owing to large thermal vibrations of the atoms, the number of reflexions observed at room temperature was insufficient for satisfactory resolution of carbon and oxygen peaks. Weissenberg photographs of crystals maintained at the temperature of liquid air are being taken to obtain enough reflexions to refine the (010) projections and to investigate the (001) projection.

In summary, the results of this preliminary investigation favour a triangular arrangement of platinum and ethylene rather than the 'end on' linkage implied by Chatt's ethylidene structure (Chatt, 1951).

* Axial ratios derived from the above cell parameters, though not identical with those determined by Jorgensen, are consistent with them.

References

CHATT, J. (1949). *J. Chem. Soc.*, p. 3340.
CHATT, J. (1951). *Research, Lond.* **4**, 180.
JORGENSEN, S. M. (1900). *Z. anorg. Chem.* **24**, 153.
ZEISE, W. C. (1827). *Ann. Phys., Lpz.* **9**, 632 (Abstract).