Conclusions

It has already been found in two dimensions that, for structures with large unit cells, difficulties arising from the increased complexity of the molecule are to some extent offset by the increase in the number of points at which the transform is sampled, and it seems probable that the same consideration will apply in three dimensions. The ease with which the two separate sets of columns can be identified in the present model suggests the possibility of detecting the existence of planar portions of more complicated molecules, and of specifying their orientation. Similarly, it may be possible to detect the presence of long chains and to determine their directions, as they give rise to flat discs in reciprocal space.

Since only approximate intensity data are required and the labour of preparing a model of the type described is not very great, the technique might prove to be a useful preliminary to a full three-dimensional structure determination.

References

ABRAHAMS, S. C., ROBERTSON, J. M. & WHITE J. G. (1949). *Acta Cryst.* **2** 233.
HANSON, A. W., LIPSON, H. & TAYLOR, C. A. (1953). *Proc. Roy. Soc.* A, **218**, 371.
KNOTT, G. (1940). *Proc. Phys. Soc., Lond.* **52**, 229.
PATTERSON, A. L. (1935). *Z. Krystallogr.* **90**, 517.
ROBERTSON, J. H. & BEEVERS, C. A. (1951). *Acta Cryst.* **4**, 270.
SHOEMAKER, D. P., DONOHUE, J., SCHOMAKER, V. & COREY, R. B. (1950). *J. Amer. Chem. Soc.* **72**, 2328.
TAYLOR, C. A. (1952). *Nature, Lond.* **169**, 1086.

Acta Cryst. (1953). **6**, 746

Bonding in benzene iododichloride and related molecules.

By JAMES D. MCCULLOUGH, *Department of Chemistry, University of California at Los Angeles, Los Angeles* 24, *California, U.S.A.*

(*Received* 18 *May* 1953)

In the recent investigation of the structure of benzene iododichloride, $C_6H_5ICl_2$, (Archer & van Schalkwyk, 1953) the authors reported what they considered to be a rather long I–Cl bond distance. If one draws the analogy between this substance, the diarylselenium dihalides, and related compounds pointed out by the present author (McCullough, 1942), the long I–Cl distance, the molecular structure and the chemical properties (dissociation into iodobenzene and chlorine) are all to be expected. It is reasonable to expect that compounds of the general type R_3(P,As,Sb,Bi)X_2, R_2(S,Se,Te)X_2 and RIX_2 should have the structure of a trigonal bipyramid with the halogen atoms at the apices and the three equatorial positions occupied by the R groups and unshared electron pairs. The X–M–X bond angle should be nearly linear and the M–X distance longer than the sum of the normal single covalent bond radii. The nature of the bonding in the *p*-tolylselenium dihalides and related molecules has been discussed by McCullough & Marsh (1950). Data on compounds of this general type which have been studied by X-ray diffraction methods are given in Table 1.

Semi-quantitative predictions based on the data in the table are probably of little value since selenium is in the row above that occupied by antimony and iodine. Data on compounds of the type R_2TeX_2 now under investigation in this laboratory should be of more use in this connection and the trends in the M–X distances in trigonal bipyramidal structures both horizontally and vertically in the periodic chart should be of interest.

References

ARCHER, E. M. & SCHALKWYK, T. G. D. VAN (1953). *Acta Cryst.* **6**, 88.
MCCULLOUGH, J. D. (1942). *J. Amer. Chem. Soc.* **64**, 2672.
MCCULLOUGH, J. D. & HAMBURGER, G. (1941). *J. Amer. Chem. Soc.* **63**, 803.
MCCULLOUGH, J. A. & HAMBURGER, G. (1942). *J. Amer. Chem. Soc.* **64**, 508.
MCCULLOUGH, J. D. & MARSH, R. E. (1950). *Acta Cryst.* **3**, 41.
WELLS, A. F. (1938). *Z. Krystallogr.* **99**, 367.

Table 1. *M–X distances in some organometallic dihalide molecules having the trigonal bipyramid structure*

Compound	Reference	Observed M–X distance (Å)	Sum of single covalent bond radii (Å)	Difference (Å)
$(CH_3)_3SbCl_2$	Wells (1938)	2·49	2·40	0·09
$(CH_3)_3SbBr_2$	Wells (1938)	2·63	2·55	0·08
$(C_6H_5)_2SeCl_2$	McCullough & Hamburger (1942)	2·30*	2·16	0·14*
$(C_6H_5)_2SeBr_2$	McCullough & Hamburger (1941)	2·52	2·31	0·21
$(p\text{-Tolyl})_2SeCl_2$	McCullough & Marsh (1950)	2·38	2·16	0·22
$(p\text{-Tolyl})_2SeBr_2$	McCullough & Marsh (1950)	2·55	2·31	0·24
$C_6H_5ICl_2$	Archer & van Schalkwyk (1953)	2·45	2·32	0·13

* Subject to greater error than that in the *p*-tolyl compound owing to there being 8 molecules per unit cell as compared to 2 in *p*-tolylselenium dichloride.