The Crystal Structure of Bispentafluorophenylmercury

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THE crystal structures of diphenylmercury[1] and di-*p*-tolylmercury[2] which have been solved show that they contain colinear C–Hg–C bonds and the whole molecule is planar. In the present compound (supplied by Prof. G. E. Coates) all hydrogens of the diphenylmercury have been replaced by

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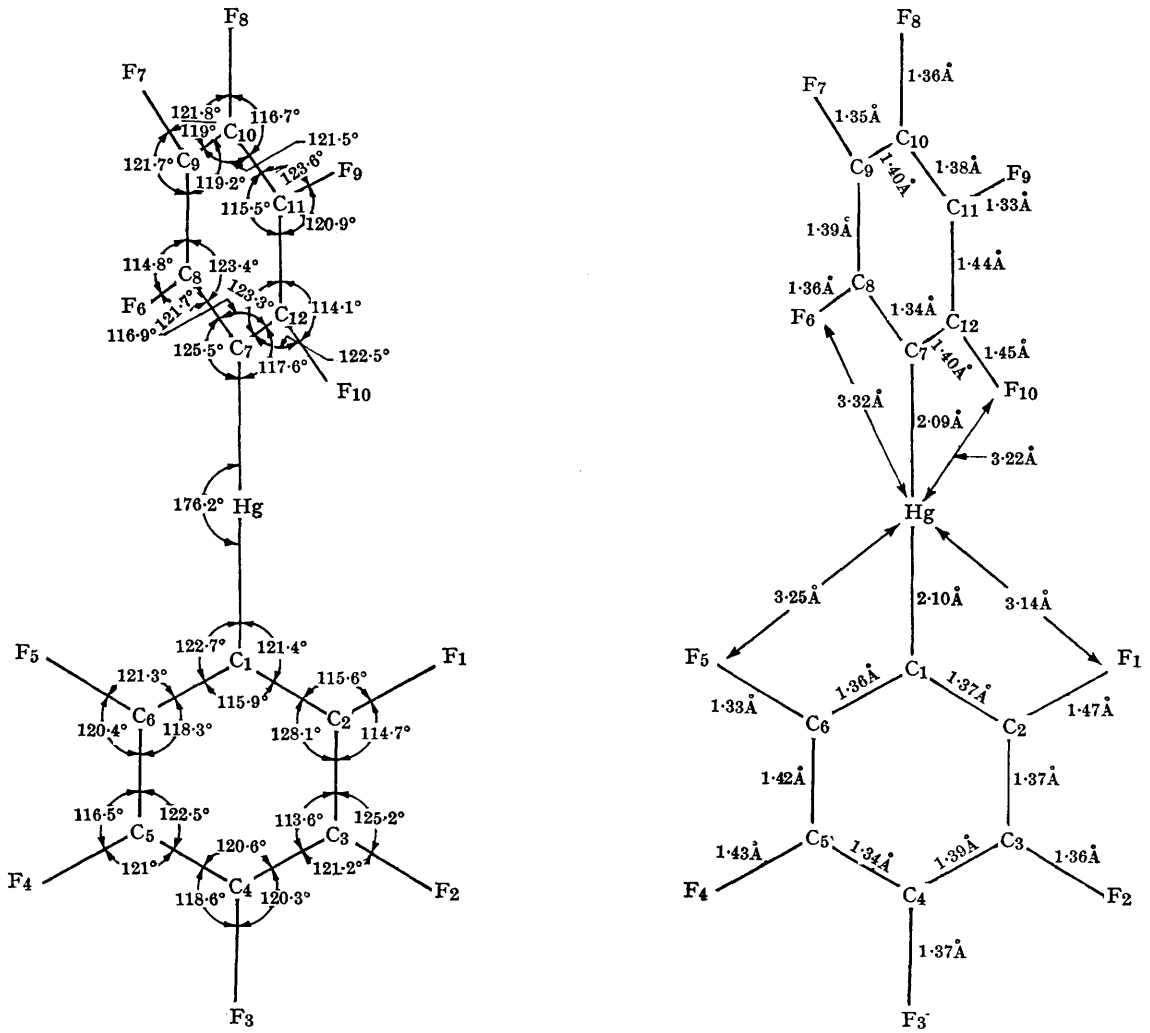
fluorine atoms to form bis-pentafluorophenylmercury. The effects of this substitution are interesting.

Bispentafluorophenylmercury, $Hg(C_6F_5)_2$ crystallizes in the orthorhombic system with $a = 20{\cdot}52 \pm 0{\cdot}02$, $b = 10{\cdot}79 \pm 0{\cdot}01$, $c = 5{\cdot}89 \pm 0{\cdot}01$ Å. The space group is $P2_12_12_1$ with four molecules in the unit cell. The intensity data were collected photographically by the Weissenberg method using Cu–$K\alpha$ radiation. 1155 out of 1335 possible reflections were observed and their intensities were measured visually. The positions of mercury were found from the Patterson projections and the light atoms were located by performing three-dimensional mercury-phased Fourier synthesis. The structure was refined by six cycles of full-matrix least-squares refinement which refined the three positional and six thermal parameters for each atom and the individual layer scale factor. Corrections for the anomolous dispersion of mercury were applied. The final R-factor was 0·086 for all reflections (0·081 for observed reflections only). The R-factor for mercury alone was 0·20.



FIGURES 1 and 2.

Bond lengths and bond angles of bispentafluorophenylmercury.

The dimensions of the molecule are as shown in Figures 1 and 2. A comparison of this structure with other similar structures[1,2] is interesting. The C–Hg–C bonds in this case are non-linear, the angle being 176·2 ± 1·2°. Each of the two fluorophenyl rings is planar, but they are tilted with respect to each other in such a way as to make an angle of 59·4 ± 1·2° between them. This tilting of the rings increases the distance between the fluorine atoms of the two rings and thus reduces the electrostatic repulsion. There are no intermolecular approaches of any significance and the crystal lattice is of molecular type. The results of this investigation contradict the calculations of Sipos and co-workers,[3] who have proposed that the angle C–Hg–C should be 130—150°.

(*Received, January 3rd*, 1966; *Com.* 003.)

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