The Crystal Structure of Bis-(π-cyclopentadienyldicarbonyliron) diphenylsulphonyltin

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THE product formed by the reaction of sulphur dioxide with bis-(π-cyclopentadienyldicarbonyliron)diphenyltin[1] has been shown by single-crystal *X*-ray analysis to be bis-(π-cyclopentadienyldicarbonyliron)diphenylsulphonyltin.

Crystals are orthorhombic, space group $P2_12_12_1$, $Z = 4$, $a = 17{\cdot}08$, $b = 12{\cdot}24$, $c = 13{\cdot}38$ Å, all $\pm$ 0·02 Å. There are 1030 significantly above background as measured by Mo-*K* radiation with balanced filters from a single crystal mounted so as to rotate about b^* on a Hilger–Watts linear diffractometer.

The heavy-atom method of phase-determination was used and the structural parameters refined by means of Fourier and block-diagonal least-squares methods. The *R* value is 0·12, with individual isotropic thermal parameters for all atoms and no corrections applied for absorption.

From the structure found, it is clear that insertion of SO_2 into the parent compound has taken place in the Sn–C bonds to give Sn–O–(SO)–C units. The geometry at the S atom is approximately tetrahedral in each case with a lone pair of electrons presumably occupying the fourth arm of the tetrahedron. O–S=O angles average 115°, O–S–C 101°, and O=S–C 98°, each with e.s.d 3°.

The two Sn–Fe distances are equal within the limits of experimental error, 2·490 and 2·507 Å (e.s.d. 0·01 Å). They are much shorter than the value of 2·56 Å found[2] for Fe–Sn in $[\pi\text{-}C_5H_5Fe(CO)_2]_2Sn(ONO)_2$ and shorter even than the 2·537 Å found[4] as an average value in $[\pi\text{-}C_5H_5Fe(CO)_2]SnPh_3$ where there is only one metal–metal bond in the molecule. This difference in bond lengths emphasises the extreme sensitivity of this type of bond to substituent differences on the Group IV metal but as yet not enough information is available on related structures to suggest a convincing explanation.

Other features of the geometry at the tin atom may be compared with those found by the Russian group[2] for the nitrito-compound. The Fe–Sn–Fe angle is 129° closely similar to the value of 126° found there. By contrast the O–Sn–O angle in our case is 81° whereas in the NO_2 compound it is given as 67°. Only one value for the Fe–Sn–O angle is given in ref. 2, 77°; in contrast the average angle of this type in this structure is 108°. Similar geometry is found in the structure of $[\pi\text{-}C_5H_5Fe(CO)_2]_2GeCl_2$ where the Cl–Ge–Cl angle is given as 96° and the Fe–Ge–Fe angle given as 96°.[4]

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