Crystal Structure of Dicarbonylbis-(π-cyclopentadienyl)irondimethyltin

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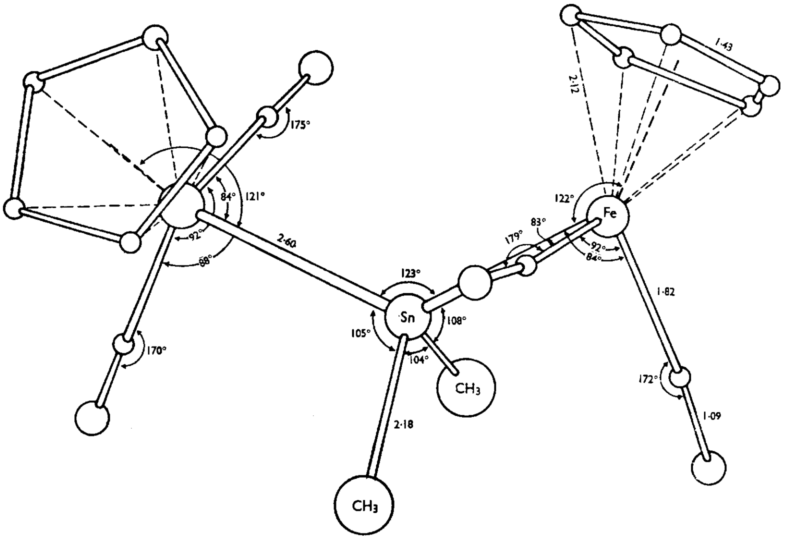
RECENTLY we have[1] undertaken a preliminary *X*-ray study of a series of polymetallic organoelement compounds with the Fe–Sn bond and of the general formula $[\pi\text{-}C_5H_5Fe(CO)_2]_2SnX_2$ (I) (where X denotes an inorganic or organic ligand), and have described the crystal and molecular structure of (I) with X = ONO (Ia). The structure of (I) with X = Cl (Ib) has already been reported.[2] In our *X*-ray study of these compounds, we intended to determine the metal-to-metal bond distances, to establish the general stereochemistry of such complexes, *e.g.*, a co-ordination type and bond angles at metal atoms, and finally to elucidate a general mode of Sn–X bonding.

Here we report the crystal and molecular structure of (I) with X = Me. The orange, plate-like crystals, elongated along *a*-axis, are monoclinic. Space group is $P2_1/n$, $a = 15{\cdot}59 \pm 0{\cdot}01$, $b = 9{\cdot}69 \pm 0{\cdot}01$, $c = 11{\cdot}66 \pm 0{\cdot}01$ Å, $\beta = 107 \pm 0{\cdot}5°$, $U = 1684$ Å^3, $D_m = 1{\cdot}8$, $D_c = 1{\cdot}9$ g.cm.$^{-3}$ for $Z = 4$, $M = 503{\cdot}4$.

The intensities of *ca.* 800 non-zero independent reflexions were estimated visually from Weissenberg diagrams taken with unfiltered Cu-K_α radiation. An absorption correction was neglected. The structure was determined by standard heavy-atom method and refined by a full-matrix least-squares method with individual isotropic temperature factors. At the present stage of refinement, the discrepancy index is $0{\cdot}13_3$ with an overall temperature factor $B = 3{\cdot}0$ Å^2, and the standard deviations in bond length are: Fe–Sn ± 0·005, Sn–C ± 0·02, Fe–C ± 0·02, C–C ± 0·03, and C–O ±0·025 Å.

The crystal is built up of discrete molecules (see Figure) with a severely distorted tetrahedral co-ordination of the Sn atom. Because the volume of the $C_5H_5(CO)_2Fe$ ligand is large, the bond angle Fe–Sn–Fe (123 ± 0·5°) is considerably increased in



FIGURE

(Ia) and (Ib) (126° and 128·6° respectively) and in the analogous germanium compound[3] with X = Cl (∠Fe–Ge–Fe = 128°). The geometry of the Sn–$Fe(CO)_2C_5H_5$ fragment is similar to that found in (Ia), (Ib), and π-$C_5H_5Fe(CO)_2SnPh_3$ (II).[4] The Fe-atom co-ordination is a "piano stool", a typical one for semi-sandwiches. The Fe–Sn bond length $2{\cdot}60_2$ and $2{\cdot}60_5$ Å are longer than in (Ia) and (Ib) (2·492 and 2·56 Å respectively) and shorter than the sum of Fe octahedral and of Sn tetrahedral radii (*ca.* 2·67 Å).[5] In (II), the Fe–Sn bond is 2·537 Å, and in $[\pi$-$C_5H_5Fe(CO)_2]_2[\pi$-$C_5H_5Mo(CO)_3]$-SnCl,[6] the mean Fe–Sn bond length is 2·59 Å. In the more complicated structure of $Me_4Sn_3Fe_4(CO)_{16}$, the terminal Fe–Sn bonds are 2·64 Å but the bridging ones are much longer (2·75 Å).[7] The mean Sn–C bond length 2·18 Å does not differ from the sum of the tetrahedral radii (*ca.* 2·18 Å).[5] The mean Fe–C (cyclopentadienyl) interatomic distance 2·12 Å is distinctly longer than that in ferrocene (2·045 Å) and near to the corresponding value in (Ia) and (II) (2·11 and 2·095 Å, respectively). The mean Fe–C(carbonyl) and C–O bond lengths are 1·82 and 1·09 Å respectively. The molecular point group symmetry in the solid state, C_1, differs from that found for (Ia) and (Ib) (C_2).

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