The Crystal Structure of Bis(dicarbonyl-π-cyclopentadienyliron)dichlorogermane

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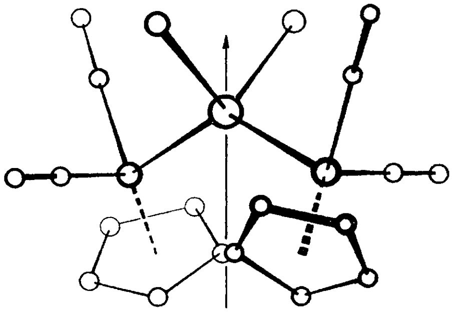
COMPOUNDS of the type $X_2M[Fe(CO)_2(\pi\text{-}C_5H_5)]_2$, where X = halogen or alkyl and M = Sn or Ge, have recently been reported.[1,2] We have undertaken a single-crystal *X*-ray study of $Cl_2Ge[Fe(CO)_2(\pi\text{-}C_5H_5)]_2$ to establish the molecular configuration in the solid state and to give the first determination of a Ge–Fe bond distance.

Crystal data: $Cl_2Ge[Fe(CO)_2(\pi\text{-}C_5H_5]_2$; $M = 497{\cdot}3$; monoclinic, $a = 14{\cdot}79$, $b = 7{\cdot}63$, $c = 15{\cdot}04$ Å, $\beta = 96° \, 5'$; $U = 1689{\cdot}3$ Å^3; $D_m = 1{\cdot}96$ g. cm.$^{-3}$; $Z = 4$, $D_c = 1{\cdot}96$ g. cm.$^{-3}$; space group $C2/c$.

The structural determination is based on 918 independent non-zero reflections and has been refined to an R-value of 8·2%.

The molecules are arranged in the crystal in such a way that the Ge atoms occur at special positions (e) of space group $C2/c$, (C^6_{2h}, No. 15).[3] This requires that the two halves of the molecule are related to one another by a two-fold axis of symmetry, and as no additional symmetry elements are present in the molecules, they must have point-group symmetry C_2 (see Figure). Important bond distances and angles are:—



FIGURE

Ge–Fe, 2·36 ± 0·01 Å; Ge–Cl, 2·26 ± 0·01 Å;
Fe–C(carbonyl), 1·74 ± 0·03 Å (mean);
Fe–C(π-C_5H_5), 2·09 ± 0·03 Å (mean);
C–O, 1·17 ± 0·04 Å (mean);
C–C(π-C_5H_5), 1·42 ± 0·04 Å (mean).
Cl–Ge–Cl, 96 ± 1°; Fe–Ge–Fe, 128 ± 1°;
Fe–Ge–Cl, 107 ± 1°;
Ge–Fe–C(carbonyl), 87 ± 2° (mean);
C–Fe–C, 92 ± 2°; Fe–C–O, 172 ± 3° (mean);
C–C–C (π-C_5H_5), 108 ± 3° (mean).

It will be seen, therefore, that the Ge atoms show distorted tetrahedral bonding, with enlargement of the Fe–Ge–Fe angle at the expense of the Cl–Ge–Cl angle (though the planes defined by these trios remain approximately mutually perpendicular), while the Fe atoms show octahedral bonding if, as is customary,[4] three of the six bonds are considered to be used in interaction with the π-C_5H_5 ring. Moreover, the Fe–C–O bond angles are probably significantly different from 180°.

Examination of the solution infrared spectra of this series of compounds has led to the conclusion[2] that the molecular symmetry for the alkyl compounds is C_s (m) and for the halogen compounds is C_1 (1). The possible symmetry C_2 (2) was not considered in this connection. Our crystal structure results do not, of course, invalidate these conclusions, and it may be inferred that a change of molecular configuration from C_2 to C_1 occurs on dissolution.

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[1] F. Bonati and G. Wilkinson, *J. Chem. Soc.*, 1964, 179.

[2] N. Flitcroft, D. A. Harbourne, I. Paul, P. M. Tucker, and F. G. A. Stone, *J. Chem. Soc.* (*A*), 1966, 1130.

[3] "International Tables for *X*-Ray Crystallography", vol. 1, Kynoch Press, 1952.

[4] See, for example, M. R. Churchill and R. Mason, *Proc. Roy. Soc.*, 1964, *A*, **279**, 191.