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STRUCTURAL STUDY OF IRON CARBONYL DERIVATIVES

IV *. SYNTHESIS AND CRYSTAL AND MOLECULAR STRUCTURE OF *syn*-$[\mu\text{-}(SCH_3)Fe(CO)_2P(CH_3)_3]_2$

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Summary

The preparation of the compound $[\mu\text{-}(SCH_3)Fe(CO)_2L]_2$, with $L = P(CH_3)_3$, is described. Spectroscopic studies show that this compound exists as *syn* and *anti* isomers, with respect to the orientation of the SCH_3 groups relative to the metal—metal bond. The crystal and molecular structure of the *syn* isomer has been determined by a single-crystal X-ray study. The complex crystallizes in the tetragonal space group $P4_12_12$ (or $P4_32_12$) with $Z = 8$. The intensities were measured on a Nonius CAD-4 automatic diffractometer. The structure has been refined to R and R'' values of 0.058 and 0.050 respectively, for 2156 independent reflections. The molecular structure contains two $Fe(CO)_2P(CH_3)_3$ moieties (with the phosphine ligands in axial positions) bridged through the sulfur atoms of the *syn*-SCH_3 groups. The iron—iron bond length is 2.518(1) Å. A comparison is made with similar iron carbonyl derivatives without phosphine substituents.

Introduction

Several structures of iron carbonyl derivatives containing an Fe_2S_2 core, i.e. a symmetrical double S-bridge between two $Fe(CO)_3$ groups linked by a metal—metal bond, have been determined by X-ray studies; for exemple: $[C_2H_5SFe(CO)_3]_2$ (II) [2], $[C_6H_5CSFe(CO)_3]_2$ (III) [3], and $[CH_3SFe_2(CO)_6]_2S$ (IV) [4]. But, to our knowledge, there have been no structural studies of similar complexes where one of the CO of each $Fe(CO)_3$ group has been replaced by

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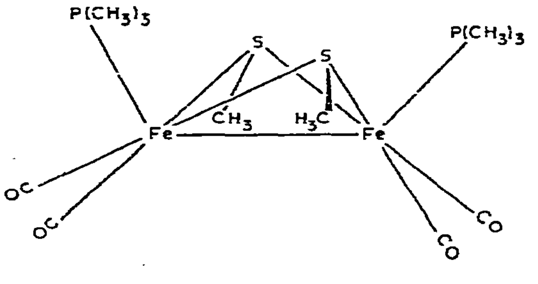
* For part III, see ref. 1.

a phosphine ligand L. We have determined the crystal structure of one such compound, $[\mu\text{-}(SCH_3)Fe(CO)_2P(CH_3)_3]_2$, in order to compare the two types of derivatives and to assess the influence of the ligand L = $P(CH_3)_3$ on the molecular structure, particularly on the metal—metal bond.

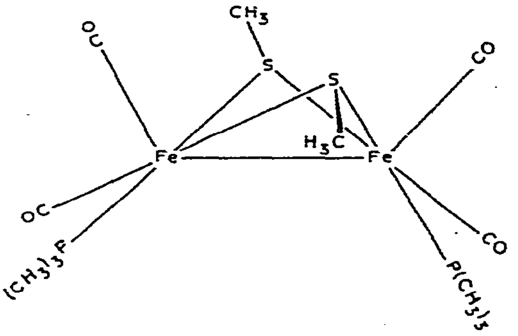
Preparative details and structural hypothesis

The compound $[\mu\text{-}(SCH_3)Fe(CO)_2P(CH_3)_3]_2$ (I) was prepared from the reaction of a slight excess of $P(CH_3)_3$ (0.6 ml) with $[\mu\text{-}(SCH_3)Fe(CO)_3]_2$ (1 g) in boiling hexane during ten hours. Crystallization in n-hexane gave air-stable brown crystals of various sizes, but with clean faces.

The compound shows three active infrared bands in the ν(CO) stretching region (1987.6 (s); 1943.1 (ms) and 1923.1 cm^{-1} (s) in hexadecane solution) and the proton NMR spectra shows one doublet in the P—CH_3 region (τ 8.50 ppm; ^2J(PH) 8.4 Hz) and one triplet in the S—CH_3 region (τ 8.09 ppm; ^4J(PH) 1 Hz). From these two observations, we conclude that the complex has a C_{2v} symmetry (structure A), in accordance with the observations of Haines et al. on the $[\mu\text{-}(SCH_3)Fe(CO)_2L]_2$ complexes with L = $P(C_2H_5)_3$ or $P(OCH_3)_3$ [5]. However, in our case, the examination of the infrared spectra of the mother liquor of crystallization shows the existence of a second isomer for which, from the infrared and NMR data, and by comparison with the studies of Haines et al. [5], structure B can be proposed. The crystallographic study of this second complex is in progress.



(A)



(B)

X-ray data collection and structure determination

Crystal data

$C_{12}H_{24}O_4P_2S_2Fe_2$ (*syn* isomer); mol. wt. 470.09. Tetragonal system: $a = b$ = 13.278(2); c = 23.942(7) Å. V = 4221 Å^3. d_c = 1.48. Z = 8.

Space group: $P4_12_12$ (or $P4_32_12$ enantiomorph; we have not attempted to determine the absolute structure).

The unit-cell parameters, obtained from Weissenberg and precession photographs, were refined using the θ angles of 15 reflections measured on a Nonius CAD-4 automatic diffractometer.

Collection of X-ray diffraction data

The intensities of 6430 reflections (with equivalent measurements for *hkl* and *khl*) were collected at room temperature, for $2 < \theta < 30°$, on the automatic diffractometer. The crystal used had such dimensions as $\mu R < 1$ for the Mo-K_α radiation (0.71069 Å). Consequently, no absorption corrections were deemed necessary. The characteristics of the diffractometer measurements were as follows: graphite monochromator, ω—2θ scan technique, scan angle: $S = 0.90 + 0.30 \text{ tg } \theta$ (in degrees), detector aperture: $D = 2.50 + 0.40 \text{ tg } \theta$ (in mm).

Intensities of equivalent reflections were averaged using the program MAXE [6], after the usual Lorentz and polarization corrections were applied. Reflections having $\sigma(I)/I > 1$ were considered to be unobserved. Finally, 2222 independent reflections were retained and used in the subsequent structure analysis.

Solution and refinement of the structure

The six heavy atoms (2Fe, 2S and 2P) of the molecule which constitutes the asymmetric unit were located using the multisolution method with MULTAN

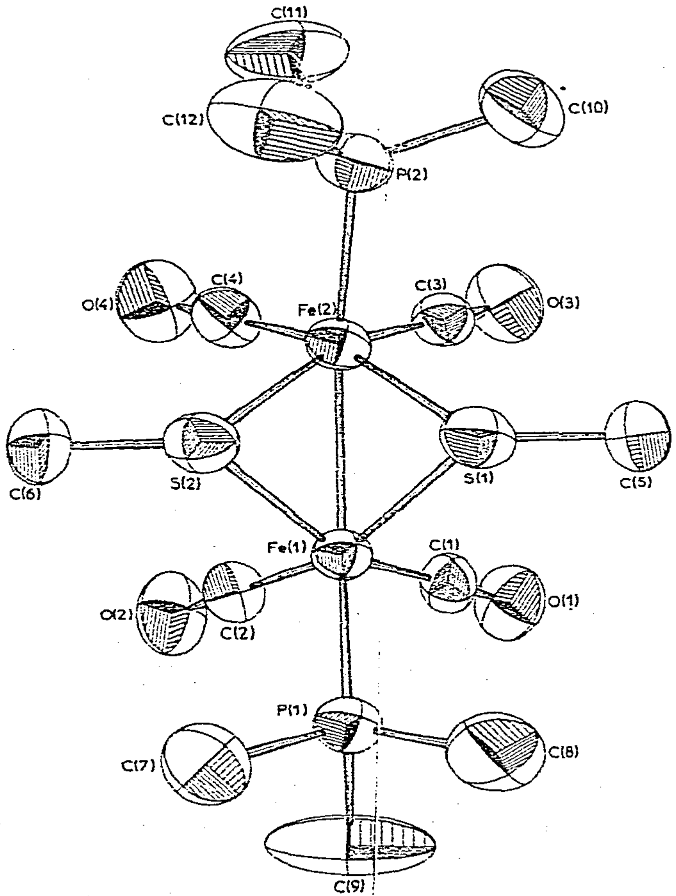


Fig. 1. Perspective view of the $[\mu\text{-}(SCH_3)Fe(CO)_2P(CH_3)_3]_2$ molecule showing the pseudo-symmetry C_{2v}.

TABLE 1

ATOMIC PARAMETERS ($\times 10^4$)

Estimated standard deviations are given in parentheses. The anisotropic thermal parameters are of the form: $\exp[-(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23})]$

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Fe(1)	3265.1(0.8)	1894.3(0.8)	2081.6(0.4)	53.7(0.7)	44.3(0.7)	12.1(0.2)	2.5(0.6)	−0.3(0.6)	0.2(0.3)
Fe(2)	3503.1(0.9)	2584.2(0.8)	3052.2(0.4)	60.3(0.8)	45.7(0.7)	12.7(0.2)	0.2(0.6)	1.9(0.3)	0(0.3)
S(1)	2638(2)	3401(2)	2373.3(0.8)	82(2)	49(1)	16.3(0.4)	12(1)	−1.4(0.6)	0.7(0.6)
S(2)	4646(2)	2784(2)	2365.8(0.8)	64(1)	64(2)	15.6(0.4)	−13(1)	3.4(0.6)	−1.7(0.6)
P(1)	3299(2)	2166(2)	1163.4(0.8)	58(1)	64(1)	13.5(0.4)	0(1)	1.7(0.6)	−0.1(0.6)
P(2)	3774(2)	3920(2)	3585.3(0.9)	71(2)	61(2)	17.0(0.4)	−4(1)	3.7(0.7)	−6.8(0.7)
O(1)	1370(4)	830(5)	2162(3)	61(4)	104(6)	34(2)	−24(4)	4(2)	6(3)
O(2)	4287(5)	− 22(5)	2096(3)	90(5)	63(4)	45(2)	21(4)	−2(3)	−1(3)
O(3)	1742(5)	1933(5)	3670(3)	86(5)	109(6)	30(2)	−12(5)	20(2)	8(3)
O(4)	4768(6)	1107(6)	3644(3)	114(6)	102(6)	32(2)	20(5)	−2(3)	17(3)
C(1)	2111(6)	1260(6)	2136(3)	49(5)	70(6)	17(2)	3(5)	3(4)	5(3)
C(2)	3891(6)	730(6)	2090(3)	61(5)	46(5)	20(2)	2(4)	2(3)	5(3)
C(3)	2436(7)	2192(6)	3418(3)	67(6)	60(6)	15(2)	6(5)	−2(3)	0(3)
C(4)	4256(7)	1737(7)	3406(3)	82(7)	66(7)	16(2)	14(6)	2(3)	4(3)
C(5)	1292(7)	3405(7)	2485(4)	80(7)	87(8)	26(2)	33(6)	−8(3)	−8(3)
C(6)	5786(6)	2040(8)	2441(4)	49(5)	127(9)	26(2)	−5(6)	3(3)	−4(4)
C(7)	4475(8)	2538(10)	871(4)	76(8)	217(13)	22(2)	−7(9)	11(3)	3(5)
C(8)	2499(9)	3168(9)	915(3)	162(11)	173(11)	15(2)	85(9)	0(4)	17(4)
C(9)	2963(13)	1119(10)	734(4)	352(20)	116(11)	19(2)	−106(12)	4(5)	−12(4)
C(10)	2688(8)	4649(9)	3731(5)	82(9)	124(10)	62(4)	10(7)	−1(5)	−54(5)
C(11)	4256(9)	3683(9)	4277(4)	206(13)	121(11)	17(2)	−1(9)	−24(4)	−7(4)
C(12)	4645(10)	4859(8)	3330(5)	158(12)	97(9)	32(3)	−61(8)	27(5)	−12(4)

TABLE 2

INTERATOMIC BOND LENGTHS AND BOND ANGLES

Estimated standard deviations are given in parentheses.

(a) Bond lengths (Å)

Fe(1)—Fe(2)	2.518(1)	C(1)—O(1)	1.139(10)
		C(2)—O(2)	1.129(10)
Fe(1)—S(1)	2.276(2)	C(3)—O(3)	1.154(10)
Fe(1)—S(2)	2.278(2)	C(4)—O(4)	1.166(11)
Fe(2)—S(1)	2.267(2)		
Fe(2)—S(2)	2.270(2)	S(1)—C(5)	1.807(9)
		S(2)—C(6)	1.819(9)
Fe(1)—P(1)	2.228(2)		
Fe(2)—P(2)	2.215(2)	P(1)—C(7)	1.781(10)
S(1)—S(2)	2.790(3)	P(1)—C(8)	1.804(11)
		P(1)—C(9)	1.786(12)
Fe(1)—C(1)	1.754(8)	P(2)—C(10)	1.772(11)
Fe(1)—C(2)	1.755(7)	P(2)—C(11)	1.804(9)
Fe(2)—C(3)	1.745(8)	P(2)—C(12)	1.807(12)
Fe(2)—C(4)	1.726(8)		

(b) Bond angles (°)

Fe(1)—S(1)—Fe(2)	67.31(0.09)	Fe(1)—P(1)—C(7)	116.7(0.3)
Fe(1)—S(2)—Fe(2)	67.22(0.09)	Fe(1)—P(1)—C(8)	115.7(0.3)
S(1)—Fe(1)—S(2)	75.56(0.07)	Fe(1)—P(1)—C(9)	115.9(0.4)
S(1)—Fe(2)—S(2)	75.91(0.07)	Fe(2)—P(2)—C(10)	114.8(0.3)
		Fe(2)—P(2)—C(11)	116.6(0.3)
Fe(1)—S(1)—C(5)	114.2(0.3)	Fe(2)—P(2)—C(12)	117.5(0.3)
Fe(2)—S(1)—C(5)	113.4(0.2)		
Fe(1)—S(2)—C(6)	114.9(0.3)	C(7)—P(1)—C(8)	100.5(0.5)
Fe(2)—S(2)—C(6)	114.2(0.3)	C(8)—P(1)—C(9)	103.7(0.6)
		C(9)—P(1)—C(7)	102.1(0.6)
Fe(1)—C(1)—O(1)	178.4(0.7)	C(10)—P(2)—C(11)	101.7(0.5)
Fe(1)—C(2)—O(2)	179.5(0.7)	C(11)—P(2)—C(12)	101.8(0.5)
Fe(2)—C(3)—O(3)	178.6(0.7)	C(12)—P(2)—C(10)	102.2(0.5)
Fe(2)—C(4)—O(4)	179.7(0.7)		

program [7]. Some oxygen and carbon atoms also appear on a Fourier synthesis computed with the normalized structure factors E of the set of phases having the best "figure of merit". Their positions, as those of the remaining non-hydrogen atoms, were obtained unambiguously from a series of difference-Fourier maps computed on the basis of the heavy atoms parameters. Refinement of positional and isotropic thermal parameters of the 22 independent non-hydrogen atoms led to a value for the index $R = \Sigma(|F_o| - K|F_c|)/\Sigma|F_o|$ of 0.097.

Least-squares refinements were performed using SFLS-5 program [8]. The quantity minimized was $\Sigma w(|F_o| - K|F_c|)^2$. Atomic scattering factors, $\Delta f'$ and $\Delta f''$ coefficients of anomalous dispersion for Fe, S and P atoms, and the weighting scheme used are described in a previous publication [9].

Although the positions of all 24 hydrogen atoms were not confirmed from a difference-Fourier synthesis, we have included their contribution in the refinement, with positions calculated assuming idealized tetrahedral geometry for the methyl groups. The parameters of hydrogen atoms were held fixed in further cycles of refinement. The contribution of hydrogen atoms reduces the R index

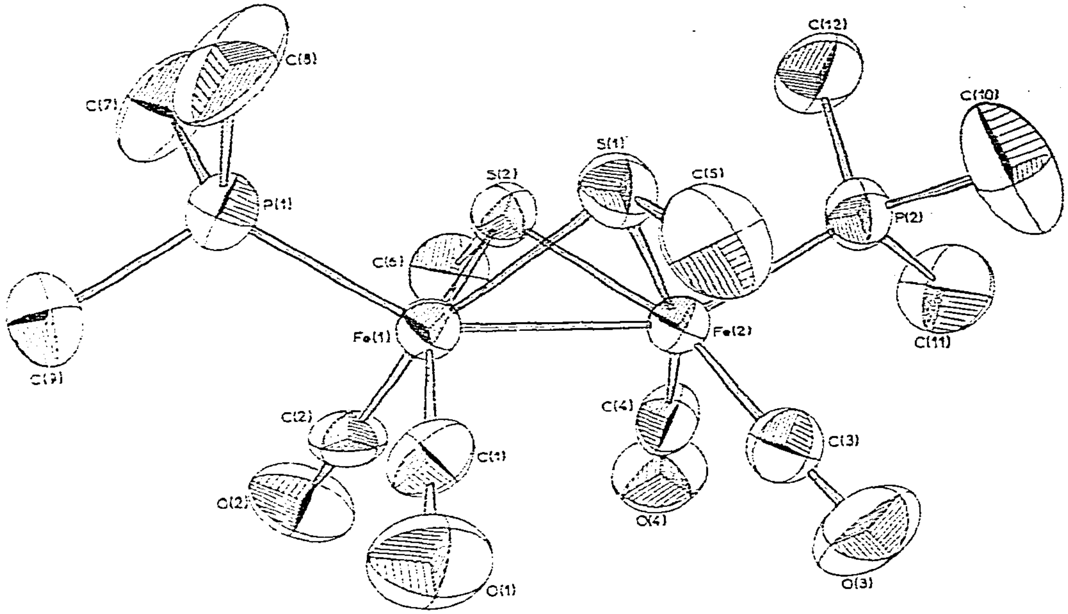


Fig. 2. Perspective view of the $[\mu\text{-}(SCH_3)Fe(CO)_2P(CH_3)_3]_2$ molecule showing the disposition of SCH_3 and $P(CH_3)_3$ groups relatively to the iron—iron bond.

in a significant way and gives rise to a more homogeneous set of bond distances and angles for the remaining atoms.

Anisotropic thermal parameters were then introduced for the 22 non-hydrogen atoms, and two further cycles of refinement of positional and anisotropic thermal parameters for these atoms reduced R to a final value of 0.058 for 2156 independent reflections (66 weak reflections exhibiting large disagreements between $|F_o|$ and $|F_c|$ were rejected). The value of the weighted index $R'' = [\Sigma\omega(|F_o| - K|F_c|)^2/\Sigma\omega|F_o|^2]^{1/2}$ is 0.050. In the last refinement cycle, no parameter shifts were greater than 0.20 of the corresponding estimated standard deviations. A table of observed and calculated structure factors is available on request.

Final coordinates and anisotropic thermal parameters for the 22 non-hydrogen atoms, with estimated standard deviations in parentheses, are given in Table 1. The atomic numbering scheme used can be seen on Fig. 1 and 2, which give two perspective views of the molecule along two perpendicular directions, plotted with program ORTEP [10]. Interatomic distances and bond angles are given in Table 2.

Description of the structure and discussion

The molecular structure of *syn*-$[\mu\text{-}(SCH_3)Fe(CO)_2P(CH_3)_3]_2$ is wholly consistent with the IR and NMR spectrographic data given above. The two ligands $L = P(CH_3)_3$ are *trans* to the metal—metal bond, axially coordinated to each iron atom, and the CH_3 groups of the bridging sulfur atoms are in a *syn-endo* position, as can be seen from Fig. 2.

The molecular geometry can be described, as in the case of similar

$[Fe(CO)_3$-μ-$(SR)]_2$ derivatives [2—4], as arising from the junction of the basal planes of two distorted tetragonal pyramids along the S···S edge. The iron atoms are displaced from their basal planes, respectively, by 0.33 and 0.27 Å in the direction of the apical atoms P(1) and P(2). The dihedral angle between the planes Fe(1)—S(1)—S(2) and Fe(2)—S(1)—S(2) is 90.9°. Furthermore, the two iron atoms are linked by a metal—metal bond of length 2.518(1) Å.

It is interesting to compare this geometry with that found in similar complexes containing Fe_2S_2-bridged systems, without direct S—S bond, and without phosphine ligands. This comparison of the main structural characteristics is given in Table 3. It appears that the replacement of one CO group on each iron atom by the ligand $P(CH_3)_3$ does not alter in a significant way the geometrical parameters of the Fe_2S_2-bridged core. The main differences compared with the nearest derivative, $[C_2H_5SFe(CO)_3]_2$ (II) [2], involve the mean S—Fe—S angle and the dihedral angle between the two Fe—S—S planes. However, it is interesting to note that the values of these two angles for compound II are also greater than corresponding values in the three other non-substituted derivatives of Table 3. No doubt, these differences may be due, in part, to the non-bonding S···S distance, which is greater in the first derivative than in the other four, possibly in connection with the *anti-syn* problem.

Let us consider now the influence of the substitution of one CO by a $P(CH_3)_3$ ligand on Fe—C(O) and C—O distances of the two remaining carbonyl groups.

The mean value of Fe—C(O) bond lengths is 1.745(1) Å in $[\mu$-(SCH_3)-$Fe(CO)_2P(CH_3)_3]_2$, while it is 1.81(2) Å in the nearest non-substituted derivative II. For the other compounds of Table 3, the mean Fe—C(O) value is also greater than in the present structure, except for $[CH_3SFe_2(CO)_6]_2S$ (IV) [4], but the low value found in this derivative seems surprising, and is probably due to the poor precision of the structural results. In another compound for which we have determined the structure with a precision analogous to that of the present work, viz. $(C_6H_4SNH)Fe_2(CO)_6$ [9], the mean Fe—C(O) distance is 1.788(3) Å.

The observed significant shortening of the remaining Fe—C(O) bond lengths, caused by the replacement of one CO by a phosphine ligand, agrees well with the π-acceptor character weaker for a phosphine than for CO. Such a shortening of M—C(O) bond lengths has also been noted in chromium carbonyl derivatives. specially for the CO groups *trans* to phosphine ligands [12,13]. On the other hand, in some mononuclear iron carbonyl derivatives having phosphine ligands, whose structural characteristics have been tabulated by Haymore and Ibers [14], there is not such a significant shortening of Fe—C(O) bond lengths as that observed in the present study.

Concerning C—O distances, the mean value in the present complex (1.147(5) Å) is not significantly different from values found in the non-substituted derivatives of Table 3. The mean value for Fe—C—O angles is 179.0(3)°, nearer 180° than in most other iron carbonyl derivatives where the current values are in the range 177—178°.

The mean S—C bond length is 1.813(6) Å, and the mean Fe—S—C angle is 114.2(2)°, in good agreement with corresponding values in compounds II and IV of Table 3. The mean Fe—P distance is 2.221(1) Å, a value which agrees well with reported ones in some mononuclear iron carbonyl derivatives possessing

TABLE 3

COMPARISON OF THE MAIN MOLECULAR PARAMETERS OF $[\mu\text{-}(SCH_3)Fe(CO)_2P(CH_3)_3]_2$ (I) WITH THOSE OF IRON CARBONYL DERIVATIVES WITH Fe_2S_2 CORE[a]

References	$[C_2H_5SFe(CO)_3]_2$ (II) [2]	$[C_6H_5CSFe(CO)_3]_2$ (III) [3]	$[CH_3SFe_2(CO)_6]_2S$ (IV) [4]	$(py)Fe_2(CO)_6\text{-}\mu_4\text{-}S\text{-}Fe_2(CO)_6S(py)$ (V) [11]	Present work
Fe—Fe	2.537(10)	2.507(5)	2.540(5)	2.532(1)	2.518(1)
Fe—S	2.259(7)	2.259(3)	{ 2.274(4) 2.248(4)	{ 2.281(1) 2.255(1)	2.273(1)
S···S	2.932(14)	2.876(7)	2.817(6)	2.804(2)	2.790(3)
Fe—S—Fe	68.3(3)	67.4(1)	68.3(1)	67.9(1)	67.3(1)
S—Fe—S	81.0(3)	78.7(1)	77.1(1)	76.4(1)	75.7(1)
Dihedral angle $(Fe_1-S_1-S_2)-(Fe_2-S_1-S_2)$	95.2(5)	91.8(5)	88.3(3)	90.5(3)	90.9
Fe—C(O)	1.81(2)	1.778(9)	1.74(2)	1.795(3)	1.745(4)
C—O	1.15(2)	1.152(12)	1.18(2)	1.142(4)	1.147(5)

[a] Distances are in Å and bond angles in degrees. The values given are mean ones, ESD's shown in parentheses are the mean of individual ESD's divided by the square root of the number of observations.

TABLE 4

DISTANCES (Å) OF ATOMS FROM SELECTED LEAST-SQUARES PLANES OF THE MOLECULE

Plane I: Plane through Fe(1), Fe(2) and the midpoint of S(1)—S(2).
Equation: $0.9595\,X - 0.2948\,Y - 0.0137\,Z - 3.3326 = 0$ [a]

P(1)	−0.033(2)	C(1)	−1.217(8)	C(7)	1.323(11)
P(2)	−0.197(2)	C(2)	1.250(8)	C(8)	−1.432(12)
O(1)	−1.991(6)	C(3)	−1.212(9)	C(9)	−0.036(17)
O(2)	2.047(6)	C(4)	1.275(9)	C(10)	−1.865(11)
O(3)	−1.999(7)	C(5)	−3.108(9)	C(11)	0.485(12)
O(4)	2.140(8)	C(6)	3.130(9)	C(12)	0.549(13)

Plane II: Plane through S(1), S(2) and the midpoint of Fe(1)—Fe(2).
Equation: $-0.1257\,X - 0.3619\,Y - 0.9237\,Z + 7.3227 = 0$ [a]

P(1)	3.159(2)	C(1)	1.642(8)	C(7)	3.429(10)
P(2)	−3.120(2)	C(2)	1.701(8)	C(8)	3.361(9)
O(1)	1.914(7)	C(3)	−1.696(8)	C(9)	4.667(10)
O(2)	1.984(7)	C(4)	−1.753(8)	C(10)	−3.611(13)
O(3)	−2.014(7)	C(5)	−0.025(9)	C(11)	−4.617(9)
O(4)	−2.091(7)	C(6)	−0.022(9)	C(12)	−3.152(11)

[a] X, Y, Z are coordinates in Å in the orthonormal system: a, $c^* \wedge a$, c^*.

phosphine ligands [14]. The mean P—C bond length of 1.792(4) Å is appreciably lower than values found in the same mononuclear compounds, and than those which are observed in a few binuclear compounds having one or more phosphine ligands whose structures have been determined. Concerning the mean Fe—P—C and C—P—C angles, respectively 116.2(1)° and 102.0(2)°, the values are in very good agreement with the ones found in the literature. These angles around P atoms deviate from ideal tetrahedral geometry in the usual way.

Examination of Fig. 1 shows that the molecular symmetry of $[\mu\text{-}(SCH_3)Fe(CO)_2P(CH_3)_3]_2$ is close to C_{2v}, at least in its central part. Deviation from this

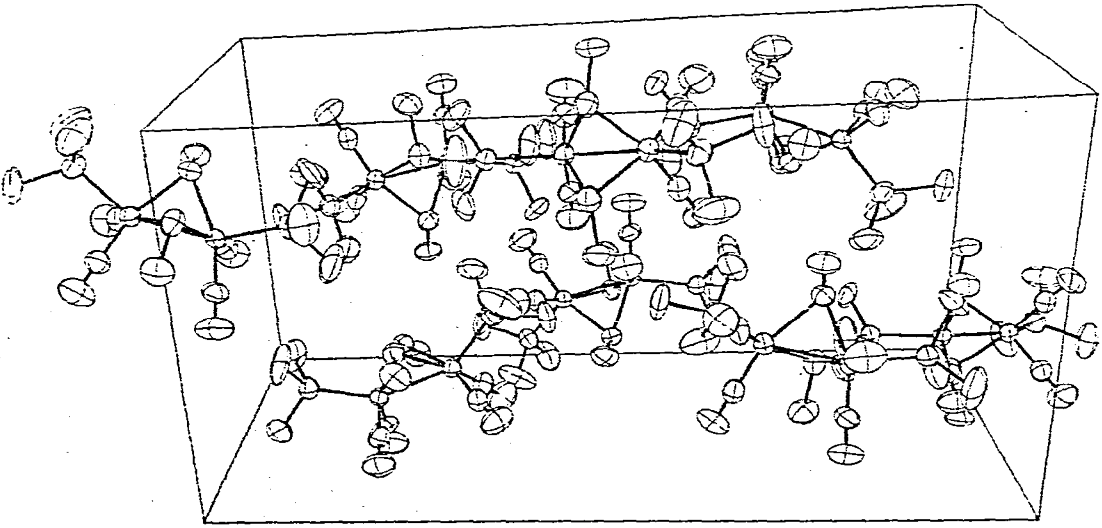


Fig. 3. Molecular packing of $[\mu\text{-}(SCH_3)Fe(CO)_2P(CH_3)_3]_2$.

TABLE 5

SHORTEST INTERMOLECULAR DISTANCES, REFERRED TO MOLECULE I (x, y, z) [a]

S(1)···C(9^{VI})	3.91 Å	O(3)···C(7^{V})	3.47 Å
S(2)···C(12^{IV})	3.82	O(3)···C(11^{IX})	3.57
O(1)···C(7^{V})	3.67	C(1)···C(7^{V})	3.81
O(1)···C(10^{VIII})	3.71	C(3)···C(7^{V})	3.59
O(1)···C(11^{VIII})	3.73	C(4)···C(7^{V})	3.88
O(2)···C(5^{III})	3.63	C(5)···C(10^{VIII})	3.91
O(2)···C(8^{VII})	3.60	C(11)···C(11^{II})	3.63

[a] Numbering of molecules. II: $y, x, \bar{z}+1$; III: $\bar{y}+1, \bar{x}, \bar{z}+\frac{1}{2}$; IV: $\bar{y}+1, \bar{x}+1, \bar{z}+\frac{1}{2}$; V: $\bar{y}+\frac{1}{2}, x-\frac{1}{2}, z+\frac{1}{4}$; VI: $\bar{x}+\frac{1}{2}, y+\frac{1}{2}, \bar{z}+\frac{1}{4}$; VII: $\bar{x}+\frac{1}{2}, y-\frac{1}{2}, \bar{z}+\frac{1}{4}$; VIII: $y-\frac{1}{2}, \bar{x}+\frac{1}{2}, z-\frac{1}{4}$; IX: $x-\frac{1}{2}, \bar{y}+\frac{1}{2}, \bar{z}+\frac{3}{4}$.

symmetry is essentially produced by the $P(CH_3)_3$ groups which clearly are not in an eclipsed conformation as would be the case with a true C_{2v} symmetry for the whole molecule. This is also evident from Table 4 which gives deviations of atoms from the mean least-squares planes I and II of the two pseudo-mirror planes, one through Fe(1), Fe(2) and the midpoint of S(1)—S(2), and the other through S(1), S(2) and the midpoint of Fe(1)—Fe(2). The angle between these two planes is exactly 90.0°.

The crystal packing in $[\mu\text{-}(SCH_3)Fe(CO)_2P(CH_3)_3]_2$ is shown in Fig. 3, and the shortest intermolecular distances are given in Table 5. The packing arises from normal Van der Waals interactions; none of the intermolecular distances are below the sum of Van der Waals radii of corresponding atoms.

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