Crystal and Molecular Structure of Di-μ-carbonyl-*cis*-μ-(1—5-η : 1′—5′-η-dicyclopentadienyldimethylsilane)bis(carbonyliron)(*Fe–Fe*)

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Crystals of the title compound are monoclinic, space group $P2_1/n$, with $Z = 4$ in a unit cell of dimensions: $a = 11{\cdot}66$, $b = 13{\cdot}27$, $c = 10{\cdot}82$ Å, $\beta = 105° 50'$. The structure was determined from diffractometer data by the symbolic addition method and refined to R 0·072 for 1309 independent reflections. The silicon atom is tetrahedrally σ bonded to two methyl groups and to two cyclopentadienyl rings; the latter are in turn each π-bonded to one iron atom. The two iron atoms are bonded to one another (2·51 Å) and are also linked by two symmetrical carbonyl bridges; the four-membered ring so defined is non-planar, being folded along the Fe–Fe axis away from the C_5 rings at an angle of *ca.* 160°. Each iron atom also carries one terminal carbonyl group, which makes the overall co-ordination approximately octahedral.

The Si atom does not lie in the $Fe_2(CO)_2$(terminal) plane, nor are the cyclopentadienyl rings symmetrically related to it (though their centroids lie in it), and the overall symmetry of the molecule is only $C_s(m)$. Reasons for this configuration are discussed. The Fe–C and C–O distances are as expected; the four Si–C distances relatively equal, mean 1·88 Å.

CRYSTALS of the title compound $Fe_2[\pi\text{-}C_5H_4{\cdot}Si(Me_2){\cdot}C_5H_4](CO)_4$ were prepared by heating under reflux a mixture of $(C_5H_5)_2SiMe_2$ and $Fe(CO)_5$ in octane for 20 h under nitrogen.[1] The structural interest of the compound lies in its relation to the known structures of compounds such as $[Fe(CO)_2(\pi\text{-}C_5H_5)]_2$,[2,3] in which the cyclopentadienyl rings are not connected to one another, $[(\pi\text{-}C_5H_5)_2Fe_2(CO)_3]_2{\cdot}Ph_2PCCPPh_2$,[4] which contains a similar iron carbonyl cyclopentadienyl moiety, and $[Fe\{\pi\text{-}C_5H_4{\cdot}[CH(NMe_2)]_2{\cdot}C_5H_4\}(CO)_4]$,[5] in which the cyclopentadienyl rings are linked by two-carbon bridges.

EXPERIMENTAL

Dark red crystals were obtained as thin plates developed in the (010) plane. The dimensions of the crystal chosen for *X*-ray diffraction (0·36 × 0·06 × 0·41 mm) were measured on a binocular microscope and the crystal mounted on *b* as rotation axis. Lattice parameters were measured from Weissenberg and precession photographs, and Mo-K_α radiation was used throughout. Intensities were measured for reciprocal layers $h0$—$9l$ on a Buerger–Supper–Pace 0·01°-incrementing two-circle autodiffractometer, with equi-inclination geometry and a stationary-background–ω-scan–stationary-background sequence. The diffractometer angular settings Υ and ϕ were input from punched paper tape prepared on an Atlas computer.[6] For each reflection hkl a scan interval of $(2{\cdot}0 + 0{\cdot}4/L)°$ was used, where L is the Lorentz correction, with a scan speed of 1° min^{-1}; during this scan a total count, N_3, was recorded. The stability of the apparatus and of the crystal were monitored by remeasuring the intensity of one particular reflection on each layer between every 20 measured intensities. No deviation $>3\ .\ N_3^{\frac{1}{2}}$ was observed. Peak profiles were checked on a chart recorder; this also served to confirm the accuracy of centring of ϕ. Background counts were taken for 0·5 min both before and after each scan (N_1 and N_2 respectively). The intensity of the reflection $I(hkl)$ is then proportional to $[N_3 - t_s(N_1 + N_2)]$ and the structure factor $F(hkl) =$

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[1] S. Moorhouse, Ph.D. Thesis, University of Bristol, 1971.

[2] O. S. Mills, *Acta Cryst.*, 1958, **11**, 620.

[3] R. F. Bryan and P. T. Greene, *J. Chem. Soc.* (*A*), 1970, 3068.

[4] A. J. Carty, T. W. Ng, W. Carter, G. J. Palenik, and T. Birchall, *Chem. Comm.*, 1969, 1101.

[5] F. S. Stephens, *J. Chem. Soc.* (*A*), 1970, 1722.

[6] J. C. Cuppola, TAPSET, A Fortran programme for calculation of diffractometer setting angles.

$[I(hkl)]^{\frac{1}{2}}(s/Lp)^{\frac{1}{2}}$, where s is a scale factor arbitrarily assessed at 10, p is the polarisation correction and t_s is the scan time in min; the standard deviation $\sigma_F(hkl) = (s/Lp)[N_3 + t_s^2(N_1 + N_2)]^{\frac{1}{2}}/2F(hkl)$. Structure factors and their standard deviations were computed from the punched paper tape output of the diffractometer by means of a specially written data reduction programme on an Atlas computer.[7] Reflections for which $[N_3 - t_s(N_1 + N_2)]/[N_3 + t_s(N_1 + N_2)]^{\frac{1}{2}} \leqslant 2{\cdot}0$ were regarded as 'unobserved' and were not included in the final refinement; the total number of 'observed' reflections was 1403.

RESULTS

Crystal Data.—$C_{16}H_{14}Fe_2SiO_4$, $M = 410{\cdot}1$, Monoclinic, $a = 11{\cdot}66(1)$, $b = 13{\cdot}27(1)$, $c = 10{\cdot}82(1)$ Å, $\beta = 105° 50'$ (10′), D_m (by flotation) $= 1{\cdot}60$, $Z = 4$, $D_c = 1{\cdot}65$, $F(000) = 832$. Space group $P2_1/n$. Mo-K_α X-radiation, $\lambda = 0{\cdot}7107$ Å; μ(Mo-K_α) $= 11{\cdot}44$ cm^{-1}.

TABLE 1

Atomic positional and thermal parameters, with standard deviations in parentheses

Atom	x/a	y/b	z/c	$U \times 10^2$ (Å^2) *
Fe(1)	0·5129(2)	0·1657(1)	0·2219(2)	3·35(5)
Fe(2)	0·5806(1)	0·3462(1)	0·2419(2)	3·14(6)
Si	0·4655(3)	0·2775(3)	0·4914(3)	3·16(9)
Carbonyl groups				
C(1)	0·5120(11)	0·1357(9)	0·0652(13)	4·1(3)
O(1)	0·5090(9)	0·1179(7)	−0·0405(10)	6·7(3)
C(2)	0·6014(11)	0·3734(10)	0·0957(14)	4·9(4)
O(2)	0·6157(10)	0·3955(9)	−0·0063(11)	7·9(3)
C(3)	0·6678(11)	0·2262(9)	0·2532(11)	3·8(3)
O(3)	0·7692(8)	0·1961(7)	0·2734(9)	5·4(3)
C(4)	0·4314(10)	0·2873(9)	0·1640(11)	3·2(3)
O(4)	0·3319(9)	0·3138(7)	0·1094(9)	5·9(3)
Methyl groups				
C(5)	0·3079(12)	0·3193(11)	0·4584(13)	5·1(4)
C(6)	0·5417(11)	0·2552(9)	0·6664(12)	4·3(5)
Cyclopentadienyl rings				
C(11)	0·4686(9)	0·1585(8)	0·3984(10)	2·6(2)
C(12)	0·5724(10)	0·0978(9)	0·4058(11)	3·6(3)
C(13)	0·5413(11)	0·0219(10)	0·3103(12)	4·5(3)
C(14)	0·4211(12)	0·0363(10)	0·2472(12)	4·3(3)
C(15)	0·3733(10)	0·1183(9)	0·2995(11)	3·6(3)
C(21)	0·5491(10)	0·3743(8)	0·4237(11)	3·0(3)
C(22)	0·6756(10)	0·3754(9)	0·4377(12)	4·0(3)
C(23)	0·6967(12)	0·4507(10)	0·3539(13)	4·6(3)
C(24)	0·5863(11)	0·4980(9)	0·2917(12)	3·8(3)
C(25)	0·4962(10)	0·4510(9)	0·3347(11)	3·3(3)
Hydrogen atoms (not refined)				
H(12)	0·665	0·111	0·475	4·4
H(13)	0·595	−0·039	0·289	4·4
H(14)	0·374	−0·011	0·166	4·4
H(15)	0·279	0·143	0·269	4·4
H(22)	0·744	0·320	0·500	4·4
H(23)	0·784	0·472	0·337	4·4
H(24)	0·574	0·564	0·228	4·4
H(25)	0·395	0·467	0·302	4·4

* $B = 8\pi^2U$.

The structure was solved by the symbolic addition method[8] and by successive electron-density difference syntheses. Attempts to refine the structure with isotropic thermal parameters for all atoms gave R 0·119 (R' 0·074); the quantity minimised was $\Sigma\{w|F_o| - |F_c|)^2\}$, and in the first instance w was taken as $1/\sigma_F(hkl)^2$. Further improvement in R was obtained by 'smoothing' the background count so as to reduce the effect of random variations; reflections for which N_1 and N_2 differed by $>[3\sigma(N_1) + 3\sigma(N_2)]$ were also deleted at this stage. The number of measured intensities used in the final refinement was thereby reduced to 1309. Individual weights were then recalculated according to the scheme: $1/w = \sigma^2 = \sigma_F^2 + |F_o| + 0{\cdot}002\ |F_o|^2$, devised so as to keep $w(\Delta F)^2$ as nearly constant as possible for ranges of F_o and of $(\sin\theta/\lambda)$. Convergence was obtained at R 0·072 (R' 0·082), and the value of the 'error-of-fit' $(=[\Sigma w(\Delta F)^2/n_o - n_v]^{\frac{1}{2}}$, where n_o = number (1309) of observations and n_v = number of variables) was 1·09. As there was no evidence on the electron-density maps for anisotropic thermal motion of either the iron or silicon atoms, no correction was applied. Finally the hydrogen atoms of the cyclopentadienyl rings were incorporated at calculated positions, assuming a C–H 1·10 Å and an isotropic thermal parameter of 3·5 Å^2. Neither the positional nor thermal parameters of the hydro-

TABLE 2

Molecular geometry *

(*a*) Distances (Å)

Fe(1)–Fe(2)	2·512(3)		
Fe(1)–C(1)	1·74(1)	Fe(2)–C(2)	1·70(1)
Fe(1)–C(3)	1·92(1)	Fe(2)–C(3)	1·87(1)
Fe(1)–C(4)	1·89(1)	Fe(2)–C(4)	1·88(1)
C(1)–O(1)	1·16(1)	C(2)–O(2)	1·20(2)
C(3)–O(3)	1·21(1)	C(4)–O(4)	1·21(1)
Fe(1)–C(11)	2·11(1)	Fe(2)–C(21)	2·13(1)
Fe(1)–C(12)	2·12(1)	Fe(2)–C(22)	2·13(1)
Fe(1)–C(13)	2·11(1)	Fe(2)–C(23)	2·08(1)
Fe(1)–C(14)	2·08(2)	Fe(2)–C(24)	2·08(1)
Fe(1)–C(15)	2·11(1)	Fe(2)–C(25)	2·10(1)
C(11)–C(12)	1·43(2)	C(21)–C(22)	1·43(2)
C(12)–C(13)	1·41(2)	C(22)–C(23)	1·40(2)
C(13)–C(14)	1·38(2)	C(23)–C(24)	1·42(2)
C(14)–C(15)	1·40(2)	C(24)–C(25)	1·40(2)
C(15)–C(11)	1·41(2)	C(25)–C(21)	1·41(2)
Si–C(11)	1·88(1)	Si–C(21)	1·88(1)
Si–C(5)	1·86(1)	Si–C(6)	1·88(1)

(*b*) Some intramolecular non-bonding distances (Å)

Fe(1) · · · Si	3·448(5)	Fe(2) · · · Si	3·449(5)
C(11) · · · C(21)	3·00(2)		
C(5) · · · C(6)	3·14(2)		
C(3) · · · C(4)	2·77(2)		
Si · · · C(3)	4·00(1)	Si · · · C(4)	3·45(1)

* Estimated standard deviations (in parentheses) include cell parameter errors.

(*c*) Angles (°)

Fe(1)–C(1)–O(1)	178·1(11)	C(12)–C(13)–C(14)	106·8(13)
Fe(1)–C(3)–O(3)	136·1(11)	C(13)–C(14)–C(15)	110·7(13)
Fe(1)–C(4)–O(4)	138·0(10)	C(14)–C(15)–C(11)	107·1(12)
Fe(2)–C(2)–O(2)	178·5(13)	C(25)–C(21)–C(22)	106·6(11)
Fe(2)–C(3)–O(3)	140·8(10)	C(21)–C(22)–C(23)	108·2(12)
Fe(2)–C(4)–O(4)	138·2(10)	C(22)–C(23)–C(24)	108·1(13)
C(1)–Fe(1)–C(3)	91·4(5)	C(23)–C(24)–C(25)	107·9(12)
C(1)–Fe(1)–C(4)	90·3(5)	C(24)–C(25)–C(21)	109·2(11)
C(1)–Fe(1)–Fe(2)	102·8(4)	Si–C(11)–C(15)	127·1(9)
C(2)–Fe(2)–C(3)	91·9(6)	Si–C(11)–C(12)	125·8(8)
C(2)–Fe(2)–C(4)	91·4(6)	Si–C(21)–C(25)	126·0(9)
C(2)–Fe(2)–Fe(1)	104·3(5)	Si–C(21)–C(22)	126·8(9)
C(3)–Fe(1)–C(4)	93·5(5)	C(11)–Si–C(21)	106·3(5)
C(3)–Fe(2)–C(4)	95·3(5)	C(5)–Si–C(6)	114·2(6)
Fe(1)–C(3)–Fe(2)	83·0(5)	C(5)–Si–C(11)	108·0(6)
Fe(1)–C(4)–Fe(2)	83·7(5)	C(5)–Si–C(21)	108·2(6)
C(15)–C(11)–C(12)	106·8(11)	C(6)–Si–C(11)	109·4(5)
C(11)–C(12)–C(13)	108·5(11)	C(6)–Si–C(21)	110·2(6)

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[7] S. F. Watkins, SPADD, a Fortran data reduction programme for use on an Atlas computer.

[8] M. M. Woolfson, 'Direct Methods in Crystallography,' Clarendon Press, Oxford, 1961, pp. 88—92.

gen atoms were refined. The final R 0·072 (R' 0·082) resulted from a refinement in which the average shift-to-error was 0·01, and a final electron-density difference synthesis showed no peaks $>0{\cdot}7$ or $<-0{\cdot}6$ eÅ^{-3}. Bond lengths and angles with their respective standard deviations were computed from the full variance–covariance matrix obtained in the last refinement cycle. Positional and thermal parameters are in Table 1, interatomic distances in Table 2, and some least-squares planes in Table 3. No absorption correction was applied, and the atomic scattering factors used were those of ref. 9. All computational work was carried out on an Atlas computer using the '*X*-Ray System' of programs.[10] Observed and calculated structure factors are listed in Supplementary Publication No. SUP 20703 (5 pp.).†

TABLE 3

(*a*) Some least-squares planes and lines: distances (Å) of relevant atoms from these planes are given in square brackets

Plane (1): Cyclopentadienyl ring 1

[C(11) −0·007, C(12) −0·001, C(13) 0·010, C(14) −0·014, C(15) 0·013]

$$-5{\cdot}1676x - 8{\cdot}0150y + 8{\cdot}2036z = -0{\cdot}4236$$

Plane (2): Cyclopentadienyl ring 2

[C(21) 0·017, C(22) −0·006, C(23) −0·008, C(24) 0·018, C(25) −0·022]

$$-0{\cdot}7140x + 8{\cdot}7537y + 7{\cdot}9782z = 6{\cdot}2816$$

Plane (3): Fe_2 and $(CO)_2$(terminal)

[Fe(1) 0·008, Fe(2) 0·015, C(1) 0·008, C(2) 0·002, O(1) −0·017, O(2) 0·003, Centroid ring (1) −0·002, Centroid ring (2) −0·017]

$$10{\cdot}4846x - 3{\cdot}9552y + 0{\cdot}6800z = 4{\cdot}8663$$

Plane (4): Fe_2 and μ-(CO) group (1)

[Fe(1) 0·006, Fe(2) 0·005, C(3) −0·022, O(3) 0·011]

$$-2{\cdot}0678x - 0{\cdot}4170y + 10{\cdot}7628z = 1{\cdot}2553$$

Plane (5): Fe_2 and μ-(CO) group (2)

[Fe(1) 0·002, Fe(2) 0·003, C(4) −0·012, O(4) 0·006]

$$-5{\cdot}7431x + 0{\cdot}9945y + 10{\cdot}4796z = -0{\cdot}4559$$

Plane (6): Fe(1), Fe(2), Si

$$9{\cdot}2711x - 3{\cdot}8166y + 3{\cdot}2105z = 4{\cdot}8371$$

Plane (7): Si, C(11), C(21)

$$8{\cdot}1368x - 3{\cdot}8018y + 4{\cdot}7734z = 5{\cdot}0812$$

Plane (8): Si, C_2(Me), μ-$(CO)_2$

[Si 0·022, C(3) −0·044, O(3) 0·015, C(4) 0·045, O(4) −0·017, C(5) −0·020, C(6) −0·0001]

$$3{\cdot}4199x + 12{\cdot}6305y + 0{\cdot}0676z = 5{\cdot}1271$$

Line (9): Si, C(11)

$x = 0{\cdot}4662$, $y = 0{\cdot}2186 + 0{\cdot}0632T$,* $z = 0{\cdot}4439 + 0{\cdot}0504T$

* T is a parameter which can assume all real values.

Line (10): Si, C(21)

$x = 0{\cdot}5086 + 0{\cdot}0448T$, $y = 0{\cdot}3278 + 0{\cdot}0518T$, $z = 0{\cdot}4586 - 0{\cdot}0352T$

Line (11): Fe(1), Fe(2)

$x = 0{\cdot}5467 + 0{\cdot}0268T$, $y = 0{\cdot}2558 + 0{\cdot}0719T$, $z = 0{\cdot}2321 + 0{\cdot}0079T$

(*b*) Angles (°) between least-squares planes and lines

(1)–(2)	97·2	(1)–(9)	5·4	(2)–(9)	8·2
(1)–(11)	49·5	(2)–(11)	47·7	(3)–(6)	13·7
(3)–(7)	22·8	(3)–(8)	89·5	(4)–(5)	159·7
(1)–(3)	89·6	(2)–(3)	89·3		

DISCUSSION

Our crystallographic study confirms that the overall gross structure of the molecule is that expected from spectroscopic considerations.[1] The silicon atom is tetrahedrally σ-bonded to two methyl groups and to two cyclopentadienyl rings, while the latter are in turn each π-bonded to one iron atom. The two iron atoms are bonded to one another (Fe–Fe 2·51 Å) and are also linked by two symmetrical carbonyl bridges. The Fe_2C_2 ring so defined is non-planar, with an angle between the two Fe–C–Fe planes of *ca.* 160°. Each iron atom carries one terminal carbonyl group on the side away from the cyclopentadienyl ring. The co-ordination state of the iron atoms can be regarded as octahedral if the cyclopentadienyl rings are assumed to occupy three sites and any iron–iron interaction is ignored; the 18-electron rule is obeyed only if the presence of an iron–iron bond is assumed. A stereoscopic view of the molecule drawn by computer[11] is given in Figure 1. The position of the molecule in its monoclinic unit cell, its relation to the symmetry elements of the space group, and the system of numbering the atoms, are illustrated by a view along the *b* direction of the cell (Figure 2).

The tetrahedral co-ordination around the silicon atom, coupled with the equivalence of the two iron atoms, constrains the cyclopentadienyl rings to an eclipsed (*cis*) configuration as seen along a line parallel to the Fe–Fe bond. Indeed, the whole molecule possesses idealised mirror symmetry about the plane which is the perpendicular bisector of the Fe–Fe bond, as shown in Figure 3, which also illustrates the most surprising feature of the molecule: that there is no second plane of symmetry. In fact the silicon atom lies more than 0·5 Å away from the plane defined by the iron atoms and the terminal carbonyl groups, although it is, of course, equidistant from both iron atoms. Furthermore, although the cyclopentadienyl rings are necessarily placed asymmetrically with respect to the $Fe_2(CO)_2$(terminal) plane, their centroids lie in this plane and the ring planes are perpendicular to it. We must ask why the silicon atom also does not lie in this plane to give the whole molecule C_{2v} ($2mm$) symmetry instead of its actual C_s (m) symmetry?

If it can be assumed that in the compound $[Fe(CO)_2(\pi\text{-}C_5H_5)]_2$[3] the cyclopentadienyl rings take up the optimum configuration with respect to the iron atoms because they are not otherwise bonded to extraneous atoms, then the 'natural' position is one in which the

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† For details of Supplementary Publications see Notice to Authors No. 7 in *J.C.S. Dalton*, 1972, Index issue. Items less than 10 pp. are sent as full-sized copies.

[9] H. P. Hanson, F. Herman, J. D. Lea, and S. Skillman, *Acta Cryst.*, 1964, **17**, 1040.

[10] J. M. Stewart, F. A. Kundell, and J. C. Baldwin, 'The *X*-ray System of Crystallographic Programmes for any Computer,' Computer Science Centre, University of Maryland, 1970.

[11] C. K. Johnson, ORTEP, a Fortran programme for crystal structure illustrations, Oak Ridge National Laboratory Report, ORNL 3794.

dihedral angle between the two ring planes is very close to 90°. In the compound $Fe_2\{\pi\text{-}C_5H_4\cdot CH(NMe_2)\cdot CH(NMe_2)\cdot C_5H_4\}(CO)_4$, where there is a relatively flexible two-carbon bridge between the two rings, the dihedral angle again remains close to 90° (88·8°). In our silicon-bridged structure, however, the angle between the ring planes has increased to 97·2°, doubtless primarily because of the added constraint imposed by the lengths of the Si–C bonds which, at 1·88(1) Å, are not significantly different from other tetrahedral Si–C bonds.[12] In pulling the rings closer to one another, however, the silicon atom becomes constrained to a bond angle equal to the dihedral angle between the two cyclopentadienyl ring planes, except in so far as the Si–C bonds deviate (i) from the plane of the ring to which they are attached and (ii) from the $Fe_2(CO)_2$ plane in which the Si atom would lie if the overall symmetry were C_{2v}. By swinging out of this plane, the Si atom forces the cyclopentadienyl rings even closer together (thus making the dihedral angle nearer to the tetrahedral value), and in conjunction with the deviation of the Si–C bond from the plane of the C_5 rings towards the Fe_2 axis, achieves an environment which is very close to ideal tetrahedral (see Table 2 and Figure 4).

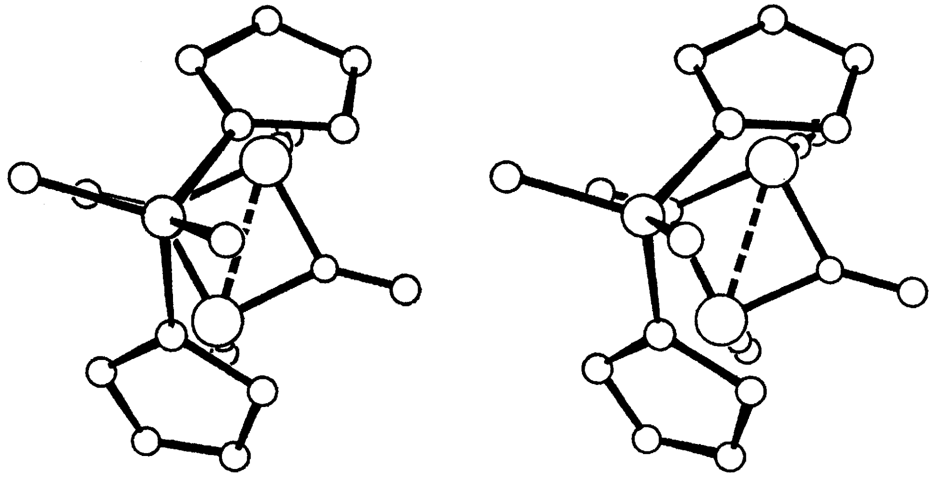

FIGURE 1 A stereoscopic view of the molecule

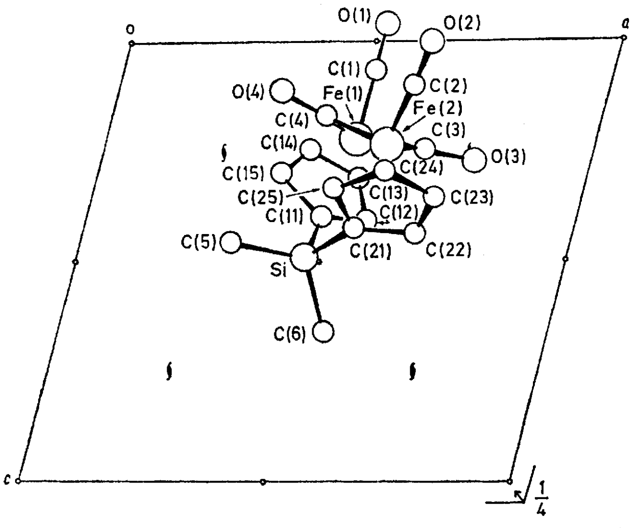

FIGURE 2 A view of the molecule in its monoclinic cell seen in projection along *b* looking towards the origin. Only one molecule is shown, but the symmetry elements of $P2_1/n$ show how the three symmetry-related molecules are placed

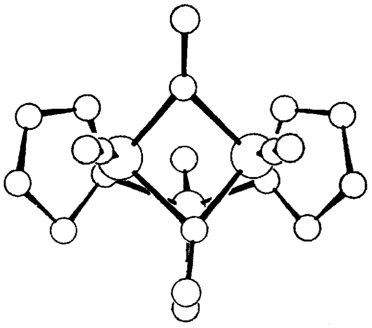

FIGURE 3 A view of the molecule along the *c* direction of the monoclinic cell, showing the displacement of the silicon atom from the central $Fe_2(CO)_2$(terminal) plane.

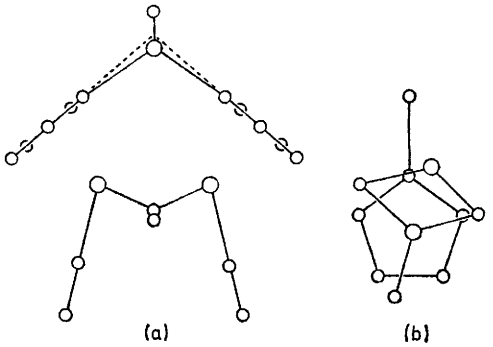

FIGURE 4 Diagrammatic representations of the molecule to show geometrical relationships, (a) in section through the $Fe_2(CO)_2$(terminal) plane, and (b) along the vector perpendicular to the cyclopentadienyl ring passing through the centroid

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[12] Chem. Soc. Special Publ., No. 18, 1965.

The Fe–Fe *Interaction*.—The value of the Fe–Fe bond distance [2·512(3) Å] is close to those found in other structures containing two iron atoms bridged by two carbonyl groups: *e.g.*, 2·510(1) $Fe_2\{(\pi\text{-}C_5H_4\cdot CH(NMe_2)\cdot CH(NMe_2)\cdot C_5H_4\}(CO)_4$,[5] 2·531(2) *cis*$[(\pi\text{-}C_5H_5)Fe(CO)_2]_2$,[3] 2·534(2) *trans*$[(\pi\text{-}C_5H_5)Fe(CO)_2]_2$,[13] 2·55(1) $Fe_3(CO)_{12}$,[14] 2·54 $[(\pi\text{-}C_5H_5)_2Fe_2(CO)_3]_2\cdot Ph_2PCCPPh_2$,[4] and 2·53 Å $[(\pi\text{-}C_5H_5)Fe(CO)]_2CO\cdot CNPh_5$.[15]

The Carbonyl Groups.—The geometry of the $Fe_2(CO)_4$ portion of the molecule is identical (within experimental error) to that of the similar units in the compounds of refs. 3 and 5. The terminal groups show no significant deviation from linearity and form a coplanar unit with the two iron atoms. The bridging carbonyl groups likewise form individual coplanar units with the two iron atoms, but the two planes so defined are not themselves coplanar: the dihedral angle between these planes is 160°. The individual Fe–C and C–O distances are as expected. The mean Fe–C–Fe angle for the carbonyl bridge is 82·5°.

The Silicon–Carbon Bonds.—These have a mean length of 1·88(1) Å and the silicon atom achieves a closely tetrahedral environment (Table 2). The two links to the cyclopentadienyl rings deviate from the planes of the rings towards the Fe–Fe axis (see Table 3). The plane defined by the two Si–(C_5-ring) bonds is, of course, parallel to the Fe · · · Fe vector but does not include the two iron atoms; it is at an angle of *ca.* 23° to the $Fe_2(CO)_2$(terminal) plane.

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