lated trinuclear metal carbonyl complexes, is given elsewhere.[41]

The apical group in each of the diamagnetic complexes $Co_3(CO)_9CCH_3$ and $Ir_4(CO)_{12}$ is formally a three-electron donor such that each metal of the $M_3(CO)_9$ fragment achieves a closed-shell electronic configuration, whereas in the paramagnetic complex $SCo_3(CO)_9$ the sulfur effectively contributes *four* electrons to the $Co_3(CO)_9$ fragment such that the entire molecule contains one electron in excess of the "krypton" configuration for each cobalt atom.

A salient structural feature of the SCO_3 fragment of $SCo_3(CO)_9$ is that the average distance of 2.64 A for the Co–Co bonds is longer by 0.1–0.2 A than the Co–Co distances found in $Co_3(CO)_9CCH_3$ (2.46 A) and in other polynuclear cobalt carbonyl complexes.[41] The average Co–S length of 2.14 A is at least 0.1 A shorter than other Co–SR bond lengths in complexes containing triply bridging and/or doubly bridging metal-coordinated mercapto groups[12,20] but agrees closely with Co–S bond lengths in other complexes in which the sulfur is symmetrically coordinated to cobalt atoms.[20]

A preliminary X-ray investigation of the diamagnetic complex $SCo_2Fe(CO)_9$, recently prepared by Khattab, Markó, Bor, and Markó,[15] showed that the crystals of this cobalt–iron complex (in which an iron atom is substituted for one cobalt atom) are isomorphous with those of $SCo_3(CO)_9$. A complete structural determination of this diamagnetic complex is in progress in order to determine the effect of the one unpaired electron on the metal–metal bonds in $SCo_3(CO)_9$. Also, a single-crystal esr study of the paramagnetic $SCo_3(CO)_9$ diluted in the diamagnetic host $SCo_2Fe(CO)_9$ is being carried out in collaboration with Professor John E. Harriman at the University of Wisconsin for the purpose of unraveling the electron density distribution of the unpaired electron. Details of these investigations will be reported in later papers.

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CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY, THE OHIO STATE UNIVERSITY, COLUMBUS, OHIO 43210,
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Preparation and Structure of $[CH_3SFe_2(CO)_6]_2S$: an Organometallic Complex Containing a Tetrahedral-like Sulfur Atom Coordinated to Four Metal Atoms[1]

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The reaction of $Fe_3(CO)_{12}$ with methyl thiocyanate has yielded as a condensation by-product the diamagnetic tetramer $[CH_3SFe_2(CO)_6]_2S$. This complex has been characterized by chemical and physical means including a three-dimensional single-crystal X-ray study which not only unambiguously established the actual composition but also revealed the first known example of an organometallic complex containing a tetrahedral-like sulfur atom bridging four metal atoms. The compound crystallizes with two molecules in a triclinic unit cell of symmetry $P\bar{1}$ and of reduced cell parameters $a = 8.93$ A, $b = 9.28$ A, $c = 16.04$ A, $\alpha = 81° 40'$, $\beta = 80° 05'$, and $\gamma = 66° 35'$. A full-matrix, anisotropic–isotropic, least-squares refinement has resulted in discrepancy factors of $R_1 = 9.1\%$ and $R_2 = 9.3\%$. The molecular configuration of approximate C_2-2 symmetry consists of two essentially identical $[CH_3SFe_2(CO)_6]$ fragments bridged by a metal-coordinated tetrahedral-like sulfur atom which donates its *six* valence electrons to the four iron atoms. The properties and structural features are discussed and compared with those of $[C_2H_5SFe(CO)_3]_2$ and other related complexes.

Introduction

The reactions of sulfur and sulfur-containing compounds with metal carbonyls and derivatives have produced a wide variety of unusual organometallic sulfur complexes.[3–11] To date, structural investigations of a number of these compounds have shown sulfur to utilize from one to five of its six valence electrons

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(1) The structural characterization of this compound represents the VIIth paper concerning systematic structural investigations of organometallic sulfur complexes. For paper VI see: C. H. Wei and L. F. Dahl, *Inorg. Chem.*, **6**, 1229 (1967).

(2) (a) University of Wisconsin; (b) the X-ray work is abstracted in part from the Ph.D. thesis of J. M. Coleman, University of Wisconsin, 1966; (c) The Ohio State University.

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in bonding to transition metals. Metal carbonyl mercapto complexes[5,12] studied include ones in which the RS ligands are attached to one,[13] two,[14–18] and three[16,18] metal atoms by formal use of one, three, and five valence electrons, respectively. Direct crystallographic evidence of sulfur functioning as a doubly bridging, two-electron-donating group,[19] a triply bridging, four-electron-donating group,[10,11,18,20–23] and a quadruply bridging, four-electron-donating group[24] in organometallic complexes also has been recently uncovered.

This paper reports the preparation, properties, and X-ray characterization of $[CH_3SFe_2(CO)_6]_2S$ which has provided the first known example of an organometallic complex in which sulfur donates *six* electrons to *four* metal atoms. This compound was first isolated by P. J. P. and A. W. as a by-product during their investigation of the reactions between alkyl thiocyanates and triiron dodecacarbonyl in an attempt to prepare hitherto unknown dimeric bridging thiocyanato complexes of the type $[Fe(CO)_3SCN]_2$ in which each sulfur atom is coordinated to the two metal atoms. In particular, formation of $[CH_3SFe_2(CO)_6]_2S$ was observed in 1% yield on the heating of $Fe_3(CO)_{12}$ with methyl thiocyanate in benzene. The molecular weight determinations together with the elemental analysis were consistent with a tetranuclear iron carbonyl methyl mercaptan complex. The infrared spectrum indicated the presence of only terminal carbonyl groups, while the nmr spectrum established the diamagnetism of the compound and the equivalence of all hydrogen atoms. An X-ray crystallographic study was necessary in order to establish the actual composition as well as the molecular configuration of this new type of mixed mercapto–sulfur–metal complex. This latter technique directly disclosed the presence of a tetrahedral-like, four-coordinated sulfur atom linking two diiron hexacarbonyl methyl mercaptan moieties to each other by its participation as a bridging ligand in each moiety.

Experimental Section

Preparation and Properties of $[CH_3SFe_2(CO)_6]_2S$.—Methyl thiocyanate (Eastman Organic Chemicals; 5.0 g, 69 mmoles) was added to 11 g (22 mmoles) of $Fe_3(CO)_{12}$[25] in 150 ml of benzene. The reaction mixture was refluxed under nitrogen until the initial green color changed to deep red-brown (*ca.* 6 hr). The contents of the flask were then cooled to 25° and filtered to give 5 g of a brown, pyrophoric residue and a deep red filtrate. The filtrate was evaporated to dryness at 25° (~20 mm); the red solid was dissolved in *ca.* 10 ml of hexane, and the solution was filtered. Chromatography of this solution on an alumina column (60 × 2.5 cm; Woelm alumina, grade III acid) with hexane eluent gave three bands. Upon evaporation of the solvent at 25° (~20 mm), the first two eluates—red and orange in color—yielded the *anti* (1.85 g, 15%) and *syn* (0.98 g, 8%) isomers of $[CH_3SFe(CO)_3]_2$, respectively. These compounds were characterized by comparison of their infrared spectra with those reported earlier by King.[26]

Evaporation of the solvent (~20 mm) from the third eluate afforded 0.11 g (~1% yield) of deep red crystals which melt at 162–165° (uncorrected). *Anal.* Calcd for $[CH_3SFe_2(CO)_6]_2S$: S, 14.03; C, 24.55; H, 0.88; mol wt, 686. Found:[27] S, 14.23; C, 24.77; H, 1.09; mol wt (Mechrolab osmometer, Model 301 A), 662 (C_6H_6), 702 (CCl_4), 698 ($CHCl_3$). The compound is very stable to air; however, its solutions in organic solvents decompose slowly on storage. The infrared spectrum of $[CH_3SFe_2(CO)_6]_2S$ shows CO stretching bands at 2082 (m), 2059 (s), 2942 (vs), 2010 (s), and 1995 (s) cm^{-1} (1,1,2,2-tetrachloroethane solution; Beckman IR-9 spectrophotometer); other prominent absorptions are at 2948 (m), 1438 (m), 1429 (m), 1318 (m), 960 (w), 948 (vw), 700 (vw), 620 (s), 585 (s), 560 (s), 500 (m), and 461 (w) cm^{-1} (KBr pellet; Perkin-Elmer Model 337 spectrophotometer). Its proton magnetic resonance spectrum in $CDCl_3$ solution shows a sharp signal at τ 7.67 (tetramethylsilane internal standard).

X-Ray Data.—Weissenberg and precession photographs showed the compound to be triclinic. For the collection of intensity data, a small, uniformly shaped needle crystal 0.29 mm in diameter and 0.57 mm in length was cut from a larger crystal and mounted inside a thin-walled Lindemann glass capillary. Eleven layers of multiple-film equiinclination Weissenberg data obtained by rotation about the *a* axis of a B-centered unit cell resulted in 1985 visually estimated reflections. In addition, three layers of multiple-film equiinclination Weissenberg data were taken around the *a* axis of the reduced primitive unit cell. Two separate sets of intensity data (corresponding to a 360° rotation range) were collected for all nonzero reciprocal levels by which the entire accessible independent reciprocal lattice was recorded on the top half of the Weissenberg film. The intensities of only the upper half of the Weissenberg film were determined in order to eliminate the variation in area of each reflection due to spot compaction.[28] An analytical correction of these data for spot extension was made.[29] Timed-exposure precession photographs were taken for the *hk*0 and *hk*1 layers of the B-centered triclinic cell.

In order to obtain precise photographic data over a wide range of intensities, all photographs were taken with Zr-filtered Mo Kα radiation. In general, each set of Weissenberg data consisted of three (two) nine-film packets which were exposed to the X-ray beam for 70, 10, and 1.5 hr (if necessary). Timed exposures differing by a factor of 1.3 were used for the precession data with the longest exposed time being 36 hr. The intensities on each film were judged by comparison with a calibrated set of intensities of a given reflection taken from the same crystal. For each nonweak reflection at least five independent intensity measurements in the linear range were made. These measurements for each reflection in a given set were averaged with the INTAV program.[30] After corrections for Lorentz-polarization effects (*i.e.*, absorption corrections were ignored owing to the small estimated μR_{max} value of 0.36), all sets of Weissenberg and precession data, which contained 849 common reflections, were merged onto one scale by a weighted least-squares program.[31]

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The low disagreement factor of 4.7% for the merging, which yielded 2057 independent maxima, indicated that the resulting structure amplitudes did not contain serious systematic errors.

The standard deviations of the individual structure amplitudes were estimated as follows: if $I(hkl)_o < \sqrt{10}I_{\min}$, $\sigma(F(hkl)_o) = [|F(hkl)_o|/20][\sqrt{10}I_{\min}/I(hkl)_o]^2$; if $I(hkl)_o \geq \sqrt{10}I_{\min}$, $\sigma(F(hkl)_o) = |F(hkl)_o|/20$.

In order to obtain accurate lattice constants, precession photographs of the $h0l$ and $hk0$ zones of the B-centered unit cell were calibrated by the superposition of a zero-level NaCl exposure on the same film.

Crystal Data.—The measured lattice parameters for the non-Bravais B-centered triclinic cell of $[CH_3SFe_2(CO)_6]_2S$ (mol wt, 685.8) are $a_B = 10.00 \pm 0.02$ A, $b_B = 16.04 \pm 0.03$ A, $c_B = 15.23 \pm 0.03$ A, $\alpha_B = 79° 05' \pm 10'$, $\beta_B = 87° 35' \pm 10'$, and $\gamma_B = 91° 05' \pm 10'$. All results, however, are reported in terms of the primitive reduced cell, which is obtained from the B-centered cell by the following transformation: $a = 0.5(-a_B + c_B)$, $b = 0.5(a_B + c_B)$, and $c = b_B$. A Delaunay reduction[32] verified the triclinic symmetry.

The lattice parameters for this reduced cell are $a = 8.93 \pm 0.02$ A, $b = 9.28 \pm 0.02$ A, $c = 16.04 \pm 0.03$ A, $\alpha = 81° 40' \pm 10'$, $\beta = 80° 05' \pm 10'$, and $\gamma = 66° 35' \pm 10'$; the volume of this unit cell is 1,197.5 A^3. The observed density of 1.91 g cm^{-3}, measured by flotation in ethyl iodide, agrees well with the value of 1.90 g cm^{-3} calculated on the basis of two structurally determined formula species per unit cell. The total number of electrons per unit cell, $F(000)$, is 676. The linear absorption coefficient for Mo Kα radiation is 24.9 cm^{-1}. The centrosymmetric space group $P\overline{1}$ was inferred from the distribution of heavy-atom vectors in the Patterson map and subsequently confirmed by the structural determination. Hence, the crystallographically independent unit consists of four iron, three sulfur, twelve oxygen, fourteen carbon, and six hydrogen atoms which comprise one molecule. All atoms were found from the X-ray determination to occupy the general twofold set of positions $\pm(x, y, z)$ of $P\overline{1}$.

Determination of the Structure.—Application of the usual combination of three-dimensional Patterson and Fourier syntheses eventually led to the location of 33 nonhydrogen atoms which thereby established the exact composition of the compound. The resulting atomic parameters were refined with a local version of the Busing–Martin–Levy full-matrix, least-squares program.[33] Five cycles of isotropic refinement of the unmerged Weissenberg data were performed until all parameter shifts except for those of two light atoms were less than one standard deviation. For this refinement the unweighted R_1 equals 11.3% and the weighted R_2 equals 12.1%. At this point the merged data became available for refinement. Three least-squares cycles with an isotropic thermal parameter per atom and one scale factor lowered R_1 to 9.8% and R_2 to 10.4%. A three-dimensional difference Fourier synthesis based on these refined atomic parameters showed neither residual peaks greater than 1 electron/A nor troughs less than -1.5 electrons/A^3. Since some anisotropic density was observed around the iron positions on this map, two further cycles of least-squares refinement with anisotropic temperature factors for only the iron atoms were computed; the discrepancy values were reduced to $R_1 = 9.1\%$ and $R_2 = 9.5\%$. Two final cycles then were run with anisotropic temperature factors applied to the iron and sulfur atoms and isotropic thermal parameters to all other atoms; the final R_1 and R_2 values for this last anisotropic–isotropic refinement were 9.1 and 9.3%, respectively. An inspection of these refinements with the merged data revealed no differences greater than 1σ for the corresponding atomic parameters either between the completely isotropic refinement and the final anisotropic–isotropic refinement or between the two anisotropic–isotropic refinements.

The positional and thermal parameters for the last mixed anisotropic–isotropic refinement are given in Table I. The observed and calculated structure factors based on the output parameters of the last cycle of this refinement are given in Table II. On the basis of the minimum intensities recorded on the photographs, unobserved structure factors were generated to the edge of the observed reciprocal lattice corresponding to $(\sin\theta)/\lambda = 0.6$. Structure factor calculations for these unobserved reflections verified the over-all correctness of the structure; these F_c values for the unobserved but experimentally accessible reflections were omitted from Table II, since none of them was greater than $1.4F_o$(min).

TABLE I

FINAL ATOMIC PARAMETERS AND STANDARD DEVIATIONS FOR $[CH_3SFe_2(CO)_6]_2S$ FROM ANISOTROPIC–ISOTROPIC LEAST-SQUARES REFINEMENT

Atom	x ($10^4\sigma_x$)	y ($10^4\sigma_y$)	z ($10^4\sigma_z$)	B ($10^2\sigma_B$)
Fe(1)	1.1250 (2)	0.7825 (3)	0.1632 (1)	*a*
Fe(2)	0.9460 (2)	0.6269 (3)	0.2229 (2)	*a*
Fe(3)	1.3302 (2)	0.4718 (3)	0.3657 (1)	*a*
Fe(4)	1.4128 (2)	0.3181 (3)	0.2355 (1)	*a*
S(1)	1.0836 (5)	0.6129 (6)	0.0899 (3)	*a*
S(2)	1.2440 (5)	0.2765 (6)	0.3524 (3)	*a*
S(3)	1.2087 (4)	0.5553 (6)	0.2460 (2)	*a*
$H_3C(1)$	0.9426 (22)	0.7075 (26)	0.0076 (12)	4.22 (42)
$H_3C(2)$	1.3362 (20)	0.0914 (26)	0.4146 (12)	4.00 (41)
C(1-1)	1.2967 (21)	0.8005 (26)	0.0968 (12)	3.80 (40)
O(1-1)	1.4058 (17)	0.8101 (21)	0.0472 (9)	5.93 (34)
C(1-2)	0.9717 (19)	0.9546 (24)	0.1222 (10)	2.99 (35)
O(1-2)	0.8626 (16)	1.0578 (20)	0.0951 (8)	5.38 (32)
C(1-3)	1.1213 (20)	0.8889 (27)	0.2450 (12)	3.92 (41)
O(1-3)	1.1166 (17)	0.9602 (22)	0.3026 (10)	6.50 (37)
C(2-1)	0.9126 (22)	0.4505 (30)	0.2352 (13)	4.27 (45)
O(2-1)	0.8955 (19)	0.3332 (25)	0.2426 (10)	7.25 (42)
C(2-2)	0.7627 (24)	0.7503 (30)	0.1878 (13)	4.87 (46)
O(2-2)	0.6347 (15)	0.8475 (19)	0.1625 (8)	5.54 (33)
C(2-3)	0.8709 (18)	0.6774 (23)	0.3259 (11)	2.93 (35)
O(2-3)	0.8151 (16)	0.7197 (21)	0.3938 (9)	5.84 (34)
C(3-1)	1.1861 (22)	0.5776 (28)	0.4458 (12)	4.30 (43)
O(3-1)	1.0996 (18)	0.6447 (22)	0.5046 (10)	6.87 (38)
C(3-2)	1.4773 (23)	0.3493 (28)	0.4264 (12)	4.51 (45)
O(3-2)	1.5753 (18)	0.2683 (23)	0.4707 (10)	7.06 (40)
C(3-3)	1.4377 (21)	0.5984 (26)	0.3376 (11)	3.57 (39)
O(3-3)	1.5038 (18)	0.6878 (23)	0.3213 (10)	6.58 (38)
C(4-1)	1.3599 (22)	0.2251 (28)	0.1636 (13)	4.51 (46)
O(4-1)	1.3226 (15)	0.1572 (20)	0.1207 (9)	5.46 (33)
C(4-2)	1.5884 (20)	0.1697 (25)	0.2708 (11)	3.52 (37)
O(4-2)	1.7030 (16)	0.0596 (20)	0.2949 (9)	5.58 (32)
C(4-3)	1.5322 (20)	0.3928 (24)	0.1593 (11)	3.24 (37)
O(4-3)	1.6125 (17)	0.4543 (22)	0.1107 (10)	6.59 (38)

Resulting Thermal Coefficients ($\times 10^4$) with Esd of the Last Significant Figures Given in Parentheses

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Fe(1)	104 (4)	63 (4)	23 (1)	−32 (4)	−12 (2)	−2 (2)
Fe(2)	71 (3)	74 (4)	30 (1)	−22 (4)	−17 (2)	−2 (2)
Fe(3)	90 (4)	98 (5)	17 (1)	−28 (4)	−7 (2)	−6 (2)
Fe(4)	78 (3)	83 (5)	22 (1)	−9 (4)	−10 (2)	−10 (2)
S(1)	152 (7)	95 (9)	23 (2)	−48 (7)	−28 (3)	−2 (4)
S(2)	118 (6)	82 (8)	28 (2)	−33 (7)	−19 (3)	6 (4)
S(3)	70 (6)	75 (8)	18 (2)	−26 (6)	−6 (3)	−2 (3)

[a] For the Fe and S atoms the anisotropic temperature factors are of the form: $\exp\{-[B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + 2B_{12}hk + 2B_{13}hl + 2B_{23}kl]\}$.

The intramolecular distances and angles, together with estimated standard deviations, calculated from the full inverse matrix (which included lattice parameter errors) with the Busing–

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TABLE II

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $[CH_3SFe_2(CO)_6]_2S$

H	K	L	FO	FC
0	0	3	55.0	48.4
0	0	4	20.0	20.4
0	0	5	25.6	19.5
0	0	-6	27.7	25.5
0	0	-7	72.2	74.2
0	0	-8	72.8	74.8
0	0	9	40.4	38.7
0	0	-10	49.5	55.0
0	0	-12	41.9	41.1
0	0	-13	44.3	45.4
0	0	-15	58.0	67.9
0	-1	-1	79.3	85.4
0	-1	2	31.7	29.7
0	-1	-2	134.6	132.4
0	-1	3	35.7	31.7
0	-1	4	22.1	17.9
0	-1	-4	38.0	33.9
0	-1	5	23.0	21.5
0	-1	-5	84.4	89.7
0	-1	6	26.3	26.0
0	-1	-6	49.3	51.1
0	-1	7	52.7	52.4
0	-1	-7	143.5	156.8
0	-1	8	95.6	96.8
0	-1	-8	33.0	32.4
0	-1	-9	89.5	96.3
0	-1	10	46.8	46.3
0	-1	-10	24.1	24.6
0	-1	-12	20.2	17.6
0	-1	13	42.5	42.9
0	-1	14	31.6	28.3
0	-1	15	29.0	28.2
0	-1	-15	33.8	33.0
0	-1	16	26.3	19.7
0	-1	17	22.2	14.0
0	-1	-17	24.4	23.6
0	-1	18	29.4	29.3
0	-2	-4	56.5	58.0
0	-2	-5	70.2	73.6
0	-2	6	69.6	66.7
0	-2	-6	41.6	40.7
0	-2	7	34.7	32.6
0	-2	-8	63.8	66.0
0	-2	9	32.7	31.5
0	-2	-9	65.0	65.5
0	-2	10	40.1	41.4
0	-2	11	39.2	39.4
0	-2	12	40.7	35.9
0	-2	-12	40.8	40.7
0	-2	13	60.6	62.9
0	-2	16	43.3	46.2
0	-2	18	26.1	27.0
0	-3	2	24.3	20.8
0	-3	3	56.4	65.7
0	-3	-3	50.6	51.8
0	-3	4	54.3	69.2
0	-3	-4	90.2	98.6
0	-3	5	58.7	73.6
0	-3	-5	57.1	65.1
0	-3	6	49.9	49.6
0	-3	-6	39.3	35.3
0	-3	-7	65.2	69.1
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-3	-7	3	35.8	37.3
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-3	-8	-9	54.3	60.5
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9	4	2	50.8	50.9
9	4	4	33.3	34.5
9	4	5	32.2	27.3
9	4	6	31.4	25.0
9	4	-6	29.7	23.8
9	4	7	37.5	36.9
9	5	2	31.8	31.8
9	5	7	29.4	22.0
9	5	8	32.5	33.1
9	5	9	35.4	36.3
9	6	5	35.5	34.2
9	6	10	34.2	31.1
9	7	-2	30.3	26.3
9	7	-3	27.8	22.0
9	7	-4	32.2	27.8
9	7	5	26.2	22.2
9	7	6	29.8	32.7
9	7	7	27.4	29.3
9	7	10	27.4	18.4
9	8	-2	26.0	26.4
9	9	2	27.3	20.2
9	9	5	33.6	18.4
10	-1	-1	25.3	21.6
-10	-1	3	19.5	14.1
10	-1	-3	24.0	23.0
-10	-1	5	20.6	17.0
-10	-1	-6	27.1	24.7
10	-1	7	29.2	27.9
10	-1	9	29.8	26.2
10	-1	10	25.0	16.6
10	-1	12	23.5	24.4
10	-1	14	24.2	19.4
-10	-2	0	15.8	13.3
10	2	-2	29.6	25.5
-10	-2	2	22.4	25.3
-10	-2	-3	16.5	15.2
-10	-2	-4	21.6	23.0
10	4	1	22.7	22.4
10	5	1	35.1	31.1
10	5	-1	30.5	16.8
10	5	-2	30.8	19.8
10	5	6	30.8	25.0
10	5	7	28.9	18.2
10	5	8	38.2	34.5
10	8	0	27.2	23.6
10	8	2	26.9	26.3
10	9	2	29.8	32.0
10	9	4	30.8	30.4
-11	-1	0	25.3	24.0
-11	-1	2	24.2	17.0
-11	-1	-2	23.6	20.6
-11	-1	-5	33.1	35.2
-11	-1	-7	28.0	30.0

Martin–Levy function and error program,[34] are listed in Tables III and IV, respectively. Table V presents specified nonbonding intramolecular distances. Table VI gives the "best" molecular least-squares planes formed by certain specified atoms and the perpendicular distances of these and other atoms from these planes.[35] All Patterson and Fourier summations were computed with the Blount program.[36] The atomic scattering factors utilized

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[34] W. R. Busing, K. O. Martin, and H. A. Levy, ORFFE", A Fortran Crystallographic Function and Error Program," ORNL-TM-306, Oak Ridge National Laboratory, 1964.

[35] D. L. Smith, Ph.D. Thesis, Appendix IV, University of Wisconsin, 1962.

[36] J. F. Blount, Ph.D. Thesis, Appendix, University of Wisconsin, 1965.

TABLE III

INTRAMOLECULAR DISTANCES AND STANDARD DEVIATIONS (A) OF $[CH_3SFe_2(CO)_6]_2S^a$

Fe(1)–Fe(2)	2.543 (6)	C(1-1)–O(1-1)	1.17 (2)
Fe(3)–Fe(4)	2.536 (7)	C(1-2)–O(1-2)	1.16 (2)
Av	2.540	C(1-3)–O(1-3)	1.20 (2)
Fe(1)–S(1)	2.268 (7)	C(2-1)–O(2-1)	1.14 (3)
Fe(2)–S(1)	2.265 (8)	C(2-2)–O(2-2)	1.23 (2)
Fe(3)–S(2)	2.280 (8)	C(2-3)–O(2-3)	1.17 (2)
Fe(4)–S(2)	2.284 (7)	C(3-1)–O(3-1)	1.19 (2)
Av	2.274	C(3-2)–O(3-2)	1.17 (2)
Fe(1)–S(3)	2.247 (7)	C(3-3)–O(3-3)	1.17 (2)
Fe(2)–S(3)	2.253 (7)	C(4-1)–O(4-1)	1.16 (2)
Fe(3)–S(3)	2.254 (7)	C(4-2)–O(4-2)	1.20 (2)
Fe(4)–S(3)	2.239 (7)	C(4-3)–O(4-3)	1.20 (2)
Av	2.248	Av	1.18
Fe(1)–C(1-1)	1.76 (2)	$H_3C(1)$–S(1)	1.86 (2)
Fe(1)–C(1-2)	1.77 (2)	$H_3C(2)$–S(2)	1.82 (2)
Fe(1)–C(1-3)	1.74 (2)	Av	1.84
Fe(2)–C(2-1)	1.76 (3)	S(1)···S(3)	2.812 (9)
Fe(2)–C(2-2)	1.72 (2)	S(2)···S(3)	2.822 (9)
Fe(2)–C(2-3)	1.73 (2)	Av	2.817
Fe(3)–C(3-1)	1.75 (2)	Fe(1)···Fe(3)	4.167 (10)
Fe(3)–C(3-2)	1.70 (2)	Fe(1)···Fe(4)	4.161 (11)
Fe(3)–C(3-3)	1.76 (2)	Fe(2)···Fe(3)	4.113 (9)
Fe(4)–C(4-1)	1.76 (2)	Fe(2)···Fe(4)	4.034 (9)
Fe(4)–C(4-2)	1.74 (2)	Av	4.119
Fe(4)–C(4-3)	1.73 (2)		
Av	1.74		

[a] Standard deviations of last significant figures are enclosed in parentheses.

in this structural analysis were obtained from the International Tables;[37] corrections for both real and imaginary anomalous dispersion effects[38] were made in the least-squares refinements.

Discussion

The molecular configuration of $[CH_3SFe_2(CO)_6]_2S$ depicted in Figure 1 consists of two identical $[CH_3SFe_2(CO)_6]$ moieties joined to a unique sulfur atom such that this bridging sulfur is tetrahedrally coordinated to the four iron atoms. The idealized geometry of C_{2v} symmetry for the two $[SFe_2(CO)_6]S$ fragments (each without the alkyl group but containing the bridging sulfur atom) is identical with that of the corresponding fragment in $[C_2H_5SFe(CO)_3]_2$.[15] Although no special molecular symmetry is demanded by the space group (*i.e.*, all atoms are in general positions), the independent molecule possesses approximate C_2 symmetry with the twofold axis passing through the unique sulfur and the midpoint of S(1) and S(2). The methyl groups, then, are *syn* to each other.

The localized sulfur–carbon environment about each iron is a distorted tetragonal pyramid formed by the three carbonyl groups and two sulfur atoms. A calculation in Table VI(a–d) of the "best" basal planes (each comprised of two sulfur and two carbonyl carbon atoms) reveals the degree of distortion about each of the iron atoms from a regular tetragonal pyramid. As expected, the four iron atoms are equivalently dis-

TABLE IV

BOND ANGLES AND STANDARD DEVIATIONS (DEGREES) OF $[CH_3SFe_2(CO)_6]_2S^a$

Fe(1)–S(1)–Fe(2)	68.2 (2)	S(1)–Fe(1)–C(1-1)	98.5 (7)
Fe(3)–S(2)–Fe(4)	67.5 (2)	S(1)–Fe(2)–C(2-1)	100.2 (7)
Av	67.9	S(2)–Fe(3)–C(3-1)	103.4 (8)
Fe(1)–S(3)–Fe(2)	68.8 (2)	S(2)–Fe(4)–C(4-1)	97.8 (7)
Fe(3)–S(3)–Fe(4)	68.7 (2)	Av	100.0
Av	68.8	S(3)–Fe(1)–C(1-1)	109.0 (7)
Fe(1)–S(3)–Fe(3)	135.6 (3)	S(3)–Fe(2)–C(2-1)	105.1 (6)
Fe(1)–S(3)–Fe(4)	136.1 (2)	S(3)–Fe(3)–C(3-1)	105.8 (6)
Fe(2)–S(3)–Fe(3)	131.8 (2)	S(3)–Fe(4)–C(4-1)	105.6 (6)
Fe(2)–S(3)–Fe(4)	127.8 (3)	Av	106.4
Av	132.8	S(1)–Fe(1)–C(1-2)	95.9 (7)
S(1)–Fe(1)–S(3)	77.0 (3)	S(1)–Fe(2)–C(2-2)	92.6 (7)
S(1)–Fe(2)–S(3)	77.0 (2)	S(2)–Fe(3)–C(3-2)	92.2 (9)
S(2)–Fe(3)–S(3)	77.0 (2)	S(2)–Fe(4)–C(4-2)	93.4 (6)
S(2)–Fe(4)–S(3)	77.2 (2)	Av	93.5
Av	77.1	S(3)–Fe(1)–C(1-2)	152.8 (6)
S(1)–Fe(1)–Fe(2)	55.8 (2)	S(3)–Fe(2)–C(2-2)	155.7 (8)
S(1)–Fe(2)–Fe(1)	55.9 (2)	S(3)–Fe(3)–C(3-2)	154.7 (7)
S(2)–Fe(3)–Fe(4)	56.3 (2)	S(3)–Fe(4)–C(4-2)	151.0 (7)
S(2)–Fe(4)–Fe(3)	56.2 (2)	Av	153.6
Av	56.0	S(1)–Fe(1)–C(1-3)	161.9 (7)
S(3)–Fe(1)–Fe(2)	55.7 (2)	S(1)–Fe(2)–C(2-3)	162.0 (7)
S(3)–Fe(2)–Fe(1)	55.5 (2)	S(2)–Fe(3)–C(3-3)	157.8 (7)
S(3)–Fe(3)–Fe(4)	55.4 (2)	S(2)–Fe(4)–C(4-3)	165.2 (7)
S(3)–Fe(4)–Fe(3)	55.9 (2)	Av	161.7
Av	55.6	Fe(1)–C(1-1)–O(1-1)	174.5 (17)
S(3)–Fe(1)–C(1-3)	91.4 (7)	Fe(1)–C(1-2)–O(1-2)	173.2 (18)
S(3)–Fe(2)–C(2–3)	92.5 (5)	Fe(1)–C(1–3)–O(1-3)	178.3 (19)
S(3)–Fe(3)–C(3-3)	91.3 (6)	Fe(2)–C(2-1)–O(2-1)	178.0 (19)
S(3)–Fe(4)–C(4-3)	92.2 (6)	Fe(2)–C(2-2)–O(2-2)	175.5 (21)
Av	91.8	Fe(2)–C(2-3)–O(2-3)	176.4 (17)
C(1-1)–Fe(1)–C(1-2)	98.0 (8)	Fe(3)–C(3-1)–O(3-1)	174.1 (16)
C(2-1)–Fe(2)–C(2-2)	98.2 (10)	Fe(3)–C(3-2)–O(3-2)	177.4 (20)
C(3-1)–Fe(3)–C(3-2)	98.9 (9)	Fe(3)–C(3-3)–O(3-3)	176.9 (18)
C(4-1)–Fe(4)–C(4-2)	102.8 (10)	Fe(4)–C(4-1)–O(4-1)	175.4 (19)
Av	99.5	Fe(4)–C(4-2)–O(4-2)	174.8 (19)
C(1-1)–Fe(1)–C(1-3)	98.4 (9)	Fe(4)–C(4-3)–O(4-3)	174.6 (18)
C(2-1)–Fe(2)–C(2-3)	96.6 (10)	Av	175.8
C(3-1)–Fe(3)–C(3-3)	97.8 (10)	$H_3C(1)$–S(1)–Fe(1)	115.0 (8)
C(4-1)–Fe(4)–C(4-3)	95.0 (9)	$H_3C(1)$–S(1)–Fe(2)	112.1 (6)
Av	97.0	$H_3C(2)$–S(2)–Fe(3)	116.3 (7)
C(1-2)–Fe(1)–C(1–3)	88.1 (9)	$H_3C(2)$–S(2)–Fe(4)	114.0 (6)
C(2-2)–Fe(2)–C(2-3)	91.4 (9)	Av	114.4
C(3-2)–Fe(3)–C(3-3)	90.7 (10)		
C(4-2)–Fe(4)–C(4-3)	91.0 (8)		
Av	90.3		

[a] Standard deviations of last significant figures are enclosed in parentheses.

TABLE V

NONBONDING INTRAMOLECULAR DISTANCES (A) FOR $[CH_3SFe_2(CO)_6]_2S$

C(2-1)···C(4-1)	3.76 (3)	S(3)···C(1-2)	3.90 (2)
C(2-1)···C(2-2)	2.63 (3)	S(3)···C(3-2)	3.86 (2)
C(2-1)···C(2-3)	2.60 (3)	S(3)···C(1-3)	2.88 (2)
C(4-1)···C(4-2)	2.74 (3)	S(3)···C(3-3)	2.89 (2)
C(4-1)···C(4-3)	2.58 (3)	S(3)···C(2-1)	3.20 (2)
C(2-1)···S(1)	3.10 (2)	S(3)···C(4-1)	3.20 (2)
C(4-1)···S(2)	3.07 (2)	S(3)···C(2-2)	3.88 (2)
C(2-1)···S(2)	3.48 (2)	S(3)···C(4-2)	3.86 (2)
C(4-1)···S(1)	3.63 (2)	S(3)···C(2-3)	2.90 (2)
C(2-2)···C(2-3)	2.47 (3)	S(3)···C(4-3)	2.88 (2)
C(4-2)···C(4-3)	2.48 (3)	C(1-1)···C(1-2)	2.66 (2)
C(2-2)···S(1)	2.90 (2)	C(1-1)···C(1-3)	2.65 (3)
C(4-2)···S(2)	2.95 (2)	C(1-2)···C(1-3)	2.44 (3)
C(2-3)···S(2)	3.91 (2)	C(3-1)···C(3-2)	2.62 (3)
C(4-3)···S(1)	3.98 (2)	C(3-1)···C(3-3)	2.65 (3)
S(1)···C(1-1)	3.07 (2)	C(3-2)···C(3-3)	2.46 (3)
S(2)···C(3-1)	3.18 (2)	C(1-3)···C(3-3)	3.42 (2)
S(1)···C(1-2)	3.02 (2)	C(2-3)···C(3-1)	3.43 (2)
S(2)···C(3-2)	2.90 (2)	C(4-3)···C(1-1)	3.61 (3)
S(3)···C(1-1)	3.28 (2)		
S(3)···C(3-1)	3.21 (2)		

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(37) "International Tables for X-Ray Crystallography," Vol. III, The Kynoch Press, Birmingham, England, 1962, p 202.

(38) C. H. Dauben and D. H. Templeton, *Acta Cryst.*, **8**, 841 (1955); "International Tables for X-Ray Crystallography," Vol. III, The Kynoch Press, Birmingham, England, 1962, p 215.

TABLE VI

EQUATIONS OF BEST MOLECULAR PLANES AND DISTANCES (A) OF ATOMS FROM THESE PLANES[a]

(a) Plane through S(1), S(3), C(1-2), and C(1-3)

$0.870X - 0.070Y - 0.487Z - 9.533 = 0$

S(1)	0.01	C(1-3)	0.19	O(1-3)	0.03
S(3)	−0.01	Fe(1)	0.38	C(1-1)	2.12
C(1-2)	−0.14	O(1-2)	−0.58	O(1-1)	3.26

(b) Plane through S(1), S(3), C(2-2), and C(2-3)

$0.414X + 0.903Y - 0.118Z - 9.699 = 0$

S(1)	−0.00	C(2-3)	−0.08	O(2-3)	0.14
S(3)	0.00	Fe(2)	−0.32	C(2-1)	−2.06
C(2-2)	−0.12	O(2-2)	0.54	O(2-1)	−3.20

(c) Plane through S(2), S(3), C(3-2), and C(3-3)

$0.483X - 0.581Y - 0.656Z - 1.046 = 0$

S(2)	−0.00	C(3-3)	−0.04	O(3–3)	0.12
S(3)	0.00	Fe(3)	−0.38	C(3-1)	−2.12
C(3-2)	0.05	O(3-2)	0.30	O(3-1)	−3.28

(d) Plane through S(2), S(3), C(4-2), and C(4-3)

$-0.622X - 0.399Y - 0.674Z + 13.025 = 0$

S(2)	0.01	C(4-3)	0.23	O(4-3)	0.06
S(3)	−0.01	Fe(4)	0.34	C(4-1)	2.09
C(4-2)	−0.24	O(4-2)	−0.56	O(4-1)	3.24

(e) Plane through Fe(1), Fe(2), and the Midpoint of S(1)–S(3)

$-0.477X + 0.112Y - 0.872Z + 7.858 = 0$

S(1)	1.41	O(2-1)	0.16	C(2-2)	1.20
S(3)	−1.41	C(1-2)	1.12	C(2-3)	−1.25
C(1-1)	0.24	C(1-3)	−1.29	O(2-2)	2.05
O(1-1)	0.51	O(1-2)	1.91	O(2-3)	−2.06
C(2-1)	0.10	O(1-3)	−2.18		

(f) Plane through Fe(3), Fe(4), and the Midpoint of S(2)–S(3)

$0.126X + 0.798Y - 0.589Z - 2.048 = 0$

S(2)	−1.41	O(4-1)	−0.37	C(4-2)	−1.16
S(3)	1.41	C(3-2)	−1.20	C(4-3)	1.28
C(3-1)	−0.02	C(3-3)	1.26	O(4-2)	−2.02
O(3-1)	−0.10	O(3-2)	−2.03	O(4-3)	2.20
C(4-1)	−0.17	O(3-3)	2.11		

(g) Plane through Fe(1), S(1), and S(3)

$0.829X - 0.282Y - 0.483Z - 7.912 = 0$

C(1-2)	−0.79	O(1-3)	−0.74	Fe(4)	1.42
C(1-3)	−0.42	Fe(2)	−1.77	S(2)	−0.53
O(1-2)	−1.37	Fe(3)	0.16		

(h) Plane through Fe(2), S(1), and S(3)

$0.266X + 0.963Y - 0.034Z - 8.335 = 0$

C(2-2)	0.65	O(2-3)	0.80	Fe(4)	−1.71
C(2-3)	0.44	Fe(1)	1.76	S(2)	−2.32
O(2-2)	1.20	Fe(3)	−0.30		

(i) Plane through Fe(3), S(2), and S(3)

$0.656X - 0.528Y - 0.540Z - 4.104 = 0$

C(3-2)	0.67	O(3-3)	0.90	Fe(2)	−1.52
C(3-3)	0.57	Fe(4)	1.76	S(1)	0.30
O(3-2)	1.08	Fe(1)	−0.35		

(j) Plane through Fe(4), S(2), and S(3)

$-0.757X - 0.295Y - 0.583Z + 13.989 = 0$

C(4-2)	−0.81	O(4-3)	−0.62	Fe(2)	1.67
C(4-3)	−0.32	Fe(3)	−1.77	S(1)	2.36
O(4-2)	−1.28	Fe(1)	0.33		

(k) Plane through S(1), S(3), Fe(3), and Fe(4)

$0.825X + 0.418Y - 0.381Z - 11.766 = 0$

S(1)	−0.02	C(1-1)	2.77	O(3-2)	0.13
S(3)	0.03	C(2-1)	−2.81	C(4-2)	0.19
Fe(3)	−0.00	O(1-1)	3.79	O(4-2)	0.25
Fe(4)	0.00	O(2-1)	−3.73	C(3-1)	−0.62
$H_3C(1)$	−0.18	C(1-3)	1.59	C(3-3)	1.71
Fe(1)	1.17	C(2-3)	−1.91	O(3-1)	−1.00
Fe(2)	−1.36	O(1-3)	1.84	O(3-3)	2.84
C(1-2)	1.31	O(2-3)	−2.25	C(4-1)	−0.78
C(2-2)	−1.79	S(2)	−1.89	C(4-3)	1.61
O(1-2)	1.27	$H_3C(2)$	−2.62	O(4-1)	−1.36
O(2-2)	−2.01	C(3-2)	0.08	O(4-3)	2.76

(l) Plane through S(2), S(3), Fe(1), and Fe(2)

$-0.014X - 0.590Y - 0.808Z + 6.321 = 0$

S(2)	−0.01	C(3-1)	−2.80	O(1-2)	−0.44
S(3)	0.02	C(4-1)	2.79	C(2-2)	−0.13
Fe(1)	−0.00	O(3-1)	−3.92	O(2-2)	−0.26
Fe(2)	0.00	O(4-1)	3.72	C(1-1)	0.78
$H_3C(2)$	0.07	C(3-3)	−1.47	C(1-3)	−1.65
Fe(3)	−1.20	C(4-3)	1.97	O(1-1)	1.39
Fe(4)	1.34	O(3-3)	−1.71	O(1-3)	−2.79
C(3-2)	−1.41	O(4-3)	2.31	C(2-1)	0.73
C(4-2)	1.55	S(1)	1.86	C(2-3)	−1.64
O(3-2)	−1.62	$H_3C(1)$	2.51	O(2-1)	1.23
O(4-2)	1.81	C(1-2)	−0.30	O(2-3)	−2.77

(m) Plane through S(1), S(3), and the Midpoint of Fe(1)–Fe(2)

$0.788X + 0.490Y - 0.372Z - 11.695 = 0$

Fe(1)	1.27	C(1-2)	1.54	C(1-3)	1.75
Fe(2)	−1.27	C(2-2)	−1.58	C(2-3)	−1.75
C(1-1)	2.81	O(1-2)	1.58	O(1-3)	2.05
C(2-1)	−2.79	O(2-2)	−1.72	O(2-3)	−2.05
O(1-1)	3.79				
O(2-1)	−3.77				

(n) Plane through S(2), S(3), and the Midpoint of Fe(3)–Fe(4)

$-0.071X - 0.590Y - 0.804Z + 7.060 = 0$

Fe(3)	−1.27	C(3-2)	−1.54	C(3-3)	−1.62
Fe(4)	1.27	C(4-2)	1.47	C(4-3)	1.84
C(3-1)	−2.83	O(3-2)	−1.78	O(3-3)	−1.91
C(4-1)	2.77	O(4-2)	1.64	O(4-3)	2.12
O(3-1)	−3.93				
O(4-1)	3.74				

[a] The equations of the planes are given in an orthogonal Ångström coordinate system (X, Y, Z) which is related to the fractional unit cell coordinate system (x, y, z) as follows: $X = xa + yb \cos \gamma + zc \cos \beta$, $Y = yb \sin \gamma + zc \cos \mu$, $Z = zc \cos \sigma$, where $\cos \mu = (\cos \alpha - \cos \beta \cos \gamma)/\sin \gamma$ and $\cos \sigma = 1 - \cos^2 \beta - \cos^2 \mu$.

placed by 0.36 A (*i.e.*, the average of 0.38, 0.32, 0.38, and 0.34 A) from their respective basal planes in the direction of their apical carbonyl groups. Similar displacements of the iron atoms were also observed in $[C_2H_5SFe(CO)_3]_2$ (0.38 A for both irons)[15] and $[SFe(CO)_3]_2$ (0.34 and 0.32 A).[39] As in these previously reported structures, each of the two $[SFe_2(CO)_6]S$ fragments is formed by the intersection of the two basal planes at the S···S edge; the resulting dihedral angles of 69.3 and 68.1° compare favorable to that of 69.5° for $[C_2H_5SFe(CO)_3]_2$. The approximate C_{2v} symmetry for a given $[SFe_2(CO)_6]S$ fragment is shown from a calculation of its two vertical mirror planes (Table VI, (e) and (m), (f) and (n)) which are approximately perpendicular to each other (dihedral angle between (e) and (m), 89.8°; between (f) and (n), 90.3°). The pairs of corresponding atoms related by these four mirror

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(39) C. H. Wei and L. F. Dahl, *Inorg. Chem.*, **4**, 1 (1965).

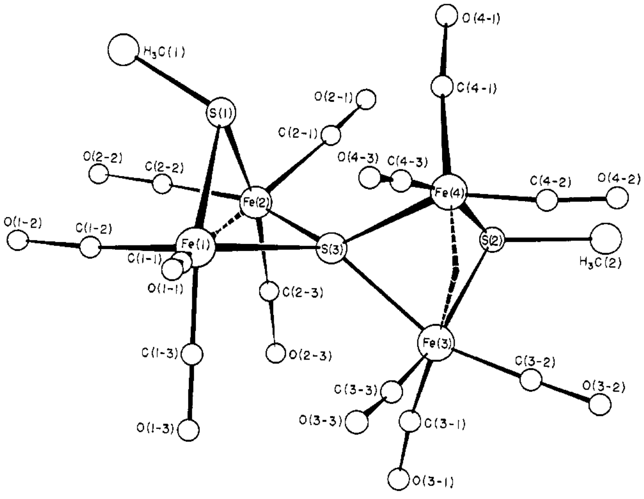

Figure 1.—The molecular configuration of $[CH_3SFe_2(CO)_6]_2S$.

planes are essentially equidistant from these symmetry planes. These results indicate that the two $[SFe_2(CO)_6]S$ fragments are not appreciably distorted upon formation of the tetrameric molecule.

The six intramolecular Fe···Fe distances may be divided into two molecularly equivalent bonding ones of 2.54-A (av) length and four nonbonding ones of 4.12-A (av) length. The two bonding Fe–Fe distances are identical with those in $[C_2H_5SFe(CO)_3]_2$ (2.54 A) and $[SFe(CO)_3]_2$ (2.55 A). The mean value for the four Fe–SR bonds is 2.274 A (individual esd, 0.008 A), while the mean value for the bonds from the unique sulfur to the four iron atoms is 2.248 A (individual esd, 0.007 A). The mean Fe–C and C–O distances of 1.74 and 1.18 A, respectively, are not dissimilar within their standard deviations from the mean Fe–C and C–O distances reported for $[C_2H_5SFe(CO)_3]_2$ (1.81 and 1.15 A)[15] and $[SFe(CO)_3]_2$ (1.78 and 1.14 A).[39] The individual Fe–C–O bond angles are approximately linear.

Figure 2 shows the [100] projection of the $[CH_3SFe_2(CO)_6]_2S$ unit cell. The closest intermolecular distances of 3.0 A for C···O and O···O contacts, 3.4 A for S···O contacts, and 3.2 A for H_3C···O contacts correspond to van der Waals separations. As expected, some of the nonbonding intramolecular distances listed in Table V are somewhat shorter than these minimum intermolecular values.

The ability of a tetrahedral atom to link metal carbonyl entities was first reported by Fritchie, *et al.*,[40–42] who found for crystalline $(CH_3)_4Sn_3Fe_4(CO)_{16}$ a

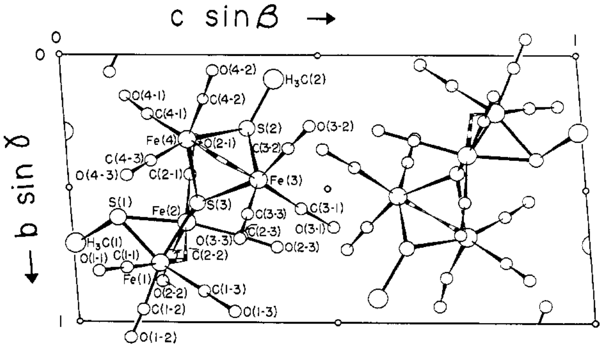

Figure 2.—[100] projection of the unit cell of $[CH_3SFe_2(CO)_6]_2S$.

structure consisting of a linear array of tetrahedral tin atoms bridged by $Fe(CO)_4$ groups such that the unique tin atom is surrounded by a distorted tetrahedron of $Fe(CO)_4$ groups and the two terminal $(CH_3)_2Sn$ groups are each bonded to two $Fe(CO)_4$ moieties. The stereochemical environment of the unique central tin atom coordinated to the four iron atoms is significantly different from that around the two $Sn(CH_3)_2$ groups as shown both by a bond length difference of 0.15 A for the average Fe–$Sn(CH_3)_2$ bond length (2.625 ± 0.008 A) compared to the average Fe–Sn (central) bond length (2.774 ± 0.008 A) and by a difference of 6.4° in the average Fe–Sn–Fe bond angles (*i.e.*, 105.2° for the $Sn(CH_3)_2$ groups compared to 98.8° for the central tin atom). However, no such trend is noted in $[CH_3SFe_2(CO)_6]_2S$; the acute Fe–S–Fe angles at the unique sulfur (68.8 and 68.7°) are equivalent to those at the mercapto sulfur atoms (68.2 and 67.5°), while the previously mentioned average value of the four Fe–S(central) bonds is slightly shorter (and not considerably longer) than the average value of the four Fe–SCH_3 bonds.

This structure represents the first known example of an organometallic complex in which a tetrahedral-like sulfur utilizes all six valence electrons in forming σ bonds to four metal atoms. Similar tetrahedral-like metal-coordinated sulfur atoms are known for the simple metal sulfides MS which possess the zinc blende and wurtzite structures.[43] It is noteworthy that FeS possesses the nickel arsenide structure with a coordination number of six for both the iron and sulfur atoms.[43]

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(40) R. M. Sweet and C. J. Fritchie, Jr., Abstracts of Annual Meeting of the American Crystallographic Association, Austin, Texas, Feb 28–March 2, 1966, p 51; R. M. Sweet, C. J. Fritchie, Jr., and R. A. Schunn, *Inorg. Chem.*, **6**, 749 (1967).

(41) A recent crystallographic investigation[42] of $SnFe_4(CO)_{16}$ has produced another example of a tin atom tetrahedrally coordinated to four $Fe(CO)_4$ groups which in turn are linked in two pairs by iron–iron bonds. No details of this structural analysis are yet available.

(42) P. Woodward, private communication to L. F. Dahl, 1966; *cf.* M. I. Bruce, J. Cotton, D. A. Harbourne, S. A. R. Knox, I. Paul, D. T. Rosevear, and F. G. A. Stone, "Proceedings of the IXth International Conference on Coordination Chemistry," W. Schneider, Ed., Verlag Helvetica Chimica Acta, Basel, Switzerland, 1966, pp 173, 174.

(43) *Cf.* A. F. Wells, "Structural Inorganic Chemistry," 3rd ed, Oxford at the Clarendon Press, London, 1962, for the crystal structures of these metal sulfides.