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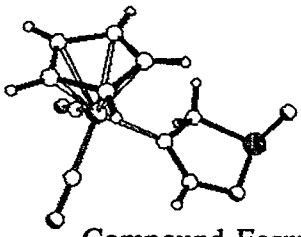
Organometallics, 1998, 17(13), 2832-2838, DOI:10.1021/om980006l



CRYSTAL STRUCTURE ANALYSIS REPORT[1]

Compound Formula: $CpFe(CO)_2(C_3H_3SO_2)$ Reference Code: MWA4-0897

Description of Single-Crystal Sample and Mounting Used for Data Collection:

1) Color: Yellow
2) Shape: Rectangular parallelepiped
3) Dimensions: 0.35 mm. x 0.40 mm. x 0.40 mm.
4) Indices of Faces:
5) Crystal Mount: Crystal was sealed inside a thin-walled glass capillary with epoxy.
6) Crystal Orientation: Crystal was oriented with one of its longest edges nearly parallel to the phi axis of the diffractometer.
7) Comments:

Space Group and Cell Data:

1) Crystal System: Monoclinic Space Group and Number[2]: $P2_1/c$ - C_{2h}^5 (No. 14)
2) Number of Computer-Centered Reflections Used in the Least-Squares Refinement of the Cell Dimensions: 40 measured at: 293 °K
3) Lattice Constants with esd's:

a= 10.3532(9)Å	α= 90.00°	V= 2228.2(3)Å^3
b= 9.5692(7)Å	β= 97.961(6)°	Z= 8 formula units
c= 22.708(2)Å	γ= 90.00°	λ= 0.71073 Å

4) Molecular Weight: 280.08 amu Calculated Density: 1.670 g·cm^{-3}
5) Linear Absorption Coefficient[3a]: 1.534mm^{-1} F(000) = 1136.
6) Comments:

Description of Data Collection:

1) Instrument: Siemens P4 Autodiffractometer
2) X-ray Tube: Normal focus Take-Off-Angle (TOA): 6°
3) Radiation: MoK$\bar{\alpha}$
4) XX Monochromator: XX Graphite ___Other (Specify:)
   ___Filter: ___Nickel ___Niobium ___Other (Specify:)
5) Incident Beam Collimator Diameter: 1.5 mm Temperature: 293 °K
6) Scanning Technique: XX ω Scan ___θ-2θ Scan
7) Scan Range (= low range + high range + separation between Kα_1 and Kα_2) :
   Low range = 0.45° High range = 0.45°
8) Ratio of Background Counting Time to Net Scanning Time: 0.50
9) 2θ Ranges of Data and Scan Rates for a Total of 2 shells:

Shell#	2θ Min.	2θ Max.	Scan Rate	Comments
1	3.0°	43.0°	6° /min	0.0-0.5 CuK$\bar{\alpha}$ spheres
2	43.0°	50.8°	4° /min	0.5-0.8 CuK$\bar{\alpha}$ spheres

11) Total Number of Reflections Collected: 4336
12) Number of Independent Reflections Collected: 4096
13) Number of Check Reflections Monitored and Frequency:
    Number: 3 Frequency: 300
14) Data Collected: $0 \leq h \leq 12$, $0 \leq k \leq 11$, $-27 \leq l \leq 27$
15) $R_{int} = 0.022$
16) Comments: Background counts were measured at each end of the scan range.

Data Reduction:

1) Lorentz and Polarization Corrections? Yes
2) Correction for Check Reflection Intensity Changes? None
3) Absorption Correction: Yes
   ____Spherical[4] (μr=)
   _XX_ Psi-scan (_16_ Reflections used)
   Range of relative transmission factors: 0.843 - 1.000
   ____Numerical (Gaussian Grid)
4) Comments:

Structure Solution:

1) Method(s) Used in Structure Solution
   ___Heavy-atom Patterson Techniques
   _XX_ Direct Methods
      a) _XX_ SHELXTL-PC
      b) ___Other
   ___Other Techniques
2) Hydrogen Atom Position Located? Yes
   After Refinement Cycle #_2_ by ___Difference Fourier
   _XX_ Calculated
3) Comments:

CRYSTAL STRUCTURE ANALYSIS REPORT Reference Code: MWA4-0897

Structure Refinement:[5] (see next page for summary of refinement cycles)

1) Final Scale Factor: 0.1506(3)
2) Extinction Parameter[6] Refined? Yes Final Value: x = 0.0012(2)
   Form: $k[1+0.001(x)(F_c^2)(\lambda^3)/\sin(2\theta)]^{-1/4}$
3) Anomalous Dispersion Corrections[3b] for Which Atoms: Fe, S, O
4) Variable Occupancies for Which Atoms? None

Atom	Final Occupancy	Atomic Form Factor[3c] Used

5) Refinement Constraints/Restraints: The hydrogen atoms were included in the structure factor calculations as idealized atoms (assuming sp^3- or sp^2-hybridization of the carbon atoms and a C-H bond length of 0.98Å) "riding" on their respective carbon atoms. The isotropic thermal parameters for the hydrogen atoms were fixed at values 1.2 times the equivalent isotropic thermal parameters of the carbon atoms to which they are covalently bonded.
6) Shift/Error Analysis for Final Least-Squares Cycle[7]:
   Maximum Shift for all Parameters: 0.001 σ_p
   Average Shift for all Parameters: 0.000 σ_p
7) Peaks found in Final Difference Fourier Map: There were no peaks present in the final difference Fourier map above the background level ($0.285e^-/Å^3$). The minimum and mean electron density in the final difference Fourier were -0.315 and 0.00 $e^-/Å^3$, respectively. The rms deviation from the mean electron density was 0.06 $e^-/Å^3$.

Summary of Full Matrix Least-Squares Refinement[5] Cycles

Cycle Number	sin θ /λ Minimum	sin θ /λ Maximum	Anisotropic[8] Atoms Number and Type	Isotropic Atoms Number and Type	Isotropic Atoms Positions Refined	Isotropic Atoms Thermal Parameters	# Refined Parameters	R_1 (unweighted,based on F) R_1[10]	# Observed Reflections	$F_o/\sigma(F_o)$ Cutoff	R_2 (weighted,based on F^2)[9] R_2[11]	Total # Independent Reflections	'Goodness-of-fit' (Goof)[12]	Extinction Correction
1	0.00	0.60	2 Fe, 2 S	8 O, 20 C	X	X	149	0.088	2449	4.0	0.184	3566	1.86	
2	0.00	0.60	2 Fe, 2 S 8 O, 20 C				289	0.060	2449	4.0	0.122	3566	1.28	
3	0.00	0.60	2 Fe, 2 S 8 O, 20 C	16 H*	X	X	290	0.050	2449	4.0	0.095	3566	1.007	X

* See Item 5 on page 4 regarding the treatment of the hydrogen atoms.

Final Statistics from Cycle #3 for All of the Reflection Data: $R_1 = 0.110$; $R_2 = 0.106$; GOOF = 1.038 for 4096 reflections

References and Notes

1. All calculations were performed on an IBM compatible 586 personal computer using the Siemens SHELXTL-PC (Version 5.0) interactive software package.

2. "International Tables for X-Ray Crystallography", Vol. A, Kluwer Academic Publishers, Dordrecht, 1995.

3. "International Tables for X-Ray Crystallography", Vol. C, Kluwer Academic Publishers, Dordrecht, 1992; a) Tables 4.2.4.2 pp. 193-199; b) Tables 4.2.6.8 pp 219-222; c) Tables 6.1.1.4 pp 500-502.

4. $R_{int} = \Sigma | F_o^2 - F_o^2(mean) | \ / \ \Sigma[F_o]^2$

5. Refinement on F^2 for all reflections except for 530 with negative F^2 or flagged as potentially having systematic errors. Weighted R-factors wR_2 and all goodnesses of fit S are based on F^2, conventional R-factors R_1 are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2sigma(F^2)$ is used only for calculating "R-factor obs" etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on all data will be even larger.

6. A. C. Larson in "Crystallographic Computing", **1970**, Ed. F. R. Ahmed, Munksgaard, Copenhagen, pp 291-294.

7. σ_p is the estimated standard deviation of the parameter in question.

8. The anisotropic thermal parameter is of the form:
$\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)]$.

9. The weighting scheme used is defined as: $w = 1 / [\sigma^2(F_o^2) + (a^*P)^2 + b^*P + d + e^*\sin(\theta)]$ where $P = [F_o^2 + 2F_c^2]/3$. In this case, a= 0.0415, b= 0, d = 0 and e = 0.

10. $\underline{R}_1 = \Sigma | \ |F_o| - |F_c| \ | / \Sigma |F_o|$

11. $w\underline{R}_2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$

12. GooF = $S = [\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)]^{1/2}$ where n is the total number of reflections and p is the number of parameters refined.

Table S1. Atomic Coordinates for Atoms in Crystalline $CpFe(CO)_2(C_3H_3SO_2)$ **14a** [a]

Atom Type[b]	Fractional Coordinates 10^4x	10^4y	10^4z	Equivalent Isotropic Thermal Parameter, U, $Å^2 \times 10^3$ [c]
		Molecule 1		
Fe_1	3337(1)	8082(1)	170(1)	40(1)
S_1	-1019(1)	7615(2)	240(1)	72(1)
O_1	-318(3)	8568(4)	794(2)	67(1)
O_2	-1014(4)	6151(5)	433(2)	90(1)
O_3	2881(4)	9557(5)	-947(2)	88(1)
O_4	3907(4)	10602(4)	866(2)	72(1)
C_1	1501(4)	8211(5)	305(2)	39(1)
C_2	1052(5)	8604(5)	786(2)	52(1)
C_3	373(5)	7780(6)	-156(2)	61(2)
C_4	3039(5)	8981(6)	-502(2)	53(1)
C_5	3677(5)	9602(6)	595(2)	51(1)
C_6	4223(7)	6659(6)	800(3)	73(2)
C_7	5130(5)	7122(6)	436(3)	68(2)
C_8	4679(6)	6765(6)	-145(3)	68(2)
C_9	3501(6)	6042(6)	-142(3)	66(2)
C_{10}	3239(6)	5986(6)	430(3)	72(2)
		Molecule 2		
Fe_2	-1695(1)	5961(1)	7698(1)	46(1)
S_2	-6091(1)	5250(2)	7490(1)	64(1)
O_{11}	-5583(3)	5939(4)	8138(2)	71(1)
O_{12}	-6493(4)	6394(4)	7078(2)	76(1)
O_{13}	-2566(4)	7688(4)	6672(2)	77(1)
O_{14}	-1468(4)	8228(4)	8546(2)	82(1)
C_{11}	-3558(4)	5713(5)	7793(2)	39(1)

Table S1. (continued)

Atom Type[b]	Fractional Coordinates 10^4x	10^4y	10^4z	Equivalent Isotropic Thermal Parameter, U, $Å^2 \times 10^3$ [c]
C_{12}	-4223(5)	6270(6)	8179(2)	58(2)
C_{13}	-4451(5)	4788(5)	7381(2)	58(2)
C_{14}	-2217(5)	7015(6)	7080(2)	53(1)
C_{15}	-1562(5)	7338(6)	8211(2)	54(1)
C_{16}	-403(7)	4630(7)	8225(3)	85(2)
C_{17}	239(7)	5335(9)	7811(7)	142(5)
C_{18}	-328(14)	5010(14)	7269(6)	174(8)
C_{19}	-1288(9)	4068(9)	7329(4)	107(3)
C_{20}	-1329(6)	3850(6)	7910(3)	69(2)

[a] The numbers in parentheses are the estimated standard deviations in the last significant digit.
[b] Atoms are labeled in agreement with Figure 1.
[c] This is one-third of the trace of the orthogonalized U_{ij} tensor.

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Table S2. Anisotropic Thermal Parameters for Nonhydrogen Atoms in Crystalline $CpFe(CO)_2(C_3H_3SO_2)$ **14a** [a,b]

Atom Type[c]	Anisotropic Thermal Parameters ($Å^2 \times 10^3$) U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
			Molecule 1			
Fe_1	40(1)	37(1)	42(1)	1(1)	5(1)	3(1)
S_1	37(1)	92(1)	86(1)	-5(1)	1(1)	-4(1)
O_1	47(2)	73(3)	86(3)	-21(2)	25(2)	-1(2)
O_2	88(3)	78(3)	105(3)	-18(3)	15(3)	-39(3)
O_3	92(3)	113(4)	60(2)	33(3)	14(2)	23(3)
O_4	78(3)	57(3)	83(3)	-23(2)	17(2)	-19(2)
C_1	40(3)	38(3)	40(3)	-1(2)	6(2)	1(2)
C_2	37(3)	53(3)	68(3)	-9(3)	12(3)	-5(2)
C_3	43(3)	81(4)	55(3)	5(3)	-4(3)	1(3)
C_4	51(3)	56(3)	55(3)	0(3)	16(3)	6(3)
C_5	48(3)	51(3)	53(3)	-2(3)	9(3)	-6(3)
C_6	86(5)	63(4)	65(4)	20(3)	-1(4)	26(4)
C_7	43(3)	52(4)	104(5)	4(4)	-4(3)	9(3)
C_8	79(5)	55(4)	79(4)	11(3)	39(4)	26(4)
C_9	67(4)	38(3)	91(5)	-14(3)	-1(3)	11(3)
C_{10}	66(4)	44(4)	113(5)	23(4)	35(4)	14(3)
			Molecule 2			
Fe_2	45(1)	40(1)	51(1)	5(1)	7(1)	6(1)
S_2	47(1)	52(1)	90(1)	3(1)	-2(1)	-4(1)
O_{11}	54(2)	91(3)	72(2)	8(2)	21(2)	0(2)
O_{12}	70(3)	63(3)	89(3)	4(2)	-15(2)	17(2)
O_{13}	100(3)	71(3)	58(2)	17(2)	2(2)	15(2)
O_{14}	90(3)	79(3)	74(3)	-27(2)	0(2)	-16(3)
C_{11}	42(3)	31(3)	42(3)	2(2)	3(2)	-5(2)
C_{12}	54(4)	66(4)	52(3)	1(3)	4(3)	-7(3)

Table S2. (continued)

Atom Type[c]	Anisotropic Thermal Parameters ($Å^2 \times 10^3$) U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C_{13}	46(3)	41(3)	84(4)	-3(3)	-4(3)	7(3)
C_{14}	61(4)	44(3)	54(3)	-5(3)	10(3)	-1(3)
C_{15}	46(3)	58(4)	55(3)	5(3)	-2(3)	-6(3)
C_{16}	84(5)	70(5)	89(5)	7(4)	-25(4)	40(4)
C_{17}	31(4)	65(5)	330(16)	69(9)	29(7)	14(4)
C_{18}	208(15)	159(12)	192(11)	119(10)	157(11)	146(11)
C_{19}	150(9)	87(6)	74(5)	-19(4)	-15(5)	79(6)
C_{20}	56(4)	36(3)	113(5)	18(3)	5(4)	16(3)

[a] The numbers in parentheses are the estimated standard deviations in the last significant digit.

[b] The form of the anisotropic thermal parameter is: $\exp[-2pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)]$.

[c] Atoms are labeled in agreement with Figure 1.

Table S3. Atomic Coordinates for Hydrogen Atoms in Crystalline $CpFe(CO)_2(C_3H_3SO_2)$ **14a** [a]

Atom Type[b]	Fractional Coordinates 10^4x	10^4y	10^4z
		Molecule 1	
H_2	1614(5)	8902(5)	1117(2)
H_{3a}	557(5)	6897(6)	-336(2)
H_{3b}	211(5)	8482(6)	-465(2)
H_6	4297(7)	6747(6)	1233(3)
H_7	5952(5)	7605(6)	572(3)
H_8	5128(6)	6930(6)	-492(3)
H_9	2970(6)	5629(6)	-489(3)
H_{10}	2476(6)	5536(6)	560(3)
		Molecule 2	
H_{12}	-3827(5)	6867(6)	8473(2)
H_{13a}	-4282(5)	3811(5)	7477(2)
H_{13b}	-4323(5)	4946(5)	6971(2)
H_{16}	-184(7)	4654(7)	8659(3)
H_{17}	996(7)	5950(9)	7906(7)
H_{18}	-48(14)	5313(14)	6895(6)
H_{19}	-1836(9)	3599(9)	7002(4)
H_{20}	-1926(6)	3213(6)	8076(3)

[a] The hydrogen atoms were included in the structure factor calculations as idealized atoms (assuming sp^3- or sp^2-hybridization of the carbon atoms) "riding"on their respective carbon atoms. The isotropic thermal parameters of the hydrogen atoms were fixed at values 1.2 or 1.5 times the equivalent isotropic thermal parameters of the carbon atoms to which they are covalently bonded.

[b] Hydrogen atoms which are covalently bonded to carbon are labeled with the same numerical subscript(s) as their carbon atoms with an additional literal subscript (a or b) where necessary to distinguish between hydrogens bonded to the same carbon atom.

Table S4. Bond Lengths in Crystalline $CpFe(CO)_2(C_3H_3SO_2)$ **14a** [a]

Type[b]	Length, Å	Type[b]	Length, Å
Molecule 1		Molecule 2	
Fe_1-C_4	1.741(6)	Fe_2-C_{15}	1.750(6)
Fe_1-C_5	1.754(5)	Fe_2-C_{14}	1.752(6)
Fe_1-C_1	1.971(4)	Fe_2-C_{11}	1.984(5)
Fe_1-C_8	2.075(5)	Fe_2-C_{18}	2.040(8)
Fe_1-C_7	2.084(5)	Fe_2-C_{19}	2.064(7)
Fe_1-C_9	2.091(5)	Fe_2-C_{17}	2.072(7)
Fe_1-C_6	2.093(5)	Fe_2-C_{16}	2.098(5)
Fe_1-C_{10}	2.098(5)	Fe_2-C_{20}	2.099(5)
Fe_1-C_{p1}	1.722(-)[c]	Fe_2-C_{p2}	1.726(-)[c]
S_1-O_1	1.638(4)	S_2-O_{11}	1.632(4)
S_1-O_2	1.468(4)	S_2-O_{12}	1.464(4)
S_1-C_3	1.807(5)	S_2-C_{13}	1.804(5)
O_1-C_2	1.421(5)	O_{11}-C_{12}	1.434(6)
O_3-C_4	1.143(5)	O_{13}-C_{14}	1.144(5)
O_4-C_5	1.145(5)	O_{14}-C_{15}	1.139(6)
C_1-C_2	1.301(6)	C_{11}-C_{12}	1.300(6)
C_1-C_3	1.514(6)	C_{11}-C_{13}	1.509(6)

Table S4. (continued)

Type[b]	Length, Å	Type[b]	Length, Å
C_6-C_{10}	1.386(8)	C_{16}-C_{20}	1.341(8)
C_6-C_7	1.406(8)	C_{16}-C_{17}	1.397(11)
C_7-C_8	1.380(7)	C_{17}-C_{18}	1.325(14)
C_8-C_9	1.403(8)	C_{18}-C_{19}	1.362(14)
C_9-C_{10}	1.365(8)	C_{19}-C_{20}	1.341(9)

[a] The numbers in parentheses are the estimated standard deviations in the last significant digit.

[b] Atoms are labeled in agreement with Figure 1.

[c] The symbols C_{p1} and C_{p2} are used to represent the centers of gravity for the two cyclopentadienyl rings designated by carbon atoms C_6-C_{10} and C_{16}-C_{20} for Molecules 1 and 2, respectively. These values are therefore listed without estimated standard deviations.

Table S5. Bond Angles Involving Nonhydrogen Atoms in Crystalline $CpFe(CO)_2(C_3H_3SO_2)$ **14a** [a]

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
Molecule 1		Molecule 2	
$C_4Fe_1C_5$	94.0(2)	$C_{15}Fe_2C_{14}$	95.0(2)
$C_4Fe_1C_1$	92.7(2)	$C_{15}Fe_2C_{11}$	90.4(2)
$C_5Fe_1C_1$	89.2(2)	$C_{14}Fe_2C_{11}$	87.7(2)
$C_{p1}Fe_1C_1$	119.9(-)[c]	$C_{p2}Fe_2C_{11}$	122.7(-)[c]
$C_{p1}Fe_1C_4$	125.3(-)[c]	$C_{p2}Fe_2C_{14}$	125.4(-)[c]
$C_{p1}Fe_1C_5$	126.0(-)[c]	$C_{p2}Fe_2C_{15}$	125.2(-)[c]
$C_4Fe_1C_8$	92.6(2)	$C_{15}Fe_2C_{18}$	131.1(6)
$C_5Fe_1C_8$	126.9(3)	$C_{14}Fe_2C_{18}$	91.8(3)
$C_1Fe_1C_8$	142.9(2)	$C_{11}Fe_2C_{18}$	138.4(6)
$C_4Fe_1C_7$	121.0(2)	$C_{15}Fe_2C_{19}$	158.2(3)
$C_5Fe_1C_7$	95.9(2)	$C_{14}Fe_2C_{19}$	103.8(3)
$C_1Fe_1C_7$	145.3(2)	$C_{11}Fe_2C_{19}$	101.3(3)
$C_8Fe_1C_7$	38.8(2)	$C_{18}Fe_2C_{19}$	38.8(4)
$C_4Fe_1C_9$	100.2(2)	$C_{15}Fe_2C_{17}$	98.6(4)
$C_5Fe_1C_9$	160.2(2)	$C_{14}Fe_2C_{17}$	116.9(4)
$C_1Fe_1C_9$	103.7(2)	$C_{11}Fe_2C_{17}$	152.8(3)
$C_8Fe_1C_9$	39.4(2)	$C_{18}Fe_2C_{17}$	37.6(4)
$C_7Fe_1C_9$	64.9(2)	$C_{19}Fe_2C_{17}$	63.1(4)
$C_4Fe_1C_6$	158.2(2)	$C_{15}Fe_2C_{16}$	95.3(3)
$C_5Fe_1C_6$	97.3(2)	$C_{14}Fe_2C_{16}$	155.3(3)
$C_1Fe_1C_6$	106.0(2)	$C_{11}Fe_2C_{16}$	114.7(3)
$C_8Fe_1C_6$	65.8(2)	$C_{18}Fe_2C_{16}$	64.6(3)
$C_7Fe_1C_6$	39.3(2)	$C_{19}Fe_2C_{16}$	63.2(3)
$C_9Fe_1C_6$	64.9(2)	$C_{17}Fe_2C_{16}$	39.1(3)
$C_4Fe_1C_{10}$	135.2(3)	$C_{15}Fe_2C_{20}$	125.2(3)
$C_5Fe_1C_{10}$	130.7(3)	$C_{14}Fe_2C_{20}$	139.7(3)
$C_1Fe_1C_{10}$	86.0(2)	$C_{11}Fe_2C_{20}$	90.4(2)

Table S5. (continued)

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
$C_8Fe_1C_{10}$	65.0(2)	$C_{18}Fe_2C_{20}$	64.2(3)
$C_7Fe_1C_{10}$	64.7(2)	$C_{19}Fe_2C_{20}$	37.6(2)
$C_9Fe_1C_{10}$	38.0(2)	$C_{17}Fe_2C_{20}$	63.4(3)
$C_6Fe_1C_{10}$	38.6(2)	$C_{16}Fe_2C_{20}$	37.3(2)
$O_2S_1O_1$	108.6(2)	$O_{12}S_2O_{11}$	107.6(2)
$O_2S_1C_3$	105.2(3)	$O_{12}S_2C_{13}$	106.6(3)
$O_1S_1C_3$	92.0(2)	$O_{11}S_2C_{13}$	91.7(2)
$C_2O_1S_1$	109.9(3)	$C_{12}O_{11}S_2$	109.8(3)
$C_2C_1C_3$	109.1(4)	$C_{12}C_{11}C_{13}$	108.7(5)
$C_2C_1Fe_1$	127.9(4)	$C_{12}C_{11}Fe_2$	129.6(4)
$C_3C_1Fe_1$	123.0(3)	$C_{13}C_{11}Fe_2$	121.6(3)
$C_1C_2O_1$	118.5(5)	$C_{11}C_{12}O_{11}$	118.3(5)
$C_1C_3S_1$	105.8(3)	$C_{11}C_{13}S_2$	106.2(3)
$O_3C_4Fe_1$	177.8(5)	$O_{13}C_{14}Fe_2$	179.0(5)
$O_4C_5Fe_1$	179.0(5)	$O_{14}C_{15}Fe_2$	179.5(4)
$C_{10}C_6C_7$	106.5(5)	$C_{20}C_{16}C_{17}$	106.3(7)
$C_8C_7C_6$	108.6(5)	$C_{18}C_{17}C_{16}$	108.7(10)
$C_7C_8C_9$	107.3(5)	$C_{17}C_{18}C_{19}$	107.4(9)
$C_{10}C_9C_8$	108.1(6)	$C_{20}C_{19}C_{18}$	108.9(9)
$C_9C_{10}C_6$	109.4(6)	$C_{16}C_{20}C_{19}$	108.7(7)
$C_{10}C_6Fe_1$	70.9(3)	$C_{20}C_{16}Fe_2$	71.4(3)
$C_7C_6Fe_1$	70.0(3)	$C_{17}C_{16}Fe_2$	69.4(4)
$C_8C_7Fe_1$	70.2(3)	$C_{18}C_{17}Fe_2$	69.9(5)

Table S5. (continued)

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
$C_6C_7Fe_1$	70.7(3)	$C_{16}C_{17}Fe_2$	71.4(4)
$C_7C_8Fe_1$	71.0(3)	$C_{17}C_{18}Fe_2$	72.5(6)
$C_9C_8Fe_1$	71.0(3)	$C_{19}C_{18}Fe_2$	71.6(5)
$C_{10}C_9Fe_1$	71.2(3)	$C_{20}C_{19}Fe_2$	72.6(4)
$C_8C_9Fe_1$	69.7(3)	$C_{18}C_{19}Fe_2$	69.7(5)
$C_9C_{10}Fe_1$	70.7(3)	$C_{16}C_{20}Fe_2$	71.3(3)
$C_6C_{10}Fe_1$	70.5(3)	$C_{19}C_{20}Fe_2$	69.8(4)

[a] The numbers in parentheses are the estimated standard deviations in the last significant digit.

[b] Atoms are labeled in agreement with Figure 1.

[c] The symbols C_{p1} and C_{p2} are used to represent the centers of gravity for the two cyclopentadienyl rings designated by carbon atoms C_6-C_{10} and C_{16}-C_{20} for Molecules 1 and 2, respectively. These values are therefore listed without estimated standard deviations.