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PREPARATION AND CRYSTAL STRUCTURE OF BIS [BIS(PENTAMETHYLCYCLOPENTADIENYL)YTTERBIUM(III)]UNDECACARBONYLTRIFERRATE, $[(C_5Me_5)_2Yb]_2$ $[Fe_3(CO)_{11}]$; A COMPOUND WITH FOUR ISOCARBONYL (Fe-CO-Yb) INTERACTIONS

T. Don Tilley and Richard Andersen

November 1981

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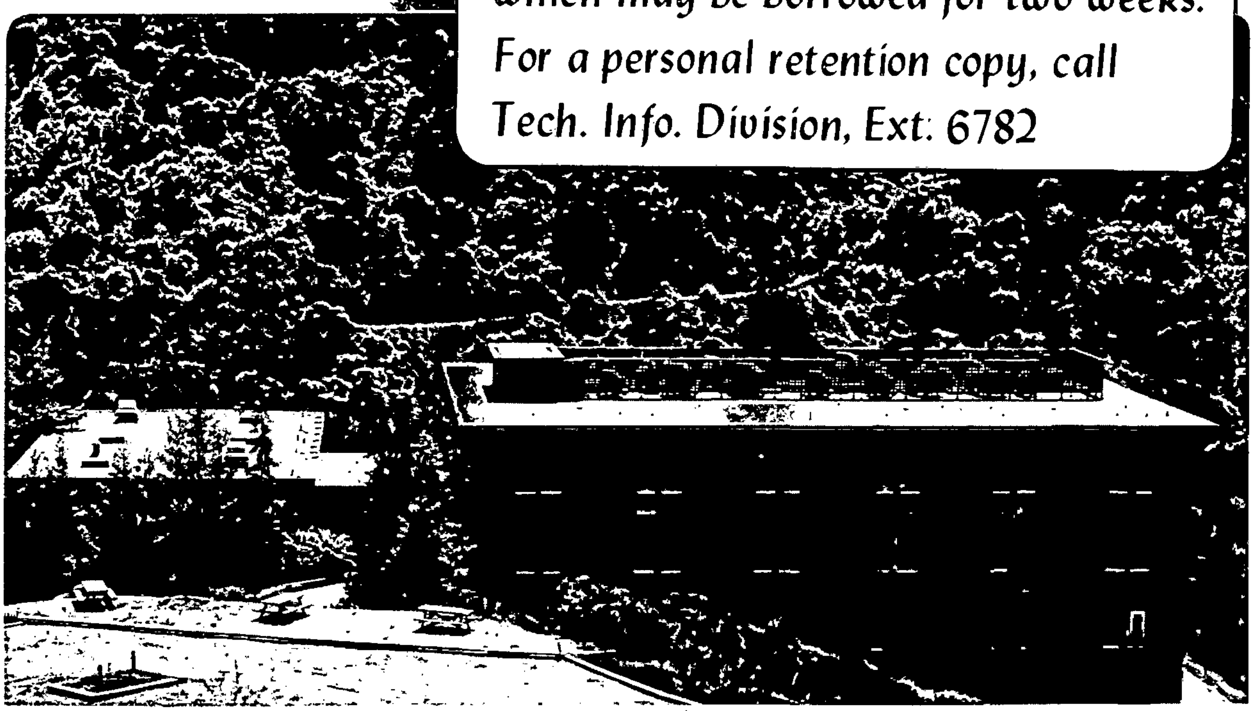

Prepared for the U.S. Department of Energy under Contract W-7405-ENG-48

LBL-13612

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LBL-13612

Preparation and Crystal Structure of Bis [bis(pentamethylcyclopentadienyl)ytterbium(III)]Undecacarbonyltriferrate, $[(C_5Me_5)_2Yb]_2 [Fe_3(CO)_{11}]$; A Compound with Four Isocarbonyl (Fe-CO-Yb) Interactions

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This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under Contract Number W-7405-ENG-48.

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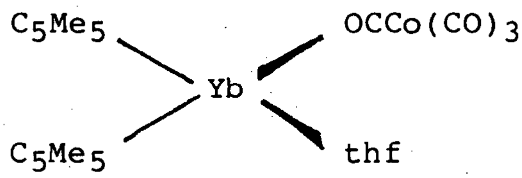
Abstract

The $Fe_2(CO)_9$ and $Fe_3(CO)_{12}$ clusters react with two molar equivalents of the divalent, f-block metallocene, $(Me_5C_5)_2Yb(OEt_2)$, to give the complex, $[(Me_5C_5)_2Yb]_2[Fe_3(CO_7)(\mu\text{-}CO)_4]$ as shown by X-ray crystallography. The cluster anion has four bridging CO groups arranged so as to form two trans-metalloacetonylacetonate-like groups about the Fe_3 atom. Mononuclear $Fe(CO)_5$ reacts with the ytterbium-metallocene to give $[(Me_5C_5)_2Yb]_2[Fe(CO)_4]$.

It has been shown recently that the divalent lanthanide complex $(C_5Me_5)_2Yb(OEt_2)$ reduces $Co_2(CO)_8$, cleaving the metal-metal bond to give I.[1] The tetracarbonylcobaltate anion is



(I)

bonded to the trivalent Lewis acid fragment $[Yb(C_5Me_5)_2(thf)]^+$, by donation of a lone pair of electrons on one of the carbon monoxide groups. Infrared and X-ray data suggest that the carbon-oxygen bond of the bridging carbonyl ligand was significantly weakened, resulting in a charge disparity in the sense, $Co(\delta-)-C(\delta+)-O(\delta-)-Yb(\delta+)$. This should enhance the reactivity of the bridging carbon monoxide group toward nucleophilic and/or electrophilic reagents. Such carbon- and oxygen-bonded carbonyl ligands have been shown to exhibit unique physical properties and reactivity patterns.[2]

In investigating the utility of $(C_5Me_5)_2Yb(OEt_2)$ in preparing complexes of transition metal carbonyl anions that contain M-CO-M' bonds, it was of interest to examine reactions of carbonyl clusters having bridging carbon monoxide groups. Carbonyl ligands that bridge two or more transition metals have a lower C-O bond order than terminal ones, and are better σ-donors toward hard Lewis acids. As a result, some Lewis acids induce terminal-to-bridge CO shifts.[2] Such interactions will result in further charge disparity in the bridging carbon monoxide group and activate the C-O bond to an even greater extent.

Reaction of two molar equivalents of $(C_5Me_5)_2Yb(OEt_2)$ with $Fe_3(CO)_{12}$ in toluene, or stoichiometric amounts of $(C_5Me_5)_2Yb(OEt_2)$ and $Fe_2(CO)_9$ in toluene, results in a dark red solution, from which violet prisms (m.p. 307-310°C) of $[(C_5Me_5)_2Yb]_2[Fe_3(CO)_{11}]$ may be crystallized.[3] The infrared spectrum shows that the carbonyl ligands are significantly perturbed relative to the electronically equivalent $[Et_4N]_2$-$[Fe_3(CO)_9(\mu\text{-}CO)(\mu_3\text{-}CO)]$, which has ν(CO)(thf) at 1938 s, 1910 ms, 1890 sh, and 1670 w cm^{-1}.[4] The ytterbium complex shows two low energy C-O stretching frequencies at 1667 and 1604 cm^{-1}, suggesting the presence of η^2,η^1-triply bridging carbonyl ligands.

In order to unequivocably establish the structure of this novel complex, a crystal structure analysis was performed.[5] Of the three discrete molecules in the unit cell, two are well-ordered and related by an inversion center while the third is disordered about the center of inversion. An ORTEP view of the ordered molecule is shown in Figure I. The molecule has approximate C_{2v} symmetry about the Fe(1)-C(1) vector. The C_5Me_5 groups are inequivalent in the solid state as well as in solution since they give two equal-area resonances in the ^1H NMR spectrum at 26°C.[3] The two iron-iron distances [Fe(1)-Fe(2) and Fe(1)-Fe(3)] of 2.524(1) and 2.538(1) Å, respectively, are essentially equal as are the four ytterbium-oxygen distances (average, 2.243(5) Å). The average ytterbium-carbon(C_5Me_5) bond length of 2.573(13) Å is similar to those found in ytterbium(III) metallocenes of the same coordination number $[Yb(C_5Me_5)_2S_2CNEt_2$, 2.63(3)[6a] and

$Yb(C_5Me_5)_2(thf)Co(CO)_4$, 2.596(1) Å[1]]. However, this average bond length is significantly longer than that found in the ytterbium(II) species of identical coordination number, $Yb(C_5Me_5)_2(py)_2$, 2.742(7) Å.[6b] This difference is expected since the ionic radius of Yb(III) is ca. 0.16 Å smaller than that of Yb(II) when both ions have the same coordination number.[7] Thus, the paramagnetism of the complex is explained, since Yb(II) is an f^{13} ion whereas Yb(II) is an f^{14} ion and the complex can be viewed as a tight ion-pair of the form $[Yb(C_5Me_5)_2]^+_2[Fe_3(CO)_7-(\mu-CO)_4]^=$.

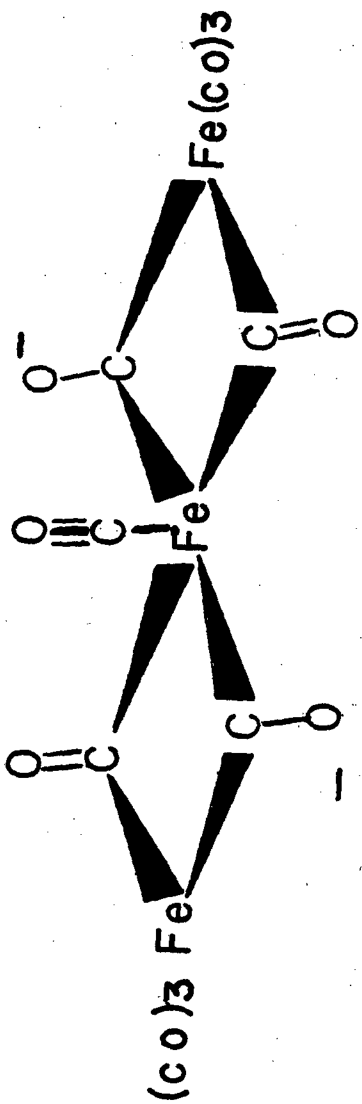
The Fe(2)-Fe(1)-Fe(3) angle is 161.8° and there is no direct interaction between Fe(2) and Fe(3). The two planes defined by the carbonyls bound to Yb(1) and Yb(2) are inclined with respect to each other, with a dihedral angle of 168.1° away from the unique carbonyl bonded to Fe(1). Thus, the overall shape of the cluster might be described as an inverted umbrella, the handle being the unique carbonyl bound to Fe(1). The least-squares plane defined by the bridging carbonyl carbon atoms C(2), C(3), C(4) and C(5) is 0.36 Å below Fe(1) and above Yb(1) and Yb(2) by 0.56 and 0.48 Å, respectively. The terminal Fe(2) and Fe(3) atoms are slightly below this plane, by 0.06 and 0.02 Å, respectively.

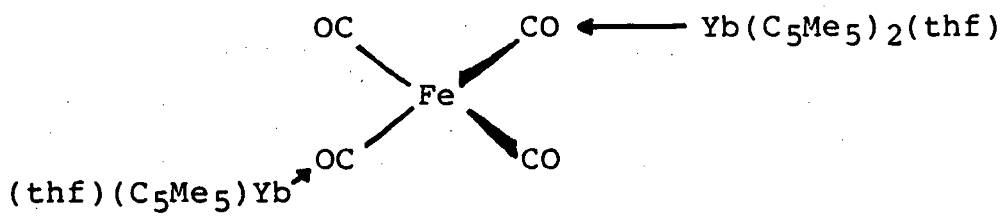
The bonding iron-iron distances are similar to those found in the electronically equivalent (48 electron) tri-iron clusters $[Fe_3(CO)_9(\mu-CO)(\mu_3-CO)]^{=4}$, $[Fe_3(CO)_{10}(\mu-H)(\mu-CO)]^-$,[8a] and $Fe_3(CO)_{10}(\mu-CO)_2$.[8b] The latter three clusters have their iron atoms at the corners of an isosceles triangle, the geometry usually found for tri-metallic cluster molecules.[9] The geometry of the $[Fe_3(CO)_7(\mu\text{-}CO)_4]^=$ cluster (Figure II shows the averaged bond angles and lengths within the cluster) has been greatly perturbed by the presence of the two $[Yb(C_5Me_5)_2]^+$ units, which have forced four carbonyl groups into bridging positions. The Fe(1)CO(4)CO(5) and Fe(1)CO(2)CO(3) fragments may be viewed as metalloacetonylacetonate groups coordinated in a chelating fashion to the two ytterbium(III) centers.[10] Thus, the $Fe_3(CO)_{11}^=$ cluster may be viewed, in an electronic sense, by the valence bond structure shown below. In order to act as a chelating ligand, the $[Fe_3(CO)_{11}]^=$ distorts by breaking an Fe-Fe bond. This process does not require much energy since the Fe-Fe bond energy in $Fe_3(CO)_{12}$ is estimated to be ca. 19 kcal mol^{-1},[11] most certainly less than that of four ytterbium-oxygen bonds.

(See illustration, next page)

A rich reaction chemistry is suggested by the 'opened' geometry of the $[Fe_3(CO)_{11}]^=$ cluster. However, toluene solutions of the $[(C_5Me_5)_2Yb]_2[Fe_3(CO)_{11}]$ cluster did not react with H_2 nor CO at 18 atm during a 24 h period.

In order to examine reactions of the complete set of binary iron carbonyls with the ytterbium(II) metallocene, we have studied the reaction of $Fe(CO)_5$ with two molar equivalents of $Yb(C_5Me_5)_2(OEt_2)$. The reaction gives $[Yb(C_5Me_5)_2(thf)]_2[Fe(CO)_4]$ after crystallization from tetrahydrofuran.[12] The complex gives $Fe(CO)_4(SnPh_3)_2$ upon reaction with Ph_3SnCl, as shown by infrared spectroscopy.[13] Thus, the complex may be formulated as the tetracarbonylferrate, shown below, analogous to the well-known sodium salt, $Na_2Fe(CO)_4$.[14]





Acknowledgement.

This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U. S. Department of Energy under contract Number W-7406-ENG-48. We also thank the N.S.F. for a grant to the Chemistry Department used to purchase the X-ray diffractometer.

Supplementary Material.

A list of thermal and positional parameters (5 pages) is available. Ordering information is given on any current masthead page.

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3. Anal. Calcd. for $C_{51}H_{71}Fe_3O_{11}Yb$: C, 44.6; H, 5.21. Found: C, 44.9; H, 4.63. IR(Nujol): ν(CO) = 2048 w, 1998 s, 1973 s, 1667 w, 1604 bs s cm^{-1}. ^1H NMR (PhMe-d_8, 26°C): δ 8.09 ($\nu_{1/2}$ = 130 Hz) and 6.11 ($\nu_{1/2}$ = 130 Hz) due to the two inequivalent C_5Me_5 groups. μ_B (solid state, 4-60 K): 3.91 B. M. per ytterbium. Mp. 307-310°C.

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5. The structure was solved by Dr. F. J. Hollander, staff crystallographer at the U. C. Berkeley X-ray crystallographic facility (CHEXRAY). Crystal data: $(C_5Me_5)_4Yb_2Fe_3(CO)_{11}$, F_w = 1362.7; Space group, $P\bar{1}$, triclinic; a = 14.525(2), b = 18.058(2), c = 18.324(2) Å; α = 72.151(11); β = 84.050(11), γ = 72.151(11)°; V = 4321(1) Å^3; ρ_{calc} = 1.571 gcm^{-3}; Z = 3; μ(Mo-K_α) = 40.05 cm^{-1}; λ = 0.71073 Å. The structure was solved by Patterson and Fourier methods and refined using 8622 data [$F^2 > 3\sigma(F^2)$] measured on a Nonius CAD 4 diffractometer. The R and R_w for all data were 5.76 and 8.33%, respectively.

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12. Anal. Calcd. for $C_{52}H_{76}FeO_6Yb_2$: C, 52.1; H, 6.39. Found: C, 51.6; H, 6.42. ^1H NMR (thf-d_8, 26°C); a single resonance was observed at δ 9.52 ($\nu_{1/2}$ = 144 Hz). Hydrolysis of a sample dissolved in benzene gave a mixture of Me_5C_5H and tetrahydrofuran in area ratio

2:1 by ^{1}H NMR spectroscopy. ν(CO)(Nujol): 2004 w, 1980 w, 1961 w, 1928 s, 1922 s, 1753 m sh, 1741 s, 1711 s, 1648 m sh and 1608 s br cm^{-1}.

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Figure Captions

Figure 1. An ORTEP drawing of $[(Me_5C_5)_2Yb]_2[Fe_3(CO)_7(\mu\text{-}CO)_4]$.

Figure 2. A line-drawing showing some average bond lengths and distances. The average Fe(2,3)-C(terminal) and their associated C-O bond lengths are 1.741 ± 0.013 and 1.176 ± 0.014 Å, respectively. The Fe(1)-C(1) and C(1)-O(1) bond lengths are 1.698(8) and 1.161(9) Å, respectively. The average Me_5C_5(centroid)-Yb-Me_5C_5-(centroid) angle is $141.6 \pm 0.004°$ and the Me_5C_5-(centroid)-Yb bond length is 2.289 ± 0.019 Å.

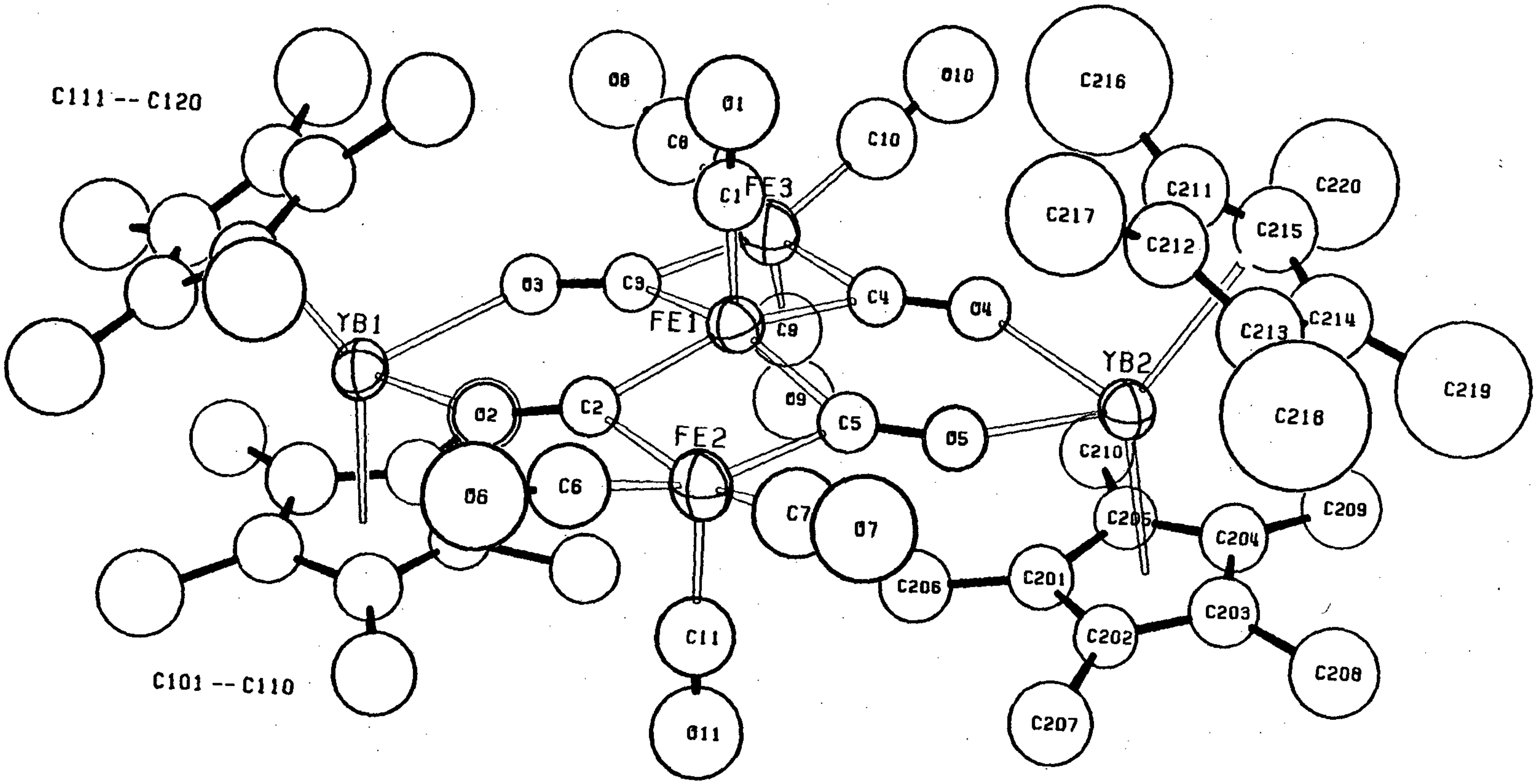

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Figure 1

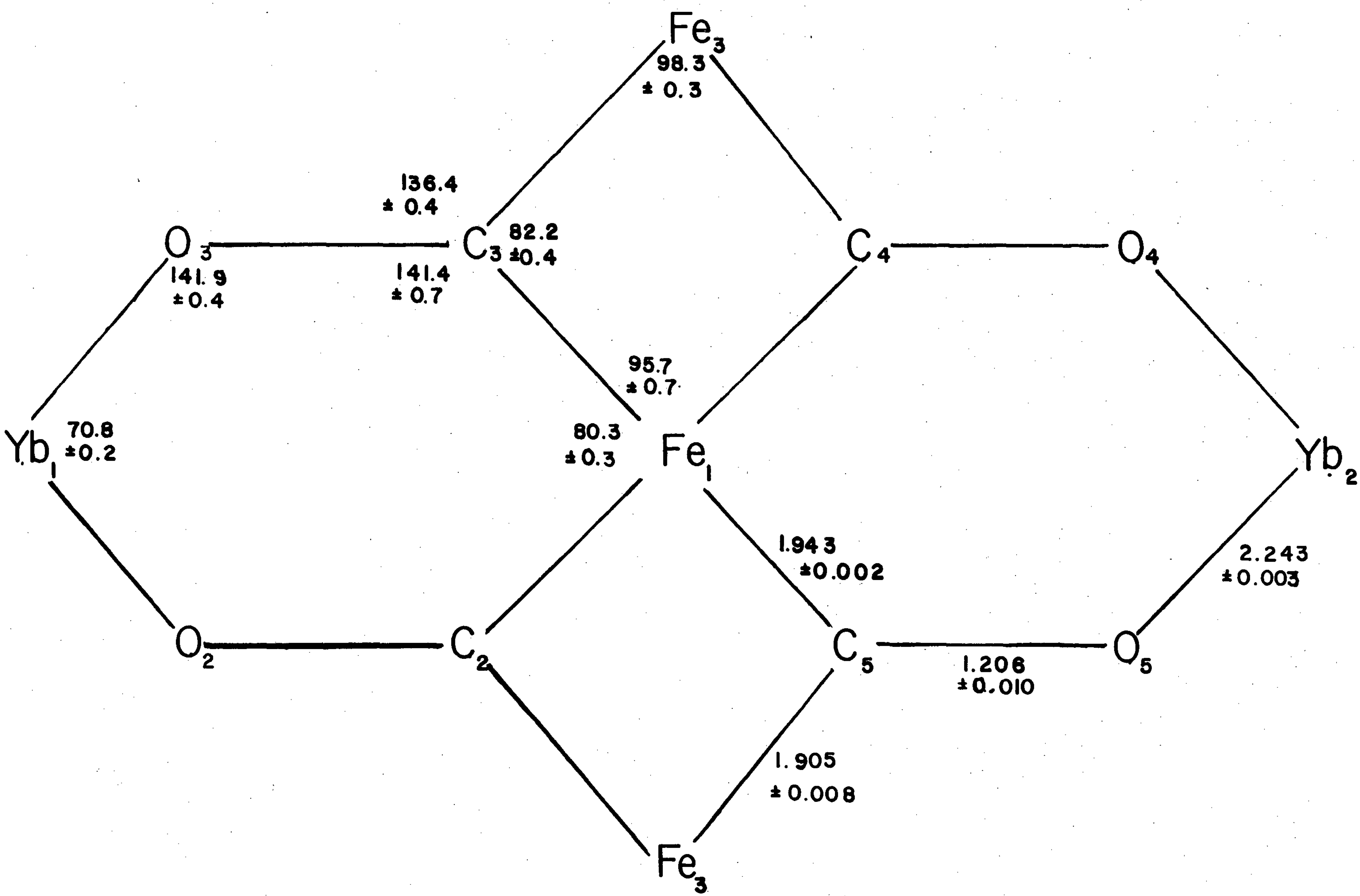
Fe3
98.3
± 0.3
136.4
± 0.4
O3
C3
82.2
±0.4
C4
O4
141.9
±0.4
141.4
± 0.7
95.7
± 0.7
Yb1
70.8
±0.2
80.3
±0.3
Fe1
Yb2
1.943
±0.002
2.243
±0.003
O2
C2
C5
O5
1.206
±0.010
1.905
±0.008
Fe3

Figure 2

Supplementary Materials for

Preparation and Crystal Structure of Bis[bis(pentamethylcyclopentadienyl)ytterbium(III)]Undecacarbonylferrate, $[(C_5Me_5)_2Yb]_2$-$Fe_3(CO)_{11}]$; A Compound with Four Isocarbonyl (Fe-CO-YB) Interactions

by T. Don Tilley and Richard A. Andersen

1. The Yb(1), Yb(2) and Fe(1), Fe(2), Fe(3) are the metal atoms in the ordered molecule. The Yb(3) and Fe(4) are the ordered metal atoms in the disordered molecule on the inversion at 1/2,1/2,1/2 and Fe(5) is the central (disordered) iron atom of that molecule. O(1-11) and C(1-11) are the CO groups in the ordered molecule and O(21-26) and C(21-26) are the ordered CO groups in the disordered molecule and O(24P) and C(24P-26P) are the disordered CO groups of the latter molecule. O(25P, 26P) were not located. C(101-120) and C(201-220) are the carbon atoms of the Me_5C_5 groups in the ordered molecule, see Figure 1 of the manuscript for the numbering scheme. C(301-320) are the ordered Me_5C_5 ordered carbon atoms inn the disordered molecule. The numbering scheme is symmetrical to that of the molecule.

2. HCP1-HCP6 are the centroids of the Me_5C_5 groups calculated from the position of the ring carbon atoms. Again, HCP1-HCP4 are the ordered rings of the ordered molecule and HCP5-HCP6 are the ordered rings on the disordered molecule. C101-C110 are the atoms of Cp1 on Yb(1). C111-C120 are the atoms of Cp2 on Yb(2), etc.

3. The following atoms were given occupancy factors of 0.50: Fe(5), C(23), O(23), C(24), O(24), C(25), O(25), C(26), O(26), C(24P), O(24P), C(25P), and C(26P).

POSITIONAL AND THERMAL PARAMETERS AND THEIR ESTIMATED STANDARD DEVIATIONS.

ATOM	X	Y	Z	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
YB1	-0.25170(4)	-0.04093(3)	0.32917(3)	0.00521(3)	0.00371(2)	0.00263(2)	-0.00403(4)	0.00098(4)	-0.00258(3)
YB2	0.18944(4)	0.19643(3)	0.07925(3)	0.00488(3)	0.00294(2)	0.00258(2)	-0.00269(4)	0.00049(4)	-0.00150(3)
YB3	0.41087(5)	0.54710(4)	0.25849(3)	0.00617(4)	0.00342(2)	0.00277(2)	-0.00306(4)	-0.00144(4)	-0.00144(3)
FE1	-0.0367(1)	0.1041(1)	0.2381(1)	0.0043(1)	0.00272(6	0.00248(6	-0.0017(1)	-0.0001(1)	-0.00146(9)
FE2	0.0954(1)	-0.0232(1)	0.3038(1)	0.0047(1)	0.00323(7	0.00286(6	-0.0020(1)	-0.0010(1)	-0.00034(11)
FE3	-0.1645(1)	0.2075(1)	0.1417(1)	0.0045(1)	0.00316(8	0.00374(7	-0.0009(1)	-0.0009(2)	-0.00039(12)
FE4	0.3901(2)	0.6364(1)	0.4992(1)	0.0106(2)	0.00317(8	0.00400(7	0.0015(2)	-0.0048(2)	-0.00277(11)
FE5	0.5338(3)	0.5101(2)	0.4868(2)	0.0052(2)	0.00235(12	0.00280(12	-0.0010(3)	-0.0008(3)	-0.00153(18)
O1	-0.0523(9)	0.1914(7)	0.3458(7)	7.7(3)					
O2	-0.0984(6)	-0.0417(5)	0.3369(5)	3.8(2)					
O3	-0.2327(6)	0.0789(5)	0.2525(5)	3.7(2)					
O4	0.0295(6)	0.2195(5)	0.1019(5)	3.9(2)					
O5	0.1649(6)	0.1011(5)	0.1877(5)	3.7(2)					
O6	0.0794(11)	-0.1302(9)	0.4604(8)	9.3(4)					
O7	0.2857(11)	-0.0247(8)	0.3407(8)	9.1(4)					
O8	-0.3704(12)	0.2611(9)	0.1744(9)	10.6(5)					
O9	-0.1757(10)	0.1569(8)	0.0065(7)	8.0(3)					
O10	-0.1684(11)	0.3771(9)	0.0703(9)	9.9(4)					
O11	0.1524(10)	-0.1448(8)	0.2217(7)	8.1(3)					
O21	0.3910(7)	0.6005(6)	0.3550(5)	4.8(2)					
O22	0.5045(7)	0.4557(6)	0.3571(6)	5.3(2)					
O23	0.6923(20)	0.5772(16)	0.4287(16)	8.7(7)					
O24	0.5085(28)	0.7420(23)	0.4602(22)	13.4(12)					
O25	0.7056(21)	0.3122(17)	0.3687(16)	9.1(8)					
O26	0.2140(22)	0.7386(17)	0.4016(17)	9.7(8)					
O24P	0.3176(32)	0.7778(26)	0.3674(25)	15.5(14)					

C1	-0.0483(10)	0.1548(8)	0.3033(8)	4.5(3)
C2	-0.0427(9)	-0.0026(7)	0.3067(7)	3.3(3)
C3	-0.1710(9)	0.1131(7)	0.2240(7)	3.4(3)
C4	-0.0279(9)	0.1891(7)	0.1420(7)	3.3(3)
C5	0.1027(9)	0.0740(7)	0.2244(7)	3.4(3)
C6	0.0855(12)	-0.0843(10)	0.3995(9)	5.8(4)
C7	0.2100(13)	-0.0251(11)	0.3254(10)	6.6(4)
C8	-0.2875(15)	0.2382(12)	0.1616(12)	8.1(5)
C9	-0.1723(13)	0.1802(10)	0.0609(10)	6.1(4)
C10	-0.1685(13)	0.3085(11)	0.0978(10)	6.9(5)
C11	0.1305(12)	-0.0987(10)	0.2569(9)	5.6(4)
C101	-0.1702(11)	-0.1572(9)	0.2738(8)	4.8(3)
C102	-0.1849(10)	-0.0856(8)	0.2109(8)	4.1(3)
C103	-0.2846(11)	-0.0500(9)	0.1971(8)	4.8(3)
C104	-0.3319(12)	-0.1010(10)	0.2517(9)	5.7(4)
C105	-0.2626(11)	-0.1666(9)	0.2987(9)	5.1(4)
C106	-0.0747(14)	-0.2162(11)	0.3059(10)	7.0(5)
C107	-0.1041(12)	-0.0570(9)	0.1610(9)	5.2(4)
C108	-0.3319(13)	0.0258(11)	0.1312(10)	6.5(4)
C109	-0.4397(14)	-0.0932(11)	0.2476(11)	7.0(5)
C110	-0.2842(15)	-0.2457(12)	0.3608(12)	8.0(5)
C111	-0.3804(11)	0.0444(9)	0.3991(9)	5.1(4)
C112	-0.2885(12)	0.0328(9)	0.4314(9)	5.3(4)
C113	-0.2528(11)	-0.0483(9)	0.4723(8)	4.9(3)
C114	-0.3198(11)	-0.0867(9)	0.4679(9)	5.0(3)
C115	-0.3971(12)	-0.0288(9)	0.4233(9)	5.4(4)
C116	-0.4515(18)	0.1258(14)	0.3505(14)	10.0(7)
C117	-0.2380(15)	0.1027(12)	0.4234(11)	7.9(5)
C118	-0.1643(17)	-0.0811(14)	0.5192(13)	9.3(6)
C119	-0.3116(16)	-0.1719(13)	0.5166(13)	8.9(6)
C120	-0.4965(16)	-0.0395(13)	0.4126(13)	8.9(6)
C201	0.1623(10)	0.0963(8)	0.0174(8)	4.3(3)
C202	0.2619(10)	0.0694(8)	0.0335(8)	3.9(3)

C203	0.3047(11)	0.1272(9)	-0.0114(8)	5.0(3)
C204	0.2314(11)	0.1935(9)	-0.0607(8)	4.8(3)
C205	0.1458(10)	0.1750(8)	-0.0432(8)	4.3(3)
C206	0.0897(12)	0.0501(10)	0.0488(9)	5.6(4)
C207	0.3138(13)	-0.0140(11)	0.0899(10)	6.7(4)
C208	0.4146(15)	0.1186(12)	-0.0219(11)	7.8(5)
C209	0.2480(14)	0.2616(11)	-0.1282(10)	6.9(5)
C210	0.0497(13)	0.2258(10)	-0.0804(10)	6.4(4)
C211	0.1559(14)	0.3214(11)	0.1264(11)	7.1(5)
C212	0.2174(13)	0.2612(10)	0.1781(10)	6.2(4)
C213	0.3042(13)	0.2437(11)	0.1412(10)	6.7(4)
C214	0.2877(14)	0.2966(11)	0.0672(11)	7.1(5)
C215	0.1945(14)	0.3421(11)	0.0634(10)	6.8(5)
C216	0.0511(33)	0.3587(27)	0.1551(26)	21.1(17)
C217	0.2011(21)	0.2229(17)	0.2629(17)	12.5(9)
C218	0.4017(30)	0.1873(25)	0.1738(23)	19.3(14)
C219	0.3839(28)	0.3030(23)	0.0116(21)	17.5(13)
C220	0.1536(28)	0.4154(22)	-0.0105(21)	17.0(13)
C301	0.2905(15)	0.4697(12)	0.3311(11)	7.9(5)
C302	0.3284(15)	0.4375(12)	0.2788(12)	7.9(5)
C303	0.3038(15)	0.4845(12)	0.2093(12)	8.1(5)
C304	0.2411(13)	0.5634(11)	0.2146(10)	6.7(4)
C305	0.2351(14)	0.5468(12)	0.2957(11)	7.6(5)
C306	0.2988(23)	0.4348(18)	0.4257(18)	14.1(10)
C307	0.3972(33)	0.3492(27)	0.2881(26)	21.1(17)
C308	0.3297(29)	0.4454(23)	0.1405(22)	18.0(14)
C309	0.1769(26)	0.6438(21)	0.1617(20)	16.2(12)
C310	0.1768(28)	0.6099(23)	0.3373(21)	16.7(13)
C311	0.4542(16)	0.6711(13)	0.1615(12)	8.7(6)
C312	0.5225(14)	0.6389(12)	0.2091(11)	7.4(5)
C313	0.5788(13)	0.5583(11)	0.2011(10)	6.5(4)
C314	0.5350(13)	0.5521(10)	0.1447(10)	6.1(4)
C315	0.4585(17)	0.6246(14)	0.1221(13)	9.3(6)

C316	0.3672(33)	0.7582(27)	0.1249(26)	21.3(17)
C317	0.5749(39)	0.6312(31)	0.2757(31)	25.1(22)
C318	0.6708(28)	0.4990(22)	0.2367(21)	17.3(13)
C319	0.5652(21)	0.4821(17)	0.1020(16)	12.4(9)
C320	0.4059(26)	0.6198(22)	0.0379(20)	16.3(12)
C21	0.4186(12)	0.5846(9)	0.4215(9)	5.4(4)
C22	0.5266(12)	0.4477(10)	0.4227(9)	5.8(4)
C23	0.6286(23)	0.5476(18)	0.4504(18)	5.4(7)
C24	0.4526(31)	0.7014(25)	0.4790(24)	8.2(11)
C25	0.6760(21)	0.3337(17)	0.4204(16)	4.6(7)
C26	0.2767(24)	0.7004(19)	0.4439(18)	5.6(8)
C24P	0.3558(39)	0.7147(32)	0.4246(31)	11.4(15)
C25P	0.5696(48)	0.2814(38)	0.4356(36)	14.8(21)
C26P	0.7350(39)	0.3803(32)	0.4516(30)	11.2(16)
HCP1	-0.2468(0)	-0.1121(0)	0.2464(0)	4.0000(0)
HCP2	-0.3277(0)	-0.0173(0)	0.4388(0)	4.0000(0)
HCP3	0.2212(0)	0.1323(0)	-0.0129(0)	4.0000(0)
HCP4	0.2319(0)	0.2930(0)	0.1153(0)	4.0000(0)
HCP5	0.2798(0)	0.5004(0)	0.2659(0)	4.0000(0)
HCP6	0.5098(0)	0.6090(0)	0.1677(0)	4.0000(0)

THE FORM OF THE ANISOTROPIC THERMAL PARAMETER IS:

EXP[-(B(1,1)*H*H + B(2,2)*K*K + B(3,3)*L*L + B(1,2)*H*K + B(1,3)*H*L + B(2,3)*K*L)].

This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

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