LBL-21982
Preprint c.2

Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

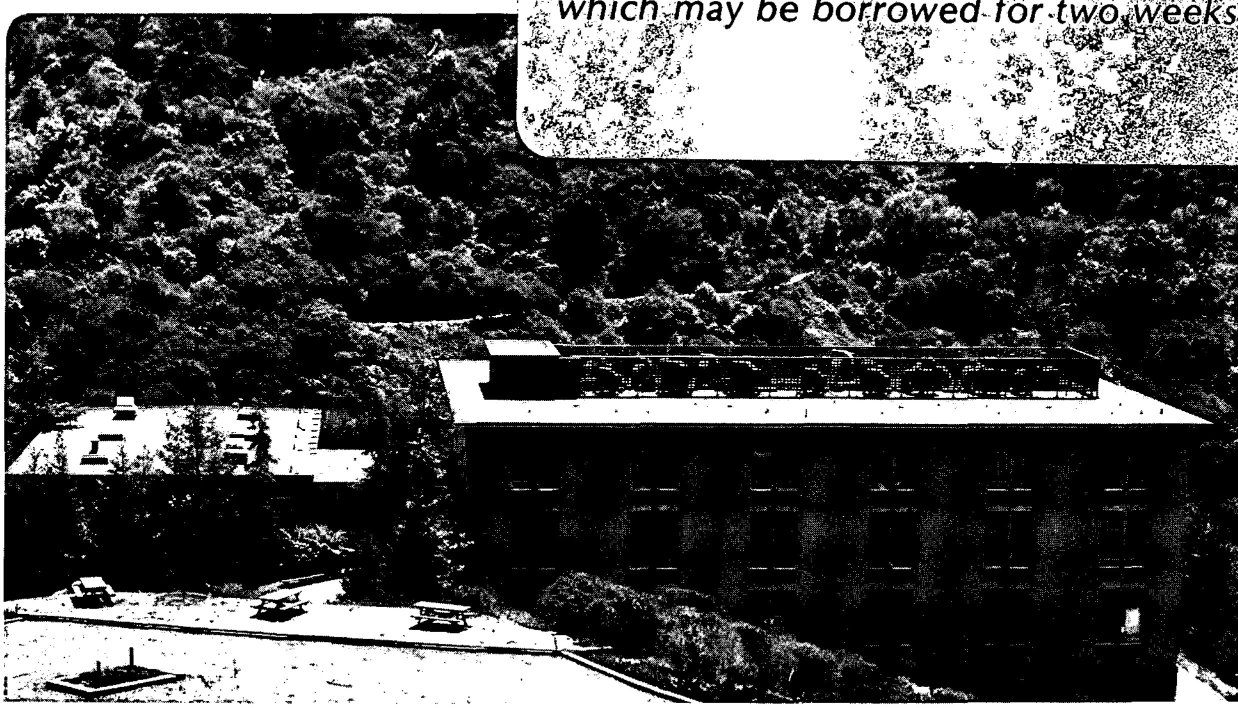
Materials & Molecular Research Division

Submitted to Inorganic Chemistry

BIS(PENTAMETHYLCYCLOPENTADIENYL) YTTERBIUM (II) AS A LEWIS ACID AND AN ELECTRON-TRANSFER LIGAND; PREPARATION AND CRYSTAL STRUCTURE OF $[Yb(C_5Me_5)_2(\mu\text{-}OC)_2Fe(C_5H_4Me)]_2$

J.M. Boncella and R.A. Andersen

August 1986



Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

LBL-21982

Bis(Pentamethylcyclopentadienyl) Ytterbium (II) as a Lewis Acid and an Electron-Transfer Ligand; Preparation and Crystal Structure of $[Yb(C_5Me_5)_2(\mu\text{-}OC)_2Fe(C_5H_4Me)]_2$

James M. Boncella and Richard A. Andersen*

Chemistry Department and Materials and Molecular Research Division of Lawrence Berkeley Laboratory, University of California, Berkeley, California 94720

*Address correspondence to this author at Chemistry Department, UCB.

ABSTRACT

The divalent ytterbium metallocene, $Yb(C_5Me_5)_2(OEt_2)$, reacts with $M_2(C_5H_4R)_2(CO)_4$ to give dimers of composition $M_2(C_5H_4R)_2(CO)_4Yb_2(C_5Me_5)_4$, where M is Fe and R = H, Me, and Me_3Si or M is Ru and R = Me_3Si. X-Ray crystallographic studies with M = Fe and R = Me, show that the molecule is a centrosymmetric dimer of the structure $[(Me_5C_5)_2Yb(\mu\text{-}OC)_2(FeC_5H_4Me)]_2$. The space group is $P2_1/n$ with a = 10.6069(15)Å, b = 23.4930(31)Å, c = 10.8730(20)Å, β = 92.041(13)°, V = 2707.7(13)Å^3, and Z = 2.

In an earlier paper, we outlined an approach for using the divalent metallocene, $Yb(C_5Me_5)_2(OEt_2)$, as a Lewis acid and as a one electron-transfer reagent towards transition metal carbonyls, giving compounds in which the carbon monoxide ligand bridges the transition metal and lanthanide metal atoms (M-CO-Yb).[1] The net result of coordination and electron-transfer is reduction of the carbon-oxygen stretching frequency and bond order. For example, the lowest carbon-oxygen stretching frequency of $[(Me_5C_5)_2Yb(\mu\text{-}OC)_2Mn(CO)_3]_2$ in tetrahydrofuran is 1723 cm^{-1} whereas the lowest CO stretching frequency in $NaMn(CO)_5$ in tetrahydrofuran or $(Me_2N)_3PO$ is 1829 or 1861 cm^{-1}, respectively.[2] Thus the C-O bond order in the ytterbium-manganese contact ion-pair is lower than that in the sodium-manganese ion-pair.

One strategy for reducing the carbon-oxygen bond order to an even lower value in complexes of the general type M-CO-Yb, where M is a transition metal, is to replace the electron-withdrawing carbon monoxide ligands (terminal) with electron-donating ligands, such as the cyclopentadienide group. In order to test the validity of this suggestion, we chose to allow $Cp_2Fe_2(\mu\text{-}CO)_2(CO)_2$ to react with the diethyl ether complex of bis(pentamethylcyclopentadienyl) ytterbium (II), since the CpFe and $Mn(CO)_3$ fragments are electronically equivalent (thirteen electron fragments). Assuming that both molecules are structurally equivalent, they will differ only by the amount of electron density located on the transition metal fragment which will be manifested in the carbon-oxygen (bridging) stretching frequency and bond length. In this regard, it has been shown recently that $[(Me_5C_5)_2Zr]_2(\mu\text{-}N_2)_2(N_2)_2$ acts as a two electron-transfer reagent towards $Cp_2Fe_2(\mu\text{-}CO)_2(CO)_2$ to give $(Me_5C_5)_2ZrO_2C_2Fe_2Cp_2(\mu\text{-}CO)_2$, a complex in which a carbon-carbon bond has been formed between the two carbonyl ligands.[3]

<u>Synthetic Studies</u>. The diethyl ether complex of bis(penta-

methylcyclopentadienyl)ytterbium reacts with $Cp_2Fe_2(\mu\text{-}CO)_2(CO)_2$ in toluene to give a black, sparingly soluble material of stoichiometry $(Me_5C_5)_2YbCpFe(CO)_2$. The complex reacts with water-d_2 to give Me_5C_5D and $Cp_2Fe_2(\mu\text{-}CO)_2(CO)_2$ in a 2:1 molar ratio as shown by ^{1}HNMR spectroscopy of a benzene-d_6 extract. The infrared spectrum of the black material, recorded as a Nujol mull since the complex is essentially insoluble in saturated hydrocarbons, has two strong absorptions at 1800 and 1740 cm^{-1}. The complex is paramagnetic as shown by the shifted and broadened ^{1}HNMR resonances, see experimental section. The data suggest a formulation based upon $(Me_5C_5)_2Yb(III)$ with local C_{2v} symmetry of the $Fe(CO)_2$ unit or overall C_{2h} symmetry for a dimer unit, _i.e._ a geometry similar to the dimeric portion of $[(Me_5C_5)_2Yb(\mu\text{-}OC)_2Mn(CO)_3]_2$, in which the $Mn(CO)_3$ portion is replaced by FeCp. However, the low solubility of the complex makes further study difficult.

In order to prepare a more soluble material we allowed $(Me_5C_5)_2Yb(OEt_2)$ to react with $(MeC_5H_4)_2Fe_2(\ \text{-}CO)_2(CO)_2$ in toluene. The black solid, which is soluble in hot methylcyclohexane, is stoichiometrically identical to the cyclopentadienyl analogue, _viz._, $(Me_5C_5)_2Yb(MeC_5H_4)Fe(CO)_2$. The infrared spectrum in cyclohexane shows two strong CO stretching frequencies at 1787 and 1723 cm^{-1}, similar to those of the C_5H_5-analogue in the solid state of 1800 and 1740 cm^{-1}. The CO stretching frequencies of the MeC_5H_4-derivative are _ca._ 100 and 65 cm^{-1}, respectively, lower than those found for $(n\text{-}Bu_4N)(CpFe(CO)_2)$ in tetrahydrofuran. See Table I for other comparisons. Two other substituted cyclopentadienyliron and ruthenium derivatives were prepared, $(Me_5C_5)Yb(Me_3SiC_5H_4Fe(CO)_2)$ and $(Me_5C_5)Yb(Me_3SiC_5H_4)Ru(CO)_2$. The infrared spectra, listed in Table I, prove that all the derivatives are isostructural. Curiously, $(Me_5C_5)_2Yb(Me_5C_5)Fe(CO)_2$ is rather insoluble in hydrocarbons; the solubility is similar to the C_5H_5-derivative and is presumably related to the way these symmetrically substituted cyclopentadienyl derivatives pack in the crystalline lattice.

The magnetic susceptibility of $(Me_5C_5)_2Yb(MeC_5H_4)Fe(CO)_2$ follows Curie-Weiss behaviour $[\chi_M=C_M(T-\theta)^{-1}]$ from 5-45K with $C_M = 1.283 \pm 0.012$, $\theta = -0.50 \pm 0.10$K, and $\mu_{eff} = 3.217 \pm 0.015$ B.M. and from 90-290K with $C_M = 2.267 \pm 0.004$, $\theta = -33.78 \pm 0.39$K, and $\mu_{eff} = 4.276 \pm 0.004$ B.M. The solid state susceptibility of $(Me_5C_5)_2Yb(MeC_5H_4)Fe(CO)_2$ in conjunction with the infrared spectra suggest that all of the complexes are based upon trivalent ytterbium, i.e. electron transfer from $(Me_5C_5)_2Yb(II)$ to $Cp_2Fe_2(\mu\text{-}CO)_2(CO)_2$ has occured. As the lowest unoccupied molecular orbital in the transition metal carbonyl is metal-metal antibonding,[4] population of this orbital will break the iron-iron bond giving $(Me_5C_5)_2YbCpFe(CO)_2$. Since the $CpFe(CO)_2^-$ fragment is electronically equivalent to $Mn(CO)_5^-$, a structure related to that found for the latter is likely[2]. That this postulate is correct is shown by X-ray crystallographic analysis.

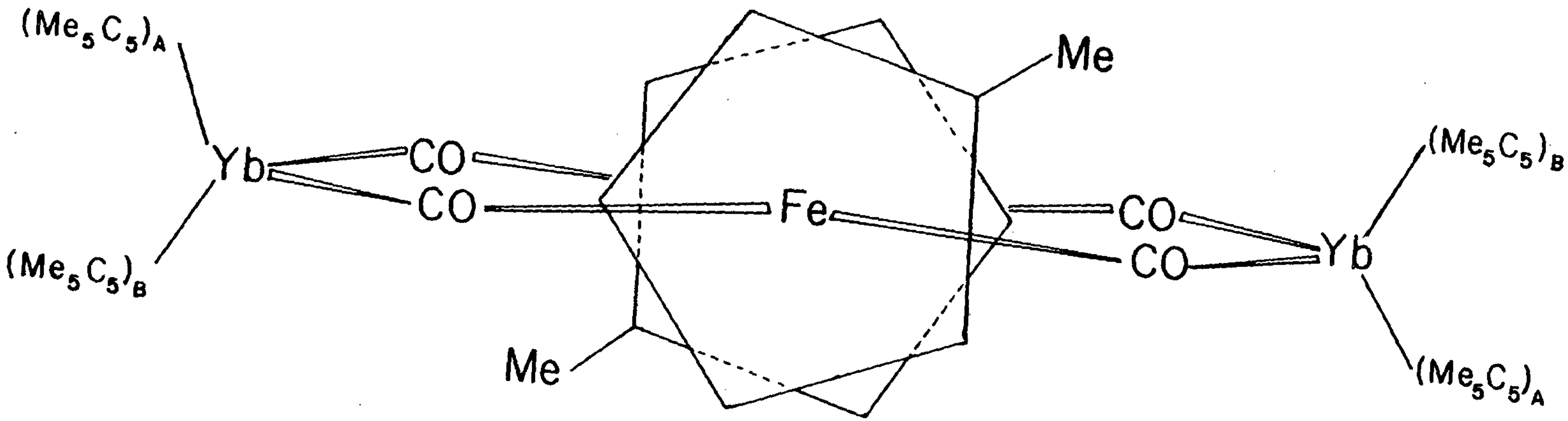
Structural Studies. An ORTEP diagram of $[(Me_5C_5)_2Yb(MeC_5H_4)Fe(CO)_2]_2$ is shown in Figure 1. As can be seen, the MeC_5H_4 and the Me_5C_5 ligands are undergoing substantial thermal motion, which contributes to the large spread in the carbon-carbon bond lengths and angles. A table of the rms thermal amplitudes is given in the Supplementary Material. The $Yb_2Fe_2C_4O_4$ core, however, does not seem to undergoing substantial thermal motion. Table II lists some bond lengths and bond angles, Table III lists the positional parameters and crystal data are given in Table IV.

The complex is a dimer, similar to that found in the dimeric portion of the electronically equivalent $[(Me_5C_5)_2Yb(\mu\text{-}OC)_2Mn(CO)_3]_2$.[1] Each of the carbonyl groups in the $(MeC_5H_4)Fe(CO)_2$ units are connected to the ytterbium atoms by way of an essentially linear Fe-C-O interation. The averaged Fe-C-O and Yb-O-C angles are 176.4 ± 0.1° and 170.3 ± 0.3°, respectively. The Yb_2Fe_2 unit is planar since the molecule has a crystallographic inversion center. The dihedral angles formed by the intersection of the Yb_2Fe_2 and YbO(1')O(2) planes is 6.1°, and between the YbO(1')O(2) planes is 5.5°. The plane defined by the FeC_2 atoms passes only 0.08Å from the inversion center at ½,0,0 but the YbO_2 plane is 0.37Å from the inversion center. Therefore, the bending direction for both planes is approximately parallel to the Fe-Fe vector. The angles formed by the MeC_5H_4 plane with the FeC_2 and Yb_2Fe_2 planes are 89.6° and 88.0°, respectively. The MeC_5H_4-rings are orientated so that C(7)C(8) are gauche relative to Fe-C(2), the C(2)FeCp(1)C(7) torsional angle being 34.3°. The Cp(1) and C(4) are eclipsed relative to Fe-C(1), the torsional angle being -0.5°, see the Newman projection down the iron-iron vector. The Me_5C_5-rings are essentially staggered with respect to each other.

(see illustration, next page)

The coordination geometry about the ytterbium atom is pseudo-tetrahedral, defining the midpoint of the Me_5C_5-group as occupying one coordination site. The centroid-Yb-centroid and O-Yb-O angles are 140° and 87.92(15)°, respectively. The averaged Yb-O bond length of 2.229 ± 0.001Å is similar to that found in the ytterbium-manganese complex of 2.277 ± 0.002Å.[1] The averaged Yb-C distance of 2.577 ± 0.016Å and the averaged Yb-centroid distance is 2.293Å, again similar to that found in the ytterbium-manganese complex.[1]

In the discussion that follows we will compare the metrical parameters of $[(Me_5C_5)Yb(\mu\text{-}OC)_2Fe(MeC_5H_4)]_2$ with the related anion $[Et_4N][CpFe(CO)_2AlPh_3]$, which contains a direct Fe-Al bond[6a], and with the electronically equivalent $[(Me_5C_5)_2Yb(\mu\text{-}OC)_2Mn(CO)_3]_2$.[1] The averaged Fe-C($MeC_5H_4$) bond length in the Yb-Fe compex of 2.097 ± 0.013Å is identical within experimental error to that

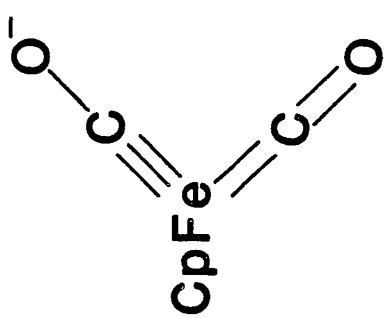

(Me5C5)A
Yb
CO
CO
Fe
Me
Me
CO
CO
Yb
(Me5C5)B
(Me5C5)B
(Me5C5)A

found in the Fe-Al compound of 2.097 ± 0.003Å. These bond lengths are also identical to those found in trans- and cis-$Cp_2Fe_2(\mu\text{-}CO)_2(CO)_2$. The averaged Fe-C(CO) distance in the Yb-Fe compound of 1.671 ± 0.002Å is shorter than that found in the Fe-Al compound (1.731 ± 0.001Å) and the C-O bond length is longer, 1.200 ± 0.001Å *vs.* 1.158 ± 0.001Å, than that found in the Fe-Al compound. Thus, the carbon monoxide ligands in the Yb-Fe compound carry significantly more negative charge, relative to the Fe-Al compound, as suggested by the carbon monoxide stretching frequencies (Table I). The bond length data suggest that the electronic structure of the Yb-Fe complex may be represented by the two resonance forms I and II and the Al-Fe complex by III.

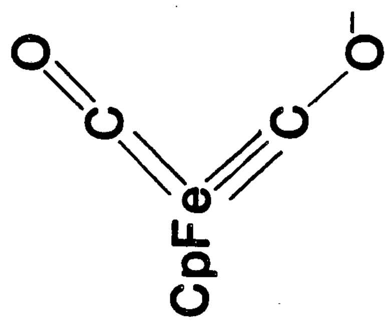
(see illustration, next page)

The averaged bridging Fe-C(CO) bond length of 1.671 ± 0.002Å in the Yb-Fe complex is shorter (1.748± 0.002Å) than that found for the Mn-C(CO) bond distance in the Yb-Mn complex. This is expected since the radius of iron is *ca.* 0.06Å smaller than that of manganese. Thus, the Yb-Fe and Yb-Mn dimers are very similar in a geometrical and electronic sense.

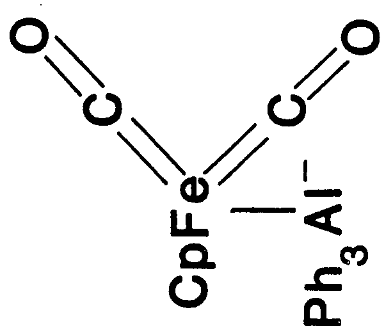
Additional studies. The Yb-Fe dimers react with methyl iodide to give $(RC_5H_4)_2Fe_2(CO)_4$ as the only metal carbonyl containing species, as shown by infrared spectroscopy. The Yb-Fe dimers also dissolve in tetrahydrofuran but the infrared spectra of the solutions show that $(RC_5H_4)_2Fe_2(CO)_4$ is the only carbonyl containing species present in solution. This is due presumably to decomposition in the infrared cells by air or moisture since when the Yb-Fe dimers are dissolved in thf in a Schlenk tube and the thf is evaporated, the infrared spectra of the solids show that the Yb-Fe dimers are intact. The latter experiment is rather informative since it suggests that thf is not as good a base towards $(Me_5C_5)_2Yb$ as is the lone pair of electrons on the carbonyl group of the $(RC_5H_4)Fe(CO)_2^-$ unit. Unfortunately, the extreme



I



II



III

moisture and air sensitivity of solutions of the Yb-Fe complexes prevent us from studying the solution equilibria in a more quantitative manner. In a qualitative manner, pyridine cleaves the dimeric unit of $(Me_3SiC_5H_4)_2Fe_2(\mu\text{-}CO)_4Yb_2(C_5Me_5)_4$ to give $(Me_3SiC_5H_4)Fe(CO)(\mu\text{-}CO)Yb(C_5Me_5)_2(py)$. The two infrared stretching frequencies, Table I, in the CO region suggest that the complex has Cs symmetry. Curiously the CO stretching frequencies of the pyridine complex at 1870 and 1678 cm^{-1} are shifted to higher and lower frequency relative to the parent dimer at 1795 and 1732 cm^{-1}. This was observed earlier in, for example, $Co(CO)_3(\mu\text{-}CO)Yb(C_5M_5)_2(thf)$.[1] The ^{1}HNMR spectra of all of the Yb-Fe and Yb-Ru dimers are listed in the experimental section and they will be discussed in detail in the following paper in this issue, since they are deceptively simple.

Experimental Section. All operations were carried out under nitrogen. Microanalyses were performed by the Microanalytical Laboratory of this department. Infrared spectra were recorded on a Perkin-Elmer 597 instrument; solid spectra were measured as Nujol mulls and solution spectra were measured on matched NaCl cells, with spacings of 0.5 mm. The magnetic susceptibility measurements were made on a SHE Corporation Model 905 Squid magnetometer, as previously described.[1]

$[FeCp(CO)_2Yb(C_5Me_5)_2]_2$. Bis(pentamethylcyclopentadienyl) ytterbium-diethyl ether (0.57 g, 0.0011 mol) in toluene (30 mL) was added to cyclopentadienyliron dicarbonyl dimer (0.20 g, 0.00056 mol) in toluene (30 mL). The mixture turned dark red and black microcrystals formed. The mixture was stirred for 12 hours and then was allowed to settle. The solution was filtered and the filtrate was saved. The residue was extracted with toluene (3 x 60 mL) and the combined extracts were filtered and the filtrate was concentrated to *ca.* 30 mL and cooled to -10°C. The combined yield of black microcrystals was 0.55 g (80%), mp 350°C (dec). Anal. Calcd for $C_{54}H_{70}Fe_2O_4Yb_2$: C, 52.3; H, 5.68. Found: C, 51.6; H, 5.70. IR (Nujol Mull): 3100 w, 2730 w, 2005 w, 1965 m, 1960 m, 1800 br, vs, 1732 br, vs, 1665 s sh, 1165 w, 1110 w, 1060 w, 1015 m, 892 w, 840 m, 810 m, 800 m, 725 w, 695 w, 655 w, 605 m sh, 583 s, 512 s, 395 sh, 378 m, 355 w, 320 s, 279 sh cm^{-1}. 1HNMR (C_6D_6, 26°C) w35.2 ($\eta_{1/2}$=13 Hz, 10 H) and 8.09 ($\eta_{1/2}$=36 Hz, 60 H).

$[Fe(C_5H_4Me)(CO)_2Yb(C_5Me_5)_2]_2$. Bis(pentamethylcyclopentadienyl) ytterbium-diethyl ether (1.3 g, 0.0024 mol) in toluene (50 mL) was added to methylcyclopentadienylirondicarbonyl dimer[8] (0.46 g, 0.0012 mol) in toluene (40 mL). The solution was stirred for 12 h, filtered and the filtrate was concentrated to ca. 40 mL and cooled (-10°C). The small black prisms were collected and dried under reduced pressure. A second crop of crystals was isolated and the combined yield was 1.2 g (78%), mp 340°C (dec.). Anal. Calcd for $C_{56}H_{74}Fe_2O_4Yb_2$: C, 53.0; H, 5.88. Found: C, 52.7; H, 5.76. IR (Nujol): 3095 w, 2730 w, 2015 w, 1972 m, 1958 sh, 1785 vs, br, 1725 vs, br, 1665 s, 1165 w, 1062 w, 1020 s br, 930 w, 885 w, 855 w, 823 w, 801 m, 725 m, 695 w, 660 m, 630 w, 585 s, 514 s, 390 m, 360 m, 325 s, and 285 sh cm^{-1}. ^{1}HNMR (C_6D_6,+25°C): w44.2 ($\eta_{1/2}$=11 Hz, 4H), 40.3 ($\eta_{1/2}$=8.6 Hz, 4 H), 38.5 ($\eta_{1/2}$=7.8 Hz, 6 H), 7.91 ($\eta_{1/2}$=45 Hz, 60 H).

$[Fe(C_5H_4SiMe_3)(CO)_2Yb(C_5Me_5)_2]_2$. Bis(pentamethylcyclopentadienyl) ytterbium-diethyl ether (0.50 g, 0.00097 mol) in toluene (20 mL) was added to trimethylsilylcyclopentadienylirondicarbonyl dimer[9] (0.24 g, 0.00048 mol) in toluene (20 mL). The mixture was stirred for 20 h, filtered, and the filtrate was concentrated to ca. 15 mL. Cooling (-10°C) yielded black prisms which were collected and dried under reduced pressure. The mother liquors afforded more black prisms on cooling. The combined yield was 0.57 g, 86%, mp 240-245 °C (dec.). Anal. Calcd for $C_{60}H_{86}O_4Fe_2Si_2Yb_2$: C, 52.0; H, 6.26. Found: C, 51.4; H, 6.13. IR (Nujol): 3170 w, 3100 w, 2720 w, 1795 s, br, 1365 m, 1243 m, 1158 m, 1059 w, 1040 m, 1017 w, 902 m, 865 m, 832 s, 798 m, 750 m, 690 m, 630 m, 620 w, 585 m, 575 sh, 508 m, 430 w, 380 m, 340 w, 315 s, 280 s cm^{-1}. ^{1}HNMR (C_6D_6, 29°C): δ50.2 ($\nu_{1/2}$=13 Hz, 4 H), 32.3 ($\nu_{1/2}$=12 Hz, 4 H), 19.5 ($\nu_{1/2}$=10 Hz, 18 H), 8.01 ($\nu_{1/2}$=37 Hz, 60 H). The complex reacts with two molar equivalents of pyridine in toluene. The pyridine complex, $Fe(C_5H_4SiMe_3)(CO)_2Yb(C_5Me_5)_2(py)$, was isolated from diethyl ether (-10°C) as red-black prisms in essentially quantitative yield. Anal. Calcd for $C_{35}H_{48}FeNO_2SiYb$: C, 54.5; H, 6.27; N, 1.81. Found: C, 52.1; H, 6.23; N, 1.61. ^{1}HNMR (C_7D_8, 26°C): δ10.2 (2 H), 9.92 (2 H), 6.30 (9 H), 4.46 (30 H).

$[Ru(C_5H_4SiMe_3)(CO)_2Yb(C_5Me_5)_2]_2$. Bis(pentamethylcyclopentadienyl)ytterbium-diethyl ether (0.72 g, 0.0014 mol) in toluene (40 mL) was added to the trimethylsilylcyclopentadienylrutheniumdicarbonyl dimer (0.41 g, 0.00070 mol) in toluene (30 mL). The red solution was stirred for 24 hours, filtered, and the filtrate was concentrated to ca. 25 mL and cooled (-10°C). The purple prisms were collected and dried under reduced pressure. Two additional crops of crystals were obtained from the mother liquor. The combined yield was 85%, mp 250-255 °C (dec). Anal. Calcd for $C_{60}H_{86}O_4Ru_2Si_2Yb_2$: C, 48.8; H, 5.87. Found: C, 48.3; H, 5.67. The infrared spectrum was essentially identical to that of its iron congener. ^{1}HNMR (C_6D_6, +27°C): δ43.8 ($\nu_{1/2}$=9.4 Hz, 4 H), 31.9 ($\nu_{1/2}$=10 Hz, 4 H), 19.6 ($\nu_{1/2}$=7.4 Hz, 18 Hz), 8.27 ($\nu_{1/2}$=41 Hz, 60 H).

$[Ru(C_5H_4SiMe_3)(CO)_2]_2$. Trimethylsilylcyclopentadiene (0.41 g, 0.0029 mol) was added to $Ru_3(CO)_{12}$ (0.52 g, 0.0024 mol) in octane (50 mL). The $Ru_3(CO)_{12}$ slowly dissolved as the mixture was refluxed and the orange-red solution turned pale yellow, ca. 45 min. The solution was cooled to room temperature , the reflux condenser was removed and the solution was stirred in air for ca. 5 min. The orange-red solution was evaporated and the brown oil was extracted with pentane (25 mL). The pentane solution was filtered and the filtrate was concentrated to ca. 5 mL and cooled (-25°C). The orange needles (60% yield) were collected, and dried under reduced pressure, mp 106-107 °C. A second crop of crystals may be obtained from the mother liquor. Anal. Calcd for $C_{20}H_{26}O_4Si_2Ru_2$: C, 40.6; H, 4.42. Found: C, 40.7; H, 4.54. NMR (C_6D_6): ^{1}H (200 MHz): The protons of the AA'BB' spin system appear as apparent triplets at δ5.01 and 4.85 with a separation between the outermost lines of 4 Hz, and the Me_3Si protons appear at δ0.311. ^{13}C: The ring carbons appear at δ95.6, 95.4, and 93.9; and, the Me_3Si carbons appear at -0.17. Ir (Nujol): 1952 s, 1935 sh, 1924 m, 1766 s, 1735 sh, 1407 w, 1356 w, 1301 w, 1245 m, 1190 w, 1156 m, 1053 w, 1037 m, 1025 sh, 928 w, 890 m, 834 s, 811 m, 753 m, 718 w, 640 m, 626 m, 610 m, 595 w, 576 w, 532 m, 519 s, 478 w, 415 w, 372 w, 275 w, 240 w cm^{-1}, ν(CO, hexane): 2005 m, 1972 s, 1963 s, 1941 s, and 1788 s cm^{-1}.[10]

X-Ray Crystallography. Crystals of $[Fe(C_5H_4Me)(CO)_2Yb(C_5Me_5)_2]_2$ suitable for X-ray crystallography were grown by cooling slowly a saturated solution of the dimer in methylcyclohexane from 60°C to room temperature over a 24 hour period. Single crystals were inserted into quartz capillaries which were then flame sealed. Preliminary precession photographs indicated monoclinic (2/n) Laue symmetry and yielded preliminary cell dimensions. The crystal used for data collection was transferred to our Enraf-Nonius CAD (for details of the CHEXRAY facility see ref. 1). Automatic peak search and indexing yielded the same unit cell as found from the photographs and confirmed the Laue symmetry. Inspection of the h0l and 0k0 zones showed systematic absences 0k0, $k \neq 2n + 1$ and h0l, $h+\ell \neq 2n + 1$ only consistent with space group $P2_1/n$. Determination of accurate cell dimensions and the orientation matrix proceeded normally, see Table IV for details of data collection.

The 3862 raw intensity data were converted to structure factor amplitudes and their esds by correction for scan speed, background and Lorentz and polarization effects. Analysis of the azimuthal scan data showed significant variation, $(I\ min)(I\ max)^{-1} = 0.86$ for the average relative intensity curve. An absorption correction based on the measured shape and size of the crystal and a 6 x 12 x 18 Gaussian grid of internal points was performed after solution of the structure. The maximum and minimum transmission factors were 0.509 and 0.430, respectively. Rejection of systematically absent and redundant data yielded a unique set of 3531 data which were used to solve and refine the structure. The structure was solved by analysis of the Patterson map followed by standard Fourier and least-squares techniques. The hydrogen atoms were not included in calculation of the structure factors.

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 DE-AC03-76SF00098. We thank Dr. F.J. Hollander, staff crystallographer of the U.C. X-ray facility (CHEXRAY), for doing the crystal structure, and the NSF for departmental grants to purchase the X-ray and magnetic susceptibility machines.

Supplementary Material. Carbon-carbon bond lengths and angles, temperature factors and structure factors (18 pages). Ordering information is given on any current masthead page.

References

(1) Boncella, J.M.; Andersen, R.A. Inorg. Chem. 1984, 23, 432.

(2) Darensbourg, M.Y.; Darensbourg, D.J.; Burns, D.; Drew, D.A. J. Am. Chem. Soc. **1976**, 98, 3127.

(3) Berry, D.H.; Bercaw, J.E.; Jircitano, A.J.; Mertes, K.B. Ibid., **1982**, 104, 4712.

(4) (a) Harris, D.C.; Gray, H.B. Inorg. Chem. **1975**, 14, 1215.

(b) For an alternative view of the bonding in $Cp_2Fe_2(\mu\text{-}CO)_2(CO)_2$ that does not invoke a direct metal-metal bond, see Mitschler, A.; Rees, B.; Lehmann, M.S. J. Am. Chem. Soc. **1978**, 100, 3390; Benard, M. Inorg. Chem. **1979**, 18, 2782.

(5) (a) Ellis, J.E.; Flom, E.A. J. Organomet. Chem. **1975**, 99, 263.

(b) Wong, A.; Harris, M.; Atwood, J.D. J. Am. Chem. Soc. **1980**, 102, 4529.

(c) Pannell, K.H.; Jackson, D. Ibid., **1976**, 98, 4443.

(d) Ulmer, S.W.; Skarstad, P.M.: Burlitch, J.M.; Hughes, R.E. Ibid. **1973**, 95, 4469.

(e) McVicker, G.B. Inorg. Chem. **1975**, 14, 2087.

(6) (a) Burlitch, J.M.; Leonowicz, M.E.; Petersen, R.B.; Hughes, R.E., Ibid. **1979**, 18, 1097.

(b) Bryan, R.F.; Greene, P.T. J. Chem. Soc. (A), **1970**, 3064.

(c) Bryan, R.F.; Greene, P.T.; Newlands, M.J.; Field, D.S. Ibid., **1970**, 3068.

(7) Shannon, R.D. Acta Cryst. **1976**, 32A, 751.

(8) (a) Reynolds, L.J.; Wilkinson, G., J. Inorg. Nucl. Chem. **1959**, 9, 86.

(b) Parker, D.J.; Stiddard J. Chem. Soc. (A), **1970**, 1040.

(9) (a) Kraihanzel, C.S.; Conville, J. J. Organometal. Chem. **1970**, 23, 357.

(b) Abel, E.W.; Moorhouse, S. Ibid., **1971**, 28, 211.

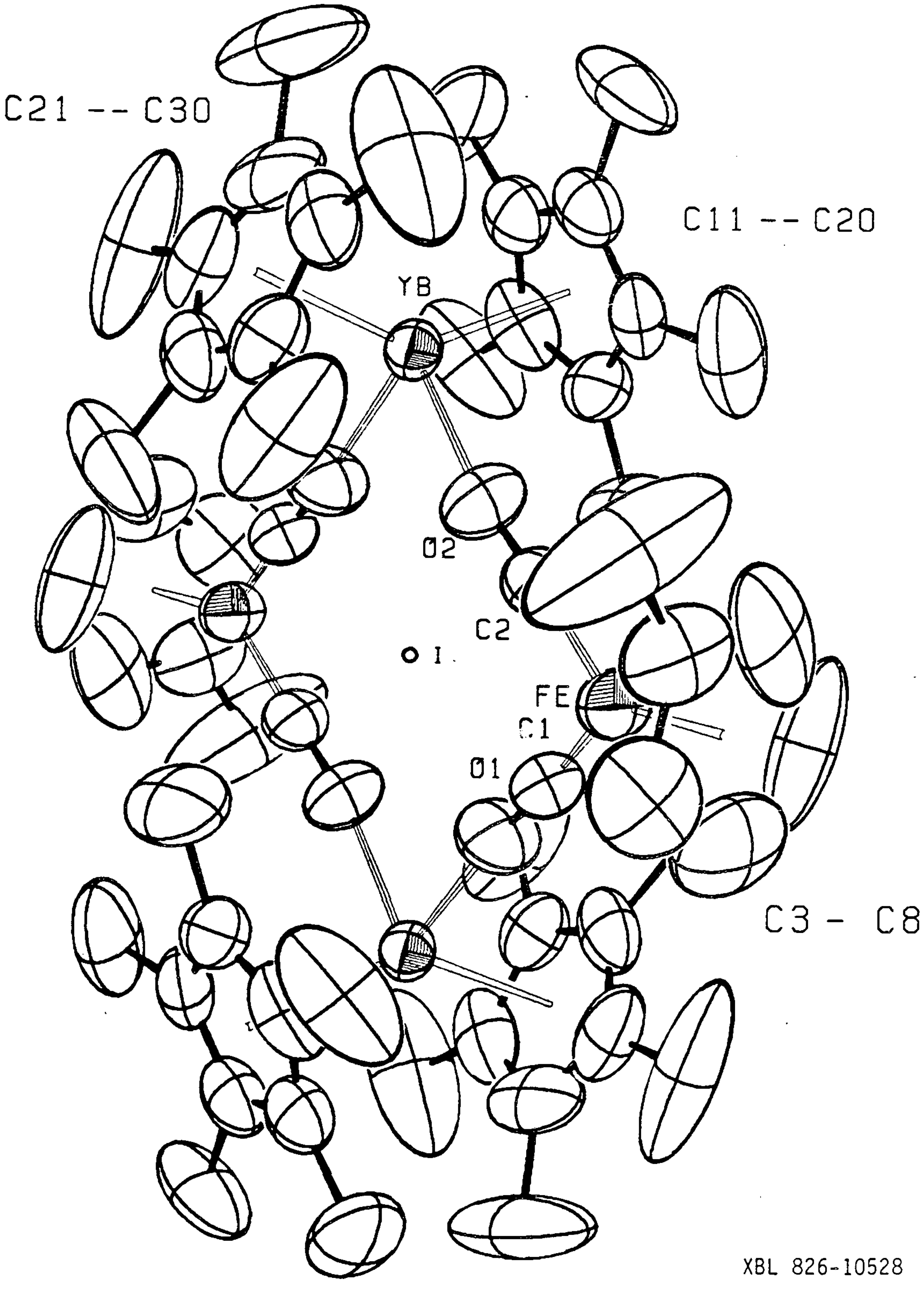
(10) The solution infrared spectrum is consistent with the presence of two isomers of C_{2h}(2 bands) and C_{2v} (3 bands) symmetry, as found for $Cp_2Ru_2(CO)_4$.

(a) Humphries, A.P.; Knox, S.A.R. J. Chem. Soc. Dalton Trans. **1975**, 1710.

(b) Cotton, F.A.; Yagupsky, G. Inorg. Chem. **1967**, 6, 15.

Figure Captions

Figure I. An ORTEP view of $[Yb(C_5Me_5)_2(\mu\text{-}OC)_2Fe(C_5H_4SiMe_3)]_2$



XBL 826-10528

Table I

Infrared Spectral Data

Compound	Medium	νCO, cm^{-1}	Reference
$[(Me_5C_5)_2Yb(C_5H_5)Fe(CO)_2]_2$	Nujol	1800s,1740s	This work
$[(Me_5C_5)_2Yb(MeC_5H_4)Fe(CO)_2]_2$	cyclohexane	1787s,1723s	This work
$[(Me_5C_5)_2Yb(Me_3SiC_5H_4)Fe(CO)_2]_2$	cyclohexane	1795s,1732s	This work
$[(Me_5C_5)_2Yb(Me_5C_5)Fe(CO)_2]_2$	Nujol	1760s,1695s	This work
$(Me_5C_5)_2YbPy(Me_3SiC_5H_4)Fe(CO)_2$	Nujol	1870s,1678s	This work
$[(Me_5C_5)_2Yb(Me_3SiC_5H_4)Ru(CO)_2]_2$	Nujol	1815s,1730s	This work
$(n\text{-}Bu_4N)CpFe(CO)_2$	thf	1865s,1788s	5a
$(Et_4N)CpFe(CO)(AlPh_3)$	Nujol	2012w,1960w,1940s, 1920wsh,1871s, 1843w	6a
$LiCpFe(CO)_2$	thf	1884s,1869s,1812s, 1788w,1750s	5b
$NaCpFe(CO)_2$	thf	1877s,1862m,1806s, 1786m,1770m	5c
$KCpFe(CO)_2$ thf	1868s,1792s,1772s		5b
$Mg[CpFe(CO)_2]_2$	thf	2010w,1948w,1916s, 1883s,1852s,1712s	5b,d,e

Table II

Some Selected Bond Lengths and Angles

INTRA-MOLECULAR DISTANCES

ATOM 1	ATOM 2	DISTANCE
YB	O1	2.228(4)
YB	O2	2.23Ø(4)
YB	C11	2.565(5)
YB	C12	2.598(5)
YB	C13	2.6Ø9(5)
YB	C14	2.572(5)
YB	C15	2.545(5)
YB	CP2 *	2.29Ø
YB	C21	2.577(6)
YB	C22	2.59Ø(6)
YB	C23	2.59Ø(5)
YB	C24	2.559(6)
YB	C25	2.567(6)
YB	CP3 *	2.296
FE	C1	1.669(6)
FE	C2	1.673(5)
FE	C3	2.1Ø6(7)
FE	C4	2.Ø86(8)
FE	C5	2.Ø89(8)
FE	C6	2.Ø83(8)
FE	C7	2.12Ø(6)
FE	CP1 *	1.733
C1	O1	1.2Ø1(6)
C2	O2	1.199(6)

INTRA-MOLECULAR ANGLES

ATOM 1	ATOM 2	ATOM 3	ANGLE
O1'	YB	O2	87.92(15)
O1'	YB	CP2 *	1Ø5.Ø
O1'	YB	CP3 *	1Ø3.Ø
O2	YB	CP2	1Ø4.9
O2	YB	CP3	1Ø4.2
CP2	YB	CP3	14Ø.Ø
C1	FE	C2	87.8Ø(23)
C1	FE	CP1 *	135.5
C2	FE	CP1	136.7
YB'	O1	C1	169.7(4)
YB	O2	C2	17Ø.8(4)
FE	C1	O1	176.6(5)
FE	C2	O2	176.2(4)

* CP1, CP2, and CP3 are the centroids of the rings C3-C7, C11-C15, and C21-C25 respectively.

' Primed atoms are related to atoms in the asymmetric unit by the inversion center at 1/2, Ø, Ø.

Table III

Positional Parameters

Atom	x	y	z
YB	0.43734(3)	0.14724(1)	-0.00014(2)
FE	0.3076(1)	-0.01754(4)	0.27073(9)
O1	0.4649(5)	-0.0848(2)	0.1181(5)
O2	0.3657(5)	0.0737(2)	0.1066(5)
C1	0.3990(7)	-0.0580(3)	0.1845(6)
C2	0.3385(7)	0.0368(3)	0.1769(6)
C3	0.1484(9)	-0.0569(5)	0.3439(9)
C4	0.2563(11)	-0.0764(5)	0.4036(10)
C5	0.3142(12)	-0.0301(7)	0.4610(8)
C6	0.2483(11)	0.0179(6)	0.4345(8)
C7	0.1449(8)	0.0061(4)	0.3663(8)
C8	0.0536(13)	0.0481(6)	0.3347(13)
C11	0.5382(8)	0.1715(4)	0.2114(6)
C12	0.5272(7)	0.2234(3)	0.1524(7)
C13	0.6084(7)	0.2241(3)	0.0527(7)
C14	0.6695(7)	0.1720(4)	0.0512(8)
C15	0.6255(7)	0.1399(3)	0.1510(7)
C16	0.4711(12)	0.1526(5)	0.3287(9)
C17	0.4596(9)	0.2754(4)	0.2030(9)
C18	0.6400(11)	0.2760(4)	-0.0269(10)
C19	0.7727(9)	0.1583(5)	-0.0345(11)
C20	0.6705(10)	0.0790(4)	0.1852(11)
C21	0.2213(8)	0.1960(4)	-0.0344(8)
C22	0.2042(8)	0.1398(4)	-0.0775(8)
C23	0.2730(8)	0.1339(4)	-0.1797(7)
C24	0.3345(9)	0.1830(4)	-0.2021(8)
C25	0.3030(8)	0.2215(4)	-0.1181(10)
C26	0.1559(11)	0.2218(7)	0.0682(12)
C27	0.1143(10)	0.0964(6)	-0.0248(11)
C28	0.2738(11)	0.0824(5)	-0.2592(10)
C29	0.4195(12)	0.1941(8)	-0.3088(10)
C30	0.3290(14)	0.2851(5)	-0.1192(16)

Table IV

Crystal Data (25°C) for $[Yb(C_5Me_5)_2(\mu\text{-}OC)_2Fe(C_5H_4SiMe_3)]_2$

Space Group	$P2_1/n$
a(Å)	10.6069(15)
b(Å)	23.4930(31)
c(Å)	10.8730(20)
β(deg)	92.041(13)
$V(Å^3)$	2707.7(13)
Z	2
Formula Wt. (amu)	1268.98
d(calc) gcm^{-3}	1.556
μ(calc) cm^{-1}	39.8
Size (mm)	0.22 x 0.27 x 0.47
Reflections, collected	3862
Reflectons, unique	3561
Reflections, $F^2>3\sigma(F^2)$	2941
R(%)	2.81
R_w(%)	4.48
Variables	289
GOF	2.190
Monochromator	highly orientated graphite
Radiation	M_oK_α, λ=0.71073 Å
Scan Range, type	3°< θ < 45°, θ-2θ
Scan Speed	0.69-6.7 (deg min^{-1})
Scan Width	$\Delta\theta = 0.55 + 0.347\tan\theta$

Supplementary Material for

Bis(Pentamethylcyclopentadienyl)Ytterbium (II) as an
Lewis Acid and an Electron-Transfer Ligand;
Preparation and Crystal Structure of
$[Yb(C_5Me_5)_2(\mu\text{-}OC)_2Fe(C_5H_4SiMe_3)]_2$

James M. Boncella and Richard A. Andersen

Table I, Carbon-carbon bond lengths and bond angles.
Table II, General Temperature Factor Expressions and rms Amplitudes
Table III, Structure Factors

INTRA-MOLECULAR ANGLES IN THE
CYCLOPENTADIENIDE LIGANDS

ATOM 1	ATOM 2	ATOM 3	ANGLE
C7	C3	C4	106.1(9)
C3	C4	C5	107.5(11)
C4	C5	C6	109.9(12)
C5	C6	C7	110.7(13)
C6	C7	C3	105.7(9)
C3	C7	C8	131.9(13)
C6	C7	C8	122.2(14)
C15	C11	C12	107.6(5)
C11	C12	C13	108.9(5)
C12	C13	C14	107.3(5)
C13	C14	C15	107.2(5)
C14	C15	C11	109.0(5)
C16	C11	C12	127.0(7)
C16	C11	C15	125.3(7)
C17	C12	C11	124.9(6)
C17	C12	C13	125.1(7)
C18	C13	C12	126.3(7)
C18	C13	C14	125.6(7)
C19	C14	C13	123.3(8)
C19	C14	C15	129.1(8)
C20	C15	C11	126.3(7)
C20	C15	C14	124.7(7)
C25	C21	C22	105.0(6)
C21	C22	C23	107.4(6)
C22	C23	C24	109.7(6)
C23	C24	C25	108.7(7)
C24	C25	C21	109.1(7)
C26	C21	C22	125.5(11)
C26	C21	C25	129.3(11)
C27	C22	C21	125.2(8)
C27	C22	C23	127.1(8)
C28	C23	C22	124.9(8)
C28	C23	C24	125.3(8)
C29	C24	C23	126.0(11)
C29	C24	C25	125.2(11)
C30	C25	C21	122.6(12)
C30	C25	C24	127.6(12)

ATOM 1	ATOM 2	DISTANCE
C3	C7	1.501(11)
C3	C4	1.374(13)
C4	C5	1.387(17)
C5	C6	1.353(17)
C6	C7	1.332(13)
C7	C8	1.415(11)
C11	C12	1.381(8)
C12	C13	1.409(8)
C13	C14	1.385(8)
C14	C15	1.414(9)
C15	C11	1.373(8)
C11	C16	1.547(9)
C12	C17	1.530(8)
C13	C18	1.540(9)
C14	C19	1.498(9)
C15	C20	1.549(8)
C21	C22	1.412(10)
C22	C23	1.358(9)
C23	C24	1.352(10)
C24	C25	1.336(11)
C25	C21	1.412(11)
C21	C26	1.466(10)
C22	C27	1.521(9)
C23	C28	1.488(9)
C24	C29	1.517(11)
C25	C30	1.519(10)

Table of General Temperature Factor Expressions - B's

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
YB	3.90(1)	3.73(1)	3.15(1)	0.47(1)	0.08(1)	0.03(1)	3.594(6)
FE	5.88(5)	4.36(4)	3.85(4)	0.27(4)	1.55(4)	0.18(4)	4.66(2)
O1	7.0(3)	5.5(3)	6.3(3)	1.4(2)	1.6(2)	-1.0(2)	6.2(1)
O2	6.7(3)	5.5(3)	6.1(2)	-0.0(2)	0.9(2)	1.7(2)	6.1(1)
C1	6.1(4)	4.2(3)	4.9(3)	-0.3(3)	0.0(3)	0.7(3)	5.0(2)
C2	5.1(3)	4.4(3)	4.4(3)	0.7(3)	0.9(3)	-0.2(3)	4.6(2)
C3	8.8(5)	12.0(7)	8.2(4)	-3.0(5)	5.3(3)	0.3(5)	9.5(3)
C4	12.0(7)	9.7(6)	9.0(5)	-0.3(6)	4.3(5)	3.1(5)	10.1(3)
C5	11.3(7)	28(1)	4.1(4)	0.5(8)	2.0(4)	6.1(6)	14.4(5)
C6	13.6(7)	16.8(9)	4.3(4)	-4.0(7)	4.7(4)	-2.7(5)	11.4(3)
C7	8.7(4)	8.7(5)	7.4(4)	1.8(4)	5.5(3)	1.7(4)	8.1(2)
C8	21.3(8)	22(1)	23.1(8)	15.0(7)	17.1(6)	14.9(7)	21.7(4)
C11	6.2(4)	7.1(4)	3.4(3)	-1.1(4)	-0.4(3)	-0.7(3)	5.6(2)
C12	4.9(4)	6.2(4)	5.6(3)	0.2(3)	-1.2(3)	-1.6(3)	5.6(2)
C13	5.7(4)	6.1(4)	5.4(4)	-1.3(3)	-1.1(3)	-0.4(3)	5.7(2)
C14	3.4(3)	8.9(5)	6.4(4)	-0.4(3)	0.6(3)	-2.7(4)	6.2(2)

Table of Root-Mean-Square Amplitudes of Thermal Vibration in Angstroms.

Atom	Min.	Int'med.	Max.	Atom	Min.	Int'med.	Max.
YB	0.200	0.206	0.233	C15	0.216	0.258	0.308
FE	0.198	0.234	0.288	C16	0.229	0.328	0.495
O1	0.214	0.296	0.322	C17	0.204	0.298	0.479
O2	0.223	0.287	0.314	C18	0.225	0.317	0.499
C1	0.216	0.257	0.281	C19	0.225	0.307	0.551
C2	0.210	0.242	0.269	C20	0.231	0.328	0.475
C3	0.185	0.374	0.434	C21	0.195	0.251	0.441
C4	0.243	0.369	0.436	C22	0.218	0.280	0.321
C5	0.172	0.382	0.610	C23	0.206	0.270	0.352
C6	0.171	0.379	0.512	C24	0.216	0.294	0.400
C7	0.182	0.310	0.424	C25	0.185	0.275	0.485
C8	0.257	0.315	0.813	C26	0.227	0.343	0.736
C11	0.198	0.269	0.315	C27	0.250	0.299	0.595
C12	0.212	0.260	0.317	C28	0.231	0.334	0.554
C13	0.215	0.279	0.307	C29	0.232	0.328	0.727
C14	0.205	0.246	0.368	C30	0.229	0.320	0.739

Fobs & Fclc (x 10.) for [(C5Me5)2 Yb (OC)2 Fe (C5H4Me)] 2 at 25 C

H	K	L	Fobs	Fcalc
0	0	2	1664	1640
0	0	4	2302	2280
0	0	6	1593	1536
0	0	8	1149	1162
0	0	10	798	780
0	1	1	1915	1937
0	1	2	118	102
0	1	3	1530	1435
0	1	4	232	218
0	1	5	812	870
0	1	6	60*	79
0	1	7	1178	1176
0	1	8	63*	68
0	1	9	414	424
0	1	10	36*	42
0	1	11	649	650
0	2	0	270	103
0	2	1	403	428
0	2	2	1897	1808
0	2	3	146	133
0	2	4	355	364
0	2	5	283	278
0	2	6	859	859
0	2	7	0*	41
0	2	8	131	94
0	2	9	0*	11
0	2	10	266	283
0	2	11	35*	31
0	3	1	3777	3938
0	3	2	117	110
0	3	3	2162	2036
0	3	4	0*	26
0	3	5	2042	2034
0	3	6	0*	6
0	3	7	906	894
0	3	8	137	103
0	3	9	1188	1161
0	3	10	87*	93
0	3	11	378	384
0	4	0	1067	1110
0	4	1	604	580
0	4	2	2588	2545
0	4	3	43*	96
0	4	4	1037	1104
0	4	5	264	281
0	4	6	1704	1715
0	4	7	77*	94

H	K	L	Fobs	Fcalc
0	4	8	890	902
0	4	9	90*	127
0	4	10	833	817
0	4	11	0*	39
0	5	1	825	655
0	5	2	498	474
0	5	3	238	266
0	5	4	185	167
0	5	5	380	395
0	5	6	301	292
0	5	7	0*	29
0	5	8	124	94
0	5	9	343	339
0	5	10	0*	59
0	5	11	88*	54
0	6	0	1908	2034
0	6	1	474	428
0	6	2	1193	1102
0	6	3	797	761
0	6	4	2164	2199
0	6	5	191	197
0	6	6	1050	1034
0	6	7	77*	116
0	6	8	790	801
0	6	9	0*	93
0	6	10	538	531
0	6	11	36*	14
0	7	1	1890	1838
0	7	2	182	178
0	7	3	2376	2348
0	7	4	163	165
0	7	5	1626	1611
0	7	6	193	189
0	7	7	1393	1406
0	7	8	160	136
0	7	9	767	768
0	7	10	91*	125
0	7	11	737	744
0	8	0	684	782
0	8	1	214	197
0	8	2	695	683
0	8	3	293	288
0	8	4	1137	1157
0	8	5	438	453
0	8	6	472	463
0	8	7	94	114
0	8	8	617	614

H	K	L	Fobs	Fcalc
0	8	9	90*	123
0	8	10	215	218
0	8	11	0*	19
0	9	1	1140	1131
0	9	2	0*	10
0	9	3	646	656
0	9	4	226	233
0	9	5	1090	1076
0	9	6	207	214
0	9	7	241	228
0	9	8	96	83
0	9	9	596	602
0	9	10	189	199
0	10	0	1736	1727
0	10	1	415	387
0	10	2	1859	1908
0	10	3	622	637
0	10	4	1386	1365
0	10	5	348	336
0	10	6	1410	1432
0	10	7	250	234
0	10	8	795	784
0	10	9	58*	33
0	10	10	684	673
0	11	1	1394	1367
0	11	2	51*	43
0	11	3	973	1005
0	11	4	370	362
0	11	5	1033	1034
0	11	6	313	304
0	11	7	725	732
0	11	8	158	142
0	11	9	537	538
0	11	10	89*	118
0	12	0	448	436
0	12	1	469	506
0	12	2	72*	55
0	12	3	305	310
0	12	4	226	229
0	12	5	265	252
0	12	6	108	118
0	12	7	96	135
0	12	8	212	225
0	12	9	144	155
0	12	10	86*	78
0	13	1	1503	1502
0	13	2	116	128

H	K	L	Fobs	Fcalc
0	13	3	1212	1227
0	13	4	271	272
0	13	5	804	820
0	13	6	323	328
0	13	7	832	842
0	13	8	186	195
0	13	9	607	590
0	13	10	134	139
0	14	0	1915	1921
0	14	1	266	309
0	14	2	1364	1370
0	14	3	414	396
0	14	4	886	898
0	14	5	251	261
0	14	6	894	920
0	14	7	290	286
0	14	8	735	754
0	14	9	74*	99
0	15	1	340	352
0	15	2	0*	84
0	15	3	270	271
0	15	4	289	301
0	15	5	310	294
0	15	6	234	214
0	15	7	183	179
0	15	8	155	169
0	15	9	164	174
0	16	0	1032	1029
0	16	1	371	374
0	16	2	689	715
0	16	3	258	251
0	16	4	696	701
0	16	5	299	304
0	16	6	536	517
0	16	7	105	65
0	16	8	442	441
0	16	9	0*	57
0	17	1	1164	1188
0	17	2	101	68
0	17	3	1033	1048
0	17	4	102	94
0	17	5	806	815
0	17	6	0*	56
0	17	7	819	822
0	17	8	160	139
0	18	0	730	728
0	18	1	337	297

H	K	L	Fobs	Fcalc
0	18	2	484	491
0	18	3	314	318
0	18	4	554	572
0	18	5	147	124
0	18	6	348	353
0	18	7	85*	74
0	18	8	411	415
0	19	1	186	183
0	19	2	0*	92
0	19	3	305	323
0	19	4	24*	20
0	19	5	324	303
0	19	6	127	157
0	19	7	45*	81
0	20	0	493	513
0	20	1	217	185
0	20	2	911	944
0	20	3	197	222
0	20	4	644	652
0	20	5	0*	46
0	20	6	717	712
0	20	7	0*	7
0	21	1	709	705
0	21	2	74*	18
0	21	3	573	686
0	21	4	89*	6
0	21	5	627	624
0	21	6	80*	29
0	22	0	0*	24
0	22	1	180	195
0	22	2	167	152
0	22	3	73*	124
0	22	4	0*	83
0	22	5	76*	84
0	23	1	438	455
0	23	2	0*	23
0	23	3	535	544
0	23	4	0*	27
0	24	0	728	711
0	24	1	85*	100
0	24	2	463	455
0	24	3	82*	62
0	25	1	227	218
1	0	-11	684	710
1	0	-9	772	786
1	0	-7	1850	1825
1	0	-5	1253	1250

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fclc (x 10.) for [(C5Me5)2 Yb (OC)2 Fe (C5H4Me)] 2 at 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
1	0	-3	1290	1372	1	2	5	347	356	1	4	6	316	328	1	6	7	718	728	1	8	8	299	308
1	0	-1	2707	2770	1	2	6	493	483	1	4	7	958	976	1	6	8	312	325	1	8	9	402	383
1	0	1	3670	3971	1	2	7	305	301	1	4	8	185	182	1	6	9	721	735	1	8	10	241	255
1	0	3	1045	996	1	2	8	413	420	1	4	9	888	861	1	6	10	214	198	1	8	11	273	268
1	0	5	1973	1951	1	2	9	251	252	1	4	10	185	174	1	6	11	418	410	1	9	-10	282	285
1	0	7	1142	1142	1	2	10	355	346	1	4	11	488	500	1	7	-11	89*	63	1	9	-9	386	371
1	0	9	1020	1007	1	2	11	0*	75	1	5	-11	358	368	1	7	-10	765	764	1	9	-8	385	401
1	0	11	653	648	1	3	-11	56*	44	1	5	-10	152	146	1	7	-9	201	187	1	9	-7	175	191
1	1	-11	196	192	1	3	-10	495	488	1	5	-9	275	273	1	7	-8	738	738	1	9	-6	521	507
1	1	-10	721	702	1	3	-9	179	158	1	5	-8	371	357	1	7	-7	53*	44	1	9	-5	657	653
1	1	-9	370	384	1	3	-8	1210	1203	1	5	-7	602	597	1	7	-6	1511	1493	1	9	-4	791	810
1	1	-8	476	478	1	3	-7	76*	113	1	5	-6	214	226	1	7	-5	394	357	1	9	-3	649	540
1	1	-7	478	474	1	3	-6	1478	1450	1	5	-5	704	696	1	7	-4	1761	1760	1	9	-2	561	582
1	1	-6	1378	1318	1	3	-5	241	256	1	5	-4	209	250	1	7	-3	132	95	1	9	-1	585	569
1	1	-5	462	437	1	3	-4	1442	1467	1	5	-3	1002	928	1	7	-2	2082	2090	1	9	0	1152	1135
1	1	-4	1138	1116	1	3	-3	572	516	1	5	-2	100	59	1	7	-1	42*	68	1	9	1	590	568
1	1	-3	476	487	1	3	-2	1762	1877	1	5	-1	850	873	1	7	0	2102	2020	1	9	2	1010	1011
1	1	-2	1795	1718	1	3	-1	428	404	1	5	0	147	90	1	7	1	354	328	1	9	3	186	172
1	1	-1	1531	1477	1	3	0	2514	2604	1	5	1	112	135	1	7	2	1384	1355	1	9	4	660	665
1	1	0	2392	2602	1	3	1	810	877	1	5	2	669	744	1	7	3	336	316	1	9	5	1140	1140
1	1	1	783	802	1	3	2	1800	1774	1	5	3	1038	1059	1	7	4	2295	2257	1	9	6	706	742
1	1	2	286	214	1	3	3	291	284	1	5	4	338	340	1	7	5	526	532	1	9	7	134	127
1	1	3	490	444	1	3	4	1323	1351	1	5	5	523	532	1	7	6	1193	1207	1	9	8	262	284
1	1	4	1286	1293	1	3	5	297	299	1	5	6	548	516	1	7	7	64*	121	1	9	9	443	439
1	1	5	489	501	1	3	6	1797	1796	1	5	7	584	595	1	7	8	1187	1201	1	9	10	443	440
1	1	6	386	367	1	3	7	67*	67	1	5	8	76*	19	1	7	9	224	223	1	10	-10	124	137
1	1	7	269	254	1	3	8	667	669	1	5	9	272	271	1	7	10	555	570	1	10	-9	822	813
1	1	8	877	859	1	3	9	223	225	1	5	10	328	308	1	7	11	71*	81	1	10	-8	150	137
1	1	9	379	358	1	3	10	930	924	1	5	11	353	348	1	8	-11	235	231	1	10	-7	707	724
1	1	10	307	296	1	3	11	36*	55	1	6	-11	474	500	1	8	-10	393	392	1	10	-6	347	354
1	1	11	271	271	1	4	-11	431	402	1	6	-10	89*	91	1	8	-9	156	145	1	10	-5	1556	1557
1	2	-11	61*	35	1	4	-10	167	156	1	6	-9	465	466	1	8	-8	76*	51	1	10	-4	472	457
1	2	-10	418	425	1	4	-9	995	1016	1	6	-8	336	345	1	8	-7	678	654	1	10	-3	1338	1354
1	2	-9	432	426	1	4	-8	346	331	1	6	-7	1045	1038	1	8	-6	763	763	1	10	-2	913	912
1	2	-8	339	344	1	4	-7	907	871	1	6	-6	71*	65	1	8	-5	70*	70	1	10	-1	1889	1880
1	2	-7	82	53	1	4	-6	305	283	1	6	-5	905	855	1	8	-4	237	89	1	10	0	116	87
1	2	-6	831	787	1	4	-5	1871	1878	1	6	-4	840	850	1	8	-3	1537	1545	1	10	1	1573	1625
1	2	-5	1127	1126	1	4	-4	581	630	1	6	-3	2639	2508	1	8	-2	1031	1040	1	10	2	466	505
1	2	-4	843	840	1	4	-3	1324	1217	1	6	-2	219	149	1	8	-1	235	314	1	10	3	1660	1662
1	2	-3	973	879	1	4	-2	121	141	1	6	-1	649	708	1	8	0	134	136	1	10	4	240	238
1	2	-2	1178	1134	1	4	-1	2960	2958	1	6	0	1019	986	1	8	1	907	879	1	10	5	1356	1364
1	2	-1	2605	2650	1	4	0	1068	1093	1	6	1	1643	1587	1	8	2	773	787	1	10	6	297	319
1	2	0	1052	1057	1	4	1	263	316	1	6	2	345	348	1	8	3	468	459	1	10	7	1093	1109
1	2	1	1038	1100	1	4	2	0*	71	1	6	3	1125	1131	1	8	4	255	207	1	10	8	139	144
1	2	2	719	708	1	4	3	2318	2273	1	6	4	763	804	1	8	5	980	955	1	10	9	734	730
1	2	3	1015	886	1	4	4	601	590	1	6	5	1551	1581	1	8	6	653	657	1	10	10	0*	67
1	2	4	578	617	1	4	5	952	938	1	6	6	341	324	1	8	7	554	546	1	11	-10	335	312

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fclc (x 10.) for [(C5Me5)2 Yb (OC)2 Fe (C5H4Me)] 2 at 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
1	11	-9	116	110	1	13	-4	855	845	1	15	5	573	564	1	18	-1	423	433	1	21	1	262	278
1	11	-8	649	645	1	13	-3	342	336	1	15	6	253	231	1	18	0	555	550	1	21	2	639	627
1	11	-7	346	350	1	13	-2	1399	1386	1	15	7	0*	28	1	18	1	605	586	1	21	3	101	99
1	11	-6	773	775	1	13	-1	711	667	1	15	8	105	113	1	18	2	32*	114	1	21	4	425	418
1	11	-5	159	121	1	13	0	1478	1504	1	15	9	397	399	1	18	3	483	499	1	21	5	194	200
1	11	-4	1063	1072	1	13	1	282	263	1	16	-9	295	303	1	18	4	456	474	1	21	6	579	564
1	11	-3	508	488	1	13	2	1046	1060	1	16	-8	43*	28	1	18	5	434	422	1	22	-5	182	163
1	11	-2	1413	1360	1	13	3	403	420	1	16	-7	446	444	1	18	6	127	165	1	22	-4	228	183
1	11	-1	586	615	1	13	4	970	990	1	16	-6	408	401	1	18	7	304	308	1	22	-3	94*	108
1	11	0	1057	1014	1	13	5	0*	67	1	16	-5	502	507	1	18	8	171	164	1	22	-2	402	396
1	11	1	52*	36	1	13	6	753	773	1	16	-4	48*	32	1	19	-7	318	298	1	22	-1	262	259
1	11	2	1202	1220	1	13	7	372	373	1	16	-3	757	776	1	19	-6	101	92	1	22	0	152	161
1	11	3	745	751	1	13	8	716	717	1	16	-2	779	754	1	19	-5	277	251	1	22	1	69*	82
1	11	4	751	760	1	13	9	0*	63	1	16	-1	735	766	1	19	-4	306	327	1	22	2	429	435
1	11	5	144	154	1	14	-9	583	553	1	16	0	75*	120	1	19	-3	360	363	1	22	3	0*	53
1	11	6	1095	1077	1	14	-8	0*	7	1	16	1	784	801	1	19	-2	208	212	1	22	4	141	151
1	11	7	498	505	1	14	-7	893	893	1	16	2	697	695	1	19	-1	396	419	1	22	5	38*	7
1	11	8	524	515	1	14	-6	430	455	1	16	3	501	515	1	19	0	168	126	1	23	-4	381	391
1	11	9	0*	87	1	14	-5	851	873	1	16	4	153	183	1	19	1	302	320	1	23	-3	228	192
1	11	10	424	431	1	14	-4	268	237	1	16	5	587	585	1	19	2	346	358	1	23	-2	435	423
1	12	-10	170	159	1	14	-3	1049	1047	1	16	6	326	318	1	19	3	508	530	1	23	-1	63*	100
1	12	-9	110	119	1	14	-2	654	643	1	16	7	472	486	1	19	4	211	208	1	23	0	480	474
1	12	-8	563	558	1	14	-1	1528	1535	1	16	8	159	179	1	19	5	193	207	1	23	1	186	201
1	12	-7	175	174	1	14	0	283	280	1	17	-8	597	597	1	19	6	310	296	1	23	2	391	401
1	12	-6	0*	86	1	14	1	1304	1332	1	17	-7	159	176	1	19	7	309	316	1	23	3	97*	110
1	12	-5	76*	40	1	14	2	465	474	1	17	-6	775	780	1	20	-7	408	421	1	23	4	479	485
1	12	-4	1116	1081	1	14	3	1038	1048	1	17	-5	0*	73	1	20	-6	0*	9	1	24	-3	603	627
1	12	-3	0*	22	1	14	4	95	66	1	17	-4	818	841	1	20	-5	727	728	1	24	-2	0*	30
1	12	-2	308	276	1	14	5	912	916	1	17	-3	68*	93	1	20	-4	227	240	1	24	-1	407	404
1	12	-1	18*	23	1	14	6	158	149	1	17	-2	980	966	1	20	-3	637	638	1	24	0	135	131
1	12	0	1003	983	1	14	7	794	799	1	17	-1	48*	40	1	20	-2	0*	75	1	24	1	642	630
1	12	1	393	389	1	14	8	0*	64	1	17	0	1107	1129	1	20	-1	794	772	1	24	2	0*	28
1	12	2	239	240	1	14	9	539	545	1	17	1	255	262	1	20	0	384	381	1	24	3	395	395
1	12	3	381	365	1	15	-9	324	323	1	17	2	990	984	1	20	1	571	590	1	25	-1	243	229
1	12	4	694	649	1	15	-8	223	213	1	17	3	150	138	1	20	2	0*	38	1	25	0	235	245
1	12	5	0*	32	1	15	-7	269	234	1	17	4	923	886	1	20	3	790	796	1	25	1	152	138
1	12	6	284	287	1	15	-6	215	210	1	17	5	203	203	1	20	4	257	268	2	0	-10	860	862
1	12	7	0*	16	1	15	-5	384	349	1	17	6	716	706	1	20	5	521	524	2	0	-8	632	645
1	12	8	401	383	1	15	-4	209	189	1	17	7	157	156	1	20	6	72*	41	2	0	-6	2119	2139
1	12	9	177	181	1	15	-3	445	381	1	17	8	649	652	1	20	7	554	547	2	0	-4	850	802
1	12	10	245	246	1	15	-2	390	376	1	18	-8	242	253	1	21	-6	399	429	2	0	-2	1222	1323
1	13	-10	444	446	1	15	-1	474	467	1	18	-7	501	515	1	21	-5	197	170	2	0	0	155	170
1	13	-9	0*	11	1	15	0	310	280	1	18	-6	151	123	1	21	-4	546	560	2	0	2	1327	1470
1	13	-8	661	686	1	15	1	609	634	1	18	-5	299	288	1	21	-3	241	238	2	0	4	870	929
1	13	-7	218	201	1	15	2	224	224	1	18	-4	505	501	1	21	-2	615	643	2	0	6	1113	1163
1	13	-6	860	883	1	15	3	245	230	1	18	-3	608	590	1	21	-1	0*	53	2	0	8	911	902
1	13	-5	107	66	1	15	4	372	374	1	18	-2	0*	31	1	21	0	543	545	2	0	10	499	508

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fclc (x 10.) for [(C5Me5)2 Yb (OC)2 Fe (C5H4Me)] 2 at 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
2	1	-11	102	86	2	3	-10	139	107	2	5	-9	39*	21	2	7	-8	0*	86	2	9	-3	244	272
2	1	-10	536	633	2	3	-9	584	597	2	5	-8	604	629	2	7	-7	650	637	2	9	-2	1636	1653
2	1	-9	668	664	2	3	-8	329	332	2	5	-7	210	183	2	7	-6	281	291	2	9	-1	452	509
2	1	-8	692	689	2	3	-7	1233	1231	2	5	-6	1228	1193	2	7	-5	1001	1013	2	9	0	849	806
2	1	-7	481	484	2	3	-6	414	400	2	5	-5	59*	66	2	7	-4	163	153	2	9	1	323	359
2	1	-6	1202	1153	2	3	-5	1350	1365	2	5	-4	1640	1577	2	7	-3	1795	1798	2	9	2	1275	1326
2	1	-5	293	306	2	3	-4	609	611	2	5	-3	639	536	2	7	-2	530	495	2	9	3	957	946
2	1	-4	944	902	2	3	-3	1148	1044	2	5	-2	1985	1820	2	7	-1	966	972	2	9	4	692	667
2	1	-3	1203	1124	2	3	-2	160	161	2	5	-1	301	278	2	7	0	144	124	2	9	5	226	249
2	1	-2	904	1008	2	3	-1	1745	1778	2	5	0	1894	1849	2	7	1	1478	1495	2	9	6	1258	1274
2	1	-1	925	926	2	3	0	215	271	2	5	1	238	241	2	7	2	540	558	2	9	7	486	496
2	1	0	898	901	2	3	1	457	372	2	5	2	1153	1079	2	7	3	911	962	2	9	8	477	478
2	1	1	1424	1611	2	3	2	2121	2022	2	5	3	916	911	2	7	4	210	208	2	9	9	210	209
2	1	2	167	235	2	3	3	1868	1919	2	5	4	1864	1845	2	7	5	1628	1655	2	9	10	549	556
2	1	3	742	658	2	3	4	188	197	2	5	5	293	273	2	7	6	482	491	2	10	-10	436	446
2	1	4	1018	1021	2	3	5	561	556	2	5	6	829	801	2	7	7	635	638	2	10	-9	285	289
2	1	5	1140	1164	2	3	6	450	441	2	5	7	310	328	2	7	8	0*	6	2	10	-8	779	804
2	1	6	803	788	2	3	7	1096	1091	2	5	8	886	885	2	7	9	760	771	2	10	-7	0*	91
2	1	7	183	182	2	3	8	240	241	2	5	9	86*	115	2	7	10	144	153	2	10	-6	677	672
2	1	8	675	669	2	3	9	573	567	2	5	10	479	455	2	8	-10	269	264	2	10	-5	577	588
2	1	9	655	650	2	3	10	263	267	2	5	11	154	156	2	8	-9	675	680	2	10	-4	1433	1409
2	1	10	566	552	2	3	11	492	492	2	6	-11	355	356	2	8	-8	228	212	2	10	-3	0*	72
2	1	11	102*	140	2	4	-11	337	338	2	6	-10	629	625	2	8	-7	436	450	2	10	-2	892	863
2	2	-11	423	429	2	4	-10	264	268	2	6	-9	180	173	2	8	-6	562	568	2	10	-1	769	710
2	2	-10	103	102	2	4	-9	[illegible]	249	2	6	-8	268	292	2	8	-5	1497	1450	2	10	0	1446	1495
2	2	-9	773	775	2	4	-8	1022	1014	2	6	-7	799	809	2	8	-4	191	171	2	10	1	98	84
2	2	-8	521	522	2	4	-7	792	810	2	6	-6	1198	1208	2	8	-3	657	615	2	10	2	1021	1063
2	2	-7	955	946	2	4	-6	450	457	2	6	-5	516	489	2	8	-2	1255	1242	2	10	3	228	238
2	2	-6	278	302	2	4	-5	477	495	2	6	-4	506	530	2	8	-1	2098	2051	2	10	4	1110	1100
2	2	-5	1337	1329	2	4	-4	1263	1245	2	6	-3	1237	1269	2	8	0	270	272	2	10	5	420	436
2	2	-4	940	949	2	4	-3	1361	1214	2	6	-2	1666	1610	2	8	1	821	886	2	10	6	905	907
2	2	-3	1669	1478	2	4	-2	1103	1058	2	6	-1	759	691	2	8	2	601	609	2	10	7	160	149
2	2	-2	397	407	2	4	-1	474	493	2	6	0	594	529	2	8	3	1405	1382	2	10	8	585	596
2	2	-1	1835	1866	2	4	0	1873	1922	2	6	1	1137	1123	2	8	4	557	553	2	10	9	106	87
2	2	0	1450	1447	2	4	1	427	383	2	6	2	654	719	2	8	5	990	984	2	10	10	419	422
2	2	1	442	522	2	4	2	1232	1190	2	6	3	770	812	2	8	6	458	445	2	11	-10	430	432
2	2	2	1504	1368	2	4	3	461	486	2	6	4	874	892	2	8	7	635	633	2	11	-9	385	379
2	2	3	1889	1816	2	4	4	1623	1622	2	6	5	944	941	2	8	8	326	314	2	11	-8	422	420
2	2	4	707	705	2	4	5	976	982	2	6	6	703	702	2	8	9	579	590	2	11	-7	553	564
2	2	5	961	951	2	4	6	843	824	2	6	7	514	505	2	8	10	150	142	2	11	-6	572	581
2	2	6	364	409	2	4	7	489	481	2	6	8	638	650	2	9	-10	357	353	2	11	-5	720	705
2	2	7	816	819	2	4	8	610	611	2	6	9	469	472	2	9	-9	283	295	2	11	-4	750	733
2	2	8	119	114	2	4	9	377	393	2	6	10	319	325	2	9	-8	581	590	2	11	-3	1132	1139
2	2	9	813	781	2	4	10	537	537	2	6	11	343	349	2	9	-7	308	310	2	11	-2	426	452
2	2	10	251	252	2	4	11	254	267	2	7	-11	305	327	2	9	-6	761	738	2	11	-1	880	832
2	2	11	477	462	2	5	-11	88*	121	2	7	-10	57*	62	2	9	-5	487	496	2	11	0	1085	1120
2	3	-11	575	575	2	5	-10	608	616	2	7	-9	724	737	2	9	-4	1263	1198	2	11	1	578	580

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fclc (x 10.) for [(C5Me5)2 Yb (OC)2 Fe (C5H4Me)] 2 at 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
2	11	2	811	822	2	13	8	475	477	2	16	-1	975	971	2	19	-3	189	203	2	22	5	348	365
2	11	3	910	916	2	13	9	383	388	2	16	0	568	559	2	19	-2	470	441	2	23	-4	296	282
2	11	4	1093	1097	2	14	-9	347	334	2	16	1	524	508	2	19	-1	258	247	2	23	-3	361	357
2	11	5	550	544	2	14	-8	537	524	2	16	2	433	433	2	19	0	802	805	2	23	-2	387	371
2	11	6	160	147	2	14	-7	0*	18	2	16	3	804	821	2	19	1	82*	140	2	23	-1	280	253
2	11	7	683	670	2	14	-6	704	719	2	16	4	366	385	2	19	2	530	531	2	23	0	171	166
2	11	8	691	722	2	14	-5	573	590	2	16	5	435	441	2	19	3	233	220	2	23	1	456	450
2	11	9	202	186	2	14	-4	668	671	2	16	6	445	458	2	19	4	672	691	2	23	2	294	309
2	11	10	90*	142	2	14	-3	143	143	2	16	7	372	375	2	19	5	135	145	2	23	3	237	226
2	12	-10	0*	66	2	14	-2	876	878	2	16	8	280	287	2	19	6	334	347	2	23	4	240	231
2	12	-9	395	393	2	14	-1	650	655	2	17	-8	0*	65	2	19	7	219	228	2	24	-3	60*	86
2	12	-8	0*	22	2	14	0	748	821	2	17	-7	489	487	2	20	-6	264	272	2	24	-2	498	483
2	12	-7	949	976	2	14	1	141	119	2	17	-6	0*	16	2	20	-5	0*	94	2	24	-1	0*	37
2	12	-6	360	350	2	14	2	862	845	2	17	-5	516	516	2	20	-4	596	619	2	24	0	300	303
2	12	-5	402	373	2	14	3	537	540	2	17	-4	67*	3	2	20	-3	332	327	2	24	1	173	173
2	12	-4	200	202	2	14	4	843	852	2	17	-3	695	692	2	20	-2	408	407	2	24	2	413	411
2	12	-3	1049	1062	2	14	5	201	187	2	17	-2	159	153	2	20	-1	0*	53	3	0	-11	0*	23
2	12	-2	110	122	2	14	6	677	684	2	17	-1	670	657	2	20	0	701	671	3	0	-9	758	744
2	12	-1	790	784	2	14	7	249	252	2	17	0	207	209	2	20	1	345	339	3	0	-7	39*	48
2	12	0	158	131	2	14	8	383	400	2	17	1	857	887	2	20	2	507	519	3	0	-5	1413	1423
2	12	1	1273	1328	2	14	9	222	201	2	17	2	367	381	2	20	3	86*	96	3	0	-3	1048	924
2	12	2	330	308	2	15	-9	120	117	2	17	3	739	737	2	20	4	513	484	3	0	-1	618	632
2	12	3	914	921	2	15	-8	586	581	2	17	4	90*	153	2	20	5	246	233	3	0	1	848	736
2	12	4	121	149	2	15	-7	158	150	2	17	5	648	640	2	20	6	410	422	3	0	3	1399	1380
2	12	5	901	914	2	15	-6	665	640	2	17	6	105	104	2	21	-6	153	148	3	0	5	473	487
2	12	6	37*	56	2	15	-5	58*	21	2	17	7	435	437	2	21	-5	347	327	3	0	7	221	234
2	12	7	713	722	2	15	-4	725	700	2	17	8	0*	129	2	21	-4	270	272	3	0	9	498	516
2	12	8	103	106	2	15	-3	114	120	2	18	-8	245	235	2	21	-3	382	387	3	0	11	106	107
2	12	9	514	514	2	15	-2	997	1012	2	18	-7	526	530	2	21	-2	389	404	3	1	-11	485	497
2	12	10	102	82	2	15	-1	170	177	2	18	-6	318	336	2	21	-1	507	524	3	1	-10	182	168
2	13	-9	462	473	2	15	0	583	584	2	18	-5	355	356	2	21	0	196	171	3	1	-9	706	691
2	13	-8	326	296	2	15	1	181	156	2	18	-4	106	105	2	21	1	281	306	3	1	-8	414	444
2	13	-7	679	694	2	15	2	1102	1110	2	18	-3	770	764	2	21	2	458	464	3	1	-7	1030	1023
2	13	-6	382	355	2	15	3	316	325	2	18	-2	509	524	2	21	3	481	484	3	1	-6	480	476
2	13	-5	737	715	2	15	4	436	446	2	18	-1	291	289	2	21	4	114	112	3	1	-5	1085	1138
2	13	-4	546	521	2	15	5	253	261	2	18	0	226	221	2	21	5	288	281	3	1	-4	338	300
2	13	-3	805	773	2	15	6	798	807	2	18	1	734	730	2	21	6	260	275	3	1	-3	1541	1478
2	13	-2	607	571	2	15	7	118	104	2	18	2	570	550	2	22	-5	482	454	3	1	-2	952	903
2	13	-1	1134	1086	2	15	8	303	304	2	18	3	427	431	2	22	-4	127	122	3	1	-1	1695	1619
2	13	0	892	908	2	15	9	0*	51	2	18	4	365	363	2	22	-3	412	410	3	1	0	425	382
2	13	1	940	967	2	16	-8	234	261	2	18	5	521	521	2	22	-2	44*	81	3	1	1	631	677
2	13	2	118	103	2	16	-7	273	248	2	18	6	266	247	2	22	-1	569	575	3	1	2	1767	1733
2	13	3	728	756	2	16	-6	425	433	2	18	7	358	370	2	22	0	146	132	3	1	3	2095	2132
2	13	4	774	799	2	16	-5	847	861	2	19	-7	97*	95	2	22	1	392	405	3	1	4	99	108
2	13	5	680	694	2	16	-4	405	422	2	19	-6	505	512	2	22	2	118	84	3	1	5	1221	1212
2	13	6	133	118	2	16	-3	344	330	2	19	-5	225	214	2	22	3	498	493	3	1	6	621	649
2	13	7	488	491	2	16	-2	650	667	2	19	-4	728	708	2	22	4	67*	34	3	1	7	943	953

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fclc (x 10.) for [(C5Me5)2 Yb (OC)2 Fe (C5H4Me)] 2 at 25 C

H	K	L	Fobs	Fcalc
3	1	8	82*	66
3	1	9	764	771
3	1	10	215	233
3	1	11	466	455
3	2	-11	303	299
3	2	-10	654	661
3	2	-9	169	161
3	2	-8	1038	1061
3	2	-7	612	617
3	2	-6	1254	1245
3	2	-5	583	565
3	2	-4	1461	1478
3	2	-3	115	161
3	2	-2	1657	1648
3	2	-1	131	110
3	2	0	1958	1881
3	2	1	50*	113
3	2	2	2838	2793
3	2	3	64*	38
3	2	4	1967	1965
3	2	5	314	313
3	2	6	1277	1277
3	2	7	299	287
3	2	8	1046	1045
3	2	9	73*	15
3	2	10	705	699
3	2	11	190	184
3	3	-11	181	195
3	3	-10	350	345
3	3	-9	290	287
3	3	-8	348	345
3	3	-7	447	436
3	3	-6	522	553
3	3	-5	945	928
3	3	-4	1221	1221
3	3	-3	582	550
3	3	-2	486	443
3	3	-1	303	303
3	3	0	1792	1702
3	3	1	1696	1505
3	3	2	205	197
3	3	3	1585	1565
3	3	4	1242	1233
3	3	5	168	180
3	3	6	133	121
3	3	7	470	462
3	3	8	518	548

H	K	L	Fobs	Fcalc
3	3	9	278	252
3	3	10	170	169
3	3	11	205	206
3	4	-11	371	393
3	4	-10	515	501
3	4	-9	135	136
3	4	-8	234	219
3	4	-7	739	760
3	4	-6	894	886
3	4	-5	150	139
3	4	-4	610	647
3	4	-3	1111	1066
3	4	-2	1328	1341
3	4	-1	357	353
3	4	0	837	762
3	4	1	1125	1140
3	4	2	524	535
3	4	3	781	781
3	4	4	1111	1128
3	4	5	361	366
3	4	6	778	755
3	4	7	501	488
3	4	8	669	672
3	4	9	187	178
3	4	10	314	309
3	4	11	269	259
3	5	-11	531	532
3	5	-10	68*	43
3	5	-9	766	782
3	5	-8	71*	19
3	5	-7	1156	1178
3	5	-6	60*	59
3	5	-5	1023	1071
3	5	-4	529	496
3	5	-3	1921	1924
3	5	-2	612	595
3	5	-1	1973	1963
3	5	0	491	497
3	5	1	2124	2200
3	5	2	158	169
3	5	3	1922	1945
3	5	4	434	461
3	5	5	1790	1819
3	5	6	377	369
3	5	7	976	978
3	5	8	97	122
3	5	9	985	959

H	K	L	Fobs	Fcalc
3	5	10	46*	79
3	6	-11	73*	84
3	6	-10	556	577
3	6	-9	487	491
3	6	-8	440	432
3	6	-7	23*	28
3	6	-6	1250	1245
3	6	-5	834	848
3	6	-4	1117	1055
3	6	-3	266	257
3	6	-2	1459	1489
3	6	-1	1141	1191
3	6	0	1217	1155
3	6	1	80	90
3	6	2	1477	1487
3	6	3	757	769
3	6	4	989	1013
3	6	5	518	515
3	6	6	691	679
3	6	7	252	260
3	6	8	681	666
3	6	9	387	387
3	6	10	343	342
3	7	-10	303	307
3	7	-9	113	92
3	7	-8	288	285
3	7	-7	81*	73
3	7	-6	400	402
3	7	-5	191	149
3	7	-4	373	334
3	7	-3	0*	20
3	7	-2	1145	1098
3	7	-1	687	735
3	7	0	414	406
3	7	1	0*	38
3	7	2	752	758
3	7	3	770	793
3	7	4	333	331
3	7	5	243	232
3	7	6	708	733
3	7	7	475	457
3	7	8	228	213
3	7	9	76*	49
3	7	10	315	318
3	8	-10	447	438
3	8	-9	302	315
3	8	-8	937	927

H	K	L	Fobs	Fcalc
3	8	-7	77*	73
3	8	-6	796	795
3	8	-5	516	510
3	8	-4	1585	1595
3	8	-3	41*	46
3	8	-2	1156	1149
3	8	-1	659	698
3	8	0	1799	1877
3	8	1	139	164
3	8	2	1359	1382
3	8	3	133	146
3	8	4	1333	1329
3	8	5	310	301
3	8	6	1098	1062
3	8	7	0*	27
3	8	8	792	805
3	8	9	135	132
3	8	10	522	502
3	9	-10	175	192
3	9	-9	740	734
3	9	-8	191	188
3	9	-7	784	781
3	9	-6	191	173
3	9	-5	1337	1312
3	9	-4	520	519
3	9	-3	1412	1369
3	9	-2	92	66
3	9	-1	1926	1945
3	9	0	401	384
3	9	1	1048	1051
3	9	2	74*	30
3	9	3	1681	1668
3	9	4	593	598
3	9	5	792	791
3	9	6	78*	95
3	9	7	1050	1071
3	9	8	288	288
3	9	9	503	499
3	9	10	95*	83
3	10	-10	85*	19
3	10	-9	282	297
3	10	-8	459	442
3	10	-7	451	447
3	10	-6	215	195
3	10	-5	293	299
3	10	-4	972	949
3	10	-3	993	992

H	K	L	Fobs	Fcalc
3	10	-2	0*	22
3	10	-1	347	367
3	10	0	176	204
3	10	1	687	696
3	10	2	40*	38
3	10	3	606	613
3	10	4	311	305
3	10	5	383	378
3	10	6	420	418
3	10	7	441	434
3	10	8	104	108
3	10	9	188	186
3	10	10	216	206
3	11	-10	195	194
3	11	-9	443	451
3	11	-8	258	268
3	11	-7	749	737
3	11	-6	149	130
3	11	-5	669	662
3	11	-4	577	555
3	11	-3	1099	1074
3	11	-2	491	470
3	11	-1	504	485
3	11	0	492	528
3	11	1	1573	1583
3	11	2	259	227
3	11	3	862	865
3	11	4	480	476
3	11	5	934	949
3	11	6	238	218
3	11	7	404	404
3	11	8	187	186
3	11	9	546	548
3	12	-9	83*	77
3	12	-8	618	620
3	12	-7	127	112
3	12	-6	1164	1152
3	12	-5	276	275
3	12	-4	867	834
3	12	-3	72*	6
3	12	-2	1771	1732
3	12	-1	205	214
3	12	0	1028	1020
3	12	1	63*	78
3	12	2	1586	1585
3	12	3	56*	49
3	12	4	1188	1208

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fclc (x 10.) for [(C5Me5)2 Yb (OC)2 Fe (C5H4Me)] 2 at 25 C

Page 7

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
3	12	5	85*	91	3	15	-5	1034	1018	3	18	-7	36*	73	3	21	0	339	343	4	1	-1	300	284
3	12	6	863	871	3	15	-4	84*	77	3	18	-6	673	680	3	21	1	230	234	4	1	0	1578	1590
3	12	7	0*	17	3	15	-3	780	771	3	18	-5	133	111	3	21	2	118	117	4	1	1	719	703
3	12	8	773	792	3	15	-2	29*	49	3	18	-4	550	561	3	21	3	437	426	4	1	2	2063	2027
3	12	9	131	121	3	15	-1	1286	1295	3	18	-3	122	141	3	21	4	238	257	4	1	3	513	500
3	13	-9	396	389	3	15	0	66*	104	3	18	-2	821	812	3	21	5	173	174	4	1	4	1749	1762
3	13	-8	292	297	3	15	1	701	693	3	18	-1	306	313	3	22	-4	620	597	4	1	5	459	453
3	13	-7	563	545	3	15	2	184	176	3	18	0	617	627	3	22	-3	90*	82	4	1	6	995	1004
3	13	-6	542	546	3	15	3	1251	1268	3	18	1	201	204	3	22	-2	575	568	4	1	7	184	198
3	13	-5	342	319	3	15	4	92*	101	3	18	2	728	720	3	22	-1	0*	102	4	1	8	810	809
3	13	-4	295	309	3	15	5	703	718	3	18	3	260	279	3	22	0	632	634	4	1	9	0*	63
3	13	-3	930	935	3	15	6	71*	97	3	18	4	580	599	3	22	1	74*	37	4	1	10	488	490
3	13	-2	484	480	3	15	7	746	766	3	18	5	93*	118	3	22	2	519	513	4	2	-11	567	576
3	13	-1	183	200	3	15	8	83*	8	3	18	6	490	504	3	22	3	0*	54	4	2	-10	260	258
3	13	0	531	524	3	16	-8	681	669	3	18	7	71*	65	3	22	4	534	521	4	2	-9	726	721
3	13	1	850	859	3	16	-7	184	196	3	19	-7	502	493	3	23	-3	317	324	4	2	-8	219	197
3	13	2	512	512	3	16	-6	456	438	3	19	-6	0*	65	3	23	-2	271	268	4	2	-7	1305	1323
3	13	3	284	277	3	16	-5	292	284	3	19	-5	627	633	3	23	-1	453	463	4	2	-6	627	588
3	13	4	364	362	3	16	-4	945	972	3	19	-4	204	193	3	23	0	91*	88	4	2	-5	1241	1228
3	13	5	805	799	3	16	-3	164	165	3	19	-3	860	847	3	23	1	223	204	4	2	-4	406	415
3	13	6	377	346	3	16	-2	407	406	3	19	-2	23*	56	3	23	2	311	299	4	2	-3	1706	1707
3	13	7	236	221	3	16	-1	389	383	3	19	-1	517	498	3	23	3	417	439	4	2	-2	108	84
3	13	8	126	144	3	16	0	976	989	3	19	0	278	303	3	24	-2	0*	91	4	2	-1	1459	1481
3	13	9	439	439	3	16	1	229	227	3	19	1	1099	1081	3	24	-1	275	260	4	2	0	68*	96
3	14	-9	193	205	3	16	2	881	908	3	19	2	0*	55	3	24	0	137	129	4	2	1	2091	2146
3	14	-8	405	408	3	16	3	222	226	3	19	3	542	542	3	24	1	143	147	4	2	2	147	139
3	14	-7	246	236	3	16	4	683	682	3	19	4	200	184	4	0	-10	246	242	4	2	3	2395	2404
3	14	-6	167	119	3	16	5	252	241	3	19	5	712	711	4	0	-8	222	266	4	2	4	0*	46
3	14	-5	359	368	3	16	6	543	557	3	19	6	98*	79	4	0	-6	602	606	4	2	5	1259	1272
3	14	-4	694	687	3	16	7	141	140	3	20	-6	329	331	4	0	-4	468	455	4	2	6	123	88
3	14	-3	428	425	3	16	8	364	358	3	20	-5	98*	126	4	0	-2	628	585	4	2	7	1069	1078
3	14	-2	57*	50	3	17	-8	227	236	3	20	-4	166	144	4	0	0	142	151	4	2	8	31*	109
3	14	-1	278	275	3	17	-7	25*	5	3	20	-3	395	411	4	0	2	258	256	4	2	9	800	787
3	14	0	649	616	3	17	-6	264	266	3	20	-2	272	284	4	0	4	176	183	4	2	10	84*	110
3	14	1	460	453	3	17	-5	100	82	3	20	-1	255	248	4	0	6	162	150	4	3	-11	64*	45
3	14	2	453	471	3	17	-4	263	281	3	20	0	69*	153	4	0	8	198	178	4	3	-10	218	223
3	14	3	471	493	3	17	-3	192	211	3	20	1	404	415	4	0	10	56*	121	4	3	-9	129	94
3	14	4	318	326	3	17	-2	466	465	3	20	2	303	307	4	1	-11	90*	47	4	3	-8	355	351
3	14	5	383	385	3	17	-1	131	132	3	20	3	296	293	4	1	-10	556	580	4	3	-7	0*	58
3	14	6	476	480	3	17	0	238	315	3	20	4	219	213	4	1	-9	126	99	4	3	-6	469	459
3	14	7	186	188	3	17	1	149	137	3	20	5	219	222	4	1	-8	689	715	4	3	-5	348	301
3	14	8	146	139	3	17	2	556	575	3	20	6	166	173	4	1	-7	58*	16	4	3	-4	994	977
3	14	9	169	141	3	17	3	319	323	3	21	-5	286	269	4	1	-6	963	991	4	3	-3	602	575
3	15	-9	493	505	3	17	4	314	315	3	21	-4	249	236	4	1	-5	502	490	4	3	-2	260	286
3	15	-8	0*	46	3	17	5	247	250	3	21	-3	279	284	4	1	-4	1340	1363	4	3	-1	523	489
3	15	-7	647	660	3	17	6	251	252	3	21	-2	172	166	4	1	-3	548	514	4	3	0	654	672
3	15	-6	0*	70	3	17	7	93*	77	3	21	-1	536	526	4	1	-2	1304	1391	4	3	1	701	716

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fclc (x 10.) for [(C5Me5)2 Yb (OC)2 Fe (C5H4Me)] 2 at 25 C

H	K	L	Fobs	Fcalc
4	3	2	968	929
4	3	3	411	388
4	3	4	358	381
4	3	5	362	365
4	3	6	199	197
4	3	7	155	177
4	3	8	390	397
4	3	9	48*	83
4	3	10	189	194
4	4	-10	209	217
4	4	-9	479	506
4	4	-8	299	308
4	4	-7	273	268
4	4	-6	436	450
4	4	-5	542	553
4	4	-4	295	292
4	4	-3	1031	1031
4	4	-2	144	137
4	4	-1	1369	1419
4	4	0	160	134
4	4	1	1049	1012
4	4	2	92	124
4	4	3	1335	1371
4	4	4	106	104
4	4	5	783	782
4	4	6	245	225
4	4	7	718	697
4	4	8	150	145
4	4	9	491	486
4	4	10	127	110
4	5	-10	716	705
4	5	-9	132	147
4	5	-8	784	807
4	5	-7	55*	32
4	5	-6	1476	1467
4	5	-5	289	280
4	5	-4	1157	1141
4	5	-3	535	539
4	5	-2	2061	2057
4	5	-1	976	992
4	5	0	1812	1849
4	5	1	552	545
4	5	2	2218	2231
4	5	3	483	495
4	5	4	1010	1004
4	5	5	179	167
4	5	6	1386	1395
4	5	7	148	162
4	5	8	973	973
4	5	9	0*	19
4	5	10	616	617
4	6	-10	90*	137
4	6	-9	663	678
4	6	-8	0*	59
4	6	-7	430	413
4	6	-6	308	308
4	6	-5	1361	1345
4	6	-4	327	314
4	6	-3	954	963
4	6	-2	181	214
4	6	-1	1294	1335
4	6	0	268	267
4	6	1	1460	1439
4	6	2	0*	76
4	6	3	695	693
4	6	4	104	78
4	6	5	848	865
4	6	6	213	207
4	6	7	559	561
4	6	8	152	143
4	6	9	576	554
4	6	10	44*	111
4	7	-10	103	92
4	7	-9	58*	89
4	7	-8	230	242
4	7	-7	265	251
4	7	-6	61*	28
4	7	-5	185	177
4	7	-4	396	409
4	7	-3	301	301
4	7	-2	171	157
4	7	-1	522	525
4	7	0	769	740
4	7	1	335	339
4	7	2	365	316
4	7	3	277	270
4	7	4	512	564
4	7	5	245	251
4	7	6	103	94
4	7	7	31*	32
4	7	8	344	340
4	7	9	0*	40
4	7	10	0*	28
4	8	-10	129	138
4	8	-9	502	514
4	8	-8	0*	45
4	8	-7	1110	1097
4	8	-6	177	179
4	8	-5	836	871
4	8	-4	120	107
4	8	-3	1754	1729
4	8	-2	82	101
4	8	-1	1757	1719
4	8	0	117	136
4	8	1	1438	1429
4	8	2	227	248
4	8	3	1408	1419
4	8	4	224	216
4	8	5	766	764
4	8	6	101	94
4	8	7	1080	1097
4	8	8	174	190
4	8	9	581	580
4	8	10	124	110
4	9	-10	593	589
4	9	-9	65*	15
4	9	-8	857	853
4	9	-7	78*	8
4	9	-6	608	594
4	9	-5	165	124
4	9	-4	1598	1568
4	9	-3	497	473
4	9	-2	1001	974
4	9	-1	372	358
4	9	0	1998	2008
4	9	1	257	274
4	9	2	1175	1145
4	9	3	54*	8
4	9	4	1270	1257
4	9	5	198	212
4	9	6	772	759
4	9	7	0*	49
4	9	8	916	895
4	9	9	0*	69
4	10	-10	86*	89
4	10	-9	0*	8
4	10	-8	106	82
4	10	-7	191	178
4	10	-6	134	73
4	10	-5	121	121
4	10	-4	70*	54
4	10	-3	578	557
4	10	-2	306	264
4	10	-1	0*	34
4	10	0	42*	79
4	10	1	171	173
4	10	2	0*	73
4	10	3	208	219
4	10	4	141	140
4	10	5	0*	26
4	10	6	110	68
4	10	7	342	355
4	10	8	0*	81
4	10	9	85*	40
4	11	-9	0*	6
4	11	-8	386	390
4	11	-7	45*	26
4	11	-6	989	986
4	11	-5	174	145
4	11	-4	579	585
4	11	-3	248	237
4	11	-2	1299	1294
4	11	-1	0*	12
4	11	0	633	619
4	11	1	70*	62
4	11	2	1371	1398
4	11	3	149	134
4	11	4	526	514
4	11	5	71*	23
4	11	6	798	806
4	11	7	103	84
4	11	8	386	396
4	11	9	0*	17
4	12	-9	847	832
4	12	-8	69*	56
4	12	-7	657	656
4	12	-6	83*	18
4	12	-5	1132	1116
4	12	-4	0*	46
4	12	-3	920	924
4	12	-2	79*	34
4	12	-1	1300	1323
4	12	0	100	102
4	12	1	1402	1411
4	12	2	104	91
4	12	3	1239	1227
4	12	4	115	109
4	12	5	1248	1213
4	12	6	32*	82
4	12	7	681	679
4	12	8	0*	34
4	12	9	697	680
4	13	-9	0*	12
4	13	-8	309	292
4	13	-7	67*	13
4	13	-6	552	569
4	13	-5	148	132
4	13	-4	331	332
4	13	-3	146	102
4	13	-2	876	878
4	13	-1	0*	23
4	13	0	218	212
4	13	1	80*	40
4	13	2	979	998
4	13	3	87*	81
4	13	4	333	353
4	13	5	36*	3
4	13	6	564	567
4	13	7	85*	71
4	13	8	256	250
4	13	9	0*	27
4	14	-8	61*	15
4	14	-7	438	453
4	14	-6	23*	11
4	14	-5	228	210
4	14	-4	129	122
4	14	-3	572	567
4	14	-2	151	94
4	14	-1	188	174
4	14	0	77*	79
4	14	1	363	383
4	14	2	0*	35
4	14	3	509	514
4	14	4	0*	92
4	14	5	310	311
4	14	6	0*	9
4	14	7	365	350
4	14	8	0*	56
4	15	-8	647	649
4	15	-7	50*	56
4	15	-6	632	649
4	15	-5	86*	80
4	15	-4	1157	1153
4	15	-3	91*	125
4	15	-2	611	609

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fclc (x 10.) for [(C5Me5)2 Yb (OC)2 Fe (C5H4Me)] 2 at 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
4	15	-1	149	158	4	18	-1	789	782	4	22	0	0*	77	5	2	-3	397	370	5	4	2	1182	1177
4	15	0	1371	1369	4	18	0	0*	41	4	22	1	570	560	5	2	-2	1398	1383	5	4	3	409	402
4	15	1	32*	30	4	18	1	696	722	4	22	2	98*	70	5	2	-1	334	335	5	4	4	192	181
4	15	2	731	749	4	18	2	0*	25	4	22	3	548	548	5	2	0	1474	1532	5	4	5	197	177
4	15	3	174	160	4	18	3	563	567	4	23	-2	307	321	5	2	1	137	173	5	4	6	667	685
4	15	4	1203	1180	4	18	4	71*	70	4	23	-1	150	111	5	2	2	1411	1418	5	4	7	506	497
4	15	5	72*	56	4	18	5	603	609	4	23	0	437	444	5	2	3	692	729	5	4	8	379	372
4	15	6	666	661	4	18	6	79*	38	4	23	1	0*	81	5	2	4	1240	1262	5	4	9	108	102
4	15	7	88*	40	4	19	-6	629	626	4	23	2	268	266	5	2	5	0*	48	5	4	10	277	283
4	15	8	565	558	4	19	-5	0*	44	5	0	-9	408	415	5	2	6	957	974	5	5	-10	0*	89
4	16	-8	0*	78	4	19	-4	614	618	5	0	-7	206	173	5	2	7	313	292	5	5	-9	697	697
4	16	-7	703	693	4	19	-3	149	132	5	0	-5	803	793	5	2	8	787	787	5	5	-8	230	219
4	16	-6	93	61	4	19	-2	869	864	5	0	-3	874	859	5	2	9	85*	71	5	5	-7	846	847
4	16	-5	620	618	4	19	-1	59*	11	5	0	-1	704	717	5	2	10	469	466	5	5	-6	142	142
4	16	-4	0*	79	4	19	0	620	620	5	0	1	1043	1069	5	3	-10	88*	47	5	5	-5	1522	1499
4	16	-3	814	822	4	19	1	192	174	5	0	3	571	570	5	3	-9	164	178	5	5	-4	303	317
4	16	-2	38*	92	4	19	2	949	972	5	0	5	705	712	5	3	-8	507	511	5	5	-3	1293	1273
4	16	-1	613	625	4	19	3	0*	38	5	0	7	209	202	5	3	-7	449	443	5	5	-2	311	306
4	16	0	92*	129	4	19	4	446	440	5	0	9	396	383	5	3	-6	189	197	5	5	-1	2050	2016
4	16	1	968	998	4	19	5	41*	92	5	1	-10	374	375	5	3	-5	342	334	5	5	0	450	448
4	16	2	83*	11	4	19	6	595	600	5	1	-9	511	531	5	3	-4	1104	1108	5	5	1	1435	1466
4	16	3	804	819	4	20	-6	106	64	5	1	-8	0*	88	5	3	-3	680	690	5	5	2	350	370
4	16	4	0*	45	4	20	-5	354	347	5	1	-7	856	879	5	3	-2	217	279	5	5	3	1085	1132
4	16	5	508	511	4	20	-4	0*	9	5	1	-6	527	504	5	3	-1	124	131	5	5	4	243	243
4	16	6	75*	5	4	20	-3	205	198	5	1	-5	996	974	5	3	0	1157	1187	5	5	5	725	709
4	16	7	511	512	4	20	-2	100*	138	5	1	-4	168	143	5	3	1	519	554	5	5	6	69*	36
4	17	-7	0*	6	4	20	-1	218	214	5	1	-3	1497	1455	5	3	2	409	403	5	5	7	1050	1081
4	17	-6	24*	99	4	20	0	0*	4	5	1	-2	956	969	5	3	3	224	253	5	5	8	88*	104
4	17	-5	0*	56	4	20	1	298	296	5	1	-1	1221	1201	5	3	4	701	694	5	5	9	573	571
4	17	-4	201	190	4	20	2	0*	56	5	1	0	198	231	5	3	5	525	531	5	5	10	0*	41
4	17	-3	0*	31	4	20	3	173	188	5	1	1	1246	1280	5	3	6	249	226	5	6	-10	327	330
4	17	-2	300	309	4	20	4	70*	50	5	1	2	850	868	6	3	7	277	288	5	6	-9	333	334
4	17	-1	0*	69	4	20	5	237	230	5	1	3	1416	1457	5	3	8	356	350	5	6	-8	544	541
4	17	0	325	321	4	21	-5	137	107	5	1	4	62*	24	5	3	9	249	270	5	6	-7	267	282
4	17	1	40*	61	4	21	-4	363	349	5	1	5	986	995	5	3	10	227	196	5	6	-6	583	569
4	17	2	180	143	4	21	-3	97*	86	5	1	6	423	402	5	4	-10	314	330	5	6	-5	549	549
4	17	3	106	83	4	21	-2	287	273	5	1	7	708	688	5	4	-9	134	170	5	6	-4	1018	977
4	17	4	72*	63	4	21	-1	144	137	5	1	8	46*	123	5	4	-8	530	556	5	6	-3	508	478
4	17	5	91*	70	4	21	0	513	526	5	1	9	514	518	5	4	-7	567	554	5	6	-2	745	763
4	17	6	149	125	4	21	1	26*	104	5	1	10	122	126	5	4	-6	363	339	5	6	-1	443	422
4	17	7	26*	33	4	21	2	196	191	5	2	-10	520	527	5	4	-5	141	139	5	6	0	1112	1122
4	18	-7	275	269	4	21	3	125	115	5	2	-9	63*	74	5	4	-4	825	819	5	6	1	696	694
4	18	-6	25*	61	4	21	4	380	371	5	2	-8	666	680	5	4	-3	656	624	5	6	2	976	975
4	18	-5	686	696	4	22	-4	85*	105	5	2	-7	331	343	5	4	-2	994	1024	5	6	3	163	173
4	18	-4	0*	55	4	22	-3	622	612	5	2	-6	1354	1371	5	4	-1	763	750	5	6	4	439	446
4	18	-3	617	606	4	22	-2	0*	33	5	2	-5	208	200	5	4	0	860	865	5	6	5	410	403
4	18	-2	0*	25	4	22	-1	642	653	5	2	-4	1550	1496	5	4	1	347	334	5	6	6	855	880

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
5	6	7	185	190	5	9	-5	591	562	5	11	4	357	352	5	14	-2	361	358	5	17	-2	417	404
5	6	8	465	467	5	9	-4	380	391	5	11	5	538	537	5	14	-1	478	495	5	17	-1	278	276
5	6	9	288	262	5	9	-3	1321	1329	5	11	6	251	245	5	14	0	276	283	5	17	0	265	253
5	7	-10	299	310	5	9	-2	0*	17	5	11	7	508	519	5	14	1	472	468	5	17	1	194	188
5	7	-9	56*	86	5	9	-1	836	866	5	11	8	204	183	5	14	2	314	296	5	17	2	414	412
5	7	-8	239	237	5	9	0	494	502	5	11	9	340	338	5	14	3	407	426	5	17	3	315	301
5	7	-7	454	472	5	9	1	1532	1547	5	12	-9	0*	24	5	14	4	582	579	5	17	4	241	258
5	7	-6	535	508	5	9	2	0*	27	5	12	-8	768	753	5	14	5	400	401	5	17	5	36*	54
5	7	-5	158	144	5	9	3	649	645	5	12	-7	72*	30	5	14	6	165	141	5	17	6	244	250
5	7	-4	238	235	5	9	4	209	207	5	12	-6	720	727	5	14	7	193	192	5	18	-6	302	308
5	7	-3	873	846	5	9	5	929	936	5	12	-5	54*	49	5	14	8	269	273	5	18	-5	170	146
5	7	-2	1127	1093	5	9	6	174	158	5	12	-4	989	956	5	15	-8	0*	103	5	18	-4	566	574
5	7	-1	119	39	5	9	7	720	726	5	12	-3	0*	21	5	15	-7	705	721	5	18	-3	242	239
5	7	0	358	349	5	9	8	86*	117	5	12	-2	848	863	5	15	-6	95*	107	5	18	-2	642	623
5	7	1	412	417	5	9	9	584	582	5	12	-1	0*	2	5	15	-5	554	567	5	18	-1	273	267
5	7	2	731	742	5	10	-9	162	167	5	12	0	1010	1057	5	15	-4	77*	20	5	18	0	612	605
5	7	3	130	156	5	10	-8	0*	42	5	12	1	66*	66	5	15	-3	1034	1011	5	18	1	238	242
5	7	4	208	199	5	10	-7	378	369	5	12	2	1136	1168	5	15	-2	144	146	5	18	2	674	659
5	7	5	142	156	5	10	-6	0*	70	5	12	3	136	159	5	15	-1	566	565	5	18	3	184	186
5	7	6	535	549	5	10	-5	376	384	5	12	4	762	777	5	15	0	283	289	5	18	4	417	396
5	7	7	130	125	5	10	-4	20*	19	5	12	5	46*	14	5	15	1	1136	1168	5	18	5	190	201
5	7	8	348	349	5	10	-3	430	409	5	12	6	972	969	5	15	2	126	125	5	18	6	471	466
5	7	9	127	151	5	10	-2	237	250	5	12	7	35*	83	5	15	3	704	685	5	19	-5	655	650
5	8	-10	573	597	5	10	-1	619	624	5	12	8	462	471	5	15	4	241	251	5	19	-4	77*	98
5	8	-9	230	218	5	10	0	343	343	5	13	-8	192	204	5	15	5	886	867	5	19	-3	481	477
5	8	-8	552	541	5	10	1	595	598	5	13	-7	150	137	5	15	6	0*	112	5	19	-2	100	111
5	8	-7	0*	50	5	10	2	117	102	5	13	-6	292	280	5	15	7	455	457	5	19	-1	762	754
5	8	-6	1066	1078	5	10	3	400	466	5	13	-5	723	722	5	16	-7	0*	56	5	19	0	56*	130
5	8	-5	305	308	5	10	4	212	230	5	13	-4	276	274	5	16	-6	623	623	5	19	1	480	501
5	8	-4	937	951	5	10	5	273	300	5	13	-3	143	142	5	16	-5	122	123	5	19	2	85*	85
5	8	-3	169	154	5	10	6	48*	11	5	13	-2	434	446	5	16	-4	667	670	5	19	3	620	618
5	8	-2	1524	1494	5	10	7	391	390	5	13	-1	904	912	5	16	-3	246	263	5	19	4	0*	67
5	8	-1	326	296	5	10	8	250	238	5	13	0	275	294	5	16	-2	543	518	5	19	5	394	392
5	8	0	1592	1597	5	10	9	141	126	5	13	1	286	283	5	16	-1	155	158	5	20	-5	144	148
5	8	1	447	456	5	11	-9	438	457	5	13	2	378	372	5	16	0	762	774	5	20	-4	232	239
5	8	2	992	1018	5	11	-8	233	239	5	13	3	645	665	5	16	1	87*	84	5	20	-3	202	171
5	8	3	159	151	5	11	-7	358	337	5	13	4	290	309	5	16	2	504	509	5	20	-2	149	169
5	8	4	877	872	5	11	-6	165	126	5	13	5	328	346	5	16	3	187	183	5	20	-1	245	254
5	8	5	343	331	5	11	-5	924	929	5	13	6	243	233	5	16	4	673	660	5	20	0	141	119
5	8	6	683	683	5	11	-4	587	575	5	13	7	337	328	5	16	5	196	176	5	20	1	229	225
5	8	7	0*	96	5	11	-3	448	444	5	13	8	141	116	5	16	6	364	363	5	20	2	255	242
5	8	8	784	782	5	11	-2	124	120	5	14	-8	66*	46	5	16	7	0*	79	5	20	3	191	190
5	8	9	187	187	5	11	-1	1174	1144	5	14	-7	298	269	5	17	-7	103	123	5	20	4	0*	85
5	9	-9	492	484	5	11	0	704	688	5	14	-6	350	353	5	17	-6	256	248	5	21	-4	302	281
5	9	-8	271	274	5	11	1	421	435	5	14	-5	305	298	5	17	-5	123	129	5	21	-3	387	390
5	9	-7	841	844	5	11	2	459	484	5	14	-4	287	278	5	17	-4	235	216	5	21	-2	174	187
5	9	-6	126	136	5	11	3	983	954	5	14	-3	364	353	5	17	-3	87*	114	5	21	-1	268	262

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
5	21	0	365	351	6	2	-2	201	178	6	4	6	621	632	6	7	-4	83*	107	6	9	5	405	390
5	21	1	403	404	6	2	-1	1144	1112	6	4	7	437	430	6	7	-3	514	520	6	9	6	596	616
5	21	2	82*	115	6	2	0	516	513	6	4	8	580	583	6	7	-2	546	572	6	9	7	257	249
5	21	3	215	177	6	2	1	823	826	6	4	9	191	188	6	7	-1	1394	1419	6	9	8	425	421
5	22	-2	497	503	6	2	2	79	63	6	5	-9	181	200	6	7	0	121	107	6	10	-9	183	174
5	22	-1	103	90	6	2	3	847	869	6	5	-8	650	640	6	7	1	650	638	6	10	-8	443	440
5	22	0	568	579	6	2	4	429	448	6	5	-7	225	216	6	7	2	263	268	6	10	-7	0*	11
5	22	1	77*	34	6	2	5	901	885	6	5	-6	641	653	6	7	3	829	808	6	10	-6	577	570
5	22	2	412	418	6	2	6	73*	66	6	5	-5	180	169	6	7	4	0*	99	6	10	-5	46*	58
6	0	-10	306	317	6	2	7	541	553	6	5	-4	1100	1068	6	7	5	824	823	6	10	-4	713	737
6	0	-8	606	607	6	2	8	253	239	6	5	-3	343	337	6	7	6	148	137	6	10	-3	73*	30
6	0	-6	602	593	6	2	9	402	416	6	5	-2	667	662	6	7	7	618	649	6	10	-2	629	644
6	0	-4	1170	1130	6	3	-10	133	140	6	5	-1	155	156	6	7	8	0*	111	6	10	-1	147	118
6	0	-2	1141	1129	6	3	-9	226	206	6	5	0	1292	1302	6	7	9	459	449	6	10	0	886	913
6	0	0	612	631	6	3	-8	162	146	6	5	1	331	312	6	8	-9	474	476	6	10	1	379	356
6	0	2	1502	1497	6	3	-7	845	848	6	5	2	860	891	6	8	-8	242	230	6	10	2	654	652
6	0	4	663	657	6	3	-6	518	525	6	5	3	82	60	6	8	-7	586	589	6	10	3	80*	101
6	0	6	914	900	6	3	-5	433	431	6	5	4	589	608	6	8	-6	315	318	6	10	4	764	746
6	0	8	426	421	6	3	-4	228	214	6	5	5	357	370	6	8	-5	646	625	6	10	5	281	282
6	1	-10	329	324	6	3	-3	1460	1461	6	5	6	790	796	6	8	-4	340	359	6	10	6	548	573
6	1	-9	538	557	6	3	-2	533	536	6	5	7	115	112	6	8	-3	662	691	6	10	7	65*	72
6	1	-8	458	464	6	3	-1	565	569	6	5	8	524	543	6	8	-2	555	566	6	10	8	491	469
6	1	-7	151	185	6	3	0	74*	67	6	5	9	0*	35	6	8	-1	832	799	6	11	-8	447	459
6	1	-6	735	740	6	3	1	1235	1292	6	6	-9	281	292	6	8	0	365	377	6	11	-7	455	444
6	1	-5	900	914	6	3	2	178	168	6	6	-8	442	456	6	8	1	1033	1066	6	11	-6	227	234
6	1	-4	837	844	6	3	3	639	639	6	6	-7	470	496	6	8	2	486	484	6	11	-5	529	535
6	1	-3	368	358	6	3	4	515	512	6	6	-6	429	443	6	8	3	479	470	6	11	-4	800	791
6	1	-2	994	972	6	3	5	754	750	6	6	-5	547	548	6	8	4	246	256	6	11	-3	657	690
6	1	-1	954	975	6	3	6	322	322	6	6	-4	602	621	6	8	5	833	851	6	11	-2	267	291
6	1	0	901	922	6	3	7	599	605	6	6	-3	568	546	6	8	6	418	421	6	11	-1	532	544
6	1	1	335	354	6	3	8	174	165	6	6	-2	845	860	6	8	7	429	431	6	11	0	743	732
6	1	2	820	815	6	3	9	360	370	6	6	-1	693	687	6	8	8	177	174	6	11	1	783	805
6	1	3	699	722	6	4	-9	331	333	6	6	0	479	507	6	8	9	462	455	6	11	2	341	311
6	1	4	693	686	6	4	-8	439	466	6	6	1	576	567	6	9	-9	67*	75	6	11	3	458	493
6	1	5	478	462	6	4	-7	455	466	6	6	2	841	871	6	9	-8	302	306	6	11	4	641	648
6	1	6	595	608	6	4	-6	657	657	6	6	3	701	706	6	9	-7	358	356	6	11	5	460	474
6	1	7	443	446	6	4	-5	280	289	6	6	4	251	246	6	9	-6	795	817	6	11	6	429	417
6	1	8	358	367	6	4	-4	783	786	6	6	5	444	457	6	9	-5	79*	65	6	11	7	338	331
6	1	9	263	265	6	4	-3	649	635	6	6	6	728	728	6	9	-4	303	274	6	11	8	306	300
6	2	-10	219	222	6	4	-2	835	851	6	6	7	562	555	6	9	-3	432	423	6	12	-8	0*	27
6	2	-9	405	403	6	4	-1	557	579	6	6	8	267	256	6	9	-2	1014	1005	6	12	-7	547	566
6	2	-8	117	119	6	4	0	1223	1256	6	6	9	210	205	6	9	-1	115	85	6	12	-6	0*	15
6	2	-7	721	707	6	4	1	536	537	6	7	-9	607	619	6	9	0	655	656	6	12	-5	664	655
6	2	-6	339	351	6	4	2	439	477	6	7	-8	0*	58	6	9	1	402	394	6	12	-4	82*	48
6	2	-5	951	943	6	4	3	424	442	6	7	-7	436	438	6	9	2	827	839	6	12	-3	613	589
6	2	-4	312	307	6	4	4	897	897	6	7	-6	388	397	6	9	3	243	255	6	12	-2	73*	32
6	2	-3	1084	1094	6	4	5	115	98	6	7	-5	836	849	6	9	4	519	527	6	12	-1	921	919

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc
6	12	0	55*	60
6	12	1	552	548
6	12	2	103	91
6	12	3	825	834
6	12	4	71*	13
6	12	5	488	492
6	12	6	61*	94
6	12	7	533	543
6	12	8	93*	0
6	13	-8	338	329
6	13	-7	353	366
6	13	-6	0*	34
6	13	-5	535	541
6	13	-4	444	425
6	13	-3	502	517
6	13	-2	82*	70
6	13	-1	577	580
6	13	0	653	650
6	13	1	561	574
6	13	2	0*	95
6	13	3	541	547
6	13	4	416	407
6	13	5	508	523
6	13	6	232	234
6	13	7	316	311
6	14	-7	0*	99
6	14	-6	509	504
6	14	-5	233	231
6	14	-4	631	620
6	14	-3	484	507
6	14	-2	598	610
6	14	-1	195	184
6	14	0	657	650
6	14	1	407	400
6	14	2	644	644
6	14	3	249	248
6	14	4	608	600
6	14	5	316	329
6	14	6	431	416
6	14	7	87*	89
6	15	-7	170	169
6	15	-6	657	677
6	15	-5	222	213
6	15	-4	405	403
6	15	-3	96*	145
6	15	-2	786	782
6	15	-1	263	262

H	K	L	Fobs	Fcalc
6	15	0	472	494
6	15	1	204	188
6	15	2	773	758
6	15	3	97	102
6	15	4	495	508
6	15	5	218	204
6	15	6	430	443
6	16	-6	170	181
6	16	-5	414	399
6	16	-4	291	276
6	16	-3	412	408
6	16	-2	396	396
6	16	-1	291	288
6	16	0	267	254
6	16	1	474	471
6	16	2	372	358
6	16	3	230	221
6	16	4	309	303
6	16	5	505	505
6	16	6	208	182
6	17	-6	152	140
6	17	-5	468	473
6	17	-4	249	228
6	17	-3	525	517
6	17	-2	0*	8
6	17	-1	624	635
6	17	0	262	260
6	17	1	455	435
6	17	2	94*	47
6	17	3	562	534
6	17	4	104	104
6	17	5	401	393
6	18	-5	303	318
6	18	-4	273	283
6	18	-3	369	366
6	18	-2	417	438
6	18	-1	529	521
6	18	0	296	292
6	18	1	322	339
6	18	2	284	297
6	18	3	496	484
6	18	4	236	243
6	18	5	235	231
6	19	-4	496	494
6	19	-3	87*	115
6	19	-2	254	254
6	19	-1	0*	56

H	K	L	Fobs	Fcalc
6	19	0	481	481
6	19	1	175	189
6	19	2	299	289
6	19	3	0*	15
6	19	4	386	385
6	20	-3	46*	43
6	20	-2	369	371
6	20	-1	120	146
6	20	0	463	477
6	20	1	89*	8
6	20	2	293	283
6	20	3	165	180
6	21	-2	308	310
6	21	-1	328	321
6	21	0	191	196
6	21	1	403	385
7	0	-9	594	588
7	0	-7	728	724
7	0	-5	976	976
7	0	-3	938	975
7	0	-1	1167	1172
7	0	1	678	688
7	0	3	1368	1375
7	0	5	677	671
7	0	7	798	801
7	1	-9	191	185
7	1	-8	609	615
7	1	-7	226	207
7	1	-6	207	203
7	1	-5	268	257
7	1	-4	942	968
7	1	-3	333	337
7	1	-2	360	366
7	1	-1	491	515
7	1	0	851	868
7	1	1	283	273
7	1	2	539	540
7	1	3	383	388
7	1	4	617	619
7	1	5	378	398
7	1	6	591	593
7	1	7	204	205
7	1	8	302	311
7	2	-9	149	157
7	2	-8	214	215
7	2	-7	253	242
7	2	-6	347	331

H	K	L	Fobs	Fcalc
7	2	-5	166	152
7	2	-4	331	327
7	2	-3	360	363
7	2	-2	484	484
7	2	-1	0*	33
7	2	0	296	283
7	2	1	655	645
7	2	2	400	426
7	2	3	0*	29
7	2	4	373	368
7	2	5	291	290
7	2	6	399	411
7	2	7	0*	45
7	2	8	178	168
7	3	-9	95*	71
7	3	-8	395	386
7	3	-7	40*	61
7	3	-6	954	942
7	3	-5	243	238
7	3	-4	644	676
7	3	-3	96	95
7	3	-2	1103	1110
7	3	-1	248	261
7	3	0	784	804
7	3	1	163	191
7	3	2	1116	1120
7	3	3	171	154
7	3	4	822	826
7	3	5	112	136
7	3	6	784	799
7	3	7	70*	58
7	3	8	586	559
7	4	-9	497	492
7	4	-8	241	236
7	4	-7	642	652
7	4	-6	110	87
7	4	-5	623	626
7	4	-4	222	210
7	4	-3	960	990
7	4	-2	183	191
7	4	-1	704	727
7	4	0	383	409
7	4	1	1155	1166
7	4	2	305	275
7	4	3	622	631
7	4	4	282	301
7	4	5	1143	1149

H	K	L	Fobs	Fcalc
7	4	6	166	142
7	4	7	539	534
7	4	8	198	196
7	5	-9	195	195
7	5	-8	164	173
7	5	-7	453	463
7	5	-6	297	302
7	5	-5	195	118
7	5	-4	68*	95
7	5	-3	510	509
7	5	-2	449	433
7	5	-1	242	219
7	5	0	0*	71
7	5	1	555	565
7	5	2	36*	68
7	5	3	445	446
7	5	4	260	257
7	5	5	318	316
7	5	6	79*	84
7	5	7	289	305
7	5	8	0*	61
7	6	-9	375	365
7	6	-8	197	190
7	6	-7	488	474
7	6	-6	110	135
7	6	-5	527	531
7	6	-4	261	282
7	6	-3	517	510
7	6	-2	168	168
7	6	-1	860	857
7	6	0	399	425
7	6	1	574	559
7	6	2	130	151
7	6	3	893	902
7	6	4	347	351
7	6	5	622	631
7	6	6	0*	51
7	6	7	580	575
7	6	8	194	184
7	7	-8	784	783
7	7	-7	0*	2
7	7	-6	578	573
7	7	-5	267	262
7	7	-4	862	854
7	7	-3	85*	106
7	7	-2	797	814
7	7	-1	313	321

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fclc (x 10.) for [(C5Me5)2 Yb (OC)2 Fe (C5H4Me)] 2 at 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
7	7	0	1099	1113	7	10	-3	846	875	7	13	-1	88*	121	7	17	-2	590	608	8	2	-8	0*	88
7	7	1	0*	73	7	10	-2	199	210	7	13	0	693	704	7	17	-1	0*	3	8	2	-7	114	81
7	7	2	852	852	7	10	-1	801	817	7	13	1	191	197	7	17	0	580	608	8	2	-6	335	336
7	7	3	123	105	7	10	0	77*	65	7	13	2	695	685	7	17	1	167	158	8	2	-5	0*	3
7	7	4	1058	1077	7	10	1	961	962	7	13	3	55*	34	7	17	2	499	475	8	2	-4	81*	87
7	7	5	130	151	7	10	2	149	168	7	13	4	540	541	7	17	3	46*	23	8	2	-3	89*	30
7	7	6	805	813	7	10	3	789	770	7	13	5	0*	129	7	17	4	572	556	8	2	-2	328	342
7	7	7	0*	90	7	10	4	89*	107	7	13	6	485	470	7	18	-4	217	223	8	2	-1	83*	20
7	7	8	480	476	7	10	5	869	875	7	14	-6	121	137	7	18	-3	313	316	8	2	0	118	135
7	8	-8	239	258	7	10	6	0*	46	7	14	-5	677	662	7	18	-2	52*	77	8	2	1	89*	129
7	8	-7	309	298	7	10	7	490	487	7	14	-4	116	109	7	18	-1	406	420	8	2	2	568	565
7	8	-6	443	428	7	11	-7	383	380	7	14	-3	625	638	7	18	0	342	328	8	2	3	31*	32
7	8	-5	466	486	7	11	-6	620	604	7	14	-2	397	402	7	18	1	231	228	8	2	4	0*	30
7	8	-4	182	137	7	11	-5	54*	55	7	14	-1	682	675	7	18	2	0*	95	8	2	5	70*	6
7	8	-3	295	291	7	11	-4	538	559	7	14	0	0*	47	7	18	3	373	360	8	2	6	254	264
7	8	-2	388	415	7	11	-3	525	541	7	14	1	645	647	7	19	-3	223	227	8	2	7	99*	13
7	8	-1	733	759	7	11	-2	709	732	7	14	2	357	347	7	19	-2	76*	141	8	3	-8	0*	14
7	8	0	398	404	7	11	-1	138	133	7	14	3	669	660	7	19	-1	53*	112	8	3	-7	431	421
7	8	1	270	247	7	11	0	640	623	7	14	4	36*	15	7	19	0	130	131	8	3	-6	0*	92
7	8	2	503	511	7	11	1	315	311	7	14	5	545	534	7	19	1	215	197	8	3	-5	867	886
7	8	3	540	542	7	11	2	679	685	7	14	6	216	212	7	19	2	90*	152	8	3	-4	50*	15
7	8	4	193	201	7	11	3	243	241	7	15	-6	198	210	8	0	-8	651	663	8	3	-3	795	811
7	8	5	293	311	7	11	4	607	607	7	15	-5	421	422	8	0	-6	560	553	8	3	-2	76*	30
7	8	6	422	428	7	11	5	241	243	7	15	-4	172	169	8	0	-4	1164	1183	8	3	-1	1016	1027
7	8	7	278	259	7	11	6	383	373	7	15	-3	188	171	8	0	-2	794	806	8	3	0	0*	35
7	8	8	151	148	7	11	7	240	237	7	15	-2	199	172	8	0	0	1213	1259	8	3	1	977	985
7	9	-8	105	113	7	12	-7	0*	9	7	15	-1	404	415	8	0	2	758	782	8	3	2	0*	4
7	9	-7	24*	86	7	12	-6	221	224	7	15	0	144	158	8	0	4	1023	1040	8	3	3	891	922
7	9	-6	344	359	7	12	-5	0*	91	7	15	1	197	194	8	0	6	687	687	8	3	4	136	108
7	9	-5	363	363	7	12	-4	390	393	7	15	2	147	142	8	0	8	600	598	8	3	5	878	861
7	9	-4	222	209	7	12	-3	0*	52	7	15	3	345	340	8	1	-8	62*	4	8	3	6	0*	39
7	9	-3	71*	85	7	12	-2	296	292	7	15	4	211	182	8	1	-7	553	559	8	3	7	518	516
7	9	-2	384	379	7	12	-1	56*	32	7	15	5	232	230	8	1	-6	47*	85	8	4	-8	434	429
7	9	-1	614	607	7	12	0	551	561	7	16	-5	264	284	8	1	-5	281	302	8	4	-7	55*	106
7	9	0	220	204	7	12	1	77*	45	7	16	-4	63*	68	8	1	-4	0*	23	8	4	-6	660	674
7	9	1	344	346	7	12	2	192	162	7	16	-3	368	359	8	1	-3	750	749	8	4	-5	160	160
7	9	2	473	464	7	12	3	0*	102	7	16	-2	261	269	8	1	-2	43*	39	8	4	-4	612	592
7	9	3	344	355	7	12	4	471	469	7	16	-1	467	461	8	1	-1	509	519	8	4	-3	144	104
7	9	4	427	434	7	12	5	0*	69	7	16	0	25*	15	8	1	0	52*	53	8	4	-2	1055	1061
7	9	5	279	284	7	12	6	131	111	7	16	1	366	338	8	1	1	630	636	8	4	-1	75*	53
7	9	6	366	391	7	12	7	152	112	7	16	2	242	259	8	1	2	74*	45	8	4	0	654	642
7	9	7	134	106	7	13	-7	252	257	7	16	3	371	377	8	1	3	579	607	8	4	1	0*	19
7	10	-8	0*	64	7	13	-6	457	480	7	16	4	18*	74	8	1	4	0*	0	8	4	2	1077	1071
7	10	-7	621	618	7	13	-5	132	146	7	16	5	240	224	8	1	5	460	467	8	4	3	0*	36
7	10	-6	73*	23	7	13	-4	714	711	7	17	-5	47*	92	8	1	6	0*	67	8	4	4	663	672
7	10	-5	691	698	7	13	-3	213	207	7	17	-4	572	579	8	1	7	461	443	8	4	5	78*	79
7	10	-4	221	219	7	13	-2	632	636	7	17	-3	207	187	8	1	8	84*	22	8	4	6	698	688

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc
8	4	7	77*	55
8	5	-8	37*	30
8	5	-7	148	136
8	5	-6	78*	68
8	5	-5	181	190
8	5	-4	115	123
8	5	-3	0*	20
8	5	-2	67*	73
8	5	-1	217	230
8	5	0	66*	112
8	5	1	116	62
8	5	2	42*	33
8	5	3	0*	63
8	5	4	0*	16
8	5	5	87*	92
8	5	6	110	95
8	5	7	0*	49
8	6	-8	464	466
8	6	-7	87*	34
8	6	-6	403	407
8	6	-5	243	232
8	6	-4	748	754
8	6	-3	105	108
8	6	-2	498	513
8	6	-1	183	172
8	6	0	987	973
8	6	1	63*	77
8	6	2	655	653
8	6	3	138	131
8	6	4	833	827
8	6	5	42*	17
8	6	6	433	449
8	6	7	26*	52
8	7	-7	797	783
8	7	-6	81*	54
8	7	-5	582	576
8	7	-4	94*	65
8	7	-3	922	909
8	7	-2	115	122
8	7	-1	942	973
8	7	0	144	143
8	7	1	962	956
8	7	2	64*	20
8	7	3	979	980
8	7	4	80*	17
8	7	5	674	710
8	7	6	100*	103

H	K	L	Fobs	Fcalc
8	7	7	456	437
8	8	-7	0*	15
8	8	-6	250	238
8	8	-5	64*	96
8	8	-4	387	406
8	8	-3	242	245
8	8	-2	333	322
8	8	-1	159	143
8	8	0	535	542
8	8	1	72*	90
8	8	2	275	266
8	8	3	92*	46
8	8	4	469	471
8	8	5	130	114
8	8	6	81*	68
8	8	7	89*	80
8	9	-7	131	142
8	9	-6	164	173
8	9	-5	409	416
8	9	-4	68*	66
8	9	-3	367	387
8	9	-2	173	172
8	9	-1	424	424
8	9	0	69*	28
8	9	1	432	421
8	9	2	71*	62
8	9	3	362	372
8	9	4	24*	80
8	9	5	412	411
8	9	6	90*	24
8	10	-7	58*	73
8	10	-6	671	675
8	10	-5	74*	90
8	10	-4	664	666
8	10	-3	156	153
8	10	-2	931	932
8	10	-1	142	191
8	10	0	744	770
8	10	1	228	231
8	10	2	919	926
8	10	3	79*	78
8	10	4	680	697
8	10	5	177	162
8	10	6	541	525
8	11	-6	176	156
8	11	-5	535	531
8	11	-4	93*	135

H	K	L	Fobs	Fcalc
8	11	-3	514	523
8	11	-2	122	103
8	11	-1	587	582
8	11	0	58*	35
8	11	1	565	552
8	11	2	34*	18
8	11	3	568	570
8	11	4	0*	19
8	11	5	406	398
8	11	6	0*	2
8	12	-6	83*	6
8	12	-5	158	140
8	12	-4	199	207
8	12	-3	206	203
8	12	-2	65*	44
8	12	-1	192	179
8	12	0	153	159
8	12	1	0*	73
8	12	2	0*	41
8	12	3	155	125
8	12	4	0*	65
8	12	5	84*	41
8	13	-6	0*	92
8	13	-5	499	504
8	13	-4	168	157
8	13	-3	609	615
8	13	-2	66*	81
8	13	-1	593	591
8	13	0	0*	33
8	13	1	631	613
8	13	2	104	116
8	13	3	546	547
8	13	4	0*	52
8	13	5	435	423
8	14	-5	88*	105
8	14	-4	599	593
8	14	-3	0*	44
8	14	-2	585	597
8	14	-1	184	172
8	14	0	545	537
8	14	1	99	125
8	14	2	566	582
8	14	3	208	195
8	14	4	499	508
8	15	-4	143	142
8	15	-3	64*	151
8	15	-2	36*	15

H	K	L	Fobs	Fcalc
8	15	-1	85*	141
8	15	0	63*	16
8	15	1	73*	126
8	15	2	0*	2
8	15	3	217	208
8	15	4	66*	13
8	16	-4	287	278
8	16	-3	59*	96
8	16	-2	319	317
8	16	-1	85*	98
8	16	0	390	400
8	16	1	182	182
8	16	2	279	272
8	16	3	0*	48
8	17	-3	501	509
8	17	-2	66*	77
8	17	-1	589	580
8	17	0	0*	45
8	17	1	504	487
8	17	2	90*	39
8	18	0	351	337
9	0	-7	595	601
9	0	-5	496	493
9	0	-3	1078	1081
9	0	-1	778	767
9	0	1	977	996
9	0	3	498	523
9	0	5	707	703
9	1	-7	159	169
9	1	-6	443	439
9	1	-5	169	197
9	1	-4	443	462
9	1	-3	173	170
9	1	-2	549	546
9	1	-1	317	318
9	1	0	559	552
9	1	1	310	312
9	1	2	449	444
9	1	3	263	280
9	1	4	424	436
9	1	5	211	213
9	1	6	279	285
9	2	-7	0*	31
9	2	-6	265	293
9	2	-5	416	425
9	2	-4	156	164
9	2	-3	0*	25

H	K	L	Fobs	Fcalc
9	2	-2	323	334
9	2	-1	377	377
9	2	0	319	347
9	2	1	115	87
9	2	2	337	346
9	2	3	332	333
9	2	4	286	290
9	2	5	83*	82
9	2	6	245	230
9	3	-7	94*	67
9	3	-6	392	397
9	3	-5	42*	132
9	3	-4	819	817
9	3	-3	108	132
9	3	-2	759	765
9	3	-1	171	164
9	3	0	790	791
9	3	1	58*	58
9	3	2	817	825
9	3	3	171	170
9	3	4	539	530
9	3	5	94*	124
9	3	6	567	550
9	4	-7	293	291
9	4	-6	0*	22
9	4	-5	680	672
9	4	-4	262	265
9	4	-3	567	553
9	4	-2	66*	14
9	4	-1	866	864
9	4	0	335	322
9	4	1	580	563
9	4	2	0*	81
9	4	3	742	747
9	4	4	82*	104
9	4	5	423	404
9	4	6	140	152
9	5	-7	222	236
9	5	-6	72*	108
9	5	-5	237	254
9	5	-4	42*	62
9	5	-3	327	320
9	5	-2	138	130
9	5	-1	314	318
9	5	0	0*	21
9	5	1	379	384
9	5	2	0*	79

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fclc (x 10.) for [(C5Me5)2 Yb (OC)2 Fe (C5H4Me)] 2 at 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
9	5	3	272	258	9	9	-1	357	345	9	14	-1	430	437	10	4	-4	511	502	10	9	-3	249	234
9	5	4	0*	15	9	9	0	388	392	9	14	0	52*	68	10	4	-3	252	266	10	9	-2	360	373
9	5	5	179	197	9	9	1	330	328	9	14	1	422	406	10	4	-2	251	242	10	9	-1	300	294
9	5	6	87*	51	9	9	2	337	340	9	14	2	59*	100	10	4	-1	157	164	10	9	0	336	321
9	6	-6	100*	71	9	9	3	180	206	9	15	-2	121	122	10	4	0	470	467	10	9	1	187	176
9	6	-5	335	345	9	9	4	236	226	9	15	-1	163	186	10	4	1	288	282	10	9	2	390	379
9	6	-4	345	346	9	9	5	260	242	9	15	0	65*	63	10	4	2	291	293	10	9	3	214	199
9	6	-3	706	703	9	10	-5	599	588	9	15	1	239	233	10	4	3	0*	122	10	10	-3	0*	8
9	6	-2	144	156	9	10	-4	89*	95	10	0	-4	308	305	10	4	4	332	325	10	10	-2	294	292
9	6	-1	448	452	9	10	-3	526	523	10	0	-2	594	577	10	5	-5	45*	67	10	10	-1	243	233
9	6	0	367	358	9	10	-2	207	216	10	0	0	425	413	10	5	-4	461	452	10	10	0	423	423
9	6	1	753	753	9	10	-1	679	653	10	0	2	494	492	10	5	-3	0*	17	10	10	1	0*	69
9	6	2	200	215	9	10	0	0*	10	10	0	4	289	278	10	5	-2	394	394	10	10	2	385	370
9	6	3	466	468	9	10	1	579	572	10	1	-5	289	281	10	5	-1	84*	86	10	11	-2	195	204
9	6	4	255	251	9	10	2	187	180	10	1	-4	321	316	10	5	0	454	461	10	11	-1	154	176
9	6	5	478	460	9	10	3	628	623	10	1	-3	320	328	10	5	1	60*	62	10	11	0	204	216
9	6	6	0*	64	9	10	4	64*	11	10	1	-2	384	387	10	5	2	398	400	10	11	1	244	246
9	7	-6	639	626	9	10	5	419	404	10	1	-1	207	214	10	5	3	49*	42	10	11	2	131	124
9	7	-5	0*	92	9	11	-5	0*	57	10	1	0	424	423	10	5	4	378	368	10	12	-1	295	279
9	7	-4	601	579	9	11	-4	427	409	10	1	1	370	354	10	6	-5	185	177	10	12	0	0*	92
9	7	-3	0*	41	9	11	-3	103*	170	10	1	2	330	325	10	6	-4	245	235	11	0	-3	0*	21
9	7	-2	702	680	9	11	-2	360	371	10	1	3	0*	131	10	6	-3	432	419	11	0	-1	277	243
9	7	-1	0*	37	9	11	-1	139	143	10	1	4	298	299	10	6	-2	405	400	11	0	1	172	176
9	7	0	742	757	9	11	0	312	296	10	1	5	279	269	10	6	-1	207	194	11	1	-3	325	321
9	7	1	62*	9	9	11	1	50*	65	10	2	-5	427	441	10	6	0	275	276	11	1	-2	161	157
9	7	2	692	689	9	11	2	451	452	10	2	-4	331	326	10	6	1	395	377	11	1	-1	421	428
9	7	3	47*	42	9	11	3	184	171	10	2	-3	374	381	10	6	2	419	414	11	1	0	53*	45
9	7	4	650	640	9	11	4	288	298	10	2	-2	0*	47	10	6	3	254	279	11	1	1	365	355
9	7	5	90*	82	9	12	-4	252	272	10	2	-1	546	529	10	6	4	228	239	11	1	2	177	173
9	7	6	335	322	9	12	-3	179	162	10	2	0	245	230	10	7	-4	59*	47	11	2	-3	124	129
9	8	-6	248	275	9	12	-2	0*	81	10	2	1	410	417	10	7	-3	376	372	11	2	-2	396	409
9	8	-5	153	146	9	12	-1	88*	104	10	2	2	35*	64	10	7	-2	0*	47	11	2	-1	93*	46
9	8	-4	88*	117	9	12	0	393	390	10	2	3	395	397	10	7	-1	341	333	11	2	0	513	495
9	8	-3	357	349	9	12	1	155	140	10	2	4	188	178	10	7	0	45*	31	11	2	1	0*	94
9	8	-2	470	480	9	12	2	0*	139	10	2	5	361	354	10	7	1	499	485	11	2	2	406	398
9	8	-1	124	116	9	12	3	29*	24	10	3	-5	360	357	10	7	2	0*	27	11	3	-3	129	140
9	8	0	141	113	9	12	4	280	270	10	3	-4	156	155	10	7	3	354	329	11	3	-2	54*	54
9	8	1	341	331	9	13	-4	415	437	10	3	-3	396	388	10	7	4	0*	30	11	3	-1	184	177
9	8	2	335	313	9	13	-3	202	197	10	3	-2	235	239	10	8	-4	0*	57	11	3	0	270	256
9	8	3	251	240	9	13	-2	477	467	10	3	-1	495	480	10	8	-3	216	228	11	3	1	162	165
9	8	4	179	179	9	13	-1	156	153	10	3	0	150	130	10	8	-2	189	168	11	3	2	99*	107
9	8	5	206	181	9	13	0	425	429	10	3	1	377	378	10	8	-1	462	457	11	4	-2	267	262
9	9	-6	156	149	9	13	1	144	138	10	3	2	192	200	10	8	0	0*	51	11	4	-1	0*	109
9	9	-5	249	262	9	13	2	438	430	10	3	3	454	443	10	8	1	236	233	11	4	0	222	220
9	9	-4	370	357	9	13	3	210	217	10	3	4	154	135	10	8	2	244	230	11	4	1	216	187
9	9	-3	183	187	9	14	-3	498	491	10	3	5	243	265	10	8	3	352	351	11	4	2	248	234
9	9	-2	343	354	9	14	-2	88*	96	10	4	-5	137	132	10	9	-4	309	313	11	5	-2	0*	10

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fclc (x 10.) for [(C5Me5)2 Yb (OC)2 Fe (C5H4Me)] 2 at 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
11	5	-1	398	385																				
11	5	0	132	121																				
11	5	1	472	473																				
11	6	-1	214	180																				
11	6	0	242	230																				
11	6	1	70*	98																				

Reflections flagged with an asterisk were considered unobserved.

LAWRENCE BERKELEY LABORATORY
TECHNICAL INFORMATION DEPARTMENT
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720