Title
A PENTAMETHYLCYCLOPENTAOIENYL, CHLORO, OXO, ETHER COMPLEX OF YB(III)

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Publication Date
1989

LBL-26603
Preprint

Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

Materials & Chemical Sciences Division

Submitted to Acta Crystallographica C

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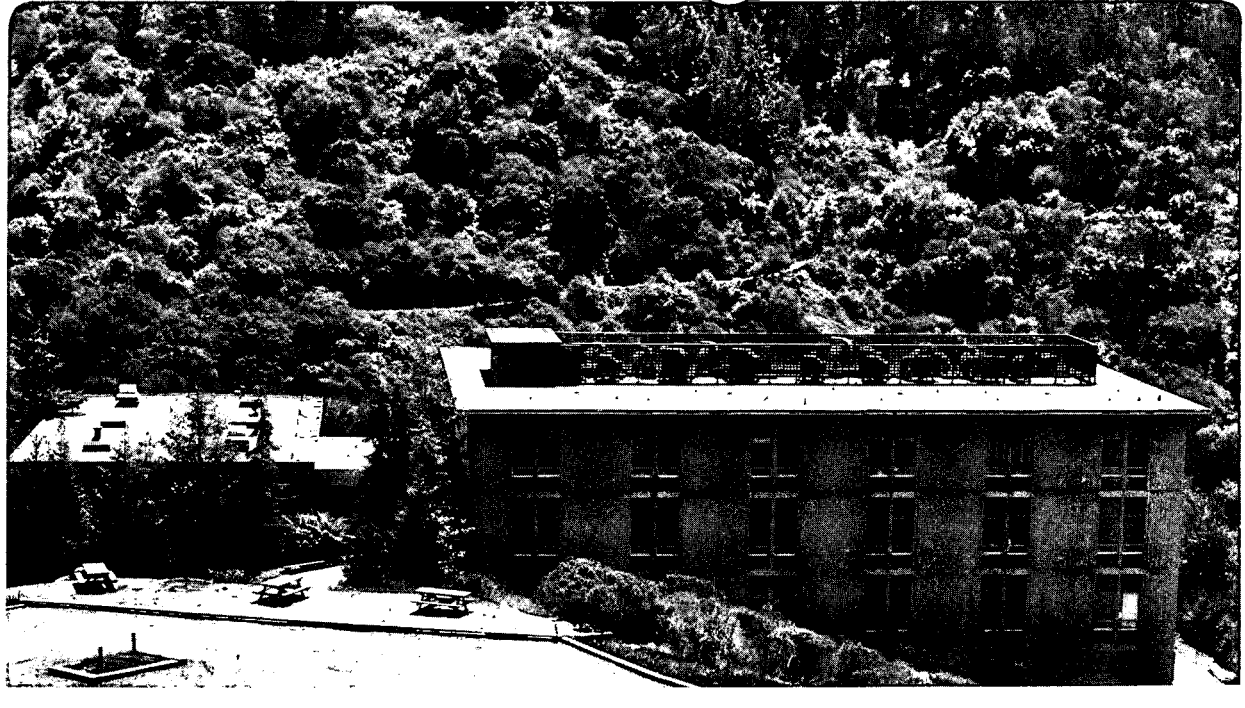

Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098.

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A Pentamethylcyclopentadienyl, Chloro, Oxo, Ether Complex of Yb(III)

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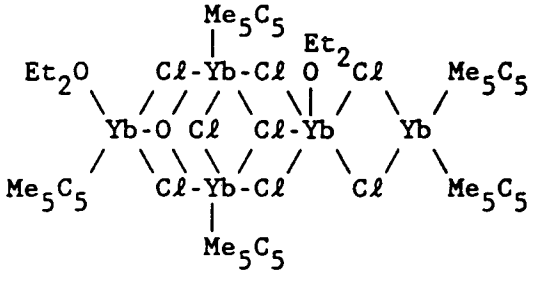
Abstract. $(Me_5C_5)_5C\ell_8(Et_2O)_2OYb_5$, $C_{58}H_{95}C\ell_8O_3Yb_5$, M_r = 1989.23, monoclinic, $P2_1/m$, a = 17.007(3) Å, b= 16.485(3) Å, c = 13.592(3) Å, β = 111.39(2)°, V = 3548.2 Å^3, Z = 2, D_x = 1.86 g/cm^3, λ(MoKα) = 0.71073 Å, μ = 68.49 cm^{-1}, F(000) = 1906, T = 296 K, R = 0.056 for 4061 [$F^2 > 2\sigma(F^2)$] of 6532 total unique data. The structure consists of a single large cluster in which the 5 ytterbium atoms are linked together by Cℓ and O bridges. The π-bonding cyclopentadienyl rings and the oxygen atoms of the ether ligands are bonded to the Yb atoms on the periphery of the cluster.

Experimental. The complex was isolated form the reaction of $Yb(C_5Me_5)_2(OEt_2)$ with $YbC\ell_3$ containing some $YbOC\ell$ as an impurity.



A blue air-sensitive crystal, 0.15x0.27x0.33 mm,was sealed inside a quartz capillary in an argon filled drybox. X-ray diffraction intensities (θ-2θ scans) were obtained using a modified Picker FACS-I automatic diffractometer equipped with a graphite monochromator. Cell dimensions from 27 reflections, $20°<2\theta<26°$; analytical absorption correction, range 2.0 to 3.1; max $\sin\theta/\lambda$ = 0.60 Å, h -20 to 20, k 0 to 19, ℓ -16 to 16; three standard reflections, 2.2%, 2.1%, 2.3% variation in standards' intensities from average, intensities adjusted isotropically; 13177 data, 6532 unique (including 4061, $F^2>2\sigma(F^2)$), R_{int}= 0.045; structure solved by Patterson and Fourier methods; refined on F, 281 parameters; hydrogen atoms not included; distance restraints on one ether (O2-C29 1.45(1), C29-C30 1.54(1)Å) and two atoms of a methyl Cp ring (C23-C23' 1.41(1), C23-C28 1.54(1)Å); anisotropic thermal parameters on 28 atoms (4 Yb, 5 Cl, 2 O & 17 C atoms), and isotropic on 16 atoms (1 O & 15 C atoms); R = 0.099 (all data), R = 0.056 ($F^2>2\sigma(F^2)$ data), wR = 0.072, S = 1.44; w = $4F^2[\sigma^2(F^2)+(0.035F^2)^2]^{-1}$; max (shift/$\sigma$) = 0.06; extinction correction - $F_{obs}(1+3.4x10^{-8}I)$, max correction 2.7%; max. & min of ΔF synthesis 2.3 and -1.9 e/Å^3; atomic f for neutral Yb, Cℓ, O & C atoms from International Tables (1974); local unpublished programs and ORTEP (Johnson, 1965).

Atomic parameters are listed in Table 1,* and distances and angles are listed in Table 2. Figure 1 shows a schematic of the structure.

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*Lists of structure factors, anisotropic thermal parameters, distances and angles, and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. XXXXX (17 pp). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Related Literature. Comparable distances for bridging Yb-Cℓ are 2.595 and 2.756 Å for $Li[YbCl_2(C_5Me_5)_2][Et_2O]$ and $Yb(C_5Me_5)_2(\mu\text{-}Cl)_2AlCl_2$ respectively (Watson, Whitney & Harlow, 1981). Bridging Yb-O distances of 2.241 and 2.21 Å have been reported for $YbFe_2O_4$ (Kato, Kamada, Kimizuka & Katsura, 1975) and YbOCℓ (Brandt & Diehl, 1974) respectively. A comparable distance for Yb-Cp is 2.347(2) Å in $(C_5Me_5)_2Yb(SC_6H_5)(NH_3)$ (Zalkin, Henly & Andersen, 1987).

Acknowledgment. Helpful discussions with Professor R. A. Andersen are appreciated. DJB gratefully acknowledges the support of the Natural Sciences and Engineering Research Council of Canada for a 1987 Postgraduate Scholarship. 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 No. DE-AC03-76SF-F00098.

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Table 1. Positional and Thermal Parameters

$$B_{eq} = 1/3\sum B_{ij} a_i^* a_j^* a_i \cdot a_j$$

Atom	x	y	z	B or B_{eq}
Yb1	0.32713(4)	0.13684(5)	0.22881(5)	3.28(2)
Yb2	0.36221(6)	1/4	0.00730(8)	3.11(3)
Yb3	0.09337(7)	1/4	0.20326(9)	4.66(4)
Yb4	-0.05438(6)	1/4	0.38927(8)	3.54(3)
Cℓ1	0.2735(3)	1/4	0.3353(4)	3.7(2)
Cℓ2	0.4502(3)	1/4	0.2580(5)	3.9(2)
Cℓ3	0.3689(3)	0.09673(28)	0.0640(3)	4.6(1)
Cℓ4	0.01739(29)	0.14491(29)	0.3001(4)	5.1(2)
Cℓ5	0.16355(27)	0.1146(3)	0.1382(4)	5.3(2)
O1	0.2820(9)	1/4	0.1067(11)	3.9(5)
O2	0.5107(12)	1/4	0.0443(14)	5.7(7)
O3	-0.0134(22)	1/4	0.0192(27)	12.4(9)
C1	0.3224(17)	-0.0077(14)	0.3108(23)	7.3(10)
C2	0.3363(18)	0.0482(19)	0.3894(22)	7.2(10)
C3	0.4156(21)	0.0822(12)	0.4123(14)	7.3(9)
C4	0.4477(12)	0.0441(18)	0.3417(23)	6.8(9)
C5	0.3891(22)	-0.0096(15)	0.2835(17)	6.8(10)
C6	0.2480(28)	-0.0638(28)	0.267(3)	15.4(13)
C7	0.2806(27)	0.0701(25)	0.452(3)	15.2(13)
C8	0.4677(25)	0.1367(23)	0.500(3)	13.1(11)
C9	0.5312(23)	0.0413(25)	0.3195(29)	13.4(11)
C10	0.4089(23)	-0.0722(23)	0.2113(28)	12.4(10)

C11	0.2336(11)	0.2079(12)	-0.1549(12)	5.6(6)
C12	0.3059(11)	0.1802(12)	-0.1785(12)	4.5(6)
C13	0.3505(19)	1/4	-0.1913(16)	4.9(9)
C14	0.4262(20)	1/4	-0.2322(24)	8.7(15)
C15	0.3279(19)	0.0903(14)	-0.1964(17)	8.9(11)
C16	0.1654(14)	0.1519(20)	-0.1448(19)	9.6(11)
C17	-0.0233(12)	0.2078(13)	0.5878(14)	6.1(7)
C18	0.0500(13)	0.1817(14)	0.5664(14)	5.8(7)
C19	0.0941(14)	1/4	0.5509(18)	4.1(7)
C20	0.1750(15)	1/4	0.5352(23)	6.2(11)
C21	0.0831(19)	0.0945(14)	0.5686(18)	9.1(11)
C22	-0.0744(18)	0.1494(22)	0.6258(23)	11.8(14)
C23	-0.1890(16)	0.2078(8)	0.2259(21)	8.6(7)
C24	-0.2022(14)	0.1778(15)	0.3139(19)	7.2(5)
C25	-0.2169(15)	1/4	0.3686(19)	4.3(5)
C26	-0.262(3)	1/4	0.446(4)	11.7(13)
C27	-0.2084(27)	0.0940(28)	0.361(3)	15.3(13)
C28	-0.193(5)	0.162(4)	0.125(4)	27.1(28)
C29	0.5504(24)	0.1788(17)	0.018(3)	14.9(13)
C30	0.5924(29)	0.1181(27)	0.105(3)	16.5(15)
C31	-0.050(3)	0.166(3)	-0.029(4)	16.6(15)
C32	-0.035(3)	0.109(4)	-0.096(4)	20.3(19)

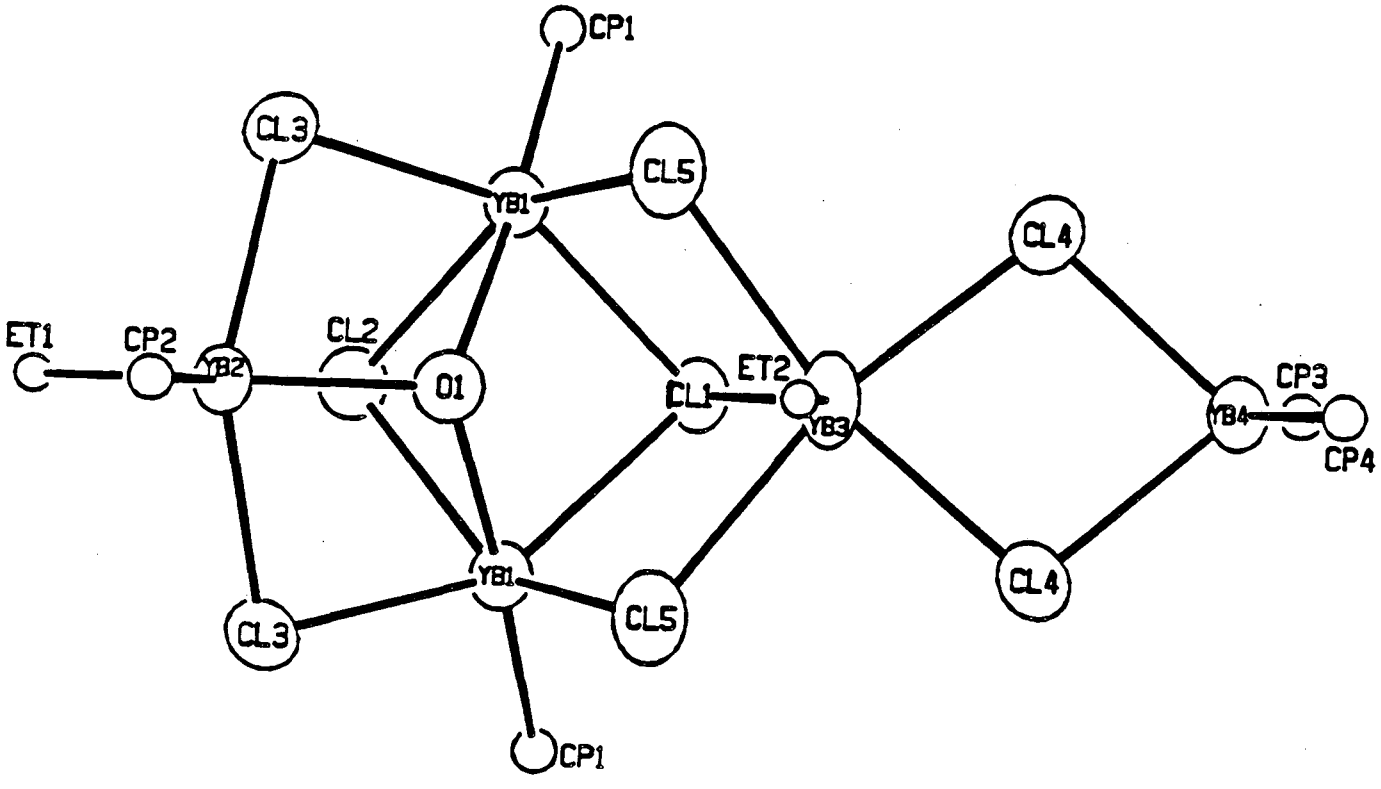
Table II. Selected Distances (Å) and Angles (°)*

Cp1 - Yb1	2.324	O2 - Yb2	2.388(18)	C17 - Yb4	2.646(17)
O1 - Yb1	2.428(9)	Cℓ2 - Yb2	3.183(6)	C18 - Yb4	2.664(18)
C1 - Yb1	2.644(18)	Cℓ3 - Yb2	2.632(5)	C19 - Yb4	2.675(20)
C2 - Yb1	2.584(17)	C11 - Yb2	2.570(16)	C23 - Yb4	2.635(26)
C3 - Yb1	2.562(16)	C12 - Yb2	2.618(15)	C24 - Yb4	2.628(24)
C4 - Yb1	2.569(17)	C13 - Yb2	2.634(19)	C25 - Yb4	2.675(24)
C5 - Yb1	2.631(20)	O3 - Yb3	2.50(3)	O1 - Cℓ1	3.163(15)
Cℓ1 - Yb1	2.715(4)	Cℓ1 - Yb3	2.932(6)	O1 - Cℓ2	2.850(15)
Cℓ2 - Yb1	2.723(4)	Cℓ4 - Yb3	2.76(3)	O1 - Cℓ3	3.087(10)
Cℓ3 - Yb1	2.669(4)	Cℓ5 - Yb3	2.82(3)	O1 - Cℓ5	3.139(11)
Cℓ5 - Yb1	2.625(4)	Cℓ4 - Yb4	2.653(5)	C29 - O2	1.463(14)
Cp2 - Yb2	2.301	Cp3 - Yb4	2.368	C31 - O3	1.57(5)
O1 - Yb2	2.243(15)	Cp4 - Yb4	2.348		

Cℓ1-Yb1-Cp1	105.79	O2 -Yb2-Cp2	111.56	Cp3-Yb4-Cp4	135.20
Cℓ2-Yb1-Cp1	108.51	Cℓ3-Yb2-Cℓ3	147.51(18)	Yb1-Cℓ1-Yb1	86.81(15)
Cℓ3-Yb1-Cp1	103.57	Cℓ3-Yb2-O1	78.14(11)	Yb1-Cℓ1-Yb3	98.79(15)
Cℓ5-Yb1-Cp1	108.13	Cℓ3-Yb2-O2	90.52(16)	Yb1-Cℓ2-Yb1	86.49(15)
O1 -Yb1-Cp1	175.06	O1 -Yb2-O2	134.6(6)	Yb1-Cℓ2-O1	51.60(17)
Cℓ1-Yb1-Cℓ2	80.88(14)	Cℓ1-Yb3-Cℓ4	105.91(13)	Yb2-Cℓ2-O1	43.2(3)
Cℓ1-Yb1-Cℓ3	149.53(13)	Cℓ1-Yb3-Cℓ5	74.02(11)	Yb1-Cℓ3-Yb2	90.66(13)
Cℓ1-Yb1-Cℓ5	80.88(16)	Cℓ1-Yb3-O3	145.9(8)	Yb3-Cℓ4-Yb4	100.43(16)
Cℓ1-Yb1-O1	75.7(3)	Cℓ4-Yb3-Cℓ4	77.61(19)	Yb1-Cℓ5-Yb3	103.87(16)
Cℓ2-Yb1-Cℓ3	82.31(16)	Cℓ4-Yb3-Cℓ5	88.74(14)	Yb1-O1 -Yb1	100.4(5)
Cℓ2-Yb1-Cℓ5	142.27(15)	Cℓ4-Yb3-Cℓ5	165.84(14)	Yb1-O1 -Yb2	107.6(4)
Cℓ2-Yb1-O1	66.9(3)	Cℓ4-Yb3-O3	100.5(6)	Yb1-O1 -Cℓ2	61.5(3)
Cℓ3-Yb1-Cℓ5	97.62(15)	Cℓ5-Yb3-Cℓ5	104.60(20)	Yb2-O1 -Cℓ2	76.3(4)
Cℓ3-Yb1-O1	74.4(3)	Cℓ5-Yb3-O3	85.5(5)	Yb2-O2 -C29	119.7(19)
Cℓ5-Yb1-O1	76.7(4)	Cℓ4-Yb4-Cℓ4	81.53(21)	C29-O2 -C29	106(3)
Cℓ2-Yb2-Cp2	174.31	Cℓ4-Yb4-Cp3	106.08	Yb3-O3 -C31	116.9(22)
Cℓ3-Yb2-Cp2	104.88	Cℓ4-Yb4-Cp4	107.47	C31-O3 -C31	125(4)
O1 -Yb2-Cp2	113.85				

* Cp1, Cp2, Cp3 & Cp4 represent the ring centers of atom groups: C1-C5; C11,C11',C12,C12',C13; C17,C17',C18,C18',C19; & C23,C23',C24,C24',C25. Primed symbols are atoms in position x,1/2-y,z.

Figure 1. ORTEP schematic drawing of ytterbium complex. Pentamethylcyclopentadienes are represented by CP: CP1 (C1-C10), CP2 (C11-C16), CP3 (C17-C22) & CP4 (C23-C28); Ethyl ethers are represented by ET: ET1 (O2, C29, C30) & ET2 (O3, C31, C32).



SUPPLEMENTAL MATERIALS

A Pentamethylcyclopentadienyl, Chloro, Oxo, Ether Complex of Yb(III)

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Abstract. $(Me_5C_5)_5C\ell_8(Et_2O)_2OYb_5$, $C_{58}H_{95}C\ell_8O_3Yb_5$, M_r = 1989.23, monoclinic, $P2_1/m$, a = 17.007(3) Å, b= 16.485(3) Å, c = 13.592(3) Å, β = 111.39(2)°, V = 3548.2 Å^3, Z = 2, D_x = 1.86 g/cm^3, λ(MoKα) = 0.71073 Å, μ = 68.49 cm^{-1}, F(000) = 1906, T = 296 K, R = 0.056 for 4061 [$F^2 > 2\sigma(F^2)$] of 6532 total unique data. The structure is a single large cluster in which the 5 ytterbium atoms are linked together by Cℓ and O bridges. The π-bonding cyclopentadienyl rings and the oxygen atoms of the ether ligands are bonded to the Yb atoms on the periphery of the cluster.

Supplementary Table 1. Thermal Parameters ($Å^2$) *

Atom	B or B11	B22	B33	B12	B13	B23
Yb1	3.31(3)	3.64(3)	3.017(29)	0.115(27)	1.299(23)	0.320(27)
Yb2	2.88(4)	3.69(5)	2.89(4)	0	1.21(3)	0
Yb3	2.85(4)	7.37(8)	3.86(5)	0	1.35(4)	0
Yb4	2.71(4)	4.33(5)	3.65(5)	0	1.24(4)	0
Cℓ1	3.82(24)	4.24(28)	3.27(24)	0	1.72(20)	0
Cℓ2	2.92(22)	4.07(28)	4.53(27)	0	1.25(20)	0
Cℓ3	6.51(24)	3.94(21)	4.17(20)	0.50(18)	2.87(18)	-0.07(17)
Cℓ4	5.37(22)	4.82(23)	5.67(23)	0.18(19)	2.74(19)	-0.75(20)
Cℓ5	3.57(18)	6.75(28)	5.31(22)	-1.23(19)	1.46(17)	-1.43(21)
O1	3.9(7)	4.3(8)	3.3(7)	0	1.1(6)	0
O2	6.1(10)	6.9(11)	6.2(10)	0	4.6(9)	0
O3	12.4(9)					
C1	8.7(15)	3.2(10)	8.2(16)	-1.7(10)	1.0(13)	3.4(10)
C2	8.9(16)	7.8(16)	7.2(14)	4.5(14)	5.4(13)	6.0(13)
C3	12.5(20)	3.1(9)	2.2(8)	0.4(11)	-2.0(10)	1.2(7)
C4	3.6(9)	8.5(16)	8.5(15)	3.0(10)	2.3(10)	6.4(14)
C5	11.4(19)	5.3(12)	4.5(10)	4.1(13)	3.9(13)	1.8(9)
C6	15.4(13)					
C7	15.2(13)					
C8	13.1(11)					
C9	13.4(11)					
C10	12.4(10)					
C11	4.2(8)	9.1(14)	2.9(7)	-2.6(8)	0.7(6)	0.1(8)
C12	5.3(9)	5.0(10)	2.2(6)	-0.3(8)	0.4(6)	-1.0(7)
C13	8.3(17)	5.6(14)	0.8(8)	0	1.7(9)	0
C14	6.0(16)	16.9(35)	5.1(15)	0	4.1(14)	0
C15	14.2(21)	4.8(11)	5.3(11)	2.3(13)	0.6(12)	-2.0(10)
C16	4.9(10)	16.5(25)	6.8(13)	-3.3(14)	1.3(9)	2.9(15)
C17	5.5(9)	9.2(15)	3.9(8)	-1.2(9)	2.1(7)	0.6(8)
C18	6.1(10)	6.7(12)	3.6(8)	1.3(10)	0.6(8)	1.6(9)
C19	3.2(10)	3.8(12)	3.6(11)	0	-0.7(8)	0
C20	2.5(10)	9.1(21)	6.6(16)	0	1.3(11)	0
C21	14.5(23)	4.1(11)	5.9(12)	1.8(13)	0.5(13)	0.7(10)
C22	8.3(16)	18.0(29)	9.4(18)	-6.3(18)	3.4(14)	3.9(18)
C23	8.6(7)					
C24	7.2(5)					
C25	4.3(5)					
C26	11.7(13)					
C27	15.3(13)					
C28	27.1(28)					
C29	14.9(13)					
C30	16.5(15)					
C31	16.6(15)					
C32	20.3(19)					

* Anisotropic temperature factor form = $\exp[-(B11\ h^2\ a^{*2}+2B12\ hka^*b^*+...)/4]$

Isotropic temperature factor form = $\exp[-B(\sin\theta/\lambda)^2]$

Supplemental Table 3. Additional Distances and Angles

C29 - O2	1.463(14)	C11 - C11	1.39(4)	C24 - C23	1.39(3)
C31 - O3	1.57(5)	C12 - C11	1.453(25)	C23 - C23	1.390(25)
C2 - C1	1.36(3)	C16 - C11	1.527(27)	C28 - C23	1.550(15)
C5 - C1	1.32(3)	C13 - C12	1.423(23)	C25 - C24	1.472(26)
C6 - C1	1.50(5)	C15 - C12	1.569(28)	C27 - C24	1.54(5)
C3 - C2	1.39(3)	C14 - C13	1.58(4)	C24 - C25	1.472(26)
C7 - C2	1.53(5)	C17 - C17	1.39(4)	C26 - C25	1.51(5)
C4 - C3	1.41(3)	C18 - C17	1.445(27)	O2 - C29	1.463(14)
C8 - C3	1.50(4)	C22 - C17	1.509(28)	C30 - C29	1.518(14)
C5 - C4	1.35(3)	C19 - C18	1.411(25)	C32 - C31	1.38(6)
C9 - C4	1.56(4)	C21 - C18	1.54(3)	O3 - C31	1.57(5)
C10 - C5	1.54(4)	C20 - C19	1.47(3)		

C29-O2-C29	106(3)	C4 -C5-C10	121(3)	C19-C1-C21	122.5(20)
C31-O3-C31	125(4)	C11-C1-C12	108.3(11)	C18-C1-C18	105.9(25)
C2 -C1-C5	108.4(23)	C11-C1-C16	127.1(15)	C18-C1-C20	126.8(12)
C2 -C1-C6	127(4)	C12-C1-C16	124.2(20)	C18-C1-C20	126.8(12)
C5 -C1-C6	124(4)	C11-C1-C13	107.7(18)	C23-C2-C24	110.9(12)
C1 -C2-C3	109.0(21)	C11-C1-C15	126.8(20)	C23-C2-C28	119.3(26)
C1 -C2-C7	129(3)	C13-C1-C15	125.2(19)	C24-C2-C28	128.5(29)
C3 -C2-C7	121(4)	C12-C1-C12	107.9(24)	C23-C2-C25	104.9(21)
C2 -C3-C4	104.7(20)	C12-C1-C14	125.6(12)	C23-C2-C27	137.2(25)
C2 -C3-C8	131(3)	C12-C1-C14	125.6(12)	C25-C2-C27	117.8(23)
C4 -C3-C8	123(3)	C17-C1-C18	107.3(13)	C24-C2-C24	107.9(25)
C3 -C4-C5	107.7(20)	C17-C1-C22	129.7(17)	C24-C2-C26	125.1(13)
C3 -C4-C9	138(3)	C18-C1-C22	121.7(23)	C24-C2-C26	125.1(13)
C5 -C4-C9	113(3)	C17-C1-C19	109.7(20)	O2 -C2-C30	117(3)
C1 -C5-C4	110.2(22)	C17-C1-C21	127.6(22)	O3 -C3-C32	137(5)
C1 -C5-C10	127(3)				

Supplemental Table 4. Least-Squares Planes

PLANE NO. 1
EQUATION OF THE PLANE: 2.89491 a - 11.73275 b + 7.78143 c = 3.44172

DISTANCE TO THE PLANE FROM ATOMS			
FORMING	THE PLANE	NOT FORMING	THE PLANE
C1	0.000(39)	Yb1	-2.320(15)
C2	-0.003(40)	C6	0.11(7)
C3	0.006(45)	C7	0.07(7)
C4	-0.004(41)	C8	0.20(7)
C5	0.004(46)	C9	0.10(7)
		C10	0.23(7)

PLANE NO. 2
EQUATION OF THE PLANE: 3.62507 a + 11.30830 c = -0.90602

DISTANCE TO THE PLANE FROM ATOMS			
FORMING	THE PLANE	NOT FORMING	THE PLANE
C11	0.002(25)	Yb2	2.302(9)
C12	-0.004(25)	C14	-0.18(5)
C13	0.013(37)	C15	-0.13(5)
C11'	0.002(25)	C16	-0.13(5)
C12'	-0.004(25)	C15'	-0.13(4)
		C16'	-0.13(5)

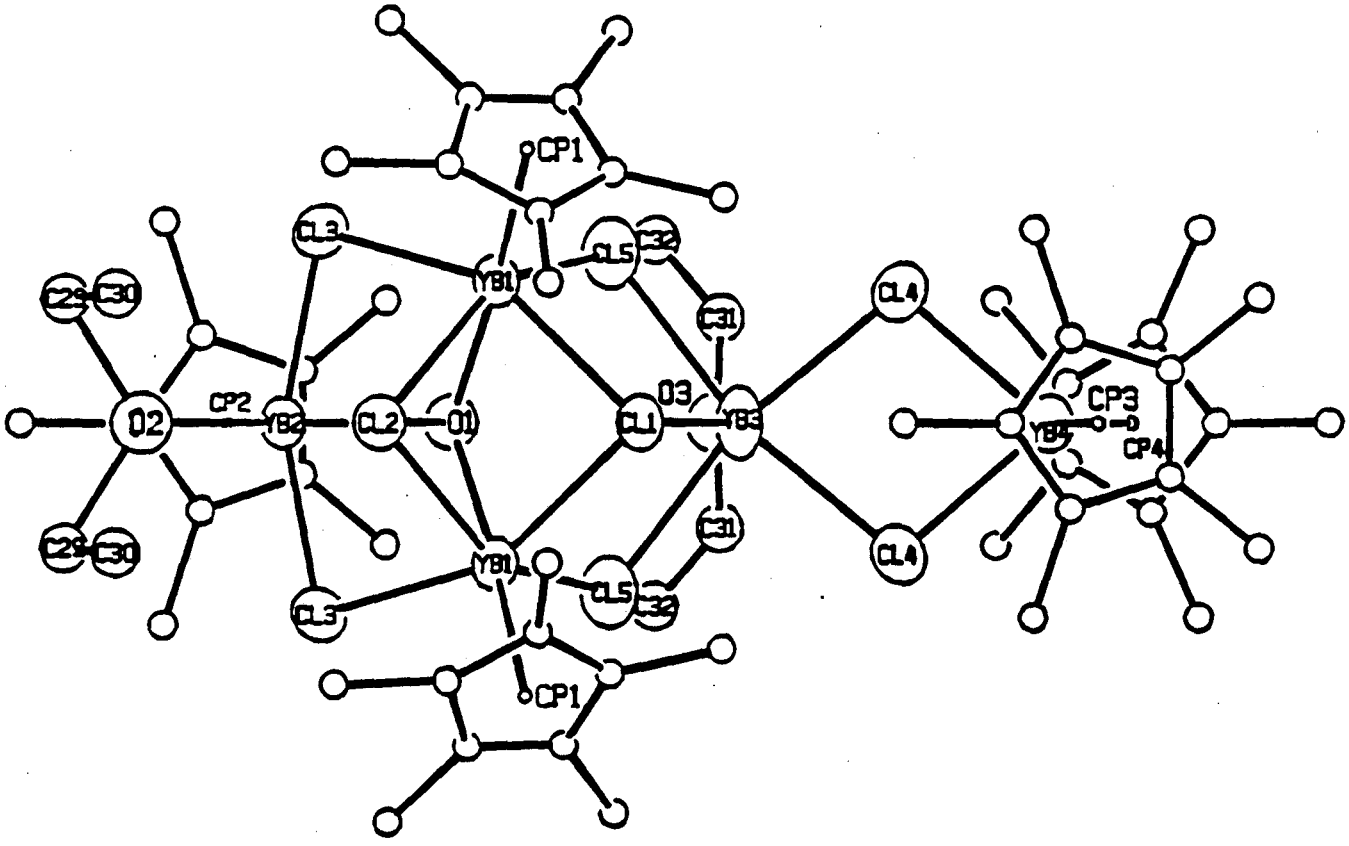
PLANE NO. 3
EQUATION OF THE PLANE: 3.50327 a + 0.03314 b + 11.36320 c = 6.60844

DISTANCE TO THE PLANE FROM ATOMS			
FORMING	THE PLANE	NOT FORMING	THE PLANE
C17	-0.00(3)	Yb4	-2.367(12)
C18	0.01)3)	C20	0.09(5)
C19	-0.01(3)	C21	0.15(5)
C17'	-0.02(4)	C22	0.25(5)
C18'	0.01(4)	C21'	0.16(5)
		C22'	0.25(5)

PLANE NO. 4
EQUATION OF THE PLANE: 14.30315 a + 0.10629 b + 2.67735 c = -2.05901

DISTANCE TO THE PLANE FROM ATOMS			
FORMING	THE PLANE	NOT FORMING	THE PLANE
C23	-0.02(4)	Yb4	2.350(13)
C24	0.03(3)	C26	-0.46(7)
C25	-0.03(3)	C27	0.06(6)
C23'	-0.01(4)	C28	-0.35(9)
C24'	0.04(4)	C27'	0.09(6)
		C28'	-0.33(5)

Supplementary Figure 1. ORTEP Drawing Showing Pentamethyl Cp Rings.



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