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BIS(PENTAMETHYLCYCLOPENTADIENYL)YTTERBIUM(III)
(PHENYLSULFIDE)(AMMONIA)$[(CH_3)_5C_5]_2Yb(SC_6H_5)\cdot NH_3$

A. Zalkin, T.J. Henley, and R.A. Andersen

April 1986

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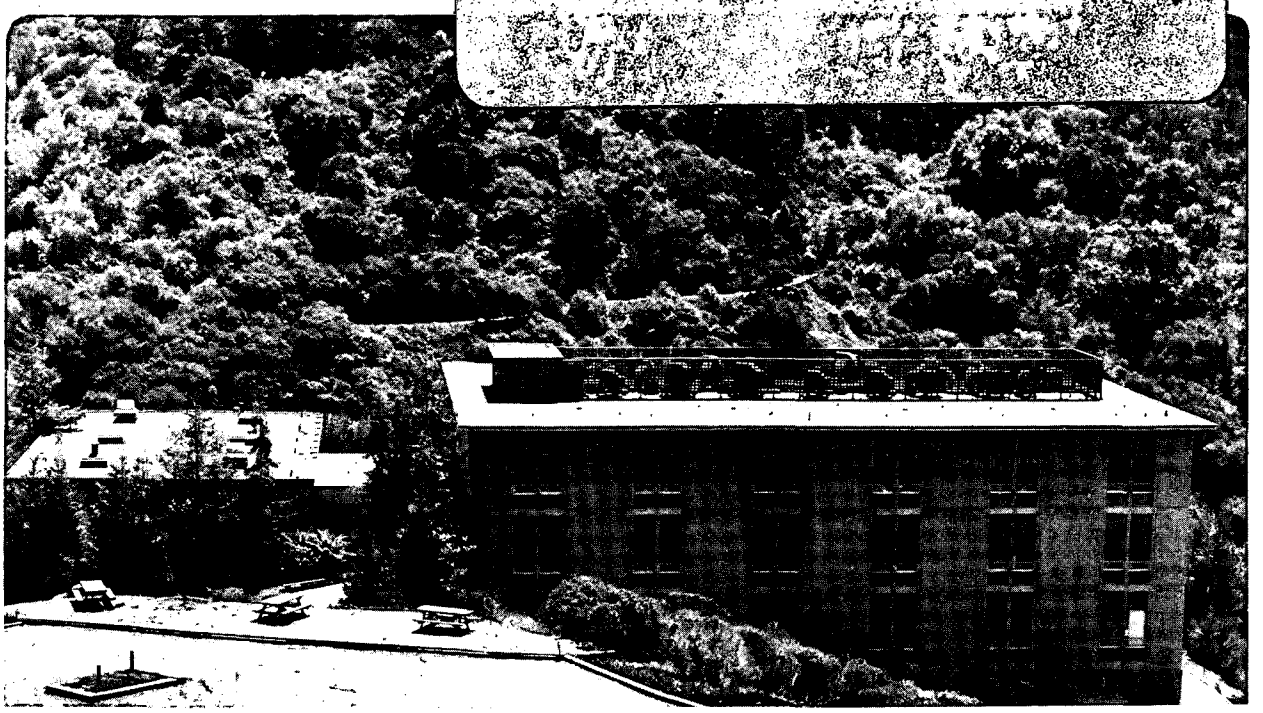

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Bis(pentamethylcyclopentadienyl)ytterbium(III)(phenylsulfide)(ammonia)

$$[(CH_3)_5C_5]_2Yb(SC_6H_5)\cdot NH_3$$

By Allan Zalkin, Timothy J. Henley & Richard A. Andersen

Materials and Molecular Research Division, Lawrence Berkeley Laboratory and

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Abstract. M_r = 569.70, triclinic, $P\bar{1}$, a = 14.091(6), b = 18.294(8), c = 10.430(6) Å, α = 104.52(6)°, β = 96.66(5)°, γ = 93.77(5)°, V = 2572.6 $Å^3$, Z = 4, D_x = 1.471 g cm^{-3}, λ(MoKα)=0.71073 Å, μ = 37.0 cm^{-1}, F(000) = 1148, T = 296 K, R = 0.038 for 6052 unique reflections with $F^2>2\sigma(F^2)$. Two independent but chemically similar molecules are found in the unit cell. The Yb is at the center of a distorted tetrahedron consisting of a S atom, a N atom and the centers of 2 pentamethylcyclopentadienyl rings. Distances are: Yb-N 2.423(8) and 2.432(8) Å; Yb-S 2.670(3) and 2.679(3) Å; ave Yb-C 2.64 ± 0.02 Å; ave Yb-Cp 2.347 ± 0.007 Å.

Introduction. The title compound was prepared as part of an extensive study of the electron-transfer and bond-cleaving properties of the divalent ytterbium metallocene, $[(CH_3)_5C_5]_2Yb$, towards transition metal carbonyls with metal to metal bonds (Boncella & Andersen, 1984) and with organic compounds with non-metal to non-metal bonds (Berg, 1986). The trivalent $[(CH_3)_5C_5]_2YbS(C_6H_5)\cdot(NH_3)$ was isolated in the reaction of $[(CH_3)_5C_5]_2Yb(NH_3)_2$ and diphenyldisulfide.

Experimental. The complex was prepared from the reaction of $[(CH_3)_5C_5]_2Yb(NH_3)_2$ and $C_6H_5SSC_6H_5$ in a 2:1 molar ratio in diethyl ether, and red crystals were obtained by crystallization from hexane (-10°C). The synthesis details and spectroscopic characterization of this and related molecules will be published in due course (Berg, 1986). The red air-sensitive crystals used in the X-ray study were picked from this batch and sealed inside quartz capillaries under argon. Crystal 0.09 x 0.19 x 0.36 mm with 6 faces; modified Picker automatic diffractometer, graphite monochromator; cell dimensions from 27 reflections, $23° < 2\theta < 34°$; analytical absorption correction, range 1.33 to 2.10; max. $(\sin\theta)/\lambda$ = 0.60 $Å^{-1}$, h -16 to 16, k -21 to 21, ℓ -12 to 7; three standard reflections, 3.8%, 4.1%, 9.1% variation in standards intensities from average, intensities adjusted isotropically; 15867 data, 9132 unique (including 6052, $F^2 < 2\sigma$), R_{int} = 0.031; structure solved by Patterson and Fourier methods; refined on F, 523 parameters; 16 hydrogen atoms in calculated positions and fixed isotropic thermal parameters; anisotropic thermal parameters for non-hydrogen atoms; R = 0.075 for 9132 data, R = 0.038 for 6052 reflections for which $F^2 > 2\sigma$, wR = 0.048, S = 1.2; $w = [\sigma(F)]^{-2}$, p = 0.06 in calc. of $\sigma(F^2)$; max (shift/σ) = 0.002; empirical extinction

correction, $F_{corr} = (1 + 8.4 \times 10^{-8} I)$; max. and min. of ΔF synthesis 0.6 and -0.7 e A^{-3}; atomic f for neutral Yb, S, N and C, and spherical bonded H 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. Figures 1 and 2 show the molecules and numbering scheme.

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*Lists of structure factors, anisotropic thermal parameters, calculated hydrogen positions, distances and angles, least-squares planes and additional ORTEP drawings have been deposited with the British Library Lending Division as Supplementary Publication No. (49 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1.2HU, England.

Discussion. The unit cell contains two crystallographically independent molecules that are chemically the same. The most obvious geometrical differences can be seen in Figures 1 and 2 in which the two molecules are in a similar orientation. The disposition of the phenylsulfide groups are such that reflection of the group through a mirror in the S-Yb-N plane in one of the molecules would bring it into near geometrical equivalence with the other molecule. Comparable distances in the two molecules are statistically equivalent with no differences exceeding 3 standard deviations. Most of the comparable angles are similar with the exception of the Yb-S-C angle that differs by 9° which is probably due to steric effects in the different environments of the phenylsulfide groups. The bond lengths in the C_6H_5S portion of the molecule are essentially unchanged from those in $C_6H_5SSC_6H_5$

(Sacerdoti & Gilli, 1975), $C_6H_5SCH_3$ (Zaripov, 1976) and $C_6H_5SC\ell$ (Zaripov, Popik & Vilkov, 1980). The Yb-S-C bond angle in the two individual molecules in the unit cell are opened ca. 15° relative to the angle at sulfur in $C_6H_5SSC_6H_5$, $C_6H_5SCH_3$ and $C_6H_5SC\ell$.

The cyclopentadienyl and phenyl rings are planar. The cyclopentadienyl rings that sandwich the Yb atom are staggered. The methyl carbon atoms are bent out of the planes of the cyclopentadienyl rings in a direction away from the Yb atom. The displacement of these carbon atoms from the least-squares planes of the cyclopentadienyl rings range from 0.0 to 0.4 Å with an average displacement for all 20 methyl carbon atoms of 0.19 ± 0.09 Å. This outward bending of the methyl groups was also observed in $[(CH_3)_5C_5]_2Yb\cdot OC_4H_8$ (Tilley, Andersen, Spencer, Ruben, Zalkin & Templeton, 1980) and in $[(CH_3)_5C_5]_2Yb\cdot(NC_5H_5)_2$ (Tilley, Andersen, Spencer & Zalkin, 1982) in which the displacement from the cyclopentadienyl planes was about half the amount reported here.

The averaged Yb-S and Yb-C distances in the two independent molecules of $[(CH_3)_5C_5]_2YbS(C_6H_5)\cdot(NH_3)$ of 2.675 ± 0.005 Å and 2.64 ± 0.02 Å are similar to those found in $[(CH_3)_5C_5]_2YbS_2CN(C_2H_5)_2$ of 2.70(1) Å and 2.63 ± 0.03 Å, respectively (Tilley, Andersen, Zalkin & Templeton, 1982). The Yb-S distance is shorter than the Lu-S distance of 2.715 ± 0.007 Å found in $Li(OC_4H_8)_2[(CH_3)_5C_5]_2Lu[SC(CH_3)_3]_2$ (Schumann, Albrecht, & Hahn , 1985) as expected since Lu(III) is ca. 0.01 Å smaller than Yb(III) (Shannon, 1976). The averaged Yb-N distance of 2.428 ± 0.003 Å is shorter than the analogous distance of 2.57 ± 0.01 Å in $[(CH_3)_5C_5]_2Yb(NC_5H_5)_2$ (Tilley, Andersen, Spencer & Zalkin, 1982) and 2.55(3) Å in $[(CH_3)_5C_5]_2Yb(NH_3)(OC_4H_8)$ (Wanda, Dye & Rogers, 1984). This trend is expected since the radius of Yb(III) is

ca. 0.15 Å smaller than that of Yb(II) for a given coordination number (Shannon, 1976).

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Table 1. Atomic Parameters

$B_{eq} = \Sigma_i \Sigma_j B_{ij} a_i^* a_j^* a_i \cdot a_j / 3, \quad Å^2.$

Atom	x	y	z	$B_{eq}(Å^2)$
YB(1)	0.19533(2)	0.63154(2)	0.21092(3)	3.40(1)
S(1)	0.16339(19)	0.52104(15)	-0.01607(24)	5.55(8)
N(1)	0.0234(5)	0.6283(5)	0.1511(8)	5.4(3)
C(1)	0.2844(7)	0.7695(5)	0.2915(9)	4.8(3)
C(2)	0.3347(6)	0.7300(5)	0.1888(10)	4.6(3)
C(3)	0.2730(7)	0.7142(5)	0.0668(9)	4.7(3)
C(4)	0.1844(7)	0.7421(5)	0.0926(9)	4.5(3)
C(5)	0.1901(7)	0.7762(4)	0.2319(10)	4.8(3)
C(6)	0.3324(9)	0.8137(6)	0.4321(10)	6.9(4)
C(7)	0.4411(7)	0.7181(6)	0.2021(13)	7.0(4)
C(8)	0.3018(10)	0.6841(6)	-0.0737(11)	7.7(4)
C(9)	0.1016(8)	0.7418(7)	-0.0161(11)	7.2(4)
C(10)	0.1120(9)	0.8142(7)	0.3055(13)	7.5(4)
C(11)	0.2897(7)	0.6030(6)	0.4250(8)	4.7(3)
C(12)	0.2572(7)	0.5315(5)	0.3334(9)	4.4(3)
C(13)	0.1557(7)	0.5191(5)	0.3205(9)	4.6(3)
C(14)	0.1252(7)	0.5861(5)	0.4054(9)	4.9(3)
C(15)	0.2075(8)	0.6362(6)	0.4678(8)	5.1(3)
C(16)	0.3927(8)	0.6313(7)	0.4850(12)	7.0(4)
C(17)	0.3217(8)	0.4715(6)	0.2710(11)	6.4(4)
C(18)	0.0928(8)	0.4479(6)	0.2423(10)	6.1(3)
C(19)	0.0213(9)	0.5968(8)	0.4378(12)	7.7(5)
C(20)	0.2035(10)	0.7069(7)	0.5879(11)	7.6(4)
C(21)	0.2477(7)	0.5024(5)	-0.1287(9)	4.4(3)
C(22)	0.2215(7)	0.5015(6)	-0.2593(10)	5.4(3)
C(23)	0.2854(11)	0.4831(7)	-0.3516(11)	7.3(4)
C(24)	0.3756(12)	0.4673(9)	-0.3098(15)	8.9(6)
C(25)	0.4020(10)	0.4690(9)	-0.1815(16)	9.0(6)
C(26)	0.3395(9)	0.4857(7)	-0.0906(11)	7.0(4)

Table 1. Atomic Parameters (continued)

YB(2)	0.23925(2)	0.08118(2)	0.16928(3)	3.39(1)
S(2)	0.10569(17)	0.09900(16)	-0.02235(25)	5.29(8)
N(2)	0.1425(5)	-0.0406(4)	0.1085(7)	4.9(2)
C(27)	0.2801(7)	0.1501(7)	0.4262(8)	5.4(3)
C(28)	0.2302(10)	0.2017(5)	0.3692(10)	6.1(4)
C(29)	0.1333(7)	0.1698(6)	0.3259(8)	5.0(3)
C(30)	0.1233(7)	0.0986(6)	0.3556(9)	5.3(3)
C(31)	0.2145(8)	0.0858(6)	0.4176(8)	5.2(3)
C(32)	0.3751(10)	0.1735(11)	0.5172(13)	11.3(6)
C(33)	0.2679(12)	0.2833(6)	0.3738(13)	9.8(6)
C(34)	0.0467(12)	0.2077(10)	0.2800(13)	12.2(7)
C(35)	0.0298(9)	0.0480(9)	0.3449(13)	9.7(5)
C(36)	0.2385(12)	0.0206(7)	0.4799(12)	9.4(6)
C(37)	0.4213(6)	0.1071(6)	0.1484(12)	6.0(4)
C(38)	0.4150(6)	0.0384(6)	0.1869(10)	5.3(3)
C(39)	0.3615(7)	-0.0170(5)	0.0818(12)	5.5(3)
C(40)	0.3347(7)	0.0164(7)	-0.0242(10)	5.8(3)
C(41)	0.3714(7)	0.0930(7)	0.0152(11)	5.6(4)
C(42)	0.4862(9)	0.1803(8)	0.2222(17)	11.1(6)
C(43)	0.4716(9)	0.0219(10)	0.3072(13)	10.0(6)
C(44)	0.3472(11)	-0.1020(7)	0.0732(20)	11.4(7)
C(45)	0.2831(10)	-0.0290(11)	-0.1633(13)	11.7(7)
C(46)	0.3727(10)	0.1478(10)	-0.0734(17)	10.8(7)
C(47)	0.1399(6)	0.1724(5)	-0.0979(8)	4.3(3)
C(48)	0.1734(8)	0.2441(6)	-0.0244(9)	5.7(3)
C(49)	0.1990(9)	0.2993(6)	-0.0860(12)	6.8(4)
C(50)	0.1906(8)	0.2850(7)	-0.2199(12)	6.4(4)
C(51)	0.1558(8)	0.2140(7)	-0.2950(10)	6.2(4)
C(52)	0.1299(7)	0.1582(6)	-0.2359(9)	5.1(3)

Table 2. Selected distances and angles

Atoms	d(Å)	Atoms	d(Å)
Yb(1) - N(1)	2.423(8)	Yb(2) - N(2)	2.432(8)
Yb(1) - S(1)	2.670(3)	Yb(2) - S(2)	2.679(3)
Yb(1) - C(1)	2.632(8)	Yb(2) - C(27)	2.637(8)
Yb(1) - C(2)	2.646(7)	Yb(2) - C(28)	2.650(8)
Yb(1) - C(3)	2.654(8)	Yb(2) - C(29)	2.661(8)
Yb(1) - C(4)	2.624(8)	Yb(2) - C(30)	2.654(8)
Yb(1) - C(5)	2.608(8)	Yb(2) - C(31)	2.635(8)
Yb(1) - C(11)	2.649(8)	Yb(2) - C(37)	2.621(8)
Yb(1) - C(12)	2.620(8)	Yb(2) - C(38)	2.646(8)
Yb(1) - C(13)	2.651(8)	Yb(2) - C(39)	2.641(8)
Yb(1) - C(14)	2.643(8)	Yb(2) - C(40)	2.632(8)
Yb(1) - C(15)	2.644(8)	Yb(2) - C(41)	2.629(8)
S(1) - C(21)	1.756(9)	S(2) - C(47)	1.786(9)
Yb(1) - Cp_1[a]	2.340	Yb(2) - Cp_3	2.355
Yb(1) - Cp_2	2.349	Yb(2) - Cp_4	2.343

Atoms	Angle°	Atoms	Angle°
S(1) - Yb(1) - N(1)	78.3(2)	S(2) - Yb(2) - N(2)	78.1(2)
Cp_1 - Yb(1) - Cp_2	136.2	Cp_3 - Yb(2) - Cp_4	136.9
Cp_1 - Yb(1) - S(1)	111.4	Cp_3 - Yb(2) - S(2)	108.6
Cp_1 - Yb(1) - N(1)	102.8	Cp_3 - Yb(2) - N(2)	103.1
Cp_2 - Yb(1) - S(1)	108.1	Cp_4 - Yb(2) - S(2)	110.7
Cp_2 - Yb(1) - N(1)	102.9	Cp_4 - Yb(2) - N(2)	101.5
Yb(1) - S(1) - C(21)	123.0(3)	Yb(2) - S(2) - C(47)	113.9(3)

[a] Cp_1, Cp_2, Cp_3 and Cp_4 represent the centroid of cyclopentadienyl atoms C(1)-C(5), C(11)-C(15), C(27)-C(31) and C(27)-C(31) respectively.

Fig.1. ORTEP (Johnson, 1965) of the molecule I showing the atomic numbering scheme; 50% probability ellipsoids.

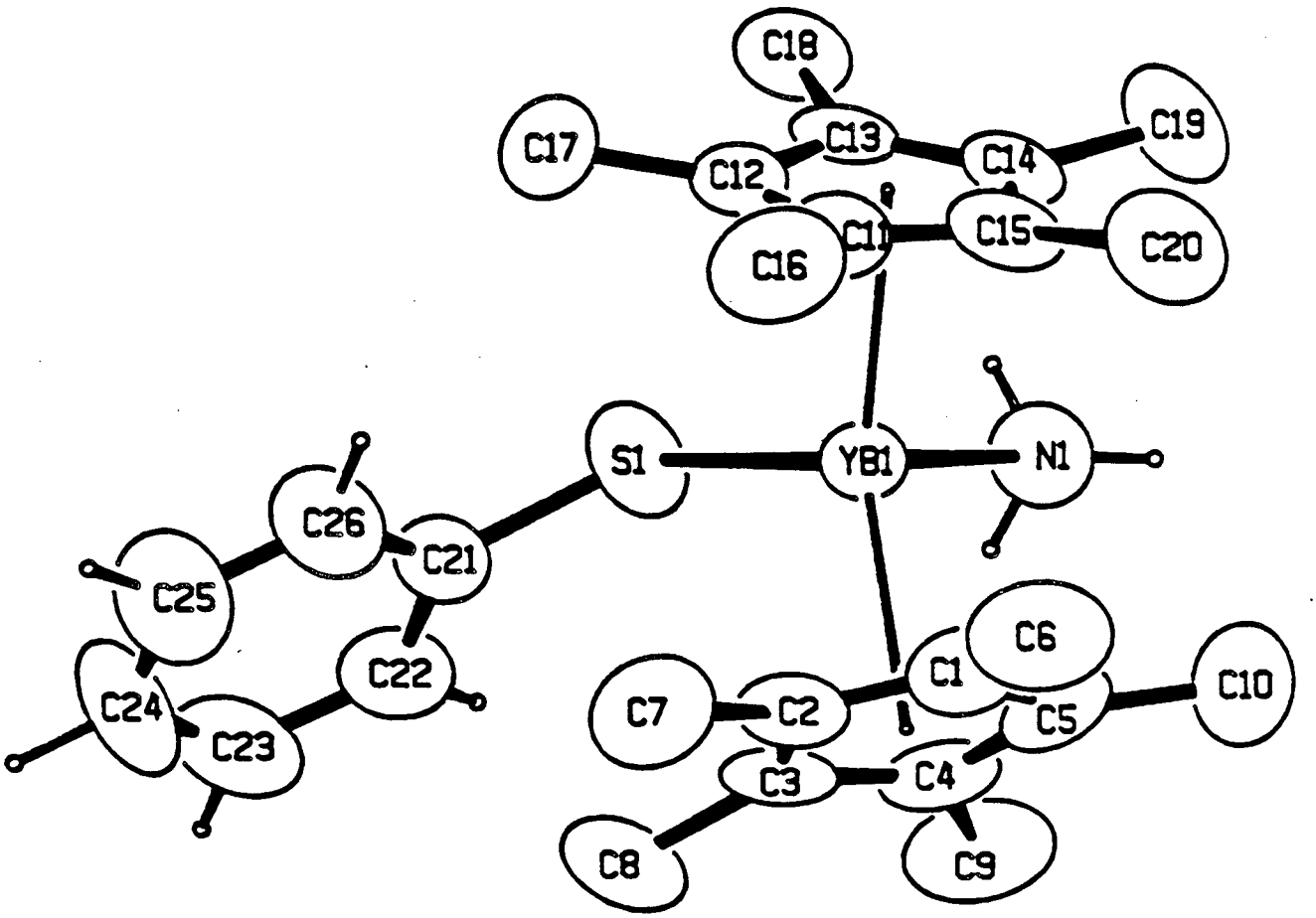
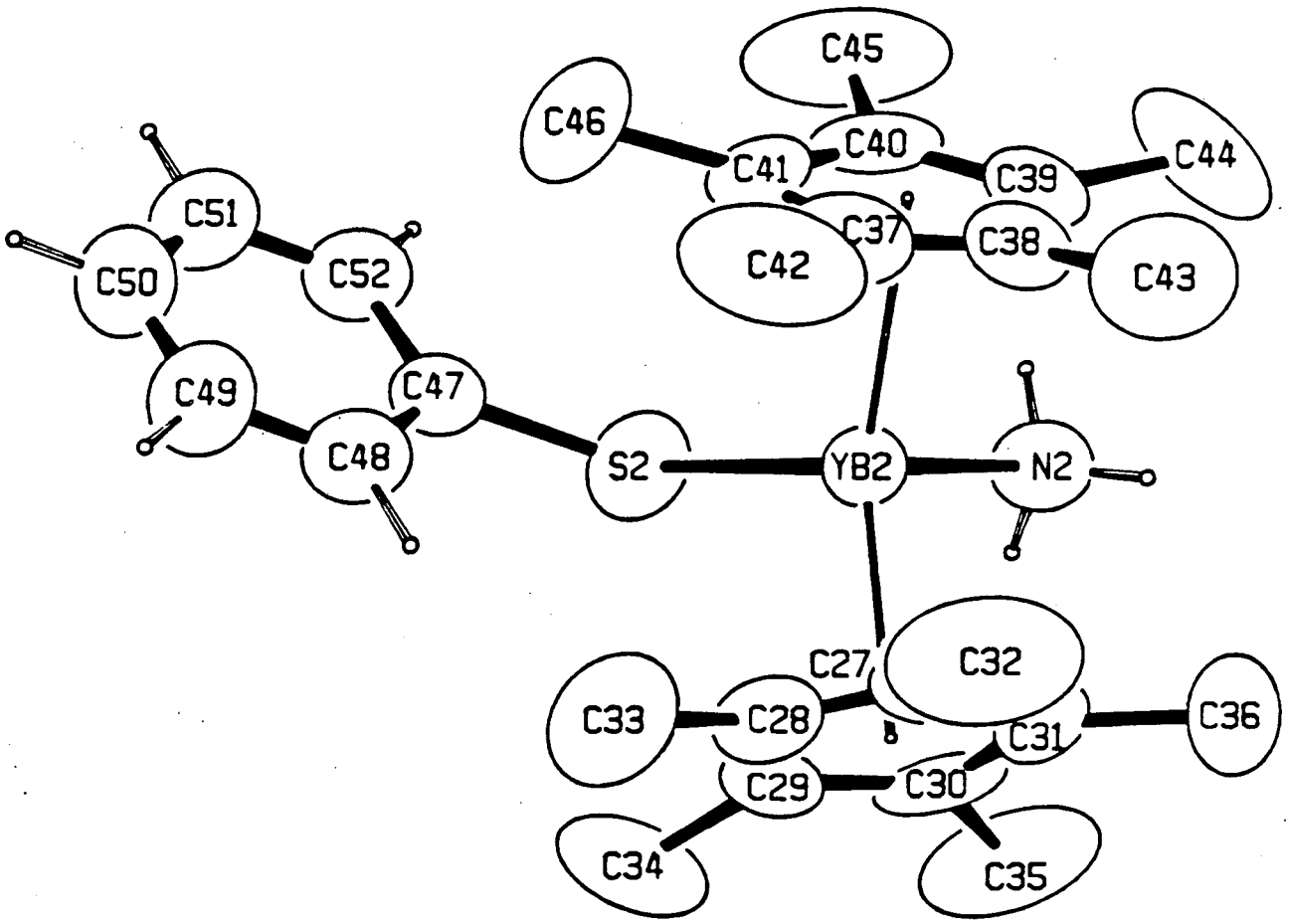


Fig.2. ORTEP (Johnson, 1965) of the molecule II showing the atomic numbering scheme; 50% probability ellipsoids.



Supplemental Material

for

Bis(pentamethylcyclopentadienyl)ytterbium(III)(phenylsulfide)(ammonia)

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Table S1. Anisotropic Thermal Parameters ($Å^2$)[a]

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
YB(1)	3.334(18)	3.453(17)	3.362(18)	-0.144(13)	0.163(13)	1.046(13)
S(1)	5.35(12)	5.61(13)	4.58(11)	-1.20(10)	1.38(9)	-0.57(9)
N(1)	4.3(4)	6.0(4)	5.9(4)	0.2(3)	0.6(3)	1.7(3)
C(1)	5.2(5)	3.5(4)	5.2(5)	-1.4(3)	-0.6(4)	1.0(3)
C(2)	3.7(4)	4.1(4)	6.3(5)	-1.6(3)	0.6(4)	2.5(4)
C(3)	6.3(5)	3.8(4)	4.6(4)	-1.3(4)	0.7(4)	2.6(3)
C(4)	5.1(5)	3.9(4)	4.8(4)	-0.6(3)	-1.2(3)	2.6(3)
C(5)	5.8(5)	2.3(3)	6.1(5)	-0.4(3)	-0.5(4)	1.3(3)
C(6)	8.6(7)	5.8(5)	4.8(5)	-2.6(5)	-2.0(5)	0.6(4)
C(7)	3.5(4)	6.5(6)	11.3(8)	-0.4(4)	0.5(5)	3.5(6)
C(8)	11.4(9)	6.3(6)	5.7(6)	-1.0(6)	3.9(6)	1.7(5)
C(9)	6.8(6)	7.5(7)	7.2(6)	-1.0(5)	-2.8(5)	3.7(5)
C(10)	6.9(7)	6.7(6)	9.3(8)	1.6(5)	2.7(6)	1.8(6)
C(11)	5.2(5)	6.1(5)	3.1(4)	0.9(4)	-0.4(3)	2.3(4)
C(12)	5.2(5)	5.1(4)	4.0(4)	1.3(4)	1.0(3)	2.8(4)
C(13)	5.4(5)	4.8(4)	4.8(4)	-0.2(4)	1.5(4)	3.3(4)
C(14)	6.0(5)	5.5(5)	4.1(4)	0.1(4)	1.9(4)	2.6(4)
C(15)	7.5(6)	5.8(5)	2.2(3)	-0.5(4)	0.5(4)	1.7(3)
C(16)	5.3(5)	7.6(7)	7.7(7)	-0.4(5)	-1.9(5)	2.9(5)
C(17)	7.4(7)	6.7(6)	6.6(6)	3.3(5)	2.0(5)	3.0(5)
C(18)	7.7(6)	4.7(5)	6.2(5)	-1.3(4)	2.1(5)	1.5(4)
C(19)	6.4(6)	9.7(8)	8.4(7)	1.2(6)	4.3(6)	3.2(6)
C(20)	11.1(9)	6.3(6)	4.6(5)	-0.7(6)	2.1(5)	-0.0(4)
C(21)	4.8(4)	4.5(4)	4.1(4)	0.1(3)	0.8(3)	1.3(3)
C(22)	6.0(5)	5.3(5)	5.0(5)	-0.4(4)	0.3(4)	1.9(4)
C(23)	9.2(8)	7.5(7)	5.3(6)	-0.9(6)	1.9(6)	2.1(5)
C(24)	9.2(9)	10.8(10)	7.3(8)	1.8(8)	5.4(7)	1.5(7)
C(25)	6.7(7)	11.9(11)	9.8(9)	2.9(7)	2.8(7)	4.0(8)
C(26)	6.6(6)	9.5(8)	5.9(6)	1.9(6)	1.6(5)	3.3(5)

Table S1. Anisotropic Thermal Parameters ($Å^2$) (continued)

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
YB(2)	2.881(17)	3.619(18)	3.569(18)	0.014(13)	0.371(13)	0.841(13)
S(2)	3.88(10)	7.13(14)	4.94(12)	-0.06(10)	-0.47(9)	2.36(10)
N(2)	4.7(4)	4.8(4)	5.2(4)	0.1(3)	1.3(3)	0.9(3)
C(27)	4.6(5)	7.8(6)	2.5(4)	0.7(4)	-0.0(3)	-0.9(4)
C(28)	9.9(8)	3.5(4)	4.3(5)	-0.2(5)	3.2(5)	-0.6(3)
C(29)	5.9(5)	6.0(5)	3.4(4)	2.9(4)	1.6(4)	0.5(4)
C(30)	4.4(5)	7.5(6)	3.2(4)	-0.9(4)	2.4(3)	-0.3(4)
C(31)	7.7(6)	5.7(5)	2.5(4)	1.4(5)	1.7(4)	1.2(3)
C(32)	6.2(7)	17.4(14)	6.3(7)	-1.2(8)	-1.6(5)	-2.1(8)
C(33)	16.2(13)	3.8(5)	8.7(8)	-2.7(6)	4.2(8)	-0.1(5)
C(34)	14.1(12)	17.8(14)	6.4(7)	12.3(12)	2.7(7)	3.0(8)
C(35)	7.4(7)	12.1(10)	7.3(7)	-4.9(7)	3.0(6)	-0.9(7)
C(36)	16.0(13)	7.4(7)	7.0(7)	5.0(8)	3.8(8)	3.8(6)
C(37)	2.2(4)	6.7(6)	8.5(7)	-0.8(4)	1.7(4)	0.6(5)
C(38)	2.9(4)	7.0(6)	6.6(6)	2.0(4)	1.2(4)	2.1(5)
C(39)	4.1(4)	4.8(5)	8.2(6)	1.6(4)	3.0(4)	1.6(4)
C(40)	3.7(4)	8.8(7)	4.6(5)	1.5(4)	2.5(4)	0.4(5)
C(41)	3.5(4)	8.1(6)	7.1(6)	1.4(4)	3.6(4)	3.9(5)
C(42)	5.5(6)	8.6(8)	16.2(13)	-3.0(6)	3.9(7)	-2.3(8)
C(43)	5.9(6)	17.4(14)	7.8(8)	4.6(8)	-0.2(5)	4.8(8)
C(44)	9.2(9)	4.4(6)	22.0(16)	2.8(6)	7.3(10)	3.1(8)
C(45)	6.7(8)	19.0(15)	5.9(7)	0.3(9)	1.3(6)	-3.1(8)
C(46)	7.2(7)	15.9(13)	15.3(12)	4.7(8)	6.7(8)	11.8(11)
C(47)	3.6(4)	5.1(4)	4.1(4)	1.1(3)	0.8(3)	1.1(3)
C(48)	6.8(6)	5.7(5)	4.0(4)	0.9(4)	1.0(4)	0.3(4)
C(49)	8.5(7)	5.9(6)	6.0(6)	0.4(5)	1.2(5)	1.5(5)
C(50)	6.6(6)	6.1(6)	7.2(7)	0.7(5)	1.5(5)	2.6(5)
C(51)	6.9(6)	7.4(7)	4.6(5)	1.3(5)	1.1(4)	1.7(5)
C(52)	5.2(5)	5.5(5)	4.1(4)	0.4(4)	0.6(4)	0.4(4)

[a] The anisotropic temperature factor has the form:

$$\exp[-0.25(B_{11}h^2a^{*2} + 2B_{12}hka^*b^* + \cdots].$$

Table S2. Estimated Hydrogen Positional and Isotropic Thermal Parameters ($Å^2$)[a]

Atom	x	y	z	B
H(1) C(22)	0.1551	0.5134	-0.2895	10.0
H(2) C(23)	0.2663	0.4815	-0.4481	10.0
H(3) C(24)	0.4220	0.4551	-0.3768	10.0
H(4) C(25)	0.4688	0.456	-0.1537	10.0
H(5) C(26)	0.3602	0.487	0.0054	10.0
H(6) C(48)	0.1791	0.2562	0.0755	10.0
H(7) C(49)	0.2243	0.3520	-0.0286	10.0
H(8) C(50)	0.2098	0.3255	-0.2645	10.0
H(9) C(51)	0.1492	0.2021	-0.3951	10.0
H(10)C(52)	0.1037	0.1064	-0.2925	10.0
H(11) N(1)	0.0341	0.6367	0.072	8.0
H(12) N(1)	0.0127	0.5788	0.1456	8.0
H(13) N(1)	-0.0207	0.6579	0.1902	8.0
H(14) N(2)	0.1646	-0.0666	0.1661	6.0
H(15) N(2)	0.1519	-0.0628	0.0257	6.0
H(16) N(2)	0.0818	-0.0316	0.117	6.0

[a] The isotropic temperature factor has the form $\exp[-B(\sin\theta/\lambda)^2]$.

Table S3. Additional Distances

C(1)	- C(2)	1.425(13)	C(11)	- C(15)	1.409(13)	C(21)	- C(22)	1.365(12)
C(1)	- C(5)	1.427(12)	C(11)	- C(12)	1.423(13)	C(21)	- C(26)	1.385(14)
C(1)	- C(6)	1.538(12)	C(11)	- C(16)	1.514(13)	C(21)	- S(1)	1.756(9)
C(2)	- C(3)	1.409(12)	C(12)	- C(13)	1.418(12)	C(22)	- C(21)	1.365(12)
C(2)	- C(1)	1.425(13)	C(12)	- C(11)	1.423(13)	C(22)	- C(23)	1.389(15)
C(2)	- C(7)	1.524(13)	C(12)	- C(17)	1.538(13)	C(23)	- C(24)	1.367(18)
C(3)	- C(4)	1.408(13)	C(13)	- C(12)	1.418(12)	C(23)	- C(22)	1.389(15)
C(3)	- C(2)	1.409(12)	C(13)	- C(14)	1.444(13)	C(24)	- C(25)	1.339(18)
C(3)	- C(8)	1.542(13)	C(13)	- C(18)	1.515(13)	C(24)	- C(23)	1.367(18)
C(4)	- C(3)	1.408(13)	C(14)	- C(15)	1.413(13)	C(25)	- C(24)	1.339(18)
C(4)	- C(5)	1.421(12)	C(14)	- C(13)	1.444(13)	C(25)	- C(26)	1.360(16)
C(4)	- C(9)	1.528(12)	C(14)	- C(19)	1.554(14)	C(26)	- C(25)	1.360(16)
C(5)	- C(4)	1.421(12)	C(15)	- C(11)	1.409(13)	C(26)	- C(21)	1.385(14)
C(5)	- C(1)	1.427(12)	C(15)	- C(14)	1.413(13)	C(22)	- H(1)	1.01
C(5)	- C(10)	1.520(14)	C(15)	- C(20)	1.568(13)	C(23)	- H(2)	1.01
C(6)	- C(1)	1.538(12)	C(16)	- C(11)	1.514(13)	C(24)	- H(3)	1.01
C(7)	- C(2)	1.524(13)	C(17)	- C(12)	1.538(13)	C(25)	- H(4)	1.01
C(8)	- C(3)	1.542(13)	C(18)	- C(13)	1.515(13)	C(26)	- H(5)	1.00
C(9)	- C(4)	1.528(12)	C(19)	- C(14)	1.554(14)	N(1)	- H(11)	0.90
C(10)	- C(5)	1.520(14)	C(20)	- C(15)	1.568(13)	N(1)	- H(12)	0.89
						N(1)	- H(13)	0.92

Table S3. Additional Distances (continued)

C(27) - C(28)	1.419(15)	C(37) - C(38)	1.412(15)	C(47) - C(48)	1.365(12)
C(27) - C(31)	1.424(14)	C(37) - C(41)	1.436(14)	C(47) - C(52)	1.386(11)
C(27) - C(32)	1.518(14)	C(37) - C(42)	1.544(15)	C(47) - S(2)	1.786(09)
C(28) - C(27)	1.419(15)	C(38) - C(39)	1.396(14)	C(48) - C(47)	1.365(12)
C(28) - C(29)	1.424(15)	C(38) - C(37)	1.412(15)	C(48) - C(49)	1.375(15)
C(28) - C(33)	1.538(14)	C(38) - C(43)	1.514(14)	C(49) - C(50)	1.345(14)
C(29) - C(30)	1.416(14)	C(39) - C(38)	1.396(14)	C(49) - C(48)	1.375(15)
C(29) - C(28)	1.424(15)	C(39) - C(40)	1.418(14)	C(50) - C(49)	1.345(14)
C(29) - C(34)	1.529(15)	C(39) - C(44)	1.534(15)	C(50) - C(51)	1.362(15)
C(30) - C(29)	1.416(14)	C(40) - C(41)	1.403(15)	C(51) - C(50)	1.362(15)
C(30) - C(31)	1.431(14)	C(40) - C(39)	1.418(14)	C(51) - C(52)	1.369(14)
C(30) - C(35)	1.535(14)	C(40) - C(45)	1.547(15)	C(52) - C(51)	1.369(14)
C(31) - C(27)	1.424(14)	C(41) - C(40)	1.403(15)	C(52) - C(47)	1.386(11)
C(31) - C(30)	1.431(14)	C(41) - C(37)	1.436(14)	C(48) - H(6)	1.00
C(31) - C(36)	1.533(14)	C(41) - C(46)	1.525(15)	C(49) - H(7)	1.01
C(32) - C(27)	1.518(14)	C(42) - C(37)	1.544(15)	C(50) - H(8)	1.01
C(33) - C(28)	1.538(14)	C(43) - C(38)	1.514(14)	C(51) - H(9)	1.00
C(34) - C(29)	1.529(15)	C(44) - C(39)	1.534(15)	C(52) - H(10)	1.00
C(35) - C(30)	1.535(14)	C(45) - C(40)	1.547(15)	N(2) - H(14)	0.90
C(36) - C(31)	1.533(14)	C(46) - C(41)	1.525(15)	N(2) - H(15)	0.89
				N(2) - H(16)	0.89

Table S4. Additional Angles

Atoms	Angle(°)	Atoms	Angle(°)
C(2) -C(1) -C(5)	108.0(08)	C(11)-C(12)-C(17)	125.7(09)
C(2) -C(1) -C(6)	124.4(09)	C(13)-C(12)-C(17)	124.0(09)
C(5) -C(1) -C(6)	126.0(10)	C(12)-C(13)-C(14)	105.8(08)
C(1) -C(2) -C(3)	107.9(08)	C(12)-C(13)-C(18)	127.2(09)
C(1) -C(2) -C(7)	126.6(09)	C(14)-C(13)-C(18)	126.8(09)
C(3) -C(2) -C(7)	124.8(10)	C(13)-C(14)-C(15)	108.4(09)
C(2) -C(3) -C(4)	108.5(08)	C(13)-C(14)-C(19)	125.8(09)
C(2) -C(3) -C(8)	126.0(10)	C(15)-C(14)-C(19)	125.4(10)
C(4) -C(3) -C(8)	124.8(09)	C(11)-C(15)-C(14)	109.0(09)
C(3) -C(4) -C(5)	108.6(08)	C(11)-C(15)-C(20)	127.6(10)
C(3) -C(4) -C(9)	124.1(09)	C(14)-C(15)-C(20)	122.1(10)
C(5) -C(4) -C(9)	127.1(10)	S(1) -C(21)-C(22)	119.4(08)
C(1) -C(5) -C(4)	107.1(09)	S(1) -C(21)-C(26)	122.1(07)
C(1) -C(5) -C(10)	125.6(09)	C(22)-C(21)-C(26)	118.5(09)
C(4) -C(5) -C(10)	127.3(09)	C(21)-C(22)-C(23)	120.4(10)
C(12)-C(11)-C(15)	107.0(08)	C(22)-C(23)-C(24)	119.3(11)
C(12)-C(11)-C(16)	126.3(09)	C(23)-C(24)-C(25)	120.5(11)
C(15)-C(11)-C(16)	125.8(09)	C(24)-C(25)-C(26)	120.7(13)
C(11)-C(12)-C(13)	109.9(08)	C(21)-C(26)-C(25)	120.6(11)

Table S4. Additional Angles (continued)

Atoms	Angle(°)	Atoms	Angle(°)
C(28)-C(27)-C(31)	108.2(09)	C(37)-C(38)-C(43)	126.7(11)
C(28)-C(27)-C(32)	122.4(12)	C(39)-C(38)-C(43)	124.1(11)
C(31)-C(27)-C(32)	126.7(12)	C(38)-C(39)-C(40)	108.4(09)
C(27)-C(28)-C(29)	107.9(09)	C(38)-C(39)-C(44)	125.8(12)
C(27)-C(28)-C(33)	126.4(12)	C(40)-C(39)-C(44)	125.1(12)
C(29)-C(28)-C(33)	124.9(12)	C(39)-C(40)-C(41)	108.5(09)
C(28)-C(29)-C(30)	108.3(09)	C(39)-C(40)-C(45)	123.7(13)
C(28)-C(29)-C(34)	128.7(12)	C(41)-C(40)-C(45)	127.6(13)
C(30)-C(29)-C(34)	122.1(12)	C(37)-C(41)-C(40)	107.0(09)
C(29)-C(30)-C(31)	107.9(08)	C(37)-C(41)-C(46)	125.7(12)
C(29)-C(30)-C(35)	127.3(11)	C(40)-C(41)-C(46)	126.6(12)
C(31)-C(30)-C(35)	124.1(12)	S(2) -C(47)-C(48)	122.3(07)
C(27)-C(31)-C(30)	107.7(09)	S(2) -C(47)-C(52)	120.0(07)
C(27)-C(31)-C(36)	124.1(11)	C(48)-C(47)-C(52)	117.6(09)
C(30)-C(31)-C(36)	127.9(11)	C(47)-C(48)-C(49)	120.8(09)
C(38)-C(37)-C(41)	108.0(09)	C(48)-C(49)-C(50)	121.4(11)
C(38)-C(37)-C(42)	126.6(12)	C(49)-C(50)-C(51)	118.7(11)
C(41)-C(37)-C(42)	124.4(12)	C(50)-C(51)-C(52)	120.9(10)
C(37)-C(38)-C(39)	108.1(09)	C(47)-C(52)-C(51)	120.6(10)

Table S5. Least-squares Planes

Plane No. 1

Equation of plane: 4.09674 a + 16.91272 b - 4.36170 c = 12.90107

Distance to the plane from atoms

in the plane			not in the plane	
atom	d(Å)	σ(d)	atom	d(Å)
C(1)	0.0073	(123)	Yb(1)	-2.340(4)
C(2)	-0.0074	(128)	C(6)	0.338(19)
C(3)	0.0040	(128)	C(7)	0.170(20)
C(4)	0.0009	(120)	C(8)	0.227(21)
C(5)	-0.0054	(125)	C(9)	0.131(19)
			C(10)	-0.004(20)

Plane No. 2

Equation of plane: -0.15660 a + 11.87613 b - 9.34229 c = 3.15060

Distance to the plane from atoms

in the plane			not in the plane	
atom	d(Å)	σ(d)	atom	d(Å)
C(11)	-0.0060	(129)	Yb(1)	2.349(05)
C(12)	0.0066	(121)	C(16)	-0.246(19)
C(13)	-0.0054	(123)	C(17)	-0.133(19)
C(14)	0.0023	(129)	C(18)	-0.110(19)
C(15)	0.0026	(138)	C(19)	-0.156(21)
			C(20)	-0.279(21)

Table S5. Least-squares Planes (continued)

Plane No. 3

Equation of plane: 3.45521 a + 17.02584 b - 0.86991 c = 9.52418

Distance to the plane from atoms

in the plane			not in the plane	
atom	d(Å)	σ(d)	atom	d(Å)
C(21)	-0.0018	(119)	Yb(1)	1.720(25)
C(22)	0.0049	(132)	S(1)	-0.074(16)
C(23)	-0.0076	(184)		
C(24)	-0.0012	(198)		
C(25)	0.0080	(199)		
C(26)	-0.0029	(165)		

Plane No. 4

Equation of plane: -5.43465 a + 4.43522 b + 8.84656 c = 2.91165

Distance to the plane from atoms

in the plane			not in the plane	
atom	d(Å)	σ(d)	atom	d(Å)
C(27)	0.0025	(154)	Yb(2)	-2.354(5)
C(28)	-0.0020	(166)	C(32)	0.395(26)
C(29)	0.0002	(139)	C(33)	0.196(25)
C(30)	0.0012	(144)	C(34)	0.232(25)
C(31)	-0.0021	(145)	C(35)	0.191(24)
			C(36)	0.128(24)

Table S5. Least-squares Planes (continued)

Plane No. 5

Equation of plane: 12.87756 a - 3.81784 b - 4.48057 c = 4.35595

Distance to the plane from atoms

in the plane			not in the plane	
atom	d(Å)	σ(d)	atom	d(Å)
C(37)	-0.0050	(156)	Yb(2)	-2.343(5)
C(38)	0.0043	(147)	C(42)	0.220(26)
C(39)	-0.0029	(154)	C(43)	0.170(25)
C(40)	-0.0002	(161)	C(44)	0.177(28)
C(41)	-0.0031	(155)	C(45)	0.131(28)
			C(46)	0.208(18)

Plane No. 6

Equation of plane: 13.50779 a - 6.33942 b - 0.20704 c = 0.80818

Distance to the plane from atoms

in the plane			not in the plane	
atom	d(Å)	σ(d)	atom	d(Å)
C(47)	0.0086	(116)	Yb(2)	1.874(21)
C(48)	-0.0080	(133)	S(2)	-0.003(15)
C(49)	0.0003	(152)		
C(50)	0.0051	(155)		
C(51)	0.0007	(151)		
C(52)	-0.0071	(125)		

Fig. S1. ORTEP drawing of molecule I viewed down a line connecting the centroids of the Cp rings to show the staggered configuration.

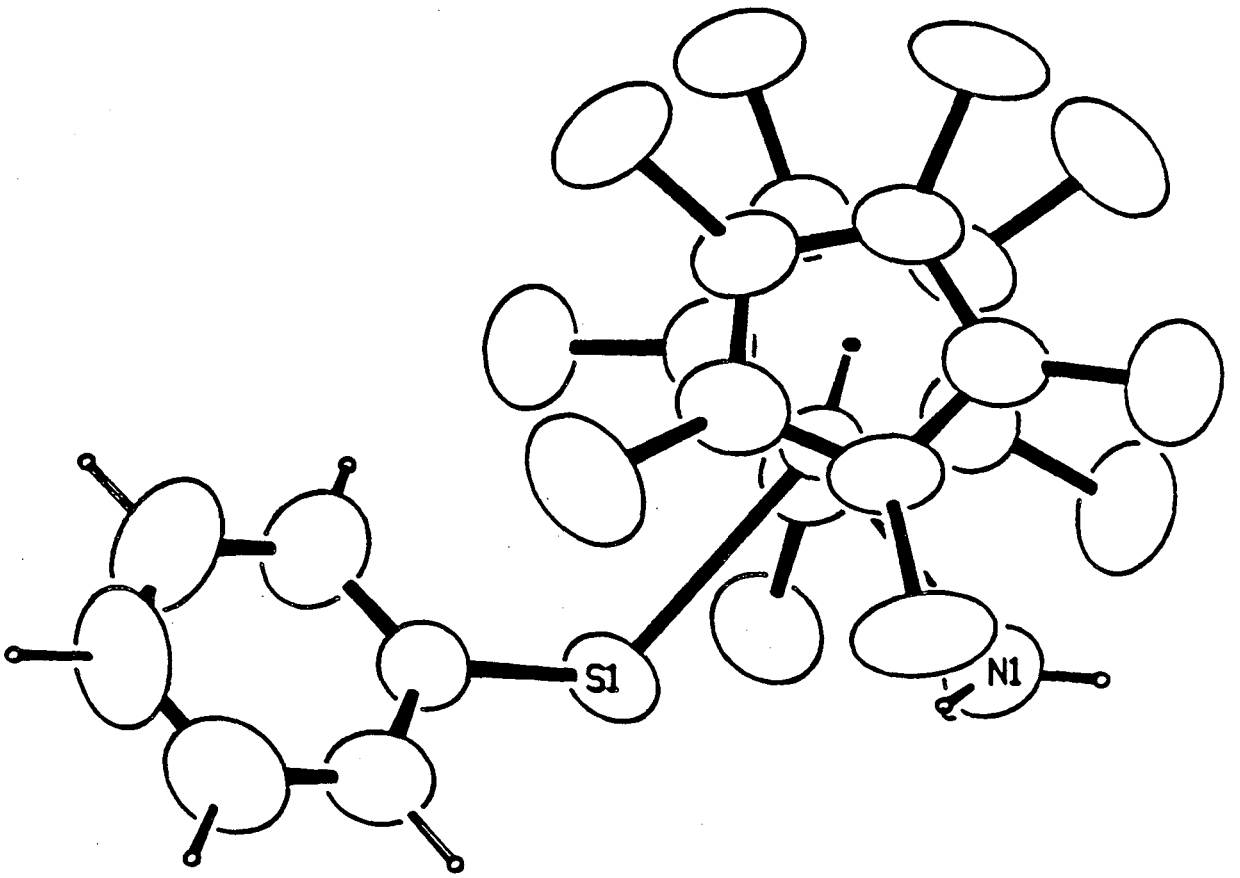


Fig. S2. ORTEP drawing of molecule 2 viewed down a line connecting the centroids of the Cp rings to show the staggered configuration.

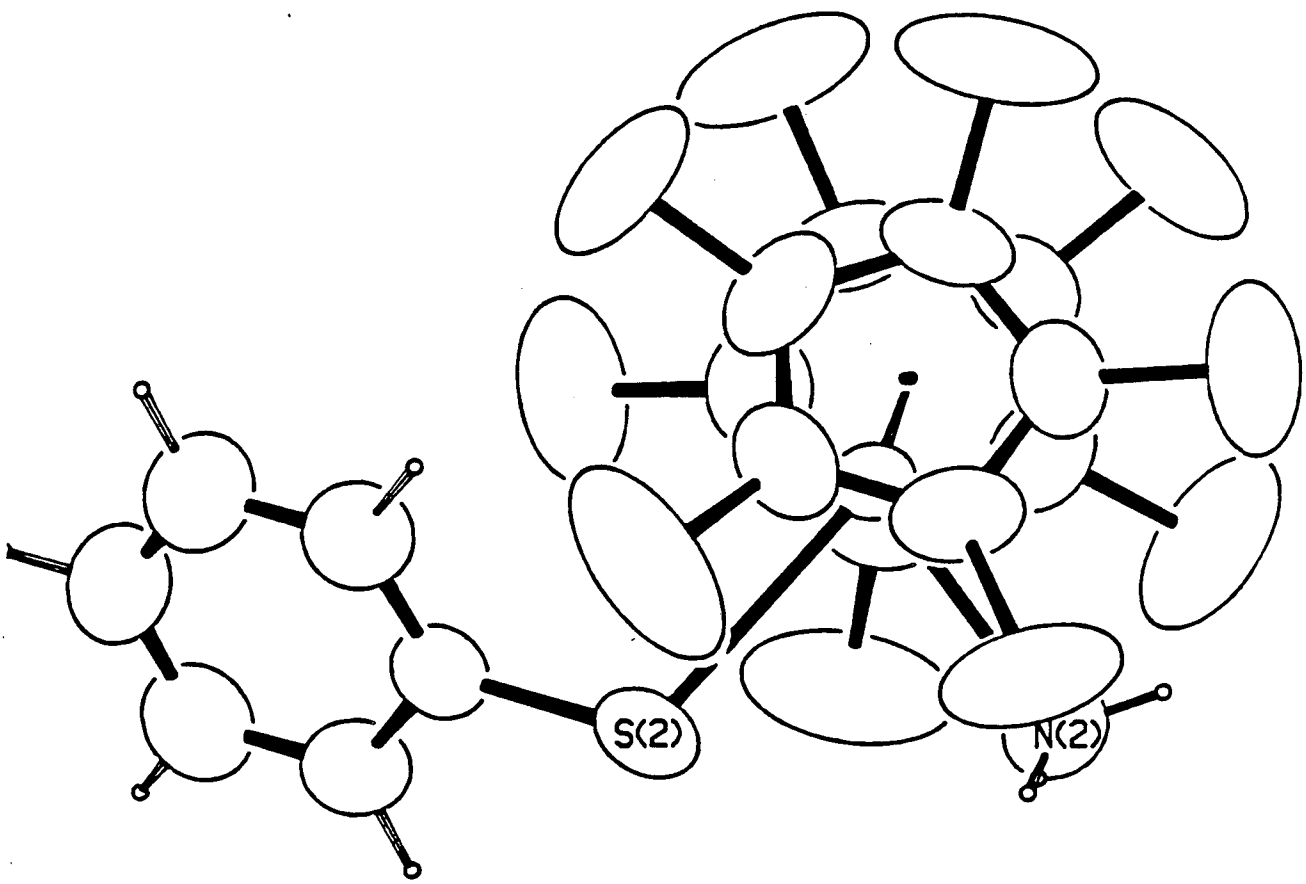


Fig. S3. ORTEP drawing of molecule 1 viewed down a line connecting the S(1) and N(1) atoms. Shows the bowing of the methyl groups away from the Cp rings.

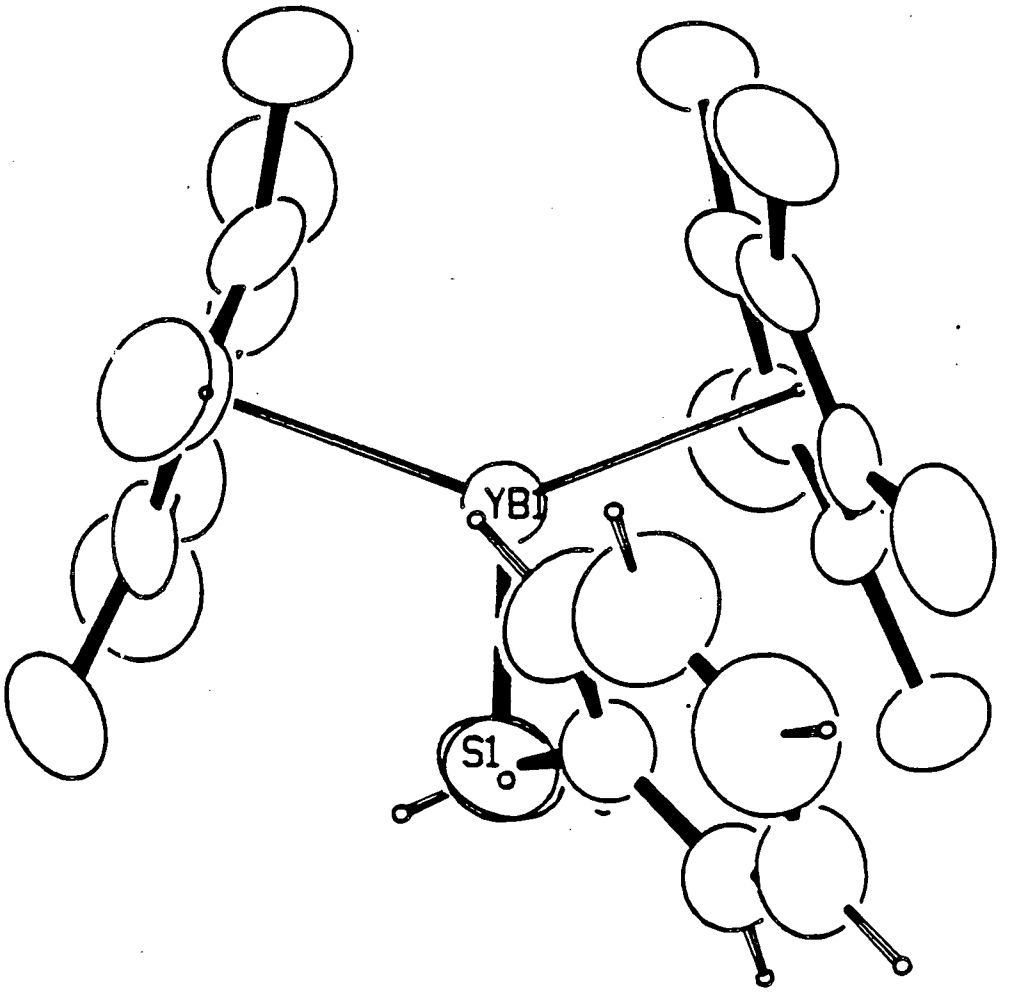
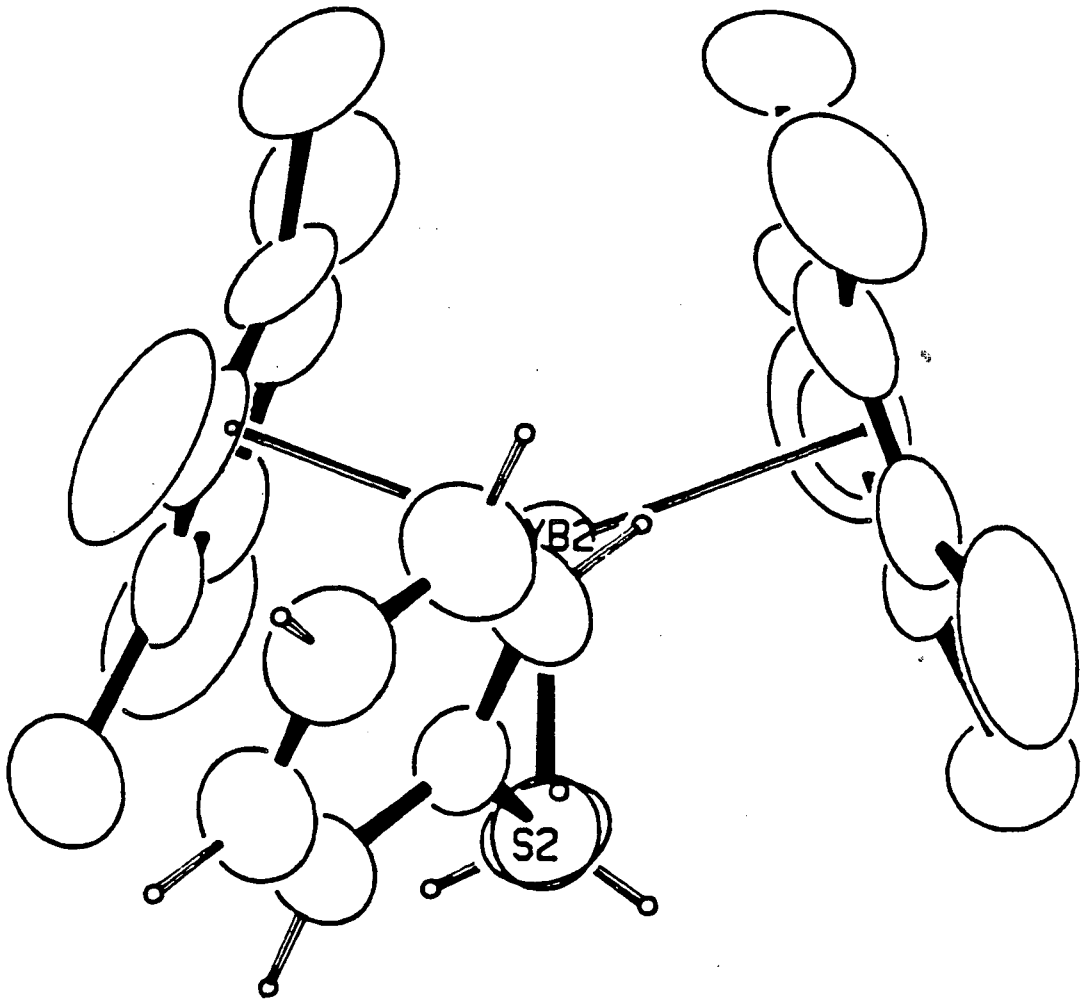


Fig. S3. ORTEP drawing of molecule 2 viewed down a line connecting the S(2) and N(2) atoms. Shows the bowing of the methyl groups away from the Cp rings.



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