N(1)	0.4866 (4)	1.1808 (6)	1.3026 (6)	0.041 (1)
N(2)	0.2711 (4)	1.3030 (6)	1.4092 (5)	0.040 (1)
C(1)	0.0434 (6)	0.8193 (9)	1.1737 (8)	0.056 (2)
C(2)	0.1891 (8)	0.7227 (9)	1.138 (1)	0.066 (3)
C(3)	0.3532 (5)	1.2195 (6)	1.2475 (6)	0.032 (1)
C(4)	0.3518 (6)	1.3152 (8)	1.5657 (7)	0.044 (2)
C(5)	0.4872 (5)	1.2406 (8)	1.4982 (7)	0.045 (2)

Table 2. *Selected geometric parameters* (Å, °)

Sn—Br(1)	2.759 (3)	S(1)—C(3)	1.711 (5)
Sn—C(1)	2.158 (7)	N(1)—C(5)	1.373 (6)
N(1)—C(3)	1.343 (6)	N(2)—C(4)	1.377 (7)
N(2)—C(3)	1.339 (6)	C(4)—C(5)	1.336 (7)
C(1)—C(2)	1.477 (9)	N(2)···Br(1^{i})	3.341 (4)
Sn—S(1)	2.771 (2)		
S(1)—Sn—C(1)	92.3 (2)	Sn—S(1)—C(3)	107.0 (2)
Br(1)—Sn—S(1)	86.19 (8)	C(3)—N(2)—C(4)	110.5 (5)
C(3)—N(1)—C(5)	110.1 (5)	N(1)—C(3)—N(2)	105.6 (4)
Sn—C(1)—C(2)	119.9 (5)	S(1)—C(3)—N(1)	126.3 (4)
S(1)—C(3)—N(2)	128.1 (4)	N(1)—C(5)—C(4)	107.3 (5)
N(2)—C(4)—C(5)	106.5 (4)	N(2)—H(1)···Br(1^{i})	145
Br(1)—Sn—C(1)	91.6 (2)		
Br(1)—Sn—C(1)—C(2)	42.8 (5)	Sn—S(1)—C(3)—N(1)	133.4 (4)

Symmetry code: (i) $-x, 2-y, 2-z$.

The crystal had a cylinder radius R of 0.1 mm. As μR = 0.63, no absorption correction was applied. The structure was solved by Patterson and subsequent difference Fourier methods. Anisotropic displacement parameters were used for all non-H atoms. H atoms were obtained from the F map except for those bonded to N atoms, which were fixed geometrically. The program used to solve and refine the structure was *SHELX*76 (Sheldrick, 1976). Molecular graphics were drawn using *ORTEP* (Johnson, 1965).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and torsion angles have been deposited with the IUCr (Reference: NA1084). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A Trinuclear Terbium(III)–Carborane Cluster, $[C_{61}H_{159}B_{24}Li_6O_5Si_{12}Tb_3].C_6H_6$

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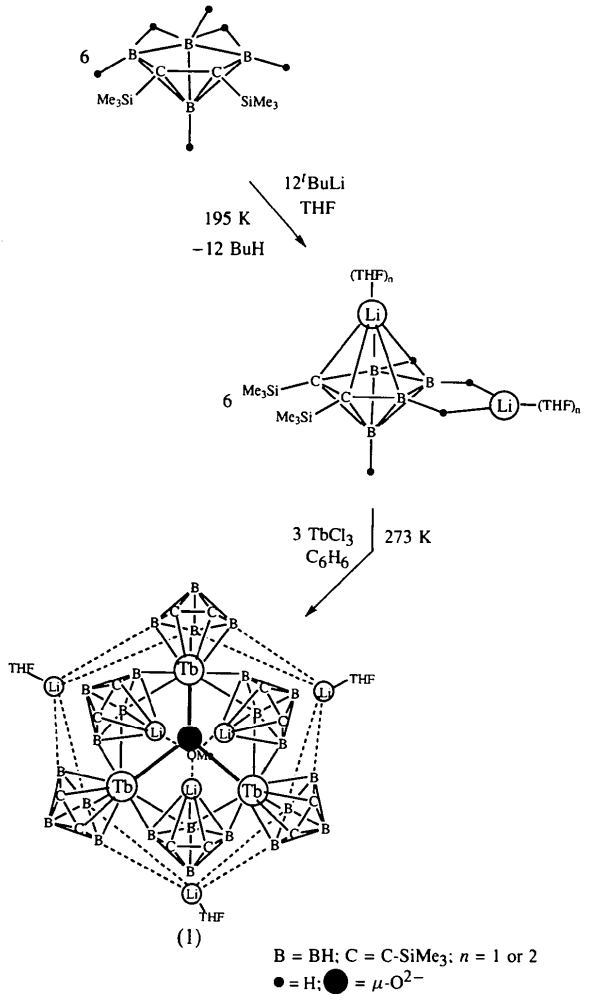
Abstract

The title compound, [{μ_3-methoxy-tris[μ-2,3-bis(trimethylsilyl)-2,3-dicarba-1-lithia-*closo*-heptaborane(6)]}-Tbκ^2B^4,B^5:Tb′κ^2B^5,B^6;Tbκ^2B^4,B^5:Tb″κ^2B^5,B^6;Tb′κ^2B^4,B^5:Tb″κ^2B^5,B^6-{μ_3-oxo-tris[μ-2,3-bis(trimethylsilyl)-2,3-dicarba-1-terba-*closo*-heptaborane(6)]}]-$Li^{THF}\kappa^2B^4,B^5$:$Li^{THF\prime}\kappa^2B^5,B^6$;$Li^{THF}\kappa^2B^4,B^5$:$Li^{THF\prime\prime}\kappa^2B^5,B^6$;$Li^{THF\prime}\kappa^2B^4,B^5$:$Li^{THF\prime\prime}\kappa^2B^5,B^6$-tris(tetrahydrofuranlithium) benzene solvate, [({μ_3-OMe-[μ-1-Li-2,3-$(SiMe_3)_2$-2,3-$C_2B_4H_4$]$_3$}-{μ_3-O-[μ-1-Tb-2,3-$(SiMe_3)_2$-2,3-$C_2B_4H_4$]$_3$})-[Li(C_4H_8O)]$_3$].C_6H_6, crystallized in the triclinic space group $P\bar{1}$. The structure of this cluster consists of three *closo*-terbacarboranes, three cage-bridged Li(THF) units, and three Tb-bridged *closo*-lithiacarboranes that form a tricapped trigonal prism with Tb atoms in the capping positions. A centrally located O atom triply bridges the Tb atoms [Tb—O = 2.185 (3), 2.170 (3) and 2.173 (3) Å], forming a nearly coplanar arrangement [Tb—O—Tb = 118.9 (2), 119.0 (2) and 120.1 (2)°]. The methoxy group in the cluster is linked to the apical Li atoms of the three *closo*-lithiacarboranes in a distorted tetrahedral fashion [average Li—O—Li = 105.9 (5)° and average C—O—Li = 112.8 (5)°].

Comment

Most of the organolanthanides that have been reported contain cyclopentadienides as ligands (Rogers & Rogers, 1991; Evans, 1985, 1987; Evans, Gonzales & Ziller, 1991; Wilkinson, Stone & Abel, 1982; Wilkinson, Gillard & McCleverty, 1987; Cotton & Wilkinson, 1988). On the other hand, the chemistry of lanthanide complexes of the C_2B_{10}, C_2B_9 and C_2B_4 carborane-ligand systems has just begun to be explored and, consequently, the carborane sandwich and half-sandwich complexes of Sm, Eu, Gd and Yb have recently been synthesized and structurally characterized (Manning, Knobler & Hawthorne, 1988; Khattar, Knobler, Johnson & Hawthorne, 1991; Manning, Knobler, Khattar & Hawthorne, 1991; Khattar, Manning, Knobler, Johnson & Hawthorne, 1992; Oki, Zhang & Hosmane, 1992). Our report on the synthesis and crystal structure of

a *closo*-gadolinium(III)–carborane cluster (Oki, Zhang & Hosmane, 1992) demonstrated that the reactivity of the C_2B_4 carborane ligands toward the lanthanide metal reagents is quite different from those of C_2B_9 and C_2B_{10} carborane systems. In order to further investigate this difference in reactivity of the C_2B_4 carborane ligands in lanthanide chemistry, we have synthesized, in 55% yield, the title compound by the treatment of the THF-solvated dilithiacarborane (Hosmane, Saxena, Barreto, Zhang, Maguire, Jia, Wang, Oki, Grover, Whitten, Dawson, Tolle, Siriwardane, Demissie & Fagner, 1993) with anhydrous $TbCl_3$ in a molar ratio of 2:1 in dry benzene, followed by extraction and recrystallization of the product from a solution containing 95% dry *n*-hexane and 5% dry THF. This resulted in the isolation of air-sensitive orange plate-shaped crystals of the title compound, (1).



Since there are no structural reports on any of the π complexes of terbium (Allen, Aspinall, Moore, Hursthouse & Karvalov, 1992; Schulz & Amberger, 1993), we carried out the X-ray diffraction analysis on a single crystal sample of (1) and report herein the results of this study.

The crystal structure (Fig. 1) reveals that (1) is isostructural with the trinuclear *closo*-gadolinium(III)–carborane cluster (Oki, Zhang & Hosmane, 1992) in that three Tb and six Li atoms form a tricapped trigonal prism with Tb atoms in the capping positions. While the methoxy O atom (O120) links the apical Li atoms of the three *closo*-lithiacarboranes in a tetrahedral fashion and is displaced from the lower Li_3 plane by 0.718 (7) Å, the central μ_3-bridged O atom (O100) deviates by only 0.180 (3) Å from the Tb_3 triangular plane. The two Li_3 planes are essentially parallel and make dihedral angles of 1.0 (3) and 0.8 (3)°, respectively, with the central Tb_3 plane. While the Tb metal atom in each *closo*-terbacarborane is η^5 bonded to the C_2B_3 face with Tb–centroid distances ranging from 2.358 (3) to 2.374 (3) Å, the Li—C_2B_3-centroid distances are unexceptional [1.80 (1)–1.83 (1) Å]. The average Tb···Tb [3.756 (1) Å], Tb—O100 [2.176 (3) Å], Li4···Li6 [2.96 (1) Å] and Li—O120 [1.86 (1) Å] distances, and the average centroid—Tb—O100 (117.1°) and average centroid—Li—O120 (167.1°) angles are all comparable with the analogous distances and angles in the *closo*-gadolinium(III)–carborane cluster (Oki, Zhang & Hosmane, 1992). To our knowledge, these results not only constitute the first structural report of any terbacarborane complex, but also the first report on any π-complexed terbium compound.

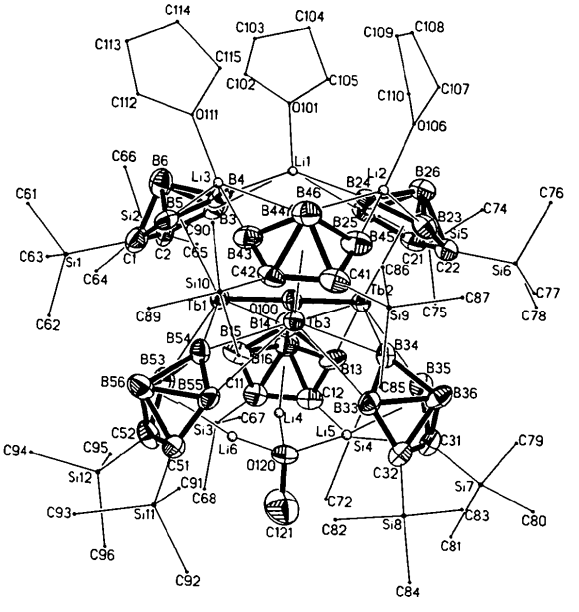


Fig. 1. Displacement ellipsoid drawing of the title compound with ellipsoids at the 40% probability level. For clarity, H atoms have been omitted; atoms of trimethylsilyl and THF, as well as Li atoms are drawn as small circles of arbitrary radii.

Experimental

Crystal data

$[C_{61}H_{159}B_{24}Li_6O_5Si_{12}Tb_3]\cdot C_6H_6$
$M_r = 2165.91$
Triclinic
$P\bar{1}$
$a = 15.976\ (4)$ Å
$b = 16.627\ (4)$ Å
$c = 23.670\ (6)$ Å
$\alpha = 90.08\ (2)°$
$\beta = 89.97\ (2)°$
$\gamma = 69.16\ (2)°$
$V = 5876\ (3)$ Å^3
$Z = 2$
$D_x = 1.224$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 24 reflections
$\theta = 9.0$–$14.0°$
$\mu = 1.944$ mm^{-1}
$T = 230\ (2)$ K
Plate
$0.25 \times 0.10 \times 0.05$ mm
Orange

Data collection

R3m/V diffractometer
$\omega/2\theta$ scans
Absorption correction: semi-empirical
$T_{min} = 0.667$, $T_{max} = 0.898$
11 202 measured reflections
10 728 independent reflections
9679 observed reflections $[I > 2\sigma(I)]$
$R_{int} = 0.013$
$\theta_{max} = 20.04°$
$h = -15 \rightarrow 15$
$k = -16 \rightarrow 16$
$l = 0 \rightarrow 22$
3 standard reflections
monitored every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0289$
$wR(F^2) = 0.0737$
$S = 1.055$
10 708 reflections
1079 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0410P)^2 + 14.4051P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = -0.001$
$\Delta\rho_{max} = 1.124$ e Å^{-3}
$\Delta\rho_{min} = -0.700$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters* (Å^2)

U_{iso} for O101–C105 (disordered THF), C131–C136 (C_6H_6); for others $U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{iso}/U_{eq}
Tb1	0.12806 (2)	0.41559 (2)	0.253671 (11)	0.03033 (10)
Tb2	0.33535 (2)	0.30432 (2)	0.168492 (11)	0.02630 (9)
Tb3	0.34421 (2)	0.29445 (2)	0.327249 (11)	0.02599 (9)
Li1	0.2405 (7)	0.5635 (7)	0.1719 (5)	0.053 (3)
Li2	0.4786 (8)	0.4259 (8)	0.2469 (4)	0.059 (3)
Li3	0.2518 (8)	0.5499 (7)	0.3427 (5)	0.057 (3)
Li4	0.1515 (7)	0.2069 (7)	0.1904 (4)	0.046 (3)
Li5	0.3280 (7)	0.1081 (6)	0.2384 (4)	0.044 (3)
Li6	0.1743 (7)	0.1881 (7)	0.3147 (4)	0.046 (3)
Si1	−0.08237 (13)	0.59523 (12)	0.34505 (8)	0.0577 (5)
Si2	−0.08888 (13)	0.62081 (13)	0.17930 (8)	0.0604 (6)
Si3	−0.06655 (13)	0.26335 (15)	0.11484 (10)	0.0681 (6)
Si4	0.15912 (14)	0.13004 (12)	0.04529 (8)	0.0583 (5)
Si5	0.34650 (13)	0.37571 (12)	−0.00374 (7)	0.0511 (5)
Si6	0.57271 (12)	0.24696 (13)	0.07081 (8)	0.0527 (5)
Si7	0.51091 (13)	−0.06273 (11)	0.16186 (8)	0.0527 (5)
Si8	0.49074 (13)	−0.05864 (11)	0.32451 (8)	0.0501 (5)
Si9	0.59526 (14)	0.21646 (14)	0.41030 (10)	0.0709 (6)
Si10	0.38437 (15)	0.34610 (14)	0.50060 (7)	0.0599 (6)
Si11	0.15966 (13)	0.12894 (12)	0.46635 (8)	0.0515 (5)
Si12	−0.04998 (13)	0.2400 (2)	0.37561 (10)	0.0711 (6)
O100	0.2727 (2)	0.3473 (2)	0.24988 (14)	0.0280 (9)
O120	0.2068 (2)	0.1295 (2)	0.2465 (2)	0.0368 (9)
C121	0.1851 (5)	0.0539 (6)	0.2488 (3)	0.089 (3)
C1	0.0130 (4)	0.5674 (4)	0.2927 (3)	0.044 (2)
C2	0.0078 (4)	0.5751 (4)	0.2295 (3)	0.043 (2)
B3	0.1001 (5)	0.5708 (4)	0.2054 (3)	0.043 (2)
B4	0.1672 (5)	0.5629 (4)	0.2587 (3)	0.043 (2)
B5	0.1077 (5)	0.5582 (4)	0.3146 (3)	0.040 (2)
B6	0.0549 (5)	0.6386 (5)	0.2642 (3)	0.051 (2)
C11	0.0475 (4)	0.2673 (4)	0.1296 (3)	0.042 (2)
C12	0.1344 (4)	0.2174 (4)	0.1003 (2)	0.041 (2)
B13	0.2077 (5)	0.2560 (4)	0.1128 (3)	0.037 (2)
B14	0.1590 (4)	0.3418 (4)	0.1511 (3)	0.034 (2)
B15	0.0570 (5)	0.3421 (5)	0.1651 (3)	0.039 (2)
B16	0.0971 (5)	0.3258 (5)	0.0926 (3)	0.042 (2)
C21	0.3772 (4)	0.3736 (3)	0.0730 (2)	0.0333 (14)
C22	0.4647 (4)	0.3237 (4)	0.1011 (2)	0.0369 (15)
B23	0.4739 (5)	0.3635 (5)	0.1590 (3)	0.035 (2)
B24	0.3823 (5)	0.4491 (5)	0.1680 (3)	0.038 (2)
B25	0.3210 (5)	0.4497 (4)	0.1118 (3)	0.035 (2)
B26	0.4349 (5)	0.4329 (5)	0.1006 (3)	0.039 (2)
C31	0.4618 (4)	0.0334 (3)	0.2094 (2)	0.0369 (15)
C32	0.4572 (4)	0.0333 (3)	0.2730 (2)	0.0366 (15)
B33	0.4365 (4)	0.1241 (4)	0.2972 (3)	0.033 (2)
B34	0.4320 (4)	0.1877 (4)	0.2425 (3)	0.030 (2)
B35	0.4418 (4)	0.1261 (4)	0.1863 (3)	0.034 (2)
B36	0.5198 (5)	0.0857 (4)	0.2432 (3)	0.038 (2)
C41	0.4871 (4)	0.3005 (4)	0.3873 (2)	0.0381 (15)
C42	0.4066 (4)	0.3477 (4)	0.4225 (2)	0.0356 (15)
B43	0.3447 (5)	0.4302 (5)	0.3922 (3)	0.041 (2)
B44	0.3953 (5)	0.4360 (4)	0.3321 (3)	0.038 (2)
B45	0.4846 (5)	0.3485 (5)	0.3304 (3)	0.038 (2)
B46	0.4609 (5)	0.4092 (5)	0.3937 (3)	0.044 (2)
C51	0.1477 (4)	0.2037 (4)	0.4049 (2)	0.0386 (15)
C52	0.0638 (4)	0.2488 (4)	0.3714 (2)	0.043 (2)
B53	0.0742 (5)	0.3225 (5)	0.3359 (3)	0.041 (2)
B54	0.1721 (4)	0.3269 (4)	0.3522 (3)	0.032 (2)
B55	0.2198 (5)	0.2436 (4)	0.3930 (3)	0.036 (2)
B56	0.1068 (5)	0.3121 (5)	0.4090 (3)	0.042 (2)
C61	−0.1575 (5)	0.7098 (5)	0.3373 (4)	0.090 (3)
C62	−0.1492 (5)	0.5242 (5)	0.3377 (3)	0.075 (2)
C63	−0.0347 (5)	0.5789 (6)	0.4174 (3)	0.083 (3)
C64	−0.1923 (5)	0.5999 (6)	0.1980 (3)	0.087 (3)
C65	−0.0538 (5)	0.5752 (5)	0.1075 (3)	0.079 (2)
C66	−0.1185 (5)	0.7391 (5)	0.1753 (3)	0.088 (3)
C67	−0.0894 (6)	0.2647 (7)	0.0380 (4)	0.109 (3)
C68	−0.0806 (6)	0.1678 (6)	0.1482 (5)	0.118 (4)
C69	−0.1539 (4)	0.3590 (5)	0.1467 (4)	0.086 (3)
C70	0.1309 (7)	0.1732 (6)	−0.0275 (3)	0.101 (3)
C71	0.2809 (6)	0.0709 (5)	0.0469 (4)	0.102 (3)
C72	0.1041 (7)	0.0507 (6)	0.0600 (4)	0.115 (4)
C73	0.2428 (6)	0.4704 (6)	−0.0173 (3)	0.102 (3)
C74	0.4337 (6)	0.3888 (6)	−0.0505 (3)	0.093 (3)
C75	0.3217 (6)	0.2797 (5)	−0.0260 (3)	0.074 (2)
C76	0.6393 (5)	0.3106 (6)	0.0433 (3)	0.086 (3)
C77	0.6407 (4)	0.1765 (5)	0.1273 (3)	0.076 (2)
C78	0.5574 (5)	0.1751 (5)	0.0144 (3)	0.083 (2)
C79	0.5364 (5)	−0.0272 (5)	0.0919 (3)	0.073 (2)
C80	0.6191 (5)	−0.1420 (5)	0.1891 (4)	0.089 (3)
C81	0.4299 (6)	−0.1175 (5)	0.1501 (3)	0.078 (2)
C82	0.4259 (5)	−0.0189 (5)	0.3903 (3)	0.073 (2)
C83	0.6127 (5)	−0.0950 (5)	0.3412 (3)	0.078 (2)
C84	0.4606 (7)	−0.1516 (5)	0.3006 (3)	0.094 (3)
C85	0.5816 (7)	0.1147 (6)	0.4345 (5)	0.136 (5)
C86	0.6476 (6)	0.2580 (6)	0.4682 (4)	0.105 (3)
C87	0.6747 (5)	0.1865 (8)	0.3496 (4)	0.141 (5)
C88	0.4373 (7)	0.2395 (7)	0.5361 (4)	0.122 (4)
C89	0.2629 (5)	0.3782 (6)	0.5125 (3)	0.087 (3)
C90	0.4249 (8)	0.4262 (7)	0.5365 (3)	0.126 (4)
C91	0.2593 (5)	0.1233 (5)	0.5087 (3)	0.068 (2)
C92	0.1772 (5)	0.0175 (4)	0.4421 (4)	0.079 (2)
C93	0.0626 (6)	0.1668 (5)	0.5163 (3)	0.088 (3)
C94	−0.1197 (5)	0.3120 (6)	0.4310 (4)	0.113 (4)
C95	−0.1046 (6)	0.2738 (7)	0.3050 (4)	0.109 (3)

C96	−0.0466 (6)	0.1278 (6)	0.3883 (5)	0.116 (4)
O101	0.2401 (4)	0.6733 (3)	0.1520 (2)	0.087 (2)
C102	0.1782 (6)	0.7509 (4)	0.1720 (4)	0.201 (6)
C103	0.1651 (7)	0.8151 (5)	0.1255 (5)	0.218 (7)
C104	0.2580 (7)	0.7862 (6)	0.1019 (4)	0.165 (5)
C105	0.2822 (5)	0.6908 (5)	0.1043 (3)	0.153 (5)
O106	0.5571 (4)	0.4877 (3)	0.2477 (2)	0.082 (2)
C107	0.5713 (7)	0.5354 (6)	0.2014 (3)	0.094 (3)
C108	0.5580 (7)	0.6217 (6)	0.2249 (4)	0.109 (3)
C109	0.5823 (7)	0.6045 (6)	0.2870 (4)	0.105 (3)
C110	0.5939 (7)	0.5147 (6)	0.2971 (4)	0.100 (3)
O111	0.2472 (4)	0.6582 (3)	0.3690 (2)	0.0753 (15)
C112	0.1739 (11)	0.7200 (9)	0.3925 (9)	0.289 (13)
C113	0.1777 (9)	0.7994 (8)	0.3957 (8)	0.190 (7)
C114	0.2573 (13)	0.7909 (8)	0.3692 (7)	0.211 (9)
C115	0.3056 (9)	0.6970 (9)	0.3649 (8)	0.231 (10)
C131	0.1882 (10)	0.0164 (9)	0.7409 (6)	0.169 (5)
C132	0.1476 (10)	0.0149 (11)	0.7916 (7)	0.208 (7)
C133	0.0562 (10)	0.0497 (10)	0.7886 (7)	0.199 (6)
C134	0.0200 (10)	0.0778 (9)	0.7367 (6)	0.167 (5)
C135	0.0606 (9)	0.0869 (10)	0.6875 (6)	0.181 (6)
C136	0.1520 (10)	0.0539 (10)	0.6909 (6)	0.188 (6)

Table 2. *Selected geometric parameters* (Å, °)

Tb1—O100	2.185 (3)	Li1—B25	2.349 (12)
Tb1—B14	2.684 (7)	Li1—B4	2.367 (12)
Tb1—B5	2.692 (7)	Li1—B24	2.386 (13)
Tb1—C1	2.700 (5)	Li2—O106	1.884 (12)
Tb1—B3	2.711 (7)	Li2—B23	2.336 (13)
Tb1—B54	2.717 (7)	Li2—B45	2.344 (13)
Tb1—C2	2.727 (5)	Li2—B24	2.362 (13)
Tb1—B4	2.737 (7)	Li2—B44	2.390 (13)
Tb1—B53	2.807 (7)	Li3—O111	1.880 (11)
Tb1—B15	2.856 (7)	Li3—B43	2.334 (13)
Tb2—O100	2.170 (3)	Li3—B5	2.354 (14)
Tb2—B34	2.664 (6)	Li3—B4	2.372 (14)
Tb2—B14	2.692 (6)	Li3—B44	2.411 (13)
Tb2—B25	2.704 (7)	Li4—O120	1.842 (11)
Tb2—C22	2.718 (5)	Li4—C12	2.150 (12)
Tb2—C21	2.728 (5)	Li4—C11	2.160 (11)
Tb2—B23	2.732 (7)	Li4—B15	2.298 (12)
Tb2—B24	2.764 (7)	Li4—B13	2.316 (12)
Tb2—B13	2.777 (7)	Li4—B14	2.472 (12)
Tb2—B35	2.876 (7)	Li5—O120	1.849 (11)
Tb3—O100	2.173 (3)	Li5—C32	2.158 (11)
Tb3—B54	2.672 (6)	Li5—C31	2.166 (11)
Tb3—B45	2.698 (7)	Li5—B35	2.302 (12)
Tb3—B34	2.712 (6)	Li5—B33	2.311 (12)
Tb3—C41	2.721 (5)	Li5—B34	2.467 (12)
Tb3—B43	2.732 (7)	Li6—O120	1.861 (11)
Tb3—C42	2.735 (5)	Li6—C52	2.158 (11)
Tb3—B44	2.754 (7)	Li6—C51	2.173 (11)
Tb3—B33	2.779 (6)	Li6—B53	2.293 (13)
Tb3—B55	2.877 (7)	Li6—B55	2.298 (13)
Li1—O101	1.884 (11)	Li6—B54	2.459 (12)
Li1—B3	2.340 (13)		
Tb2—O100—Tb3	120.07 (15)	Li4—O120—Li5	105.6 (5)
Tb2—O100—Tb1	119.01 (15)	C121—O120—Li6	108.5 (5)
Tb3—O100—Tb1	118.89 (15)	Li4—O120—Li6	106.6 (5)
C121—O120—Li4	116.1 (5)	Li5—O120—Li6	105.6 (5)
C121—O120—Li5	113.7 (5)		

Data were corrected for Lorentz, polarization and absorption effects. The structure was refined from a starting model which was based on the isostructural Gd–carborane cluster (Oki, Zhang & Hosmane, 1992). Refinement was on F^2 for all reflections except for 20 with very negative F^2 or flagged for potential systematic errors. Full-matrix least-squares refinement was performed. All non-H atoms, with the exception of those of one disordered THF (O101–C105) and the solvated benzene (C131–C136), were refined anisotropically. The disordered THF and benzene molecules were elastically restrained during final cycles of refinement. Methyl, methylene and aromatic H atoms were positioned using a riding model, while the carborane-cage H atoms were located on ΔF maps and their isotropic displacement parameters were refined as a common free variable.

Data collection, cell refinement and data reduction: *R3m/V* diffractometer control program. Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990). Software used to prepare material for publication: *SHELXL*93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry for non-H atoms have been deposited with the IUCr (Reference: NA1110). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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