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) Sn—C(1) N(1)—C(3) N(2)—C(3) C(1)—C(2) Sn_S(1)	2.759 (3) 2.158 (7) 1.343 (6) 1.339 (6) 1.477 (9) 2.771 (2)	$\begin{array}{l} S(1) & -C(3) \\ N(1) & -C(5) \\ N(2) & -C(4) \\ C(4) & -C(5) \\ N(2) & \cdot \cdot Br(1^{i}) \end{array}$	1.711 (5) 1.373 (6) 1.377 (7) 1.336 (7) 3.341 (4)
S(1) = Sn = C(1) $S(1) = Sn = C(1)$ $C(3) = N(1) = C(5)$ $Sn = C(1) = C(2)$ $S(1) = C(3) = N(2)$ $N(2) = C(4) = C(5)$ $Br(1) = Sn = C(1)$	92.3 (2) 86.19 (8) 110.1 (5) 119.9 (5) 128.1 (4) 106.5 (4) 91.6 (2)	$\begin{array}{l} Sn-S(1)-C(3)\\ C(3)-N(2)-C(4)\\ N(1)-C(3)-N(2)\\ S(1)-C(3)-N(1)\\ N(1)-C(5)-C(4)\\ N(2)-H(1)\cdots Br(1^{i}) \end{array}$	107.0 (2) 110.5 (5) 105.6 (4) 126.3 (4) 107.3 (5) 145
Br(1)—Sn—C(1)—C(2) Symm	42.8 (5) hetry code: (i)	Sn = S(1) = C(3) = N(1) -x, 2 - y, 2 - z.	133.4 (4)

The crystal had a cylinder radius R of 0.1 mm. As $\mu R = 0.63$, 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, Hatom 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, $[{\mu_3}-methoxy-tris[\mu-2,3-bis(trime$ thylsilyl)-2,3-dicarba-1-lithia-closo-heptaborane(6)]}- $\mathrm{Tb}\kappa^2 B^4, B^5$: $\mathrm{Tb}'\kappa^2 B^5, B^6$; $\mathrm{Tb}\kappa^2 B^4, B^5$: $\mathrm{Tb}''\kappa^2 B^5, B^6$; $Tb'\kappa^2 B^4, B^5: Tb''\kappa^2 B^5, B^6-\{\mu_3-\text{oxo-tris}[\mu-2,3-\text{bis}(\text{trime-}$ thylsilyl)-2,3-dicarba-1-terba-closo-heptaborane(6)]}]-Li^{THF} $\kappa^2 B^4$, B^5 : Li^{THF} $\kappa^2 B^5$, B^6 ; Li^{THF} $\kappa^2 B^4$, B^5 : Li^{THF} $\kappa^2 B^4$, Bfuranlithium) benzene solvate, [($\{\mu_3-OMe-[\mu-1-Li-2,3 (SiMe_3)_2 - 2.3 - C_2B_4H_4]_3 - \{\mu_3 - O - [\mu - 1 - Tb - 2.3 - (SiMe_3)_2 - SiMe_3 - SiMe_$ $2,3-C_2B_4H_4]_3$)-[Li(C₄H₈O)]₃].C₆H₆, crystallized in the triclinic space group $P\overline{1}$. The structure of this cluster consists of three closo-terbacarboranes, three cagebridged Li(THF) units, and three Tb-bridged closolithiacarboranes 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 = $105.9(5)^{\circ}$ and average C—O— $Li = 112.8 (5)^{\circ}$].

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 carboraneligand 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 C₂B₄ 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 THFsolvated dilithiacarborane (Hosmane, Saxena, Barreto, Zhang, Maguire, Jia, Wang, Oki, Grover, Whitten, Dawson, Tolle, Siriwardane, Demissie & Fagner, 1993) with anhydrous TbCl₃ 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 airsensitive 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 Li₃ plane by 0.718 (7) Å, the central μ_3 -bridged O atom (O100) deviates by only 0.180(3) Å from the Tb₃ triangular plane. The two Li₃ planes are essentially parallel and make dihedral angles of 1.0(3) and $0.8(3)^{\circ}$, respectively, with the central Tb₃ plane. While the Tb metal atom in each *closo*-terbacarborane is η^5 bonded to the C₂B₃ 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], $Li4 \cdot \cdot \cdot Li6$ [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.

$ \begin{array}{c} C_{7} taid data \\ (C_{1} H_{10} B_{3} Li_{0} 0_{3} Si_{1} Tb_{1} - M & Ka ration \\ C_{1} H_{10} B_{3} Li_{0} 0_{3} Si_{1} Tb_{1} - M & Ka ration \\ C_{2} H_{4} = 0.165 0_{1} & Cll parameters from 24 \\ M, = 2165 0_{1} & Cll parameters from 24 \\ Technic \\ PT & fetchins \\ PT = 0.076 (4) \\ A & = 0.014 M m^{-1} \\ = 156 0_{1} (2) \\ PT & fetchins \\$	Experimental				Si9	0.59526 (14)	0.21646 (14)	0.41030 (10)	0.0709 (6)
$ \begin{bmatrix} C_{n} H_{vv} B_{3} L_{k} O_{3} Si_{17} Tb_{1} I_{n} \\ C_{4} A_{n} \\$	Crystal data				Si10 Si11	0.38437 (13)	0.12894 (12)	0.46635 (8)	0.0599 (0)
$ \begin{array}{c} \mbox{Call} 0 \\ Call, 0 \\ Ca$	C. H. B. Li O. Si.	Thal-	Mo Ka radiation		Si12	-0.04998 (13)	0.2400 (2)	0.37561 (10)	0.0711 (6)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C.H.	[103]	$\lambda = 0.71073$ Å		O100	0.2727 (2)	0.3473 (2)	0.24988 (14)	0.0280 (9)
	M = 2165.91		Cell parameters f	from 24	C120	0.2008 (2)	0.0539 (6)	0.2488 (3)	0.089 (3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$M_r = 2105.91$		reflections		CI	0.0130 (4)	0.5674 (4)	0.2927 (3)	0.044 (2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	PI		$\theta = 9.0 - 14.0^{\circ}$		C2	0.0078 (4)	0.5751 (4)	0.2295 (3)	0.043 (2)
$ \begin{array}{c} \mathbf{x} = \mathbf{x} \in (27) (4) \mathbf{x} & \mathbf{r} = \mathbf{z} = 30 (2) \mathbf{x} & \mathbf{r} \\ \mathbf{z} = 23 670 (6) \mathbf{x} & \mathbf{Pate} & \mathbf{z} \\ \mathbf{z} = 30.08 (2)^* & 0 \cdot \mathbf{z} > \mathbf{x} 0.10 \times 0.05 \ \mathrm{nm} & \mathbf{C11} & 0 0.473 (4) & 0 \cdot \mathbf{z}^{23} (4) & 0 \cdot \mathbf{z}^{24} (6) & 0 0.041 (2) \\ \mathbf{z} = 30.08 (2)^* & 0 \cdot \mathbf{z} > \mathbf{x} 0.10 \times 0.05 \ \mathrm{nm} & \mathbf{C11} & 0 0.473 (4) & 0 \cdot \mathbf{z}^{24} (4) & 0 \cdot 1 (28 (6) & 0 \cdot \mathbf{z}^{24} (4) \\ \mathbf{z} = 50.16 (2)^* & \mathbf{z} = 25.07 (3) \mathbf{x}^{24} & \mathbf{z} = 25.07 (3) \mathbf{z}^{24} & \mathbf{z} = 25.04 (4) \mathbf{z}^{24} & $	a = 15.976 (4) Å		$u = 1.944 \text{ mm}^{-1}$		B3	0.1001 (5)	0.5708 (4)	0.2054 (3)	0.043 (2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	a = 15.970 (4) Å b = 16.627 (4) Å		T = 230(2) K		B4 B5	0.1672 (5)	0.5629(4) 0.5582(4)	0.2387(3) 0.3146(3)	0.040 (2)
$\begin{array}{c} a = 90.07 (2)^{a} & 0.25 \times 0.10 \times 0.05 \text{ nm} & C12 & 0.0475 (4) & 0.2373 (4) & 0.1296 (3) & 0.042 (2) \\ \beta = 8.997 (2)^{a} & Orange & B13 & 0.2077 (5) & 0.256 (4) & 0.1328 (3) & 0.041 (2) \\ \gamma = 69.16 (2)^{a} & Drange & B13 & 0.2077 (5) & 0.256 (4) & 0.1128 (3) & 0.037 (2) \\ \gamma = 69.16 (2)^{a} & B13 & 0.2077 (5) & 0.256 (4) & 0.1128 (3) & 0.037 (2) \\ \gamma = 58.76 (3) Å^{3} & B13 & 0.2077 (5) & 0.256 (4) & 0.1128 (3) & 0.037 (2) \\ D_{x} = 1.224 \text{ Mg m}^{-3} & C12 & 0.0447 (4) & 0.0333 (5) & 0.0493 (2) \\ D_{x} = 1.224 \text{ Mg m}^{-3} & C12 & 0.0447 (4) & 0.0333 (5) & 0.0493 (2) \\ Data collection & B24 & 0.3233 (4) & 0.0736 (5) & 0.0436 (5) & 0.0358 (2) \\ Data collection & B24 & 0.323 (5) & 0.4491 (5) & 0.1188 (3) & 0.0358 (2) \\ w/2\theta \ scans & \theta_{ms} = 20.04^{a} & C1 & 0.0418 (4) & 0.0333 (3) & 0.2794 (2) & 0.0336 (1) \\ w/2\theta \ scans & \theta_{ms} = 20.04^{a} & C1 & 0.4418 (4) & 0.0333 (3) & 0.2794 (2) & 0.0396 (1) \\ semi-empirical & k = -16 \rightarrow 16 & B33 & 0.4356 (4) & 0.1241 (4) & 0.2423 (3) & 0.0333 (2) \\ T_{ms} = 0.667, T_{ms} = 1 = 0 \rightarrow 22 & B34 & 0.4356 (4) & 0.1241 (4) & 0.2423 (3) & 0.0336 (2) \\ reflections & intensity decay: none B43 & 0.4476 (4) & 0.4384 (3) & 0.2323 (3) & 0.0336 (2) \\ reflections & intensity decay: none B44 & 0.3476 (4) & 0.4384 (4) & 0.4226 (2) & 0.0366 (1) \\ reflections & intensity decay: none B44 & 0.3476 (4) & 0.4384 (5) & 0.3321 (3) & 0.0386 (2) \\ g679 observed reflections & intensity decay: none B44 & 0.3476 (4) & 0.4386 (5) & 0.3321 (3) & 0.0386 (2) \\ reflections & intensity decay: none B44 & 0.3476 (4) & 0.4386 (5) & 0.3376 (4) & 0.0336 (2) \\ reflections & intensity decay: none B44 & 0.3476 (4) & 0.4386 (5) & 0.3376 (4) & 0.0336 (2) \\ reflections & from intersection: none (C2 - 0.43776 (4) & 0.4386 (5) & 0.3376 (4) & 0.0386 (2) \\ reflections & intensity decay: none B44 & 0.4376 (4) & 0.4386 (5) & 0.3376 (4) & 0.0386 (2) \\ reflections & from intersection: none (C2 - 0.0337 (4) & 0.4396 (4) & 0.0337 (5) & 0.0396 (5) & 0.0377 (3) & 0.0377 (3) & 0.0377 (3) & 0.0377 (3) & 0.0377 (3) & 0.0377 $	c = 23.670 (6) Å		Plate		B6	0.0549 (5)	0.6386 (5)	0.2642 (3)	0.051 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\alpha = 90.08(2)^{\circ}$		$0.25 \times 0.10 \times 0$.05 mm	C11	0.0475 (4)	0.2673 (4)	0.1296 (3)	0.042 (2)
$ \begin{array}{c} r = 69.16 \ (2)^{\circ} \\ r = 5876 \ (3) \ A^3 \\ V = 5876 \ (3) \ A^3 \\ V = 5876 \ (3) \ A^3 \\ Z = 2 \\ D_x = 1.224 \ Mg \ m^{-3} \\ C1 = 0.3772 \ (4) \ 0.3736 \ (5) \ 0.3736 \ (5) \ 0.0932 \ (6) \ 0.0936 \ (6) \\ D_x = 1.224 \ Mg \ m^{-3} \\ C2 = 0.4647 \ (4) \ 0.3237 \ (4) \ 0.0373 \ (5) \ 0.0373 \ (5) \ 0.0373 \ (6) \\ D_x = 1.224 \ Mg \ m^{-3} \\ C2 = 0.4647 \ (4) \ 0.3237 \ (4) \ 0.0373 \ (5) \ 0.0373 \ (5) \ 0.0373 \ (6) \\ D_x = 1.224 \ Mg \ m^{-3} \\ C2 = 0.4647 \ (4) \ 0.3237 \ (4) \ 0.0337 \ (5) \ 0.0333 \ (5) \ 0.0395 \ (6) \\ D_x = 1.224 \ Mg \ m^{-3} \\ C2 = 0.4647 \ (4) \ 0.3237 \ (4) \ 0.0337 \ (5) \ 0.0373 \ (5) \ 0.0373 \ (6) \ 0.0375 \ (7) \\ D_x = 2.24 \ Mg \ m^{-3} \\ M_x \ M$	$\beta = 89.97 (2)^{\circ}$		Orange		C12	0.1344 (4)	0.2174 (4)	0.1003 (2)	0.041(2) 0.037(2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\gamma = 69.16(2)^{\circ}$		0		B13	0.1590 (4)	0.3418 (4)	0.1511 (3)	0.034 (2)
$ \begin{array}{c} z = 2 \\ 2 = 2 $	$V = 5876 (3) Å^3$				B15	0.0570 (5)	0.3421 (5)	0.1651 (3)	0.039 (2)
$ \begin{array}{c} D_r = 1.224 \mbox{ Mg m}^{-3} & C1 0.47/2(4) 0.237(4) 0.237(4) 0.038(12) 0.0034(1) 0.0033(1) 0.0034(1) 0.0035(1) 0.0036(1) 0.0035(1) 0.003$	Z = 2				B16	0.0971 (5)	0.3258 (5)	0.0926 (3)	0.042 (2)
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	$D_r = 1.224 \text{ Mg m}^{-3}$				C21 C22	0.3772 (4)	0.3736(3)	0.0730(2) 0.1011(2)	0.0333(14) 0.0369(15)
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $					B23	0.4739 (5)	0.3635 (5)	0.1590 (3)	0.035 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Data collection				B24	0.3823 (5)	0.4491 (5)	0.1680 (3)	0.038 (2)
$ \begin{array}{c} \omega_{L} 2\theta \ \text{scans} \ \text{trime} \ \theta_{\max} = 20.04^{\circ} \ \text{cf} \ 0.4434(5) \ 0.4434(5) \ 0.0334(5) \ 0.0394(2)$	R3m/V diffractomete	r	$R_{\rm int} = 0.013$		B25	0.3210 (5)	0.4497 (4)	0.1118 (3)	0.035 (2)
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	$\omega/2\theta$ scans		$\theta_{\rm max} = 20.04^{\circ}$		B26 C31	0.4349 (5)	0.4329 (5)	0.2094 (2)	0.039(2) 0.0369(15)
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Absorption correction	n:	$h = -15 \rightarrow 15$		C32	0.4572 (4)	0.0333 (3)	0.2730 (2)	0.0366 (15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	semi-empirical		$k = -16 \rightarrow 16$		B33	0.4365 (4)	0.1241 (4)	0.2972 (3)	0.033 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$T_{\rm min} = 0.667, T_{\rm max}$. =	$l = 0 \rightarrow 22$		B34	0.4320 (4)	0.1877 (4)	0.2425 (3)	0.030 (2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0.898	~	3 standard reflec	tions	B35 B36	0.4418 (4)	0.1261 (4)	0.1803(3) 0.2432(3)	0.034(2) 0.038(2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	11 202 measured refl	ections	monitored eve	rv 200	C41	0.4871 (4)	0.3005 (4)	0.3873 (2)	0.0381 (15)
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	10728 independent		reflections	5	C42	0.4066 (4)	0.3477 (4)	0.4225 (2)	0.0356 (15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	reflections		intensity deca	y: none	B43	0.3447 (5)	0.4302 (5)	0.3922 (3)	0.041 (2)
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	9679 observed reflect	tions		•	B44 B45	0.3953 (5)	0.4360 (4)	0.3321(3) 0.3304(3)	0.038 (2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$[I > 2\sigma(I)]$				B46	0.4609 (5)	0.4092 (5)	0.3937 (3)	0.044 (2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $					C51	0.1477 (4)	0.2037 (4)	0.4049 (2)	0.0386 (15)
$ \begin{array}{c} \text{Refinement on } F^2 & (\Delta/\sigma)_{\text{max}} = -0.001 & \text{B53} & 0.0742(3) & 0.322(3) & 0.3327(3) & 0.032(2) \\ R[F^2 > 2\sigma(F^2)] = 0.0289 & \Delta\rho_{\text{max}} = 1.124 \text{ e} \text{Å}^{-3} & \text{B55} & 0.2198(5) & 0.2436(4) & 0.3322(3) & 0.032(2) \\ wR(F^2) = 0.0737 & \Delta\rho_{\text{min}} = -0.700 \text{ e} \text{Å}^{-3} & \text{B56} & 0.1068(5) & 0.0341(4) & 0.4902(3) & 0.042(2) \\ S = 1.055 & \text{Extinction correction: none} & C_{61} & -0.1575(5) & 0.7098(5) & 0.3373(4) & 0.090(3) \\ S = 1.057 & \text{Extinction correction: none} & C_{62} & -0.1492(5) & 0.5342(5) & 0.0373(3) & 0.075(2) \\ 10708 \text{ reflections} & \text{Atomic scattering factors} & C_{63} & -0.0347(5) & 0.5788(6) & 0.4174(3) & 0.083(3) \\ w = 1/[\sigma^2(F_{\sigma}^2) + (0.0410P)^2 & for Crystallography (1992, & C_{66} & -0.0158(5) & 0.7391(5) & 0.175(3) & 0.079(2) \\ w = 1/[\sigma^2(F_{\sigma}^2) + 4.044051P] & Vol. C, Tables 4.2.6.8 and & C_{67} & -0.0894(6) & 0.2647(7) & 0.0380(4) & 0.109(3) \\ \text{where } P = (F_{\sigma}^2 + 2F_{\sigma}^2)/3 & 6.1.1.4) & C_{68} & -0.0806(6) & 0.1678(6) & 0.1482(5) & 0.118(4) \\ \text{C70} & 0.1399(7) & 0.1732(6) & -0.0275(3) & 0.116(4) & 0.086(3) \\ \text{C70} & 0.1399(6) & 0.0799(5) & 0.0466(4) & 0.018(6) \\ \text{Uag} = (1/3)\Sigma_{L}\Sigma_{L}U_{L}a_{L}a_{L}a_{L}. & C_{77} & 0.2428(6) & 0.474(6) & -0.0275(3) & 0.101(3) \\ \text{Uso} \text{ for O101-C105} (disordered THF), C131-C136 (C_6H_6); \text{ for others} & C_{75} & 0.3217(6) & 0.2387(5) & 0.1073(3) & 0.0073(2) \\ \text{L} 2 & 0.4786(8) & 0.4259(7) & 0.1326(1) & 0.0333(10) & C79 & 0.3364(5) & -0.0275(5) & 0.0173(3) & 0.0073(2) \\ \text{L} 2 & 0.3353(2) & 0.3432(2) & 0.168492(11) & 0.02630(9) & C80 & 0.6191(5) & -0.0420(3) & 0.073(2) \\ \text{L} 2 & 0.4786(8) & 0.4259(8) & 0.2496(1) & 0.0593(3) & C27 & 0.0374(5) & 0.1371(5) & 0.0144(3) & 0.086(3) \\ 0.074(2) & 0.073(2) & 0.073(2) & 0.073(2) & 0.073(2) & 0.073(2) \\ \text{L} 2 & 0.4786(8) & 0.4259(8) & 0.2496(9) & 0.053(3) & C28 & 0.42371(6) & 0.0277(5) & 0.0390(3) & 0.073(2) \\ \text{L} 2 & 0.4786(8) & 0.4259(8) & 0.2496(9(4) & 0.053(3) & C28 & 0.42371(5) & 0.0173(3) & 0.073(2) \\ \text{L} 3 & 0.2518(8) & 0.4259(8) & 0.2496(9(4) & 0.053(3) & C28 & 0$	Refinement				C52	0.0638 (4)	0.2488 (4)	0.3714 (2)	0.043 (2)
$ \begin{array}{c} \text{Refr}^{2} & 2\sigma(F^{2}) & = 0.0289 \\ \gamma R(F^{2}) & = 0.0737 \\ \Delta \rho_{\text{min}} & = -0.700 \ \text{e}^{-3} \\ \Delta \rho_{\text{min}} & = -0.700 \ \text{min} \ \text{mi} \ \text{min} \ \text{min} \ \text{min} \ \text{min} \ \text{min} \ $	Performent on F^2		$(\Delta/\sigma) = -0$	001	B53 B54	0.0742 (5)	0.3269 (4)	0.3522 (3)	0.041(2) 0.032(2)
$ \begin{aligned} & V = 10, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0$	$R[F^2 > 2\sigma(F^2)] = 0$	0280	$\Delta_{0} = 1.124 e$	$Å^{-3}$	B55	0.2198 (5)	0.2436 (4)	0.3930 (3)	0.036 (2)
$ \begin{array}{c} \text{M}(\mathbf{r}) = 0.515 & \text{Extinction correction: none} \\ \text{S} = 1.055 & \text{Extinction correction: none} \\ \text{for } International Tables & \text{C64} = -0.1492 (5) & 0.5242 (5) & 0.3377 (3) & 0.098 (3) \\ \text{1079 parameters} & \text{from } International Tables & \text{C64} = -0.0347 (5) & 0.5798 (6) & 0.4174 (3) & 0.083 (3) \\ \text{w} = 1/[\sigma^2(F_{\sigma}^2) + (0.0410P)^2 & for Crystallography (1992, \\ + 14.4051P] & \text{Vol. C, Tables 4.2.6.8 and} \\ \text{where } P = (F_{\sigma}^2 + 2F_{\sigma}^2)/3 & 6.1.1.4) & \text{C66} = -0.0338 (5) & 0.5752 (5) & 0.1753 (3) & 0.088 (3) \\ \text{where } P = (F_{\sigma}^2 + 2F_{\sigma}^2)/3 & 6.1.1.4) & \text{C68} & -0.0896 (6) & 0.1678 (6) & 0.1467 (4) & 0.086 (3) \\ \text{c69} & -0.1539 (4) & 0.3590 (5) & 0.1467 (4) & 0.086 (3) \\ \text{c70} & 0.1390 (7) & 0.1732 (6) & -0.0275 (3) & 0.010 (3) \\ \text{equivalent isotropic displacement parameters (Å^2) & C73 & 0.2428 (6) & 0.4704 (6) & -0.0173 (3) & 0.012 (3) \\ \text{uso for O101-C105 (disordered THF), C131-C136 (C6_{H_6}); for others \\ U_{eq} = (1/3)\Sigma_i \Sigma_j U_{ij}a_i^* a_j^* a_i a_j. & C76 & 0.3391 (5) & -0.0250 (3) & 0.093 (3) \\ \text{Tb} 0 & 0.3355 (2) & 0.3432 (2) & 0.6344 (211) & 0.0250 (9) & C74 & 0.4337 (6) & 0.3888 (6) & -0.0050 (3) & 0.093 (3) \\ \text{U}_{13} & 0.34421 (2) & 0.2345 (2) & 0.03271 (11) & 0.0333 (10) & C79 & 0.554 (5) & -0.1571 (5) & 0.0144 (3) & 0.083 (2) \\ \text{Tb} 1 & 0.12806 (2) & 0.4155 (7) & 0.23771 (11) & 0.0353 (1) & C79 & 0.554 (5) & -0.0175 (5) & 0.1591 (4) & 0.088 (3) \\ \text{Tb} 1 & 0.2495 (7) & 0.5537 (7) & 0.1719 (5) & 0.053 (3) & C38 & 0.6171 (5) & 0.1391 (4) & 0.083 (2) \\ \text{Tb} 1 & 0.2495 (7) & 0.5563 (7) & 0.1719 (5) & 0.053 (3) & C38 & 0.6171 (5) & 0.1391 (4) & 0.088 (3) \\ \text{Tb} 1 & 0.2495 (6) & -0.4259 (6) & -0.0175 (5) & 0.1591 (3) & 0.073 (2) \\ \text{Tb} 1 & 0.2495 (7) & 0.5635 (7) & 0.1719 (5) & 0.0553 (3) & C38 & 0.6127 (5) & 0.3903 (3) & 0.078 (2) \\ \text{Li} 1 & 0.2495 (7) & 0.5635 (7) & 0.1719 (5) & 0.055 (3) & C38 & 0.6127 (5) & 0.3903 (3) & 0.073 (2) \\ \text{Tb} 1 & 0.02237 (13) & 0.0269 (7) & 0.0593 (3) & C88 & 0.4373 (7) & 0.2395 (7) & 0.3301 (3) & 0.078 (2) \\ \text{Li} 1 & 0.2495$	$wR(F^2) = 0.0737$.0207	$\Delta \rho_{max} = -0.700$	$e^{\AA^{-3}}$	B56	0.1068 (5)	0.3121 (5)	0.4090 (3)	0.042 (2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	S = 1.055		Extinction correct	ction: none	C61	-0.1575(5)	0.7098 (5)	0.3373 (4)	0.090 (3)
$ \begin{array}{ccccc} 1079 \ parameters & from International Tables & C64 & -0.1923 (5) & 0.5999 (6) & 0.1980 (3) & 0.087 (3) \\ w = 1/[\sigma^2(F_o^2) + (0.0410P)^2 & for Crystallography (1992, \\ + 14.4051P] & Vol. C, Tables 4.2.6.8 and & C66 & -0.0183 (5) & 0.753 (5) & 0.1075 (3) & 0.0088 (3) \\ where P = (F_o^2 + 2F_c^2)/3 & 6.1.1.4) & C68 & -0.0894 (6) & 0.2647 (7) & 0.0380 (4) & 0.109 (3) \\ where P = (F_o^2 + 2F_c^2)/3 & 6.1.1.4) & C68 & -0.0894 (6) & 0.2647 (7) & 0.0380 (4) & 0.109 (3) \\ (569 & -0.1539 (4) & 0.3590 (5) & 0.1467 (4) & 0.086 (3) \\ c70 & 0.1309 (7) & 0.1732 (6) & -0.0275 (3) & 0.010 (3) \\ equivalent isotropic displacement parameters (Å^2) & C71 & 0.2809 (6) & 0.0790 (5) & 0.0469 (4) & 0.102 (3) \\ U_{1so} for O101-C105 (disordered THF), C131-C136 (C_6H_6); for others \\ U_{eq} = (1/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*a_i.a_j. & C76 & 0.6393 (5) & 0.3106 (6) & 0.0433 (3) & 0.0086 (3) \\ U_{eq} = (1/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*a_i.a_j. & C76 & 0.6393 (5) & 0.0772 (5) & -0.0260 (3) & 0.073 (2) \\ \hline Tb1 & 0.12806 (2) & 0.4559 (2) & 0.253671 (11) & 0.0303 (10) \\ Tb3 & 0.34421 (2) & 0.29445 (2) & 0.327249 (11) & 0.02530 (9) \\ C77 & 0.6407 (4) & 0.175 (5) & 0.1273 (3) & 0.076 (2) \\ \hline x & y & z & U_{iso}/Ueq \\ C78 & 0.6393 (5) & -0.0480 (5) & 0.1991 (3) & 0.073 (2) \\ Tb1 & 0.12806 (2) & 0.4559 (2) & 0.235671 (11) & 0.02530 (9) \\ Tb3 & 0.34421 (2) & 0.29445 (2) & 0.327249 (11) & 0.02530 (9) \\ C80 & 0.6191 (5) & -0.1420 (5) & 0.1891 (4) & 0.088 (2) \\ Li3 & 0.2518 (8) & 0.5249 (8) & 0.2469 (4) & 0.057 (3) \\ Li4 & 0.1515 (7) & 0.2669 (7) & 0.1904 (4) & 0.046 (3) \\ C82 & 0.4229 (5) & -0.0189 (5) & 0.3903 (3) & 0.073 (2) \\ Li3 & 0.2518 (8) & 0.5499 (7) & 0.3427 (5) & 0.0577 (3) \\ Li4 & 0.1515 (7) & 0.0269 (7) & 0.1904 (4) & 0.046 (3) \\ C83 & 0.5816 (7) & 0.1147 (6) & 0.3425 (5) & 0.136 (5) \\ Li5 & 0.3280 (7) & 0.1818 (7) & 0.3447 (4) & 0.046 (3) \\ C83 & 0.5816 (7) & 0.1147 (6) & 0.3425 (6) & 0.136 (5) \\ Li4 & 0.1573 (13) & 0.5953 (12) & 0.3450 (8) & 0.0577 (5) \\ C93 & 0.0665 (13) & 0.0737 (13) & 0.0583 (3) & 0.077 (5) \\ C93 & 0.0665 (13)$	10708 reflections		Atomic scatterin	g factors	C62	-0.0347(5)	0.5789 (6)	0.4174 (3)	0.083 (3)
$ \begin{split} & w = 1/[\sigma^2(F_0^2) + (0.0410P)^2 & for Crystallography (1992, \\ + 14.4051P] & Vol. C, Tables 4.2.6.8 and \\ where P = (F_o^2 + 2F_c^2)/3 & 6.1.1.4 C66 & -0.0538(5) & 0.5752(5) & 0.1075(3) & 0.088(3) \\ where P = (F_o^2 + 2F_c^2)/3 & 6.1.1.4 C68 & -0.0806(6) & 0.1678(6) & 0.1482(5) & 0.118(4) \\ C69 & -0.1399(4) & 0.3590(5) & 0.1467(4) & 0.086(3) \\ C70 & 0.1309(7) & 0.1732(6) & -0.0275(3) & 0.010(3) \\ equivalent isotropic displacement parameters (Å^2) & C71 & 0.2809(6) & 0.0709(5) & 0.0469(4) & 0.102(3) \\ C71 & 0.2809(6) & 0.0709(5) & 0.0469(4) & 0.102(3) \\ C71 & 0.2437(6) & 0.3888(6) & -0.0505(3) & 0.0393(3) \\ U_{150} 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^* a_i a_j. & C75 & 0.3217(6) & 0.2797(5) & -0.0260(3) & 0.074(2) \\ V_{150} 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^* a_i a_j. & C76 & 0.6393(5) & 0.3106(6) & 0.0433(3) & 0.086(3) \\ U_{150} (2x + y + z + U_{150}/U_{eq} + C78 & 0.5574(5) & 0.1751(5) & 0.0144(3) & 0.0838(2) \\ Tb1 & 0.12806(2) & 0.41559(2) & 0.2253671(11) & 0.02530(9) & C80 & 0.6191(5) & -0.0222(5) & 0.0919(3) & 0.077(2) \\ Tb1 & 0.2485(8) & 0.4259(8) & 0.2469(4) & 0.059(3) & C83 & 0.6191(5) & -0.0172(5) & 0.1891(4) & 0.089(3) \\ Tb3 & 0.34421(2) & 0.29445(2) & 0.327249(11) & 0.02530(9) & C80 & 0.6191(5) & -0.0189(5) & 0.3303(3) & 0.078(2) \\ Li1 & 0.2405(7) & 0.1681(6) & 0.2384(4) & 0.044(3) & C88 & 0.6191(5) & -0.0189(5) & 0.3303(3) & 0.078(2) \\ Li3 & 0.2518(8) & 0.4259(8) & 0.2469(4) & 0.059(3) & C83 & 0.6127(5) & -0.0189(5) & 0.3303(3) & 0.078(2) \\ Li3 & 0.2518(8) & 0.4259(8) & 0.2469(4) & 0.059(3) & C83 & 0.6127(5) & -0.0189(5) & 0.3303(3) & 0.078(2) \\ Li3 & 0.2518(8) & 0.4259(8) & 0.2469(4) & 0.059(3) & C83 & 0.6127(5) & -0.0189(5) & 0.3303(3) & 0.078(2) \\ Li3 & 0.2518(8) & 0.4259(8) & 0.2469(4) & 0.059(3) & C83 & 0.6127(5) & -0.0189(5) & 0.3303(3) & 0.078(2) \\ Li3 & 0.2518(1) & 0.0481(6) & 0.2384(4) & 0.044(3) & C88 & 0.6476(6) & 0.2580(6) & 0.4435(5) & 0.1$	1079 parameters		from Internati	onal Tables	C64	-0.1923 (5)	0.5999 (6)	0.1980 (3)	0.087 (3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$w = 1/[\sigma^2(F_c^2)] + (0)$	$1410P)^2$	for Crystallog	raphy (1992.	C65	-0.0538 (5)	0.5752 (5)	0.1075 (3)	0.079 (2)
where $P = (F_o^2 + 2F_c^2)/3$ 6.1.1.4) where $P = (F_o^2 + 2F_c^2)/3$ 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 ₆ H ₆); for others $U_{eq} = (1/3)\Sigma_i \Sigma_j U_{ij} q_i^* a_j^* a_i a_j.$ $U_{eq} = (1/3)\Sigma_i \Sigma_j U_{ij} q_i^* a_j^* a_i a_j.$ U_{iso} for O101–C105 (disordered THF), C131–C136 (C ₆ H ₆); for others $U_{eq} = (1/3)\Sigma_i \Sigma_j U_{ij} q_i^* a_j^* a_i a_j.$ U_{iso} for O101–C105 (disordered THF), C131–C136 (C ₆ H ₆); for others $U_{eq} = (1/3)\Sigma_i \Sigma_j U_{ij} q_i^* a_j^* a_i a_j.$ U_{iso} for O101–C105 (disordered THF), C131–C136 (C ₆ H ₆); for others $U_{eq} = (1/3)\Sigma_i \Sigma_j U_{ij} q_i^* a_j^* a_i a_j.$ U_{iso} for O101–C105 (disordered THF), C131–C136 (C ₆ H ₆); for others $U_{eq} = (1/3)\Sigma_i \Sigma_j U_{ij} q_i^* a_j^* a_i a_j.$ C77 0.6407 (4) 0.1756 (5) 0.1273 (3) 0.076 (2) X Y Z U_{iso}/U_{eq} C78 0.5574 (5) 0.1751 (5) 0.0144 (3) 0.083 (2) Tb1 0.12806 (2) 0.41559 (2) 0.253671 (11) 0.02530 (9) C80 0.6191 (5) -0.1420 (5) 0.1891 (4) 0.089 (3) Tb3 0.34421 (2) 0.29445 (2) 0.327249 (11) 0.02599 (9) C81 0.4299 (6) -0.1175 (5) 0.1501 (3) 0.078 (2) Li1 0.2405 (7) 0.5633 (7) 0.1719 (5) 0.057 (3) C82 0.4259 (5) -0.0189 (5) 0.3903 (3) 0.073 (2) Li2 0.4786 (8) 0.4259 (8) 0.2469 (4) 0.059 (3) C83 0.6127 (5) -0.0189 (5) 0.3903 (3) 0.073 (2) Li3 0.2518 (8) 0.5499 (7) 0.3427 (5) 0.057 (3) C84 0.4606 (7) -0.1516 (5) 0.3906 (3) 0.094 (3) Li4 0.1515 (7) 0.2069 (7) 0.1904 (4) 0.046 (3) C87 0.6747 (5) 0.1865 (8) 0.3495 (4) 0.1414 (5) Li5 0.3280 (7) 0.1081 (6) 0.2384 (4) 0.044 (3) C86 0.6476 (6) 0.2580 (6) 0.4652 (4) 0.0136 (5) Li5 0.3280 (7) 0.01881 (7) 0.3147 (4) 0.046 (3) C87 0.6747 (5) 0.1865 (8) 0.3496 (4) 0.141 (5) Si1 -0.08237 (13) 0.59523 (12) 0.0373 (7) 0.0351 (5) 0.0377 (5) C93 0.0626 (6) 0.1668 (5) 0.5125 (3) 0.087 (3) 0.088 (3) Si3 -0.06655 (13) 0.26335 (15) 0.11484 (10) 0.0681 (6) C90 0.4249 (8) 0.4252 (7) 0.5365 (3) 0.126 (4) Si4 0.15912 (14) 0.13	+ 14 4051P	, ,	Vol. C. Tables	4.2.6.8 and	C66 C67	-0.1185(5)	0.7391 (5)	0.1753(3)	0.088(3) 0.109(3)
$ \begin{array}{c} \text{Table 1. } Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$	where $P = (F_{1}^{2} +$	$2F_{2}^{2})/3$	6.1.1.4)		C68	-0.0806(6)	0.1678 (6)	0.1482 (5)	0.118 (4)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $					C69	-0.1539 (4)	0.3590 (5)	0.1467 (4)	0.086 (3)
Table 1. Fractional atomic coordinates and isotropic orCr10.0209 (0)0.0009 (1)0.0009 (1)equivalent isotropic displacement parameters (Å ²)Cr30.2428 (6)0.0470 (6)0.0000 (4)0.102 (3) U_{iso} for O101–C105 (disordered THF), C131–C136 (C ₆ H ₆); for othersCr50.0217 (6)0.0200 (3)0.074 (2) $U_{eq} = (1/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*a_i.a_j.Cr60.6393 (5)0.3106 (6)0.0433 (3)0.0086 (3)xyZU_{iso}/UeqCr80.5574 (5)0.1715 (5)0.1273 (3)0.076 (2)XyZU_{iso}/UeqCr80.5574 (5)0.1715 (5)0.1273 (3)0.076 (2)XyZU_{iso}/UeqCr80.5574 (5)0.1715 (5)0.1273 (3)0.076 (2)XyZU_{iso}/UeqC780.5574 (5)0.175 (5)0.0144 (3)0.068 (3)0.0426 (2)0.33535 (2)0.30422 (2)$					C70	0.1309 (7)	0.1732 (6)	-0.0275(3)	0.101(3)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Table 1. Fractiona	atomic c	oordinates and	isotropic or	C72	0.2809(0) 0.1041(7)	0.0507 (6)	0.0600 (4)	0.115 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	equivalent isotr	opic displa	acement parame	ters (A ²)	C73	0.2428 (6)	0.4704 (6)	-0.0173 (3)	0.102 (3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$			-		C74	0.4337 (6)	0.3888 (6)	-0.0505(3)	0.093 (3)
$U_{eq} = (1/3) \Sigma_i \Sigma_j U_{ij} a_i^* a_j^* a_i^* a_j^*.$ C77 0.6407 (4) 0.1765 (5) 0.1273 (3) 0.076 (2) x y z U_{iso}/U_{eq} C78 0.5574 (5) 0.1751 (5) 0.0144 (3) 0.083 (2) Tb1 0.12806 (2) 0.41559 (2) 0.253671 (11) 0.03033 (10) C79 0.5364 (5) -0.0272 (5) 0.0919 (3) 0.073 (2) Tb2 0.33535 (2) 0.30432 (2) 0.168492 (11) 0.02599 (9) C80 0.6191 (5) -0.1420 (5) 0.1891 (4) 0.089 (3) Tb3 0.34421 (2) 0.29445 (2) 0.327249 (11) 0.02599 (9) C81 0.4299 (6) -0.1175 (5) 0.1501 (3) 0.078 (2) Li1 0.2405 (7) 0.5635 (7) 0.1719 (5) 0.053 (3) C82 0.4259 (5) -0.0189 (5) 0.3903 (3) 0.073 (2) Li2 0.4786 (8) 0.4259 (8) 0.2469 (4) 0.059 (3) C83 0.6127 (5) -0.0950 (5) 0.3412 (3) 0.078 (2) Li3 0.2518 (8) 0.5499 (7) 0.3427 (5) 0.057 (3) C84 0.4606 (7) -0.1516 (5) 0.3006 (3) 0.094 (3) Li4 0.1515 (7) 0.1081 (6) 0.2384 (4) 0.044 (3) C85 0.5816 (7) 0.1147 (6) 0.4345 (5) 0.136 (5) Li5 0.3208 (7) 0.1081 (6) 0.2384 (4) 0.044 (3) C85 0.6476 (6) 0.2580 (6) 0.4682 (4) 0.105 (3) Li5 0.3280 (7) 0.1081 (6) 0.2384 (4) 0.046 (3) C87 0.6747 (5) 0.1865 (8) 0.3496 (4) 0.141 (5) Si1 -0.08237 (13) 0.59523 (12) 0.34505 (8) 0.0577 (5) C88 0.4373 (7) 0.2395 (7) 0.5361 (4) 0.122 (4) Si2 -0.08888 (13) 0.62081 (13) 0.17930 (8) 0.0681 (6) C90 0.4249 (8) 0.4262 (7) 0.5361 (4) 0.122 (4) Si3 -0.06655 (13) 0.26335 (15) 0.11484 (10) 0.0681 (6) C90 0.4249 (8) 0.4262 (7) 0.5361 (4) 0.122 (4) Si5 0.34650 (13) 0.37571 (12) -0.00374 (7) 0.0511 (5) C92 0.1772 (5) 0.0175 (4) 0.4421 (4) 0.079 (2) Si6 0.57271 (12) 0.24096 (13) 0.0708 (8) 0.0527 (5) C93 0.0626 (6) 0.1668 (5) 0.5163 (3) 0.088 (3) Si7 0.51091 (13) -0.06273 (11) 0.16186 (8) 0.0527 (5) C94 -0.1177 (5) 0.3120 (6) 0.4310 (4) 0.113 (4) Si8 O 0.4971 (13) -0.06273 (11) 0.16186 (8) 0.0527 (5) C94 -0.1177 (5) 0.3120 (6) 0.4310 (4) 0.113 (4) 0.11	$U_{\rm iso}$ for O101–C105 (d	isordered TH	F), C131–C136 (C ₆	H_6 ; for others	C75	0.3217 (6)	0.2797 (5)	-0.0260(3) 0.0433(3)	0.074(2) 0.086(3)
xyz U_{iso}/U_{eq} C780.5574 (5)0.1751 (5)0.0144 (3)0.083 (2)Tb10.12806 (2)0.41559 (2)0.253671 (11)0.03033 (10)C790.5364 (5) $-0.0272 (5)$ 0.0919 (3)0.073 (2)Tb20.33535 (2)0.30432 (2)0.168492 (11)0.02599 (9)C800.6191 (5) $-0.1420 (5)$ 0.1891 (4)0.089 (3)Tb30.34421 (2)0.29445 (2)0.327249 (11)0.02599 (9)C810.4299 (6) $-0.1175 (5)$ 0.1501 (3)0.078 (2)Li10.2405 (7)0.6535 (7)0.1719 (5)0.053 (3)C820.4259 (5) $-0.0189 (5)$ 0.3903 (3)0.073 (2)Li20.4786 (8)0.4259 (8)0.2469 (4)0.059 (3)C830.6127 (5) $-0.0950 (5)$ 0.3412 (3)0.078 (2)Li30.2518 (8)0.5499 (7)0.3427 (5)0.057 (3)C840.4606 (7) $-0.1516 (5)$ 0.3006 (3)0.094 (3)Li40.1515 (7)0.2069 (7)0.1904 (4)0.046 (3)C850.5816 (7)0.1147 (6)0.4345 (5)0.136 (5)Li50.3280 (7)0.1081 (6)0.2384 (4)0.044 (3)C860.6476 (6)0.2580 (6)0.4682 (4)0.105 (3)Li60.1743 (7)0.1881 (7)0.3147 (4)0.046 (3)C870.6747 (5)0.1865 (8)0.3496 (4)0.141 (5)Si1 $-0.08237 (13)$ 0.59523 (12)0.34505 (8)0.0577 (5)C880.4373 (7)0.2395 (7)0.5361 (4)0.122 (4) <td< td=""><td>U_{eq}</td><td>$= (1/3)\Sigma_i \Sigma_i$</td><td>$a_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.</td><td></td><td>C77</td><td>0.6407 (4)</td><td>0.1765 (5)</td><td>0.1273 (3)</td><td>0.076 (2)</td></td<>	U_{eq}	$= (1/3)\Sigma_i \Sigma_i$	$a_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.		C77	0.6407 (4)	0.1765 (5)	0.1273 (3)	0.076 (2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	x	у	Ζ	$U_{\rm iso}/U_{\rm eq}$	C78	0.5574 (5)	0.1751 (5)	0.0144 (3)	0.083 (2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Tb1 0.12806 (2)	0.41559 (2)	0.253671 (11)	0.03033 (10)	C79	0.5364 (5)	-0.0272 (5)	0.0919 (3)	0.073(2)
	Tb2 0.33535 (2)	0.30432(2)	0.168492(11) 0.327249(11)	0.02630 (9)	C80	0.6191 (5)	-0.1420(3) -0.1175(5)	0.1591(4)	0.039(3) 0.078(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Li1 0.2405 (7)	0.5635 (7)	0.1719 (5)	0.053 (3)	C82	0.4259 (5)	-0.0189 (5)	0.3903 (3)	0.073 (2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Li2 0.4786 (8)	0.4259 (8)	0.2469 (4)	0.059 (3)	C83	0.6127 (5)	-0.0950 (5)	0.3412 (3)	0.078 (2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Li3 0.2518 (8)	0.5499 (7)	0.3427 (5)	0.057 (3)	C84	0.4606 (7)	-0.1516 (5)	0.3006 (3)	0.094 (3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Li4 0.1515 (7)	0.2069 (7) 0.1081 (6)	0.1904 (4)	0.046 (3)	C85 C86	0.5616(7)	0.2580(6)	0.4682 (4)	0.105 (3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Li6 0.1743 (7)	0.1881 (7)	0.3147 (4)	0.046 (3)	C87	0.6747 (5)	0.1865 (8)	0.3496 (4)	0.141 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Si1 -0.08237 (13)	0.59523 (12)) 0.34505 (8)	0.0577 (5)	C88	0.4373 (7)	0.2395 (7)	0.5361 (4)	0.122 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Si2 -0.08888 (13)	0.62081 (13)) 0.17930 (8)	0.0604 (6)	C89	0.2629 (5)	0.3/82(6)	0.5125 (3)	0.087 (3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	513 - 0.06655 (13) 514 - 0.15912 (14)	0.13004 (12)	(10) 0.11484 (10) 0.04529 (8)	0.0583 (5)	C90	0.2593 (5)	0.1233 (5)	0.5087 (3)	0.068 (2)
Si6 0.57271 (12) 0.24696 (13) 0.07081 (8) 0.0527 (5) C93 0.0626 (6) 0.1668 (5) 0.5163 (3) 0.088 (3) Si7 0.51091 (13) -0.06273 (11) 0.16186 (8) 0.0527 (5) C94 -0.1197 (5) 0.3120 (6) 0.4310 (4) 0.113 (4) Si8 0.49074 (13) -0.05864 (11) 0.32451 (8) 0.0501 (5) C95 -0.1046 (6) 0.2738 (7) 0.3050 (4) 0.109 (3)	Si5 0.34650 (13)	0.37571 (12)) -0.00374 (7)	0.0511 (5)	C92	0.1772 (5)	0.0175 (4)	0.4421 (4)	0.079 (2)
Si7 $0.51091(13) = -0.06273(11)$ $0.16186(8)$ $0.0527(5)$ $C94 = -0.1197(5)$ $0.5120(6)$ $0.4310(4)$ $0.113(4)$ Si8 $0.49074(13) = -0.05864(11)$ $0.32451(8)$ $0.0501(5)$ $C95 = -0.1046(6)$ $0.2738(7)$ $0.3050(4)$ $0.109(3)$	Si6 0.57271 (12)	0.24696 (13) 0.07081 (8)	0.0527 (5)	C93	0.0626 (6)	0.1668 (5)	0.5163 (3)	0.088 (3)
	Si7 0.51091 (13) Si8 0.49074 (13)	-0.06273 (11)) U.16186 (8)) 0.32451 (8)	0.0527(5) 0.0501(5)	C94 C95	-0.1197(5) -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)
0111	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, °)

Tb10100	2.185 (3)	Li1—B25	2 349 (12)
Tb1-B14	2.684 (7)	Lil—B4	2.367(12)
Tb1—B5	2.692 (7)	Li1-B24	2.386 (13)
Тb1—С1	2.700 (5)	Li2-0106	1.884 (12)
Tb1—B3	2.711 (7)	Li2—B23	2.336 (13)
Тb1В54	2.717 (7)	Li2	2.344 (13)
Tb1C2	2.727 (5)	Li2—B24	2.362 (13)
Tb1B4	2.737 (7)	Li2—B44	2.390 (13)
Тb1—B53	2.807 (7)	Li3—0111	1.880 (11)
Tb1B15	2.856 (7)	Li3-B43	2.334 (13)
Ть2—О100	2.170 (3)	Li3—B5	2.354 (14)
Тb2—В34	2.664 (6)	Li3—B4	2.372 (14)
Tb2—B14	2.692 (6)	Li3—B44	2.411 (13)
Tb2—B25	2.704 (7)	Li4—0120	1.842 (11)
Тb2—-С22	2.718 (5)	Li4—C12	2.150 (12)
ТЪ2—С21	2.728 (5)	Li4—C11	2.160 (11)
Tb2—B23	2.732 (7)	Li4—B15	2.298 (12)
Tb2—B24	2.764 (7)	Li4B13	2.316 (12)
Tb2—B13	2.777 (7)	Li4—B14	2.472 (12)
Тb2—В35	2.876 (7)	Li5—0120	1.849 (11)
ТЬ3—О100	2.173 (3)	Li5C32	2.158 (11)
Tb3—B54	2.672 (6)	Li5-C31	2.166 (11)
Tb3—B45	2.698 (7)	Li5B35	2.302 (12)
ТЬ3—В34	2.712 (6)	Li5-B33	2.311 (12)
Tb3C41	2.721 (5)	Li5—B34	2.467 (12)
ТЬ3—В43	2.732 (7)	Li6-0120	1.861 (11)
ТЬ3—С42	2.735 (5)	Li6-C52	2.158 (11)
ТЬ3—В44	2.754 (7)	Li6-C51	2.173 (11)
тьз—В33	2.779 (6)	Li6—B53	2.293 (13)
ТЬ3—В55	2.877 (7)	Li6B55	2.298 (13)
Li1—0101	1.884 (11)	Li6—B54	2.459 (12)
Li1—B3	2.340 (13)		
Tb2	120.07 (15)	Li4-0120-Li5	105.6 (5)
Tb2-0100-Tb1	119.01 (15)	C121-0120-Li6	108 5 (5)
Ть3—О100—Ть1	118.89 (15)	Li4-0120-Li6	106.6 (5)
C121-0120-Li4	116.1 (5)	Li5-0120-Li6	105.6 (5)
C121—O120—Li5	113.7 (5)	0.20 210	- 55.0 (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: SHELXL93 (Sheldrick, 1993). Molecular graphics: SHELXTL-Plus (Sheldrick, 1990). Software used to prepare material for publication: SHELXL93.

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Lists of structure factors, anisotropic displacement parameters, Hatom 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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