forming a four-membered chelate ring (Fig. 1). We have not found any previous reference to a structure including an analogous Hg—N—C—O chelate. In the copper complex referenced above (Cartwright, Reynolds & Skapski, 1977), the interaction is fundamentally monodentate through the N atom, as happens with the mercury complex of 1-methyl-cytosine (Authier-Martin & Beauchamp, 1977). Interatomic distances and bond angles appear in Table 2.

The geometry around the metal atom is very irregular, as expected from the constraints imposed by chelation, but may be described as intermediate between a linear Cl—Hg—Cl and a planar trigonal N(3)—Hg—Cl$_2$ with the more weakly coordinated O atom out of the HgNCl$_2$ plane. The Hg—Cl distances are similar to those in analogous compounds (Authier-Martin & Beauchamp, 1977; Authier-Martin, Hubert, Rivest & Beauchamp, 1978), whereas the Hg—N(3) and Hg—O(2) bonds are longer than in complexes where the ligand is mono-dentate (Kosturko, Folzer & Stewart, 1974), which is also a logical consequence of bidentate union.

Distances and angles within the ligand are very similar to those in free 2-pyrimidinol (Furberg & Solbakk, 1970), the appreciable distortions in bond angles that appear in its hydrochloride (Furberg & Aas, 1975) not taking place in our compound. The pyrimidine ring is planar within 0.03 Å, with the Hg atom displaced 0.371 Å out of the plane.

A hydrogen bond is formed between the only possible donor, N(1), and the carbonyl O atom of a neighbouring molecule, giving pairs related by the symmetry centre at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. The Hg atom interacts weakly with Cl atoms of neighbouring unit cells at $y + 1$ and $y - 1$ (b parameter is only 4.187 Å). This interaction together with the previous hydrogen bond generates a ladder-like structure along the b axis (Fig. 2).

References

AUTHIER-MARTIN, M & BEAUCHAMP, A. L. (1977). *Can. J. Chem.* **55**, 1213–1217.
AUTHIER-MARTIN, M., HUBERT, J., RIVEST, R. & BEAUCHAMP, A. L. (1978). *Acta Cryst.* B**34**, 273–276.
BEAUCHAMP, A. L. & SIMARD, M. (1984). *Acta Cryst.* A**40**, 67–72.
CARTWRIGHT, B. A., REYNOLDS, C. D. & SKAPSKI, A. J. (1977). *Acta Cryst.* B**33**, 1883–1887.
FURBERG, S. & AAS, J. B. (1975). *Acta Chem. Scand. Ser. A*, **29**, 713–716.
FURBERG, S. & SOLBAKK, J. (1970). *Acta Chem. Scand.* **24**, 3230–3236.
GOODGAME, D. M. L. & JEEVES, I. (1979). *Inorg. Chim. Acta*, **32**, 157–162.
KOSTURKO, D., FOLZER, C. & STEWART, R. F. (1974). *Biochemistry*, **13**, 3949–3952.
ROMERO, M. A., SALAS, J. M., SIMARD, M., QUIRÓS, M. & BEAUCHAMP, A. L. (1990). *Polyhedron*, **9**, 2733–2739.
SHELDRICK, G. M. (1987). *SHELXTL-Plus.* Release 3.4 for Nicolet *R3m/V* crystallographic system. Nicolet Instrument Corporation, Madison, Wisconsin, USA.

The First Zwitterionic and Bent-Sandwiched Hafnacarborane 4',5,5',6-Li(THF)-1,1'-*commo*-Hf(THF)Cl[2-(SiMe₃)-3-(Me)-2,3-C₂B₄H₄]₂

BY HONGMING ZHANG, LEI JIA AND NARAYAN S. HOSMANE*

Department of Chemistry, Southern Methodist University, Dallas, Texas 75275, USA

Abstract. 4',5,5',6-(Tetrahydrofuranlithium)-1-chloro-3,3'-dimethyl-1-(tetrahydrofuran-O)-2,2'-bis(tri-methylsilyl)dodecahydro-1,1'-*commo*-bis(2,3-dicarba-1-hafna-*closo*-heptaborate), $C_{20}H_{48}B_8ClHfLiO_2Si_2$, $M_r = 684.1$, monoclinic, $P2_1/c$, $a = 16.821$ (5), $b = 16.277$ (5), $c = 12.131$ (5) Å, $\beta = 90.41$ (3)°, $V = 3321$ (2) Å³, $Z = 4$, $D_x = 1.368$ Mg m⁻³, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 3.474$ mm⁻¹, $F(000) = 1376$, $T = 230$ K, final $R = 0.049$ for 2482 observed reflections. The structure shows that the title compound (2) is a zwitterion consisting of an anionic {1,1'-*commo*-Hf(Cl)(THF)[η⁵-2-(SiMe₃)-3-(Me)-2,3-C₂B₄H₄]₂}⁻ sandwich that is complexed with an *exo*-polyhedral [Li(THF)]⁺ cation for charge compensation. Bond distances in the cage structure are Hf—C 2.50 (1)–2.55 (1), Hf—B 2.52 (2)–2.56 (2), Hf—C₂B₃ centroid 2.15 and 2.16, Hf—O(THF) 2.199 (8) and Hf—Cl 2.437 (3) Å. The Hf—centroid and Hf—Cl distances, the Cl—Hf—O(THF) angle of 89.7 (2)°, and the centroid—Hf—centroid angle of 134.1° of (2) resemble those of a hafnocene derivative despite the presence of a 2− charge on each carborane ligand. As in

the cyclopentadienyl systems, the average ring centroid—Hf—O(THF) (105.8°) and ring centroid—Hf—Cl (106.3°) angles constitute the distorted tetrahedral geometry of the metal center in (2).

Introduction. In comparison with the rich and varied chemistry displayed by the more abundant members of Group IV, Ti and Zr, our knowledge of the chemistry of Hf is somewhat limited. In fact, during the last two decades or so there has been a rapidly increasing interest in the organometallic chemistry of the early transition metals, in particular Zr and, to a lesser extent, Hf (Cardin, Lappert, Raston & Riley, 1982*a,b*; Sinn & Kaminsky, 1980; Wailes, Coutts & Weigold, 1974). Consequently, a wide variety of Cp (Cp = η^5-C_5R_5, R = organic or organometallic group) complexed derivatives of Hf, formally in 4+, 3+ or 2+ oxidation states, have been reported (Cardin, Lappert, Raston & Riley, 1982*a,b*; Cardin, 1984; Cotton & Wilkinson, 1988, and references therein). However, the analogous hafnacarborane chemistry has been limited to the synthesis of a THF-solvated complex [$Et_4N]_2[4,4'$-Hf(1,6-Me$_2$-1,6-$C_2B_{10}H_{10})_2$], in which the *commo*-Hf is present in a formal oxidation state of 2+, and hence representing a 14 interstitial electron system (Salentine & Hawthorne, 1976). Nevertheless, the crystal-structure determination of this compound to confirm its molecular geometry has not been reported to date. Reported here are the synthesis and X-ray diffraction study of the first bent zwitterionic hafnium(IV) sandwich complex, which could be considered as an analogue of the hafnocene derivative.

Experimental. Treatment of the double salt Na$^+$.(THF)Li$^+$.[2-(SiMe$_3$)-3-(Me)-2,3-$C_2B_4H_4]^{2-}$ (1) (Siriwardane, Islam, West, Hosmane, Maguire & Cowley, 1987) with anhydrous HfCl$_4$ in a molar ratio of 2:1 in dry benzene (C_6H_6), and then extraction and crystallization of the product from a solution mixture of anhydrous *n*-hexane (90%) and THF (10%) resulted in the isolation of yellow, *extremely air-sensitive* crystals of the previously unknown hafnacarborane complex 1-Cl-1-(C_4H_8O)-2,2'-(SiMe$_3)_2$-3,3'-(Me)$_2$-4',5,5',6-Li(C_4H_8O)-[1,1'-*commo*-Hf($C_2B_4H_4)_2$] (2) in 65% yield as shown in the scheme below (Jia, Zhang & Hosmane, 1991, unpublished results).
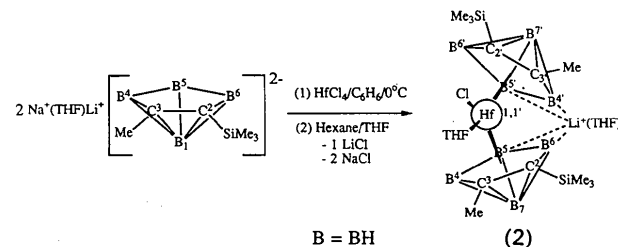
Crystals of (2) are pale yellow plates. Unit-cell parameters were determined by least-squares fit of 24 reflections in the range $10 \le 2\theta \le 25°$ for a crystal of dimensions $0.35 \times 0.15 \times 0.30$ mm (space group $P2_1/c$) on an automatic Nicolet $R3m/V$ diffractometer ($T = 230$ K) with graphite-monochromated Mo $K\alpha$ radiation and $\theta/2\theta$ scans (scan rate 5.0–25.0° min^{-1}, depending on the intensity). 3471 reflections, of which 3102 were independent, were measured in the range $3.5 \le 2\theta \le 42°$ (data collection above 42° angle was unsuccessful owing to the extreme air and/or moisture-sensitive nature of the crystal); $R_{int} = 0.030$; *hkl* range $h -16 \rightarrow 16$, $k\ 0 \rightarrow 15$, $l\ 0 \rightarrow 11$. 2482 reflections were observed with $I > 3\sigma(I)$; $\sigma(I)$ from counting statistics, three standard reflections remeasured after every 150 reflections showed a maximum fluctuation in intensity of ±0.6%; Lorentz–polarization corrections, but no extinction corrections were applied. Absorption corrections were based on ψ scans; the maximum and minimum transmission factors were 1.000 and 0.4381, respectively. The structure was solved by heavy-atom methods using Siemens *SHELXTL-Plus* (Sheldrick, 1990), and refined by full-matrix least squares, with anisotropic parameters for all non-H atoms with the exception of C atoms of the disordered THF. Boron-cage H atoms were located in difference Fourier maps, and other H atoms, except for the disordered THF, were calculated. No attempts were made to fix the H atoms on C atoms of the disordered THF. The THF molecule attached to the Li$^+$ cation [O(26), and C(27) to C(30)] is disordered and its bonds were constrained during refinements. $\Sigma w(|F_o| - |F_c|)^2$ was minimized, where $w = 1/(\sigma^2 F_o + 0.0006F_o^2)$. $R = 0.049$, $wR = 0.065$, $S = 2.15$ for 298 parameters, $(\Delta/\sigma)_{max} = 0.000$, $(\Delta\rho)_{max,min} = 0.99$, -1.67 e Å^{-3} in the final difference Fourier map. Atomic scattering factors, with anomalous-dispersion correction for heavy atoms, were those stored in *SHELXTL-Plus*.

Discussion. The final atomic parameters of the non-H atoms are given in Table 1.* Selected bond lengths and bond angles with their standard deviations are given in Table 2. The identification of the atoms and the configuration of the molecule are shown in the thermal ellipsoid (*SHELXTL-Plus*; Sheldrick, 1990) drawing of Fig. 1. The ^{1}H and ^{13}C NMR spectra of (2) were consistent with the presence of two nonequivalent SiMe$_3$ groups and two nonequivalent THF

2 Na$^+$(THF)Li$^+$ $\xrightarrow[\substack{(2)\ Hexane/THF \\ -1\ LiCl \\ -2\ NaCl}]{(1)\ HfCl_4/C_6H_6/0°C}$

B = BH   (2)

Table 1. *Atomic coordinates* ($\times 10^4$) *and isotropic or equivalent isotropic displacement coefficients* ($\text{Å}^2 \times 10^3$)

Atoms C(27) through C(30) were refined isotropically. For other atoms equivalent isotropic U is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{iso}, U_{eq}
Hf	2769 (1)	531 (1)	1301 (1)	57 (1)
Cl	3484 (2)	−564 (2)	362 (3)	70 (1)
Li	1257 (17)	1077 (18)	2967 (27)	115 (13)
Si(1)	2338 (3)	377 (3)	−1969 (4)	93 (2)
Si(2)	3019 (3)	−1518 (3)	3168 (3)	75 (2)
C(1)	2020 (8)	516 (7)	−489 (12)	68 (5)
C(2)	1627 (8)	−79 (9)	240 (12)	72 (6)
B(3)	1279 (9)	342 (11)	1276 (17)	83 (8)
B(4)	1481 (9)	1311 (10)	1094 (16)	81 (7)
B(5)	1952 (9)	1391 (9)	−46 (15)	72 (6)
B(6)	1087 (12)	800 (10)	−5 (17)	91 (8)
C(7)	1432 (10)	−978 (8)	−101 (13)	98 (7)
C(8)	1588 (12)	828 (13)	−2893 (17)	164 (12)
C(9)	3254 (11)	957 (11)	−2175 (13)	128 (9)
C(10)	2548 (15)	−701 (10)	−2364 (15)	152 (12)
C(11)	3077 (8)	−388 (9)	2954 (10)	72 (5)
C(12)	3770 (8)	147 (9)	2784 (10)	69 (5)
B(13)	3598 (11)	1096 (11)	2909 (13)	85 (7)
B(14)	2624 (11)	1117 (11)	3243 (15)	85 (7)
B(15)	2335 (10)	168 (11)	3242 (13)	74 (7)
B(16)	3222 (14)	426 (12)	3898 (15)	97 (9)
C(17)	4597 (8)	−204 (10)	2785 (12)	92 (6)
C(18)	3794 (9)	−2089 (8)	2476 (12)	92 (7)
C(19)	3095 (11)	−1690 (10)	4674 (10)	110 (8)
C(20)	2048 (9)	−1849 (9)	2627 (13)	96 (7)
O(21)	3604 (5)	1435 (5)	617 (7)	70 (4)
C(22)	4446 (8)	1250 (9)	398 (12)	84 (6)
C(23)	4762 (9)	2065 (11)	35 (14)	101 (7)
C(24)	4286 (9)	2688 (10)	592 (14)	100 (7)
C(25)	3506 (8)	2339 (8)	703 (14)	90 (7)
O(26)	431 (7)	1315 (8)	3870 (10)	123 (5)
C(27)	510 (17)	1706 (20)	4865 (23)	240 (14)
C(28)	−249 (15)	1958 (15)	5302 (20)	161 (9)
C(29)	−811 (21)	1522 (21)	4611 (26)	251 (15)
C(30)	−326 (18)	1575 (26)	3635 (28)	306 (20)

molecules. The proton-coupled ^{11}B NMR spectrum of (2) showed broad ill defined resonances at 30.03 and 21.90 p.p.m. and a broad doublet at −16.62 p.p.m. [$^1J(^{11}B-^1H) = 128$ Hz], whose relative areas indicate a 1:2:1 distribution of basal and apical BH groups, respectively. The presence of the coordinated THF and the hafnacarborane complex was also evident in the IR spectrum of (2). Unfortunately, the foregoing spectral data do not permit a distinction to be made between a *closo-* or a *commo-*complex, thus inferring that the solution spectra are not helpful in elucidating the molecular geometry of (2) (Jia, Zhang & Hosmane, 1991, unpublished results). Therefore, an X-ray analysis of (2) was undertaken.

The crystal structure reveals that the Hf atom adopts an essentially η^5-bonding posture with respect to each of the C_2B_3 faces. The metal to cage distances of 2.50 (1)–2.56 (2) Å are slightly longer than the Hf—η^5-C distances of 2.482 (4) Å in HfCl$_2$[(η^5-C$_5$H$_4$)$_2$(CH$_2$)$_3$] (Saldarriaga-Molina, Clearfield & Bernal, 1974), 2.46 (5) Å in Hf(CHPh$_2$)$_2$[(η^5-C$_5$H$_5$)$_2$] (Atwood, Barker, Holton, Hunter, Lappert & Pearce, 1977), 2.49 (3) Å in Hf(C$_4$Ph$_4$)[(η^5-C$_5$H$_5$)$_2$] (Atwood, Hunter, Alt & Rausch, 1976), and 2.45 (5) Å in Hf(CO)$_2$[(η^5-C$_5$H$_5$)$_2$] (Sikora, Rausch, Rogers & Atwood, 1979). Comparable Hf—C distances [2.50 (4) Å average] are

Table 2. *Selected interatomic lengths* (Å) *and angles* (°)

Cnt(1) represents the centroid of C(1), C(2), B(3), B(4), and B(5); Cnt(2) represents the centroid of C(11), C(12), B(13), B(14), and B(15).

Hf—Cnt(1)	2.15	Hf—Cnt(2)	2.16
Hf—Cl	2.437 (3)	Hf—C(1)	2.503 (14)
Hf—C(2)	2.510 (14)	Hf—B(3)	2.526 (16)
Hf—B(4)	2.522 (15)	Hf—B(5)	2.547 (16)
Hf—C(11)	2.552 (13)	Hf—C(12)	2.534 (13)
Hf—B(13)	2.560 (17)	Hf—B(14)	2.555 (18)
Hf—B(15)	2.540 (16)	Hf—O(21)	2.199 (8)
C(1)—C(2)	1.471 (19)	C(1)—B(5)	1.527 (19)
C(1)—B(6)	1.741 (24)	C(2)—B(3)	1.550 (24)
C(2)—B(6)	1.720 (23)	C(2)—C(7)	1.555 (20)
B(3)—B(4)	1.630 (24)	B(3)—B(6)	1.751 (28)
B(4)—B(5)	1.603 (25)	B(4)—B(6)	1.702 (26)
B(5)—B(6)	1.745 (24)	C(11)—C(12)	1.471 (19)
C(11)—B(15)	1.583 (22)	C(11)—B(16)	1.767 (23)
C(12)—B(13)	1.579 (24)	C(12)—B(16)	1.703 (23)
C(12)—C(17)	1.503 (19)	B(13)—B(14)	1.690 (27)
B(13)—B(16)	1.744 (26)	B(14)—B(15)	1.619 (25)
B(14)—B(16)	1.702 (27)	B(15)—B(16)	1.736 (27)
Li—B(3)	2.376 (37)	Li—B(4)	2.337 (37)
Li—B(14)	2.323 (34)	Li—B(15)	2.363 (34)
Li—O(26)	1.817 (32)		
Cnt(1)—Hf—Cl	106.4	Cnt(1)—Hf—O(21)	106.1
Cnt(2)—Hf—Cl	106.2	Cnt(2)—Hf—O(21)	105.5
Cnt(1)—Hf—Cnt(2)	134.1	Cl—Hf—O(21)	89.7 (2)
B(3)—Li—B(14)	96.7 (12)	B(4)—Li—B(14)	88.2 (12)
B(3)—Li—B(15)	77.9 (11)	B(4)—Li—B(15)	96.3 (12)
C(2)—C(1)—B(5)	111.6 (12)	C(2)—C(1)—B(6)	64.1 (10)
B(5)—C(1)—B(6)	64.2 (10)	C(1)—C(2)—B(3)	111.7 (12)
C(1)—C(2)—B(6)	65.6 (10)	B(3)—C(2)—B(6)	64.5 (11)
C(1)—C(2)—C(7)	123.7 (12)	B(3)—C(2)—C(7)	123.5 (12)
B(6)—C(2)—C(7)	128.9 (12)	C(2)—B(3)—B(4)	103.7 (13)
C(2)—B(3)—B(6)	62.4 (11)	B(4)—B(3)—B(6)	60.3 (11)
B(3)—B(4)—B(5)	107.5 (13)	B(3)—B(4)—B(6)	63.4 (11)
B(5)—B(4)—B(6)	63.7 (11)	C(1)—B(5)—B(4)	105.4 (12)
C(1)—B(5)—B(6)	63.9 (10)	B(4)—B(5)—B(6)	60.9 (10)
C(1)—B(6)—C(2)	50.3 (8)	C(1)—B(6)—B(3)	91.4 (11)
C(2)—B(6)—B(3)	53.0 (9)	C(1)—B(6)—B(4)	92.7 (12)
C(2)—B(6)—B(4)	94.0 (12)	B(3)—B(6)—B(4)	56.3 (10)
C(1)—B(6)—B(5)	52.0 (9)	C(2)—B(6)—B(5)	91.4 (11)
B(3)—B(6)—B(5)	96.4 (13)	B(4)—B(6)—B(5)	55.4 (10)
C(12)—C(11)—B(15)	108.6 (12)	C(12)—C(11)—B(16)	62.7 (10)
B(15)—C(11)—B(16)	62.2 (11)	C(11)—C(12)—B(13)	114.8 (12)
C(11)—C(12)—B(16)	67.2 (10)	B(13)—C(12)—B(16)	64.0 (10)
C(11)—C(12)—C(17)	120.6 (13)	B(13)—C(12)—C(17)	122.8 (13)
B(16)—C(12)—C(17)	127.4 (12)	C(12)—B(13)—B(14)	102.8 (13)
C(12)—B(13)—B(16)	61.4 (10)	B(14)—B(13)—B(16)	59.4 (11)
B(13)—B(14)—B(15)	105.8 (13)	B(13)—B(14)—B(16)	61.9 (11)
B(15)—B(14)—B(16)	63.0 (11)	C(11)—B(15)—B(14)	108.0 (13)
C(11)—B(15)—B(16)	64.1 (10)	B(14)—B(15)—B(16)	60.8 (11)
C(11)—B(16)—C(12)	50.1 (8)	C(11)—B(16)—B(13)	94.1 (11)
C(12)—B(16)—B(13)	54.5 (10)	C(11)—B(16)—B(14)	96.6 (12)
C(12)—B(16)—B(14)	97.3 (12)	B(13)—B(16)—B(14)	58.7 (11)
C(11)—B(16)—B(15)	53.7 (9)	C(12)—B(16)—B(15)	92.3 (11)
B(13)—B(16)—B(15)	98.6 (12)	B(14)—B(16)—B(15)	56.2 (11)

found in the structure of (η^5-C$_5$H$_5$)$_2$Hf(η^1-C$_5$H$_5$)$_2$ (Kulishov, Bokii & Struchkov, 1972; Rogers, Bynum & Atwood, 1981). The (C$_2$B$_3$ centroid 1)—Hf—(C$_2$B$_3$ centroid 2) angle in (2) is slightly enlarged to 134.1° when compared to 129.5° found in the structure of HfCl$_2$[(η^5-C$_5$H$_4$)$_2$(CH$_2$)$_3$] (Saldarriaga-Molina, Clearfield & Bernal, 1974). Such enlarged angles are precedented (Atwood, Hunter, Alt & Rausch, 1976; Sikora, Rausch, Rogers & Atwood, 1981; Siriwardane, Zhang & Hosmane, 1990). Nonetheless, the average Hf—centroid distance of 2.15 Å, Hf—Cl distance of 2.437 (3) Å, the Cl—Hf—O(THF) angle of 89.7 (2)°, and the bent geometry of (2) all resemble those of a hafnocene derivative despite the presence of a 2− charge on each carborane ligand. As in the Cp systems, the average ring centroid—Hf—O(THF)

(105.8°) and ring centroid—Hf—Cl (106.3°) angles indicate a distorted tetrahedral geometry of the metal center in (2) (see Fig. 1). Since Hf is bonded to a Cl atom as well as to the carborane cages, for charge compensation an additional $Li^+(THF)$ moiety is bound to two adjacent B atoms in each cage with distances ranging from 2.32 (3) to 2.38 (4) Å. In a formal sense compound (2) is a zwitterion consisting of an anionic $\{Hf(Cl)(THF)[\eta^5$-$(SiMe_3)(Me)C_2B_4$-$H_4]_2\}^-$ sandwich that is complexed with an exopolyhedral $[Li(THF)]^+$ cation. Thus, compound (2) distinguishes itself from those of structurally characterized Cp analogues (Cardin, Lappert, Raston & Riley, 1982a,b; Sinn & Kaminsky, 1980; Wailes, Coutts & Weigold, 1974; Saldarriaga-Molina, Clearfield & Bernal, 1974; Sikora, Rausch, Rogers & Atwood, 1981), and the icosahedral metallacarboranes that exhibit bent-sandwich geometries (Fronczek, Halstead & Raymond, 1977; Manning, Knobler & Hawthorne, 1988; Khattar, Knobler, Johnson & Hawthorne, 1991; Manning, Knobler, Khattar & Hawthorne, 1991). It is of interest to note that the bonding of the Li^+ cation to two adjacent B atoms of each ligand in addition to solvating with only one THF molecule and the almost eclipsed conformation of these carborane ligands make the structure of (2) quite dissimilar to that of the Zr complex 4′,5,5′-$Li^+(THF)_2$-1,1′-commo-$Zr^{IV}(THF)$-$Cl[2,3$-$(SiMe_3)_2$-2,3-$C_2B_4H_4]_2$ (3) (Siriwardane, Zhang & Hosmane, 1990) even though an identical geometry at the metal center could be found for both (2) and (3). The eclipsed conformation of the trans-C(cage)—$SiMe_3$ and Me groups of the opposing ligands in (2) could result from the presence of a $Li^+(THF)$ moiety. In any case, compound (2) represents the first hafnium(IV) sandwiched carborane complex to be reported.

The presence of a Cl atom on Hf suggests that a number of substitution reactions at the metal center could be carried out effectively. Such studies, including the catalytic applications, are currently being explored in our laboratories.

Fig. 1. Thermal ellipsoid (SHELXTL-Plus; Sheldrick, 1990) drawing of compound (2). Thermal ellipsoids are scaled to enclose 40% probability. The H atoms of $SiMe_3$ and Me groups, and of THF moleules are omitted for clarity.

References

Atwood, J. L., Barker, G. K., Holton, J., Hunter, W. E., Lappert, M. F. & Pearce, R. (1977). J. Am. Chem. Soc. 99, 6645–6652.

Atwood, J. L., Hunter, W. E., Alt, H. & Rausch, M. D. (1976). J. Am. Chem. Soc. 98, 2454–2459.

Cardin, D. J. (1984). Dictionary of Organometallic Compounds, Vol. 2 and Suppl. Vols. 1–5 (1985–1989), executive editor J. E. Macintyre. New York: Chapman and Hall.

Cardin, D. J., Lappert, M. F., Raston, C. L. & Riley, P. I. (1982a). The Chemistry of Organo-Zirconium and -Hafnium Compounds. Chichester/New York: Horwood/Wiley.

Cardin, D. J., Lappert, M. F., Raston, C. L. & Riley, P. I. (1982b). Comprehensive Organometallic Chemistry, Vol. 3, edited by G. Wilkinson, F. G. A. Stone & E. W. Abel, ch. 23.1–23.3. Oxford: Pergamon Press.

Cotton, F. A. & Wilkinson, G. (1988). Advanced Inorganic Chemistry, 5th ed. New York: John Wiley.

Fronczek, F. R., Halstead, G. W. & Raymond, K. N. (1977). J. Am. Chem. Soc. 99, 1769–1775.

Khattar, R., Knobler, C. B., Johnson, S. E. & Hawthorne, M. F. (1991). Inorg. Chem. 30, 1970–1972.

Kulishov, V. I., Bokii, N. G. & Struchkov, Yu. T. (1972). J. Struct. Chem. (USSR), 13, 1029–1032.

Manning, M. J., Knobler, C. B. & Hawthorne, M. F. (1988). J. Am. Chem. Soc. 110, 4458–4459.

Manning, M. J., Knobler, C. B., Khattar, R. & Hawthorne, M. F. (1991). Inorg. Chem. 30, 2009–2017.

Rogers, R. D., Bynum, R. V. & Atwood, J. L. (1981). J. Am. Chem. Soc. 103, 692–693.

Saldarriaga-Molina, C. H., Clearfield, A. & Bernal, I. (1974). Inorg. Chem. 13, 2880–2885.

Salentine, C. G. & Hawthorne, M. F. (1976). Inorg. Chem. 15, 2872–2882.

Sheldrick, G. M. (1990). SHELXTL-Plus Structure Determination Software Programs. Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

Sikora, D. J., Rausch, M. D., Rogers, R. D. & Atwood, J. L. (1979). J. Am. Chem. Soc. 101, 5079–5081.

Sikora, D. J., Rausch, M. D., Rogers, R. D. & Atwood, J. L. (1981). J. Am. Chem. Soc. 103, 1265–1267.

Sinn, H. & Kaminsky, W. (1980). Adv. Organomet. Chem. 18, 99–149.

Siriwardane, U., Islam, M. S., West, T. A., Hosmane, N. S., Maguire, J. A. & Cowley, A. H. (1987). J. Am. Chem. Soc. 109, 4600–4605.

Siriwardane, U., Zhang, H. & Hosmane, N. S. (1990). J. Am. Chem. Soc. 112, 9637–9638.

Wailes, P. C., Coutts, R. S. P. & Weigold, H. (1974). Organometallic Chemistry of Titanium, Zirconium and Hafnium. New York: Academic Press.