

Fig. 1. The complex cation. The intramolecular hydrogen bond is marked with the dashed line. The numbering scheme of the third anion follows those of the two anions shown.

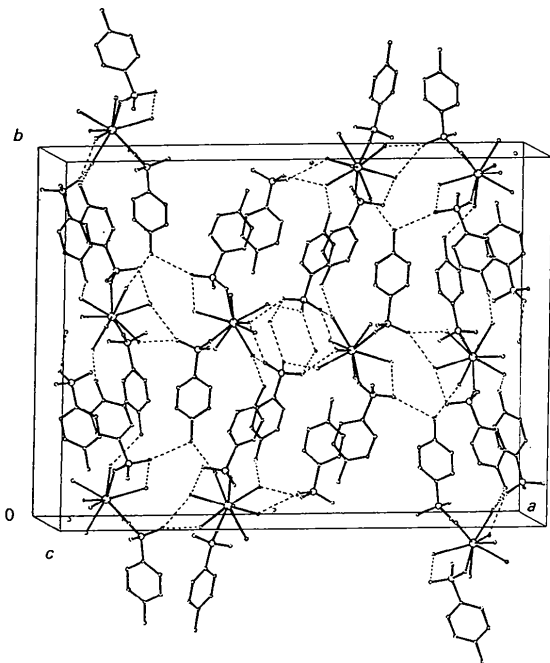


Fig. 2. View of the crystal structure. The dashed lines represent the hydrogen bonds.

difference is in the lanthanide coordination number: eight for the quoted structures, and nine for the present one. All bond distances lie within observed ranges. The coordination polyhedron of Nd1 may best be described as a tricapped trigonal prism in which upper and lower bases are defined by O11, OW6, OW1 and O12, OW7, OW4 respectively, OW2, OW3 and OW4 being the caps; $\Delta = 0.0063 \text{ \AA}^2$ [$\Delta = \sum d_i^2/9$, where d_i is the distance between the real position of the i th atom and the relevant vertex in the ideal least-squares-fitted polyhedron (Drew, 1977)]. The two best capped square antiprisms found may be described as: (i) non-capped base O12, OW2, O11, OW5; capped base OW7, OW6, OW1, OW4; cap OW3; $\Delta = 0.0644 \text{ \AA}^2$; and (ii) non-capped base OW2, OW7, OW3, OW6; capped base O12, OW4, OW1, O11; cap OW5; $\Delta = 0.0522 \text{ \AA}^2$. The structure is held together by an elaborate network of intermolecular hydrogen bonds. The crystal packing is shown in Fig. 2.

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References

- DREW, M. G. B. (1977). *Coord. Chem. Rev.* **24**, 179–275.
 JOHNSON, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
 OHKI, Y., SUZUKI, Y., NAKAMURA, M., SHIMOI, M. & OUCHI, A. (1985). *Bull. Chem. Soc. Jpn.* **58**, 2968–2974.
 OHKI, Y., SUZUKI, Y., TAKEUCHI, T. & OUCHI, A. (1988). *Bull. Chem. Soc. Jpn.* **61**, 393–405.
 SHELDRIK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.
 SHELDRIK, G. M. (1986). *SHELXS86*. Program for the solution of crystal structures. Univ. of Göttingen, Germany.
 UGOZZOLI, F. (1987). *Comput. Chem.* **11**, 109–120.

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A Permethylcyclopentadienyl Carbollide Scandium Complex, $\text{Sc}_2\text{Si}_4\text{O}_3\text{C}_{50}\text{B}_{18}\text{Li}_2\text{H}_{114}$

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Abstract. Tris(tetrahydrofuran)lithium lithium bis[3-bis(trimethylsilyl)methyl-3-(η^5 -pentamethylcyclopent-

tadienyl)-1,2-dicarba-3-scanda-*closo*-dodecaborate-(1-)], $[\text{Li}(\text{C}_4\text{H}_8\text{O})_3] \cdot \text{Li}[\text{Sc}(\text{C}_2\text{B}_9\text{H}_{11})(\text{C}_{10}\text{H}_{15})\text{CH}\{\text{Si}(\text{CH}_3)_3\}_2]_2$, $M_r = 1174.16$, triclinic, $P\bar{1}$, $a = 8.924(4)$, $b = 18.467(5)$, $c = 22.165(3) \text{ \AA}$, $\alpha = 91.42(2)$, $\beta =$

* Contribution No. 8430.

92.36 (2), $\gamma = 92.21$ (3)°, $V = 3645.6$ (18) Å³, $Z = 2$, $D_x = 1.07$ g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 2.84$ cm⁻¹, $F(000) = 1264$, room temperature, 294 K, $R = 0.064$ for 3069 reflections. Each Sc atom is bonded to one Cp* in an η^5 fashion, to one carbollide ligand in an η^5 fashion (completing a distorted icosahedron), and to one —CH(SiMe₃)₂ group in the cleft; the angle at Sc subtended by the centers of the two η^5 groups is 137.8°. Two of these complexes share an Li atom which is loosely bonded to three B atoms of each carbollide, creating a dimeric mono-anion. The counterion, a second Li atom, is coordinated to three tetrahydrofuran molecules.

Introduction. We have been studying various complexes of early-transition and lanthanide metals as catalysts for the classical homogeneous Ziegler–Natta polymerization systems. We have found that neutral alkyl or hydride complexes of Sc, such as $\{[(\eta^5\text{C}_5\text{Me}_4)\text{Me}_2\text{Si}(\eta^1\text{-NCMe}_3)]\text{Sc}(\text{PMe}_3)_2(\mu\text{-H})_2\}$, catalyze the polymerization or oligomerization of α -olefins as well as the more facile polymerization of ethylene (Shapiro, Bunel, Schaefer & Bercaw, 1990). However, these compounds are catalytically active only as monomers, whereas in solution the equilibria favor the dimers. In the hope of preventing this dimerization we have synthesized complexes of Sc containing the dianionic carbollide ligand $[\text{C}_2\text{B}_9\text{H}_{11}]$ as a substitute for the mono-anionic cyclopentadienyl or amide groups, since dimer formation would be discouraged by simple Coulombic repulsion. This carbollide ligand has recently been shown (Crowther, Baenzinger & Jordan, 1991) to support α -olefin polymerization or oligomerization catalytic activity in analogous neutral Group 4 complexes.

The carbollide ligand can be introduced either *via* the reaction of $[\text{Cp}^*\text{ScMe}_2]_x$ (Piers, Bunel & Bercaw, 1991) with $\text{C}_2\text{B}_9\text{H}_{13}$ (Crowther, Baenzinger & Jordan, 1991), followed by treatment with THF to yield $\text{Cp}^*[\text{C}_2\text{B}_9\text{H}_{11}]\text{Sc}(\text{THF})_3$ or by the reaction of $[\text{Cp}^*\text{ScCl}_2]_x$ (Piers, Bunel & Bercaw, 1991) with $\text{Na}_2[\text{C}_2\text{B}_9\text{H}_{11}]$ (Manning, Knobler, Khattar & Hawthorne, 1991), followed by addition of THF to yield the same product. Alkylation of $\text{Cp}^*[\text{C}_2\text{B}_9\text{H}_{11}]\text{Sc}(\text{THF})_3$ with $\text{LiCH}(\text{TMS})_2$ in toluene followed by precipitation in petroleum ether yields $\text{Cp}^*[\text{C}_2\text{B}_9\text{H}_{11}]\text{Sc}[\text{CH}(\text{TMS})_2]_2\text{Li}(\text{THF})_3$. X-ray-quality crystals of $[\text{Cp}^*(\text{C}_2\text{B}_9\text{H}_{11})\text{ScCH}(\text{TMS})_2]_2\text{Li}(\text{THF})_3$ were obtained by pentane diffusion into a concentrated toluene solution of $\text{Cp}^*[\text{C}_2\text{B}_9\text{H}_{11}]\text{Sc}[\text{CH}(\text{TMS})_2]_2\text{Li}(\text{THF})_3$.

Experimental. Pale yellow crystal, flat needle, $0.17 \times 0.40 \times 1.30$ mm; CAD-4 diffractometer, ω scans; 24 reflections with $20 < 2\theta < 25^\circ$ for cell dimensions; no absorption correction ($\mu r_{\text{max}} = 0.19$ and the two independent data sets merged well); $(\sin\theta/\lambda)_{\text{max}} =$

0.48 Å⁻¹; h from -8 to 8 , k from -17 to 17 , l from -21 to 21 ; three standard reflections ($\bar{1}\bar{1}4$, 040 , $\bar{1}31$) showed an early decay of about 3%, then remained constant for the remainder of data collection; first 1164 reflections deleted from data set; 13 754 reflections remained, 6801 of which were independent; goodness of fit for merging = 0.95; R_{merge} for 4195 reflections with exactly two observations = 6.4%; all 6801 reflections used in solution and refinement; Sc atoms located with a Patterson map, remaining heavy atoms found by successive structure factor, difference Fourier cycles; F^2 values used in refinement with weights $w = 1/\sigma^2(F_o^2)$; H atoms on trimethylsilyl groups, tetrahydrofuran molecules and carbollide ligands placed by calculation with C—H = 1.0, B—H = 1.05 Å, on Cp* methyl groups at idealized positions based on difference maps calculated in the expected planes, isotropic B values assigned based on displacement parameter of bonded atom; H-atom parameters not refined, but atoms repositioned once before final least-squares cycles; coordinates of all heavy atoms refined, with anisotropic displacement parameters for Sc, Si, trimethylsilyl C atoms, Cp* methyl C atoms and atoms of tetrahydrofuran; other C atoms, the B atoms and the Li atoms with isotropic thermal parameters, plus one scale factor, for a total of 532 parameters in one full matrix; final R for 5812 reflections with $F_o^2 > 0$ was 0.128, for 3069 reflections with $F_o^2 > 3\sigma(F_o^2)$ $R = 0.064$, wR (on F_o^2) = 0.013, goodness of fit = 1.45 for 6801 reflections and 532 parameters. Variances $[\sigma^2(I)]$ derived from counting statistics plus an additional term, $(0.014I)^2$; variances of the merged data by propagation of error plus another additional term, $(0.014I)^2$; ratio of maximum shift to e.s.d. in final least-squares cycle was 0.40 in a tetrahydrofuran C atom and 0.21 for other parameters; final difference Fourier map had excursions of 0.55 and -0.65 e Å⁻³; atomic scattering factors and anomalous-dispersion corrections taken from Cromer & Waber (1974) and Cromer (1974); computer programs used were those of the CRYM crystallographic computing system (Duchamp, 1964) and ORTEP (Johnson, 1976). Final parameters are given in Table 1 and selected distances and angles are listed in Table 2.† An ORTEPII drawing of the two anions and one Li atom showing the numbering system is shown in Fig. 1; Fig. 2 is a packing diagram.

† A figure showing the numbering system for the $\text{Li}(\text{THF})_3$ cation and lists of anisotropic displacement parameters, complete distances and angles, observed and calculated structure factors and assigned H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55052 (40 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH0559]

Table 1. Heavy-atom coordinates ($\times 10^4$) and equivalent isotropic ($\text{\AA}^2 \times 10^4$) or isotropic (\AA^2) thermal parameters for the Cp* carbollide scandium complex
$$U_{eq} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	U_{eq} or B^\dagger
Sc1	3815 (2)	2298 (1)	2181 (1)	503 (5)
Sc2	1785 (2)	6797 (1)	4013 (1)	463 (5)
Si1	5448 (3)	1214 (1)	1029 (1)	709 (8)
Si2	2320 (3)	650 (2)	1455 (1)	892 (10)
Si3	220 (3)	8593 (1)	4029 (1)	771 (10)
Si4	3357 (3)	8433 (1)	4684 (1)	789 (9)
C1	3992 (8)	1261 (4)	1614 (3)	4.7 (2)†
C2	1620 (8)	7964 (4)	4351 (3)	4.3 (2)†
Me1	6862 (9)	1988 (4)	1094 (4)	862 (30)
Me2	4735 (10)	1208 (6)	232 (4)	1291 (43)
Me3	6520 (10)	376 (5)	1094 (5)	1292 (41)
Me4	985 (10)	710 (5)	2082 (4)	1193 (38)
Me5	2713 (11)	-322 (5)	1396 (6)	1660 (58)
Me6	1198 (10)	835 (6)	749 (4)	1343 (43)
Me7	-1214 (9)	8146 (4)	3504 (4)	984 (32)
Me8	-890 (11)	9004 (5)	4641 (5)	1552 (45)
Me9	933 (11)	9368 (5)	3635 (6)	1911 (60)
Me10	4653 (9)	7766 (5)	5028 (4)	975 (33)
Me11	3044 (11)	9074 (6)	5323 (5)	1543 (44)
Me12	4479 (10)	8973 (4)	4149 (4)	1103 (38)
Cp1	5620 (9)	2714 (4)	3013 (3)	4.0 (2)†
Cp2	4171 (8)	2699 (4)	3270 (3)	4.3 (2)†
Cp3	3665 (9)	1972 (4)	3271 (3)	4.8 (2)†
Cp4	4741 (9)	1519 (5)	3043 (3)	4.9 (2)†
Cp5	5926 (9)	1984 (4)	2884 (3)	4.4 (2)†
Cp6	6658 (9)	3372 (4)	2947 (3)	779 (29)
Cp7	3478 (9)	3318 (4)	3594 (3)	848 (31)
Cp8	2225 (10)	1711 (5)	3561 (4)	1002 (33)
Cp9	4733 (10)	715 (5)	3068 (4)	1009 (35)
Cp10	7474 (9)	1731 (5)	2698 (4)	979 (34)
Cp11	854 (8)	6492 (4)	5036 (3)	4.1 (2)†
Cp12	-349 (8)	6374 (4)	4605 (3)	4.3 (2)†
Cp13	-43 (9)	5794 (4)	4226 (3)	4.5 (2)†
Cp14	1381 (8)	5548 (4)	4406 (3)	4.0 (2)†
Cp15	1931 (9)	5975 (4)	4890 (3)	4.1 (2)†
Cp16	870 (9)	6976 (4)	5593 (3)	783 (30)
Cp17	-1847 (9)	6752 (4)	4623 (4)	813 (29)
Cp18	-1109 (9)	5442 (4)	3740 (4)	851 (29)
Cp19	2054 (9)	4852 (4)	4205 (4)	883 (31)
Cp20	3388 (9)	5860 (5)	5264 (4)	894 (32)
Cc1	1502 (8)	2573 (4)	1529 (3)	4.5 (2)†
Cc2	2913 (8)	2759 (4)	1154 (3)	4.6 (2)†
Bc3	4004 (10)	3378 (5)	1498 (4)	3.9 (2)†
Bc4	3146 (9)	3647 (4)	2139 (4)	3.4 (2)†
Bc5	1504 (9)	3072 (5)	2164 (4)	4.0 (2)†
Bc6	1210 (11)	3046 (5)	880 (4)	5.8 (3)†
Bc7	2856 (11)	3594 (5)	854 (4)	5.6 (3)†
Bc8	2956 (10)	4180 (5)	1485 (4)	4.1 (2)†
Bc9	1359 (10)	3974 (5)	1908 (4)	4.3 (2)†
Bc10	342 (11)	3271 (5)	1528 (4)	5.2 (3)†
Bc11	1185 (10)	3955 (5)	1119 (4)	4.8 (2)†
Cc21	4076 (8)	7199 (4)	3442 (3)	3.8 (2)†
Cc22	2655 (8)	7467 (4)	3077 (3)	4.2 (2)†
Bc23	1543 (10)	6770 (5)	2853 (4)	4.1 (2)†
Bc24	2412 (9)	5993 (4)	3077 (4)	3.6 (2)†
Bc25	4059 (9)	6311 (5)	3490 (4)	3.7 (2)†
Bc26	4349 (10)	7521 (5)	2735 (4)	4.9 (2)†
Bc27	2696 (10)	7226 (5)	2329 (4)	4.8 (2)†
Bc28	2587 (10)	6282 (5)	2326 (4)	4.4 (2)†
Bc29	4183 (10)	5985 (5)	2739 (4)	3.9 (2)†
Bc30	5256 (10)	6750 (5)	2982 (4)	4.5 (2)†
Bc31	4354 (10)	6747 (5)	2271 (4)	4.6 (2)†
Li1	2786 (16)	4920 (8)	2409 (6)	5.9 (4)†
Li2	302 (18)	6795 (9)	1455 (7)	7.1 (4)†
O1	1517 (7)	6702 (5)	766 (3)	870 (22)
Cf1	2584 (17)	7227 (6)	553 (5)	1182 (43)
Cf2	3820 (15)	6767 (11)	329 (7)	1749 (71)
Cf3	3215 (22)	6095 (10)	243 (10)	2699 (103)
Cf4	1783 (14)	6027 (7)	481 (5)	1193 (44)
O2	-1143 (6)	5999 (3)	1465 (4)	863 (23)
Cf5	-1635 (11)	5620 (6)	1966 (5)	826 (36)
Cf6	-2611 (14)	4996 (7)	1737 (7)	1145 (46)
Cf7	-3038 (19)	5227 (10)	1144 (8)	1882 (76)
Cf8	-2097 (15)	5781 (9)	957 (5)	1484 (68)
O3	-751 (8)	7642 (4)	1414 (4)	1163 (27)
Cf9	-1781 (25)	7835 (10)	1769 (8)	2970 (91)
Cf10	-2623 (17)	8412 (12)	1608 (10)	2750 (93)
Cf11	-1697 (22)	8728 (7)	1261 (12)	2795 (120)
Cf12	-961 (22)	8122 (11)	971 (6)	2493 (90)

† Isotropic displacement parameter.

Table 2. Selected distances (\AA) and angles ($^\circ$) for the Cp* carbollide scandium complex

Cp*1 and Cp*2 refer to the centroids of the pentamethylcyclopentadienyl ligands, Cb1 and Cb2 to the centroids of the rings in the carbollide ligands of two C atoms and three B atoms bonded to Sc.

Sc1—C1	2.280 (7)	Si2—Me4	1.871 (10)
Sc1—Cb1	2.126	Si2—Me5	1.843 (11)
Sc1—Cp*1	2.205	Si2—Me6	1.870 (10)
Sc2—C2	2.276 (7)	Si3—Me7	1.850 (9)
Sc2—Cb2	2.142	Si3—Me8	1.873 (10)
Sc2—Cp*2	2.192	Si3—Me9	1.805 (11)
C1—Si1	1.876 (7)	Si4—Me10	1.876 (9)
C1—Si2	1.852 (8)	Si4—Me11	1.859 (10)
C2—Si3	1.870 (7)	Si4—Me12	1.867 (9)
C2—Si4	1.862 (7)	Li2—O1	1.917 (17)
Si1—Me1	1.867 (8)	Li2—O2	1.918 (17)
Si1—Me2	1.853 (10)	Li2—O3	1.859 (18)
Si1—Me3	1.857 (10)		
Cp*1—Sc1—Cb1	137.8	Si2—C1—Sc1	120.4 (4)
C1—Sc1—Cb1	111.2	Si2—C1—Si1	114.4 (4)
C1—Sc1—Cp*1	110.9	Si3—C2—Sc2	122.9 (3)
Cp*2—Sc2—Cb2	137.8	Si4—C2—Sc2	117.6 (3)
C2—Sc2—Cb2	111.0	Si4—C2—Si3	113.9 (4)
C2—Sc2—Cp*2	111.2	Si2—C1—Si1	114.4 (4)
Si1—C1—Sc1	119.5 (3)	Si4—C2—Si3	113.9 (4)

Discussion. This compound crystallizes in space group $P\bar{1}$ with four monomers in the cell, but structurally two monomer anions are loosely connected by one Li atom into one dimer (Fig. 1), with a $\text{Li}(\text{C}_4\text{H}_8\text{O})_3^+$ counterion; the cell contains two each of these two groups. There is an almost perfect non-crystallographic twofold axis relating the two halves of the anion dimer, passing through Li and the Sc1—Sc2 midpoint. The two Sc moieties are nearly identical and therefore their average structure will be discussed. The Sc atom is bonded to three centers: the Cp* centroid, the center of a pentagonal face of the carbollide and a C atom. The Sc—center distances are normal (Table 2); Sc—C distances vary slightly, being 2.502 (22) \AA to Cp* C atoms, 2.576 (22) \AA to carbollide C atoms [2.556 (14) \AA to carbollide boron atoms] and 2.278 (3) \AA to the $\text{CH}[\text{Si}(\text{CH}_3)_3]_2$ C atoms. Carbollide centroid to Sc to Cp* centroid angles are 137.8°, the same as we have found for Cp*—Sc—Cp* angles (Shapiro, Henling, Marsh & Bercaw, 1990), and the (carbollide or Cp* centroid)—Sc—C atom angles are all within 0.2° of 111.1°. These three large ligands effectively prevent the Sc atom from increasing its coordination number.

The Sc—C—Si angles average 120.1°; the sum of the angles at the C atom, however, is 354.4°, indicating a relatively small tetrahedral hybridization at the C atom. The C—Si—methyl group angles are all slightly larger than 109.5° and the methyl group—Si—methyl group angles are all slightly smaller [average 113.7 (23) and 104.9 (10)°]. The permethylcyclopentadienyl groups are also normal and regular, with C—C (ring) distances of 1.406 (16) \AA and C—C (methyl) distances of 1.518 (18) \AA . Interior C—C—C angles differ from 108° by an average of 1.7°; exterior angles range between 123.6 and 127.3°.

The carbollide ligands appear well ordered, with relatively small apparent thermal motions. The C atoms were distinguished from the B atoms on the basis of their U_{eq} values and the bond distances – the C—C distances are 1.573 (7) Å, whereas the B—B distances are 1.760 (21) Å. C—B distances in the 5-ring are significantly shorter than those to B atoms in the cap [1.646 (16) vs 1.709 (13) Å]. Refinement led to acceptable thermal parameters for all 22 atoms of the carbollide groups.

The atoms of the THF groups of the $\text{Li}(\text{THF})_3^+$ counterion show large displacement parameters, reaching r.m.s. values of 0.8 Å, and implying disorder involving non-planar configurations.

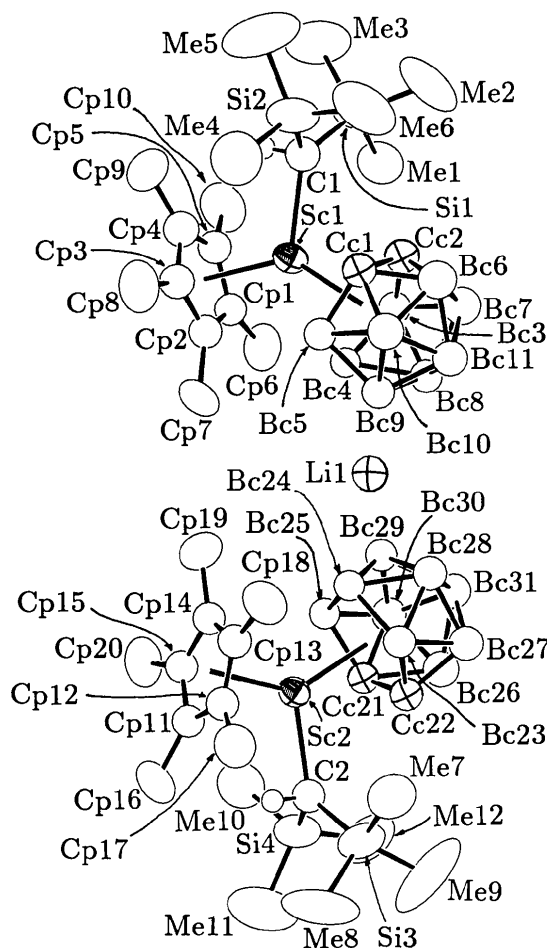


Fig. 1. An ORTEP (Johnson, 1976) drawing of the two anions and Li1 with 50% probability ellipsoids showing the numbering system. The code is: Cp(number) = permethylenecyclopentadienyl C atoms; Me(number) = methyl C atoms bonded to Si; Cc(number) = carbollide C atoms; Bc(number) = carbollide B atoms. Only two H atoms, those bonded to C1 (H1) and to C2 (H2) (neither so labeled) are shown.

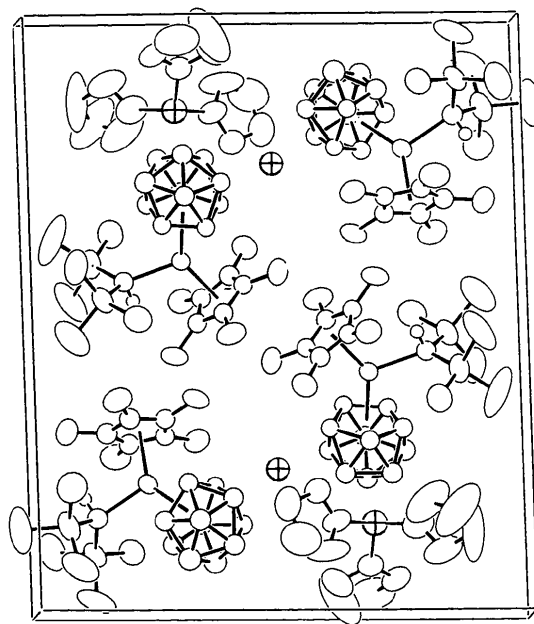


Fig. 2. An ORTEP (Johnson, 1976) drawing of the contents of one unit cell with the unit cell outlined and projected approximately down the a axis; the c axis is horizontal. Except for those on C1 and C2, H atoms are omitted. The Li atoms are shown with principal ellipses marked. Li2 , bonded to the three solvent molecules, interacts slightly with carbollide 2: Li2—Bc27 2.90, Li2—Bc28 2.95 and Li2—Bc23 3.25 Å.

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References

- CROMER, D. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, pp. 149–151. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- CROMER, D. T. & WABER, J. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, pp. 99–101. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- CROWTHER, D. J., BAENZINGER, N. C. & JORDAN, R. F. (1991). *J. Am. Chem. Soc.* **113**, 1455–1457.
- DUCHAMP, D. J. (1964). *CRYM* crystallographic computing system. Am. Crystallogr. Assoc. Meet., Bozeman, Montana. Paper B14, p. 29.
- JOHNSON, C. K. (1976). *ORTEP*. Report ORNL-3794, third revision. Oak Ridge National Laboratory, Tennessee, USA.
- MANNING, M. J., KNOBLER, C. B., KHATTAR, R. & HAWTHORNE, M. F. (1991). *Inorg. Chem.* **30**, 2009–2017.
- PIERS, W. E., BUNEL, E. E. & BERCAW, J. E. (1991). *J. Organomet. Chem.* **47**, 51–60.
- SHAPIRO, P. J., BUNEL, E., SCHAEFER, W. P. & BERCAW, J. E. (1990). *Organometallics*, **9**, 867–869, and references therein.
- SHAPIRO, P. J., HENLING, L. M., MARSH, R. E. & BERCAW, J. E. (1990). *Inorg. Chem.* **29**, 4560–4565. Note that in Table IV contained therein, Si—Cen2 should be 2.230 Å and Cen1—Sc—Cen2 should be 138.5°.