Supporting Information

Carboranylamidinates

Peter Dröse, Cristian G. Hrib and Frank T. Edelmann*

Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

Experimental Details

General Procedures. All operations were performed with rigorous exclusion of air and water in oven-dried or flame-dried glassware under an inert atmosphere of dry argon, employing standard Schlenk, high-vacuum, and glovebox techniques (MBraun MBLab; <1 ppm O_2, <1 ppm H_2O). THF, toluene, *n*-pentane, and DME were distilled from sodium/benzophenone under nitrogen atmosphere. All glassware was oven-dried at 140 °C for at least 24 h, assembled while hot, and cooled under high vacuum prior to use. The starting materials *o*-carborane, *N,N′*-diisopropylcarbodiimide, *n*-butyllithium, and anhydrous $SnCl_2$ were obtained from commercial sources and used as received. $CrCl_2(THF)_2$ was prepared according to a literature procedure[1] and stored in the glovebox. The NMR spectra were recorded in THF-d_8 solutions on a Bruker DPX 600 (^{1}H: 600 MHz; ^{13}C: 101 MHz) or a Bruker-AVANCE-DMX400 (5 mm BB, ^{1}H: 400.13 Hz; ^{13}C: 100.62 MHz), ^{1}H and ^{13}C shifts are referenced to internal solvent resonances and reported in parts per million relative to TMS. IR spectra were recorded using KBr pellets on a Perkin Elmer FT-IR spectrometer system 2000 between 4000 cm^{-1} and 400 cm^{-1} with dry KBr/sample mixtures and KBr windows. Mass spectra Massenspektroskopie (EI, 70 eV) were run on a MAT 95 apparatus. Microanalyses of the compounds were performed using a Leco CHNS 923 apparatus. Melting points: Büchi Melting Point B-540.

General remarks: The reported yields are not optimized, but it is clear that no major soluble products have been overlooked. For the Sn and Cr derivatives no meaningful ^{11}B NMR spectra could be obtained. Fairly large deviations in the found C value in the elemental analyses of **2** and **6** can be traced back to either easy loss of solvent (**2**) or high air-sensitivity (**6**).

2: A 100 mL Schlenk flask was charged with a solution of *o*-carborane (0.50 g, 3.47 mmol) in DME/*n*-pentane (1:2, 30 mL) and *n*-butyllithium (1.6 M in *n*-hexane, 2.2 mL, 3.47 mmol) was added at r.t. After stirring for 1 h, neat *N,N′*-diisopropylcarbodiimide (0.44 g, 3.47 mmol) was added and stirring at r.t. was continued for 12 h. The reaction mixture was concentrated *in vacuo* to a total volume of *ca.* 10 mL. Cooling to -32 °C for 72 h afforded colorless, block-like single-crystals suitable for X-ray diffraction. Yield: 0.62 g (65%), m.p. 112.5 °C. Anal. Calcd for $C_{13}H_{35}B_{10}LiN_2O_2$ (*M*r = 366.48 g/mol): C, 42.61; H, 9.63; N, 7.64. Found: C, 40.33; H, 9.83; N, 7.76%. **^{1}H NMR** (400 MHz, THF-d_8, 25°C): δ = 4.60 (s_{br}, 1H, (^{i}PrN=)C(N***H***^{i}Pr)), 3.70 (s_{br}, 2H, Me_2C***H***N), 3.57 (s, 4H, OC***H***$_2$), 3.26 (s, 6H, C***H***$_3$O), 1.20-3.00 (br, 10H, ***H***–B), 1.13 (s_{br}, 6H, (C***H***$_3$)$_2$CHN), 1.05 (s_{br}, 6H, (C***H***$_3$)$_2$CHN). ^{11}B NMR (128 MHz, THF-d_8, 25°C): δ = -5.15, -8.29, -11.08, -12.75, -15.15. **^{13}C{^{1}H} NMR** (100.6 MHz, THF-d_8, 25°C): δ = 156.0 ((^{i}PrN=)***C***(NH^{i}Pr), 81.3 ([***C***–CLi]$_{B10H10}$), 72.6 (O***C***H$_2$), 58.8 (***C***H$_3$O),

49.3 ([C–***C***Li]$_{B10H10}$), 48.0 ((Me$_2$***C***HN), 47.3 (Me$_2$***C***HN), 23.7 ((***C***H$_3$)$_2$CHN). **IR** (KBr cm^{-1}): ν_{max} 3407 (st, NH), 3063 (w), 3008 (w), 2969 (st, ν_s CH$_3$), 2934 (st, ν_{as} CH$_2$), 2870 (m, ν_{as} CH$_3$), 2850 (w, ν_s CH$_2$), 2832 (w), 2565 (vs, BH), 1665 (st, C=N), 1634 (vs), 1519 (vs), 1474 (st, δ_{as} CH$_3$), 1451 (st), 1413 (w), 1387 (m, δ_s CH$_3$), 1369 (m), 1320 (m), 1297 (m), 1265 (st), 1244 (st), 1192 (m), 1162 (m), 1122 (vs), 1102 (st), 1079 (vs), 1038 (m), 1027 (m), 1017 (m), 974 (w), 932 (w), 868 (st), 845 (w), 833 (w), 791 (w), 743 (m), 726 (w), 723 (w,), 706 (w), 609 (w), 527 (w), 513 (m), 498 (w), 475 (w), 409 (w). **MS** (EI): *m/z* (%) 270.2 (20) [M – Li – DME]$^+$, 227.1 (100) [(^{i}PrN=)(^{i}PrNH)C(C$_2$B$_{10}$H$_{10}$) – ^{i}Pr – H]$^+$, 170.1 (15) [N=C–C$_2$B$_{10}$H$_{10}$ – 2H]$^+$, 58.0 (95) [N^{i}Pr + H]$^+$.

3: A 100 mL Schlenk flask was charged with a solution of **2** (0.5 g, 1.4 mmol) in acetonitrile, and a few drops of water were added. The reaction mixture was stirred for 10 min at r.t., filtered and concentrated to a total volume of *ca.* 3 mL. Cooling to -32 °C for 1 week afforded colorless, needle-like single-crystals suitable for X-ray diffraction. Yield: 0.32 g (85%), m.p. 57.0 °C. Anal. Calcd for C$_9$H$_{26}$B$_{10}$N$_2$ (*M*r = 270.43 g/mol): C, 39.97; H, 9.69; N, 10.36. Found: C, 39.82; H, 9.56; N, 9.63%. **^{1}H NMR** (400 MHz, THF-*d*$_8$, 25°C): δ = 4.92 (s, 1H, [C–C***H***]$_{B10H10}$)), 4.55 (s$_{br}$, 1H, (^{i}PrN=)C(N***H***^{i}Pr)), 3.78 (sept, ^3J = 6.0 Hz, 2H, Me$_2$C***H***N), 1.40-3.20 (br, 10H, ***H***–B), 1.16 (d, ^3J = 6.1 Hz, 6H, (C***H***$_3$)$_2$CHN), 1.03 (d, ^3J = 6.1 Hz, 6H, (C***H***$_3$)$_2$CHN). ^{11}B NMR (128 MHz, THF-*d*$_8$, 25°C): δ = -3.96, -5.04, -10.03, -13.67. **^{13}C{^{1}H} NMR** (100.6 MHz, THF-*d*$_8$, 25°C): δ = 143.2 ((^{i}PrN=)***C***(NH^{i}Pr), 76.9 ([***C***–CH]$_{B10H10}$), 60.1 ([C–***C***H]$_{B10H10}$), 48.2 ((Me$_2$***C***HN), 47.3 (Me$_2$***C***HN), 24.2 ((***C***H$_3$)$_2$CHN), 23.7 ((***C***H$_3$)$_2$CHN). **IR** (KBr cm^{-1}): ν_{max} 3404 (w, NH), 3063 (m), 2969 (st, ν_s CH$_3$), 2928 (w), 2869 (w, ν_{as} CH$_3$), 2641 (m), 2630 (m), 2583 (st, BH), 2555 (m), 1665 (st, C=N), 1500 (m), 1470 (w, δ_{as} CH$_3$), 1452 (m), 1386 (w, δ_s CH$_3$), 1377 (w), 1364 (m), 1323 (m), 1303 (w), 1246 (m), 1188 (w), 1172 (w), 1121 (w), 1082 (w), 1013 (m), 730 (w), 720 (w), 509 (w), 473 (w), 451 (w). **MS** (EI): *m/z* (%) 270.3 (30) [M]$^+$, 227.2 (100) [M – ^{i}Pr – H]$^+$, 170.2 (15) [N=C–C$_2$B$_{10}$H$_{10}$ –2H]$^+$, 58.1 (70) [N^{i}Pr + H]$^+$, 43.0 (30) [^{i}Pr]$^+$.

4: In a 250 mL Schlenk flask a solution of *o*-carborane (1.00 g, 7.0 mmol) in THF (100 mL) was treated with *n*-butyllithium (1.6 M in *n*-hexane, 4.4 ml, 7.0 mmol). After stirring for 1 h, neat *N,N'*-diisopropylcarbodiimide (0.88 g, 7.0 mmol) was added and stirring at r.t. was continued for 12 h. Anhydrous SnCl$_2$ (0.66 g, 3.5 mmol) was added as solid, causing the development of a pale yellow color. After stirring for 24 h, the reaction mixture was evaporated to dryness, and the residue was extracted with toluene (50 mL). The extract was filtered and concentrated to a total volume of *ca.* 10 mL. Cooling to 5 °C for 24 afforded colorless, block-like single-crystals suitable for X-ray diffraction. Yield: 1.88 g (82%), m.p. > 260 °C. Anal. Calcd for C$_{18}$H$_{50}$B$_{20}$N$_4$Sn (*M*r = 657.55 g/mol): C, 32.88; H, 7.66; N, 8.52. Found: C, 33.01; H, 8.09; N, 8.73%. **IR** (KBr cm^{-1}): ν_{max} 3411 (vs, NH),

2974 (vs, ν_s CH_3), 2932 (st), 2871 (m, ν_{as} CH_3), 2581 (vs, BH), 1666 (m, C=N), 1599 (vs), 1516 (vs), 1458 (vs), 1390 (vs, δ_s CH_3), 1373 (st), 1164 (st), 1111 (vs), 1059 (vs), 1032 (st), 970 (m), 955 (m), 927 (m), 899 (m), 875 (w), 864 (w), 852 (m), 831 (w), 815 (m), 778 (w), 763 (w), 719 (st), 681 (w), 670 (w), 641 (w), 615 (w), 527 (w), 506 (m), 478 (m), 461 (w), 450 (m). **MS** (EI): *m/z* (%) 657.1 (20) $[M]^+$, 388.0 (20) [M – (^{i}PrN=)(^{i}PrNH)C($C_2B_{10}H_{10}$) + 2H]$^+$, 270.1 (20) [(^{i}PrN=)(^{i}PrNH)C($C_2B_{10}H_{10}$)]$^+$, 227.1 (50) [(^{i}PrN=)(^{i}PrNH)-C($C_2B_{10}H_{10}$) – ^{i}Pr – H]$^+$, 144.1 (60) $[C_2B_{10}H_{10}]^+$, 58.0 (100) [N^{i}Pr + H]$^+$.

5: In a 250 mL Schlenk flask a solution of *o*-carborane (1.00 g, 7.0 mmol) in THF (100 mL) was treated with *n*-butyllithium (1.6 M in *n*-hexane, 4.4 ml, 7.0 mmol). After stirring for 1 h, neat *N,N′*-diisopropylcarbodiimide (0.88 g, 7.0 mmol) was added and stirring at r.t. was continued for 12 h. $CrCl_2(THF)_2$ (0.94 g, 3.5 mmol) was added as solid, causing the development of a dark green color. After stirring for 48 h, the reaction mixture was evaporated to dryness, and the residue was extracted with toluene (3 x 30 mL). The combined extracts were filtered and concentrated to a total volume of *ca.* 20 mL. Cooling to 5 °C for 48 afforded blue-green, block-like single-crystals suitable for X-ray diffraction. Yield: 0.93 g (45%), m.p. 170 °C (dec.). Anal. Calcd for $C_{18}H_{50}B_{20}CrN_4$ (*M*r = 590.83 g/mol): C, 36.59; H, 8.53; N, 9.48. Found: C, 36.64; H, 8.43; N, 9.46%. **IR** (KBr cm^{-1}): ν_{max} 3902 (w), 3855 (w), 3631 (w), 3435 (m), 3403 (m, NH), 3385 (m), 2978 (m), 2972 (m, ν_s CH_3), 2933 (w), 2872 (w, ν_{as} CH_3), 2577 (vs, BH), 2344 (w), 1666 (w, C=N), 1591 (vs), 1521 (vs), 1456 (st), 1389 (m, δ_s CH_3), 1373 (m), 1323 (m), 1314 (m), 1284 (m), 1242 (m), 1181 (m), 1158 (m), 1122 (st), 1106 (m), 1059 (m), 1033 (m), 999 (w), 973 (w), 927 (w), 908 (w), 840 (w), 737 (w), 724 (w), 713 (w), 671 (w), 493 (w). **MS** (EI): *m/z* (%) 591.2 (10) $[M]^+$, 270.2 (20) [(^{i}PrN=)(^{i}PrNH)C($C_2B_{10}H_{10}$) + H]$^+$, 227.1 (100) [(^{i}PrN=)(^{i}PrNH)C(C_2B_{10}) – ^{i}Pr – H]$^+$, 58.0 (90) [N^{i}Pr + H]$^+$.

6: In a 250 mL Schlenk flask a solution of *o*-carborane (0.40 g, 2.8 mmol) in THF (100 mL) was treated with *n*-butyllithium (1.6 M in *n*-hexane, 1.7 ml, 2.8 mmol). After stirring for 1 h, neat *N,N′*-diisopropylcarbodiimide (0.35 g, 2.8 mmol) was added and stirring at r.t. was continued for 12 h. $CrCl_2(THF)_2$ (0.74 g, 2.8 mmol) was added as solid, causing the development of a dark green color. After stirring for 48 h, the reaction mixture was evaporated to dryness, and the residue was extracted with toluene (30 mL). The extract was filtered and concentrated to a total volume of *ca.* 20 mL. Cooling to -32 °C for 48 afforded blue-green block-like single-crystals suitable for X-ray diffraction. Under the microscope the crystals are dichroitic (blue/green). Yield: 0.23 g (23%), m.p. 132 °C (dec.). Anal. Calcd for $C_{18}H_{50}B_{20}Cl_2Cr_2N_4$ (*M*r = 713.73 g/mol): C, 30.29; H, 7.06; N, 7.85. Found: C, 33.14; H, 6.54; N, 7.75%. **IR** (KBr cm^{-1}): ν_{max} 3433 (m), 3403 (m, NH), 3384 (m), 2978 (m),

2972 (m, ν_s CH_3), 2933 (w), 2872 (w, ν_{as} CH_3), 2578 (vs, BH), 1667 (w, C=N), 1591 (vs), 1521 (vs), 1456 (st), 1389 (m, δ_s CH_3), 1373 (m), 1322 (m), 1289 (m), 1244 (m), 1181 (m), 1161 (m), 1122 (st), 1106 (m), 1060 (m), 1033 (m), 1000 (w), 973 (w), 737 (w), 724 (w), 493 (w). **MS** (EI): *m/z* (%) 712.8 (100) $[M]^+$, 591.1 (40) $[M - (^i PrN=)(^i PrNH)C + H]^+$, 355.9 (35) $[M - ClCr\{(^i PrN=)(^i PrNH)C(C_2B_{10})\}]^+$, 227.1 (15) $[(^i PrN=)(^i PrNH)C(C_2B_{10}H_{10}) - {}^i Pr - H]^+$, 58.0 (10) $[N^i Pr + H]^+$.

Reference

(1) Köhler, F. H.; Prössdorf, W. *Z. Naturforsch. B* **1977**, *32*, 1026.

Crystallographic Data

Crystal Data Collection, Structure Solution, and Refinement

The intensity data of **2-6** were collected on a Stoe IPDS 2T diffractometer with MoK_α radiation. The data were collected with the Stoe XAREA[2] program using ω-scans. The space groups were determined with the XRED32[2] program and the reflections were merged. The structures were solved by direct methods (SHELXS-97) and refined by full matrix least-squares methods on F^2 using SHELXL-97.[1] Data collection parameters as well as bond lengths and angles are given in Tables 1-10.

(1) (a) Sheldrick, G. M. *SHELXL-97 Program for Crystal Structure Refinement*, Universität Göttingen (Germany) **1997**; (b) Sheldrick, G. M. *SHELXS-97 Program for Crystal Structure Solution*, Universität Göttingen (Germany) **1997**.

(2) Stoe, XAREA *Program for X-ray Crystal Data collection*, (XRED32 included in XAREA) (Stoe, 2002)

Table 1. Crystallographic Data for **2**

Identification code	ip142	
Empirical formula	$C_{13}H_{35}B_{10}LiN_2O_2$	
Formula weight	366.47	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.3125(17) Å	α= 84.90(3)°
	b = 8.8541(18) Å	β= 86.31(3)°
	c = 15.564(3) Å	γ = 81.66(3)°
Volume	1127.4(4) $Å^3$	
Z	2	
Density (calculated)	1.080 Mg/m^3	
Absorption coefficient	0.061 mm^{-1}	
F(000)	392	
Crystal size	0.45 x 0.38 x 0.30 mm^3	
Theta range for data collection	2.33 to 28.28°	
Index ranges	-11<=h<=11, -11<=k<=11, -20<=l<=18	
Reflections collected	11975	
Independent reflections	5554 [R(int) = 0.0394]	
Completeness to theta = 28.00°	99.5 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5554 / 0 / 263	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0450, wR2 = 0.1012	
R indices (all data)	R1 = 0.0615, wR2 = 0.1084	
Largest diff. peak and hole	0.285 and -0.216 $e.Å^{-3}$	

Table 2. Bond lengths [A] and angles [deg] for **2**.

Li-O(1)	1.987(2)	C(7)-C(9)	1.513(2)
Li-O(2)	1.993(2)	C(7)-C(8)	1.5178(17)
Li-N(1)	2.017(2)	C(10)-C(11)	1.4989(18)
Li-C(2)	2.088(2)	B(3)-B(7)	1.754(2)
Li-C(11)	2.703(2)	B(3)-B(8)	1.7886(19)
O(1)-C(10)	1.4217(15)	B(3)-B(4)	1.7930(19)
O(1)-C(12)	1.4236(16)	B(4)-B(8)	1.765(2)
O(2)-C(11)	1.4241(15)	B(4)-B(9)	1.7664(19)
O(2)-C(13)	1.4256(14)	B(4)-B(5)	1.774(2)
N(1)-C(3)	1.2823(15)	B(5)-B(10)	1.767(2)
N(1)-C(4)	1.4763(15)	B(5)-B(9)	1.7711(19)
N(2)-C(3)	1.3620(15)	B(5)-B(6)	1.7956(19)
N(2)-C(7)	1.4699(16)	B(6)-B(11)	1.7530(19)
C(1)-C(3)	1.5282(16)	B(6)-B(10)	1.7842(19)
C(1)-C(2)	1.6751(15)	B(7)-B(11)	1.744(2)
C(1)-B(3)	1.6903(18)	B(7)-B(8)	1.7775(19)
C(1)-B(6)	1.6930(18)	B(7)-B(12)	1.7856(19)
C(1)-B(5)	1.7093(17)	B(8)-B(12)	1.785(2)
C(1)-B(4)	1.7122(17)	B(8)-B(9)	1.789(2)
C(2)-B(7)	1.7103(17)	B(9)-B(12)	1.7732(19)
C(2)-B(11)	1.7134(18)	B(9)-B(10)	1.789(2)
C(2)-B(3)	1.7200(18)	B(10)-B(11)	1.7783(19)
C(2)-B(6)	1.7206(18)	B(10)-B(12)	1.782(2)
C(4)-C(6)	1.521(2)	B(11)-B(12)	1.7735(19)
C(4)-C(5)	1.5245(17)		

O(1)-Li-O(2)	84.00(9)	C(10)-O(1)-Li	110.17(9)
O(1)-Li-N(1)	126.39(11)	C(12)-O(1)-Li	128.70(10)
O(2)-Li-N(1)	128.51(12)	C(11)-O(2)-C(13)	111.72(10)
O(1)-Li-C(2)	117.39(11)	C(11)-O(2)-Li	103.29(10)
O(2)-Li-C(2)	116.13(11)	C(13)-O(2)-Li	118.60(10)
N(1)-Li-C(2)	87.81(9)	C(3)-N(1)-C(4)	122.56(10)
O(1)-Li-C(11)	57.96(6)	C(3)-N(1)-Li	117.73(10)
O(2)-Li-C(11)	30.85(5)	C(4)-N(1)-Li	119.40(9)
N(1)-Li-C(11)	156.65(11)	C(3)-N(2)-C(7)	128.34(10)
C(2)-Li-C(11)	110.95(10)	C(3)-C(1)-C(2)	115.29(9)
C(10)-O(1)-C(12)	111.95(10)	C(3)-C(1)-B(3)	115.73(9)

C(2)-C(1)-B(3)	61.47(7)	O(2)-C(11)-Li	45.86(7)
C(3)-C(1)-B(6)	116.32(9)	C(10)-C(11)-Li	78.35(9)
C(2)-C(1)-B(6)	61.44(7)	C(1)-B(3)-C(2)	58.83(7)
B(3)-C(1)-B(6)	114.12(9)	C(1)-B(3)-B(7)	104.59(9)
C(3)-C(1)-B(5)	121.25(9)	C(2)-B(3)-B(7)	58.97(7)
C(2)-C(1)-B(5)	113.31(9)	C(1)-B(3)-B(8)	104.40(9)
B(3)-C(1)-B(5)	115.35(9)	C(2)-B(3)-B(8)	106.80(9)
B(6)-C(1)-B(5)	63.70(8)	B(7)-B(3)-B(8)	60.22(8)
C(3)-C(1)-B(4)	121.11(9)	C(1)-B(3)-B(4)	58.80(7)
C(2)-C(1)-B(4)	113.10(9)	C(2)-B(3)-B(4)	107.11(9)
B(3)-C(1)-B(4)	63.60(8)	B(7)-B(3)-B(4)	107.18(9)
B(6)-C(1)-B(4)	115.16(9)	B(8)-B(3)-B(4)	59.04(8)
B(5)-C(1)-B(4)	62.48(8)	C(1)-B(4)-B(8)	104.50(9)
C(1)-C(2)-B(7)	107.23(9)	C(1)-B(4)-B(9)	104.79(9)
C(1)-C(2)-B(11)	107.11(9)	B(8)-B(4)-B(9)	60.87(8)
B(7)-C(2)-B(11)	61.25(8)	C(1)-B(4)-B(5)	58.68(7)
C(1)-C(2)-B(3)	59.70(7)	B(8)-B(4)-B(5)	108.60(10)
B(7)-C(2)-B(3)	61.51(8)	B(9)-B(4)-B(5)	60.02(8)
B(11)-C(2)-B(3)	111.23(9)	C(1)-B(4)-B(3)	57.61(7)
C(1)-C(2)-B(6)	59.79(7)	B(8)-B(4)-B(3)	60.36(8)
B(7)-C(2)-B(6)	111.33(9)	B(9)-B(4)-B(3)	108.57(9)
B(11)-C(2)-B(6)	61.39(8)	B(5)-B(4)-B(3)	107.27(9)
B(3)-C(2)-B(6)	111.23(9)	C(1)-B(5)-B(10)	104.46(9)
C(1)-C(2)-Li	102.25(9)	C(1)-B(5)-B(9)	104.71(9)
B(7)-C(2)-Li	138.68(10)	B(10)-B(5)-B(9)	60.76(8)
B(11)-C(2)-Li	134.55(10)	C(1)-B(5)-B(4)	58.84(7)
B(3)-C(2)-Li	113.41(10)	B(10)-B(5)-B(4)	108.32(10)
B(6)-C(2)-Li	108.33(9)	B(9)-B(5)-B(4)	59.76(8)
N(1)-C(3)-N(2)	130.74(11)	C(1)-B(5)-B(6)	57.71(7)
N(1)-C(3)-C(1)	116.82(10)	B(10)-B(5)-B(6)	60.11(8)
N(2)-C(3)-C(1)	112.40(9)	B(9)-B(5)-B(6)	108.20(9)
N(1)-C(4)-C(6)	110.03(10)	B(4)-B(5)-B(6)	107.25(9)
N(1)-C(4)-C(5)	107.77(10)	C(1)-B(6)-C(2)	58.77(7)
C(6)-C(4)-C(5)	111.27(11)	C(1)-B(6)-B(11)	104.55(9)
N(2)-C(7)-C(9)	111.24(11)	C(2)-B(6)-B(11)	59.10(7)
N(2)-C(7)-C(8)	107.03(10)	C(1)-B(6)-B(10)	104.39(9)
C(9)-C(7)-C(8)	111.58(11)	C(2)-B(6)-B(10)	107.08(9)
O(1)-C(10)-C(11)	107.57(10)	B(11)-B(6)-B(10)	60.35(8)
O(2)-C(11)-C(10)	107.62(10)	C(1)-B(6)-B(5)	58.59(7)

C(2)-B(6)-B(5)	107.02(9)	B(5)-B(10)-B(9)	59.75(8)
B(11)-B(6)-B(5)	107.23(9)	B(11)-B(10)-B(9)	107.04(10)
B(10)-B(6)-B(5)	59.14(8)	B(12)-B(10)-B(9)	59.54(8)
C(2)-B(7)-B(11)	59.46(7)	B(6)-B(10)-B(9)	107.92(9)
C(2)-B(7)-B(3)	59.52(7)	C(2)-B(11)-B(7)	59.29(7)
B(11)-B(7)-B(3)	108.18(9)	C(2)-B(11)-B(6)	59.51(7)
C(2)-B(7)-B(8)	107.73(9)	B(7)-B(11)-B(6)	108.22(10)
B(11)-B(7)-B(8)	108.59(10)	C(2)-B(11)-B(12)	107.74(9)
B(3)-B(7)-B(8)	60.85(8)	B(7)-B(11)-B(12)	61.01(8)
C(2)-B(7)-B(12)	107.33(9)	B(6)-B(11)-B(12)	108.95(9)
B(11)-B(7)-B(12)	60.31(8)	C(2)-B(11)-B(10)	107.67(9)
B(3)-B(7)-B(12)	108.79(9)	B(7)-B(11)-B(10)	109.09(10)
B(8)-B(7)-B(12)	60.14(8)	B(6)-B(11)-B(10)	60.69(8)
B(4)-B(8)-B(7)	107.39(9)	B(12)-B(11)-B(10)	60.24(8)
B(4)-B(8)-B(12)	107.28(9)	B(9)-B(12)-B(11)	107.95(9)
B(7)-B(8)-B(12)	60.15(8)	B(9)-B(12)-B(10)	60.42(8)
B(4)-B(8)-B(3)	60.60(8)	B(11)-B(12)-B(10)	60.01(8)
B(7)-B(8)-B(3)	58.93(8)	B(9)-B(12)-B(8)	60.35(8)
B(12)-B(8)-B(3)	107.28(9)	B(11)-B(12)-B(8)	106.94(9)
B(4)-B(8)-B(9)	59.61(8)	B(10)-B(12)-B(8)	108.34(10)
B(7)-B(8)-B(9)	107.38(9)	B(9)-B(12)-B(7)	107.70(10)
B(12)-B(8)-B(9)	59.49(8)	B(11)-B(12)-B(7)	58.68(8)
B(3)-B(8)-B(9)	107.78(9)	B(10)-B(12)-B(7)	107.06(9)
B(4)-B(9)-B(5)	60.21(8)	B(8)-B(12)-B(7)	59.70(8)
B(4)-B(9)-B(12)	107.75(9)		
B(5)-B(9)-B(12)	107.66(9)		
B(4)-B(9)-B(8)	59.52(8)		
B(5)-B(9)-B(8)	107.68(9)		
B(12)-B(9)-B(8)	60.16(8)		
B(4)-B(9)-B(10)	107.68(9)		
B(5)-B(9)-B(10)	59.50(8)		
B(12)-B(9)-B(10)	60.04(8)		
B(8)-B(9)-B(10)	107.90(9)		
B(5)-B(10)-B(11)	107.41(9)		
B(5)-B(10)-B(12)	107.46(10)		
B(11)-B(10)-B(12)	59.75(8)		
B(5)-B(10)-B(6)	60.75(8)		
B(11)-B(10)-B(6)	58.96(8)		
B(12)-B(10)-B(6)	107.17(9)		

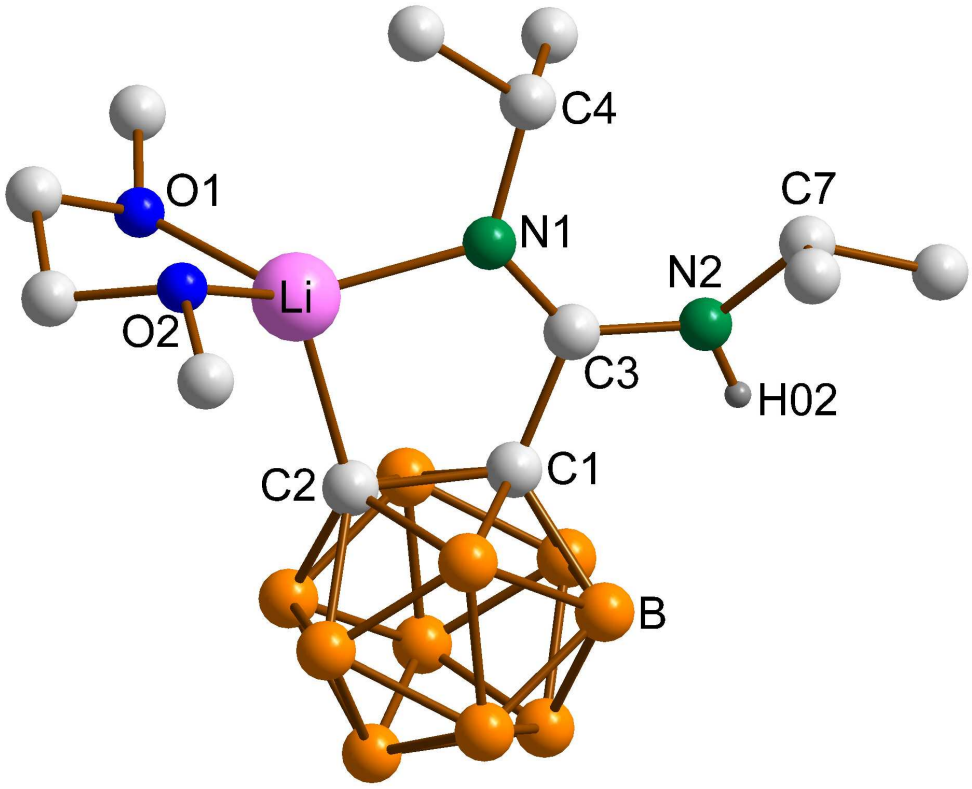

Figure 1. Molecular structure of **2**.

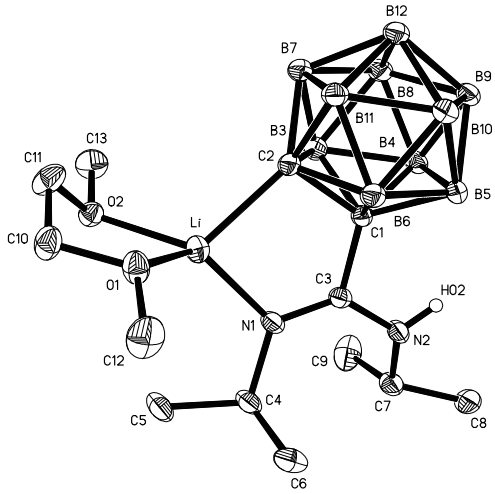

Figure 2. ORTEP drawing of the molecular structure of **2**.

Table 3. Crystallographic Data for **3**

Identification code	ip84	
Empirical formula	$C_9H_{26}B_{10}N_2$	
Formula weight	270.42	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 6.9667(14) Å	α= 90°
	b = 15.763(3) Å	β= 99.95(3)°
	c = 15.394(3) Å	γ = 90°
Volume	1665.1(6) $Å^3$	
Z	4	
Density (calculated)	1.079 Mg/m^3	
Absorption coefficient	0.054 mm^{-1}	
F(000)	576	
Crystal size	0.70 x 0.40 x 0.18 mm^3	
Theta range for data collection	2.58 to 26.37°	
Index ranges	-7<=h<=8, -19<=k<=19, -19<=l<=19	
Reflections collected	14751	
Independent reflections	3406 [R(int) = 0.1026]	
Completeness to theta = 26.00°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3406 / 0 / 242	
Goodness-of-fit on F^2	1.184	
Final R indices [I>2sigma(I)]	R1 = 0.0729, wR2 = 0.1315	
R indices (all data)	R1 = 0.1007, wR2 = 0.1400	
Largest diff. peak and hole	0.222 and -0.211 $e.Å^{-3}$	

Table 4. Bond lengths [A] and angles [deg] for **3**

N(1)-C(3)	1.274(3)	B(3)-B(4)	1.783(3)
N(1)-C(7)	1.477(3)	B(4)-B(5)	1.774(3)
N(2)-C(3)	1.365(3)	B(4)-B(9)	1.777(4)
N(2)-C(4)	1.479(3)	B(4)-B(8)	1.782(3)
C(1)-C(3)	1.529(3)	B(5)-B(10)	1.763(4)
C(1)-C(2)	1.637(3)	B(5)-B(9)	1.766(3)
C(1)-B(5)	1.705(3)	B(5)-B(6)	1.771(3)
C(1)-B(4)	1.709(3)	B(6)-B(10)	1.765(4)
C(1)-B(6)	1.728(3)	B(6)-B(11)	1.773(4)
C(1)-B(3)	1.732(3)	B(7)-B(12)	1.774(4)
C(2)-B(7)	1.693(3)	B(7)-B(8)	1.774(4)
C(2)-B(11)	1.694(3)	B(7)-B(11)	1.779(4)
C(2)-B(6)	1.722(3)	B(8)-B(9)	1.785(3)
C(2)-B(3)	1.722(3)	B(8)-B(12)	1.785(4)
C(4)-C(6)	1.514(3)	B(9)-B(12)	1.783(4)
C(4)-C(5)	1.519(3)	B(9)-B(10)	1.788(4)
C(7)-C(8)	1.515(3)	B(10)-B(11)	1.780(3)
C(7)-C(9)	1.518(3)	B(10)-B(12)	1.785(4)
B(3)-B(8)	1.770(3)	B(11)-B(12)	1.777(4)
B(3)-B(7)	1.779(4)		
C(3)-N(1)-C(7)	123.60(19)	B(6)-C(1)-B(3)	114.79(16)
C(3)-N(2)-C(4)	124.95(17)	C(1)-C(2)-B(7)	112.02(17)
C(3)-C(1)-C(2)	115.73(16)	C(1)-C(2)-B(11)	111.95(16)
C(3)-C(1)-B(5)	122.18(16)	B(7)-C(2)-B(11)	63.36(15)
C(2)-C(1)-B(5)	110.21(17)	C(1)-C(2)-B(6)	61.85(13)
C(3)-C(1)-B(4)	124.61(18)	B(7)-C(2)-B(6)	115.19(17)
C(2)-C(1)-B(4)	110.66(16)	B(11)-C(2)-B(6)	62.51(14)
B(5)-C(1)-B(4)	62.60(13)	C(1)-C(2)-B(3)	62.00(13)
C(3)-C(1)-B(6)	113.42(17)	B(7)-C(2)-B(3)	62.79(14)
C(2)-C(1)-B(6)	61.51(13)	B(11)-C(2)-B(3)	115.64(17)
B(5)-C(1)-B(6)	62.12(14)	B(6)-C(2)-B(3)	115.58(16)
B(4)-C(1)-B(6)	114.35(17)	N(1)-C(3)-N(2)	132.7(2)
C(3)-C(1)-B(3)	117.77(17)	N(1)-C(3)-C(1)	114.27(18)
C(2)-C(1)-B(3)	61.42(13)	N(2)-C(3)-C(1)	113.08(17)
B(5)-C(1)-B(3)	114.06(16)	N(2)-C(4)-C(6)	107.96(17)
B(4)-C(1)-B(3)	62.43(13)	N(2)-C(4)-C(5)	110.90(18)

C(6)-C(4)-C(5)	111.44(18)	B(10)-B(6)-B(5)	59.82(14)
N(1)-C(7)-C(8)	106.80(19)	C(2)-B(6)-B(11)	57.98(14)
N(1)-C(7)-C(9)	110.73(18)	C(1)-B(6)-B(11)	104.13(17)
C(8)-C(7)-C(9)	111.67(19)	B(10)-B(6)-B(11)	60.43(14)
C(2)-B(3)-C(1)	56.57(12)	B(5)-B(6)-B(11)	107.58(17)
C(2)-B(3)-B(8)	103.68(18)	C(2)-B(7)-B(12)	104.37(17)
C(1)-B(3)-B(8)	104.29(16)	C(2)-B(7)-B(8)	104.73(17)
C(2)-B(3)-B(7)	57.80(14)	B(12)-B(7)-B(8)	60.42(15)
C(1)-B(3)-B(7)	103.70(17)	C(2)-B(7)-B(11)	58.36(14)
B(8)-B(3)-B(7)	59.99(15)	B(12)-B(7)-B(11)	60.01(14)
C(2)-B(3)-B(4)	103.44(16)	B(8)-B(7)-B(11)	108.44(17)
C(1)-B(3)-B(4)	58.16(12)	C(2)-B(7)-B(3)	59.41(14)
B(8)-B(3)-B(4)	60.21(14)	B(12)-B(7)-B(3)	108.43(18)
B(7)-B(3)-B(4)	107.59(18)	B(8)-B(7)-B(3)	59.76(14)
C(1)-B(4)-B(5)	58.60(13)	B(11)-B(7)-B(3)	108.73(17)
C(1)-B(4)-B(9)	104.73(17)	B(3)-B(8)-B(7)	60.25(14)
B(5)-B(4)-B(9)	59.66(14)	B(3)-B(8)-B(4)	60.25(14)
C(1)-B(4)-B(8)	104.73(17)	B(7)-B(8)-B(4)	107.83(17)
B(5)-B(4)-B(8)	107.62(18)	B(3)-B(8)-B(9)	108.34(17)
B(9)-B(4)-B(8)	60.21(14)	B(7)-B(8)-B(9)	107.72(18)
C(1)-B(4)-B(3)	59.41(12)	B(4)-B(8)-B(9)	59.74(14)
B(5)-B(4)-B(3)	108.31(17)	B(3)-B(8)-B(12)	108.29(18)
B(9)-B(4)-B(3)	108.15(18)	B(7)-B(8)-B(12)	59.76(15)
B(8)-B(4)-B(3)	59.55(14)	B(4)-B(8)-B(12)	107.60(17)
C(1)-B(5)-B(10)	105.60(16)	B(9)-B(8)-B(12)	59.92(14)
C(1)-B(5)-B(9)	105.36(16)	B(5)-B(9)-B(4)	60.09(14)
B(10)-B(5)-B(9)	60.87(15)	B(5)-B(9)-B(12)	107.33(17)
C(1)-B(5)-B(6)	59.57(13)	B(4)-B(9)-B(12)	107.95(17)
B(10)-B(5)-B(6)	59.91(14)	B(5)-B(9)-B(8)	107.84(17)
B(9)-B(5)-B(6)	108.96(17)	B(4)-B(9)-B(8)	60.05(14)
C(1)-B(5)-B(4)	58.80(13)	B(12)-B(9)-B(8)	60.05(15)
B(10)-B(5)-B(4)	109.17(17)	B(5)-B(9)-B(10)	59.49(14)
B(9)-B(5)-B(4)	60.26(14)	B(4)-B(9)-B(10)	107.94(17)
B(6)-B(5)-B(4)	109.11(16)	B(12)-B(9)-B(10)	59.97(14)
C(2)-B(6)-C(1)	56.64(12)	B(8)-B(9)-B(10)	108.10(17)
C(2)-B(6)-B(10)	104.09(17)	B(5)-B(10)-B(6)	60.27(14)
C(1)-B(6)-B(10)	104.57(17)	B(5)-B(10)-B(11)	107.60(17)
C(2)-B(6)-B(5)	103.38(16)	B(6)-B(10)-B(11)	60.01(14)
C(1)-B(6)-B(5)	58.32(13)	B(5)-B(10)-B(12)	107.39(18)

B(6)-B(10)-B(12)	108.07(17)
B(11)-B(10)-B(12)	59.78(14)
B(5)-B(10)-B(9)	59.64(14)
B(6)-B(10)-B(9)	108.27(18)
B(11)-B(10)-B(9)	107.68(17)
B(12)-B(10)-B(9)	59.89(14)
C(2)-B(11)-B(6)	59.51(14)
C(2)-B(11)-B(12)	104.18(19)
B(6)-B(11)-B(12)	108.07(18)
C(2)-B(11)-B(7)	58.28(14)
B(6)-B(11)-B(7)	108.55(18)
B(12)-B(11)-B(7)	59.84(15)
C(2)-B(11)-B(10)	104.59(17)
B(6)-B(11)-B(10)	59.56(14)
B(12)-B(11)-B(10)	60.23(14)
B(7)-B(11)-B(10)	108.06(18)
B(7)-B(12)-B(11)	60.14(14)
B(7)-B(12)-B(9)	107.86(18)
B(11)-B(12)-B(9)	108.05(18)
B(7)-B(12)-B(10)	108.11(17)
B(11)-B(12)-B(10)	59.99(14)
B(9)-B(12)-B(10)	60.14(14)
B(7)-B(12)-B(8)	59.82(15)
B(11)-B(12)-B(8)	108.06(19)
B(9)-B(12)-B(8)	60.03(14)
B(10)-B(12)-B(8)	108.23(18)

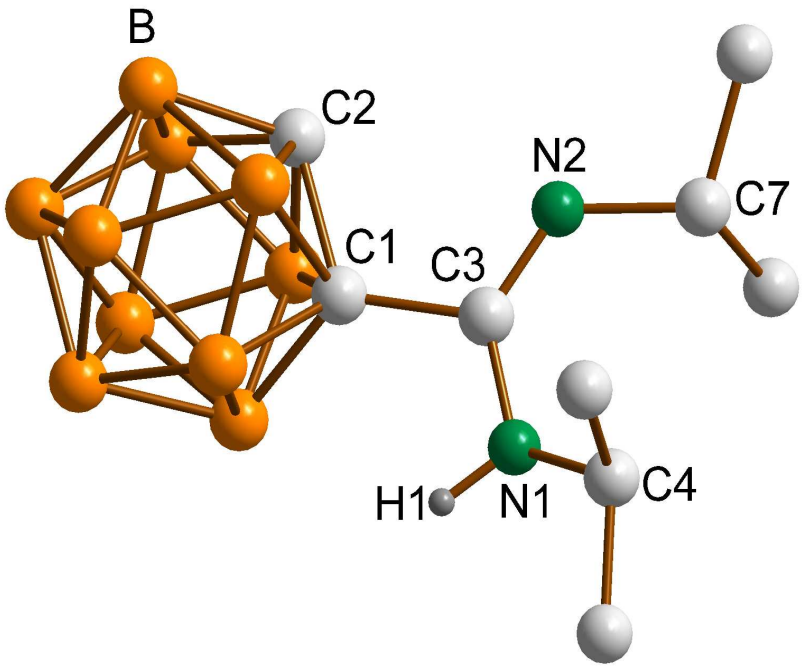

Figure 3. Molecular structure of **3**.

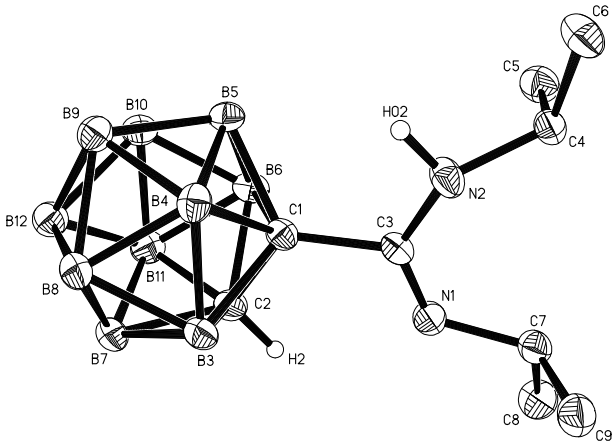

Figure 4. ORTEP drawing of the molecular structure of **3**.

Table 5. Crystallographic Data for **4**

Identification code	ip111	
Empirical formula	$C_{18}H_{48}B_{20}N_4Sn$	
Formula weight	655.49	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 22.790(5) Å	α= 90°
	b = 7.8311(16) Å	β= 101.30(3)°
	c = 19.215(4) Å	γ = 90°
Volume	3362.8(12) $Å^3$	
Z	4	
Density (calculated)	1.295 Mg/m^3	
Absorption coefficient	0.780 mm^{-1}	
F(000)	1336	
Crystal size	0.27 x 0.24 x 0.20 mm^3	
Theta range for data collection	2.54 to 28.28°	
Index ranges	-30<=h<=25, -10<=k<=9, -25<=l<=25	
Reflections collected	10800	
Independent reflections	4134 [R(int) = 0.0535]	
Completeness to theta = 28.00°	98.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4134 / 0 / 203	
Goodness-of-fit on F^2	1.085	
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.0780	
R indices (all data)	R1 = 0.0493, wR2 = 0.0806	
Largest diff. peak and hole	0.927 and -1.525 $e.Å^{-3}$	

Table 6. Bond lengths [A] and angles [deg] for **4**

Sn-C(2)	2.318(3)	B(3)-B(7)	1.759(4)
Sn-C(2)#1	2.318(2)	B(3)-B(8)	1.778(4)
Sn-N(1)	2.497(2)	B(3)-B(4)	1.789(4)
Sn-N(1)#1	2.497(2)	B(4)-B(9)	1.772(4)
N(1)-C(3)	1.287(3)	B(4)-B(5)	1.775(4)
N(1)-C(4)	1.486(3)	B(4)-B(8)	1.778(4)
N(2)-C(3)	1.347(3)	B(5)-B(9)	1.765(4)
N(2)-C(7)	1.475(3)	B(5)-B(10)	1.767(4)
C(1)-C(3)	1.528(3)	B(5)-B(6)	1.781(4)
C(1)-C(2)	1.651(3)	B(6)-B(11)	1.766(4)
C(1)-B(6)	1.694(4)	B(6)-B(10)	1.774(4)
C(1)-B(5)	1.709(4)	B(7)-B(11)	1.764(4)
C(1)-B(4)	1.716(3)	B(7)-B(12)	1.771(4)
C(1)-B(3)	1.717(4)	B(7)-B(8)	1.773(4)
C(2)-B(11)	1.709(4)	B(8)-B(12)	1.779(5)
C(2)-B(7)	1.717(4)	B(8)-B(9)	1.780(4)
C(2)-B(6)	1.730(4)	B(9)-B(12)	1.771(5)
C(2)-B(3)	1.734(4)	B(9)-B(10)	1.792(5)
C(4)-C(6)	1.521(4)	B(10)-B(11)	1.777(4)
C(4)-C(5)	1.522(4)	B(10)-B(12)	1.780(4)
C(7)-C(9)	1.518(4)	B(11)-B(12)	1.779(4)
C(7)-C(8)	1.518(4)		
C(2)-Sn-C(2)#1	96.95(12)	C(2)-C(1)-B(5)	112.89(19)
C(2)-Sn-N(1)	73.03(7)	B(6)-C(1)-B(5)	63.11(17)
C(2)#1-Sn-N(1)	94.46(8)	C(3)-C(1)-B(4)	119.9(2)
C(2)-Sn-N(1)#1	94.46(8)	C(2)-C(1)-B(4)	112.84(17)
C(2)#1-Sn-N(1)#1	73.03(7)	B(6)-C(1)-B(4)	115.20(19)
N(1)-Sn-N(1)#1	161.40(9)	B(5)-C(1)-B(4)	62.43(16)
C(3)-N(1)-C(4)	119.6(2)	C(3)-C(1)-B(3)	114.2(2)
C(3)-N(1)-Sn	119.44(16)	C(2)-C(1)-B(3)	61.94(15)
C(4)-N(1)-Sn	120.10(15)	B(6)-C(1)-B(3)	115.21(19)
C(3)-N(2)-C(7)	128.3(2)	B(5)-C(1)-B(3)	114.55(18)
C(3)-C(1)-C(2)	115.57(19)	B(4)-C(1)-B(3)	62.82(15)
C(3)-C(1)-B(6)	117.65(19)	C(1)-C(2)-B(11)	108.52(19)
C(2)-C(1)-B(6)	62.26(16)	C(1)-C(2)-B(7)	108.47(19)
C(3)-C(1)-B(5)	122.6(2)	B(11)-C(2)-B(7)	62.00(17)

C(1)-C(2)-B(6)	60.07(15)	B(5)-B(4)-B(3)	108.0(2)
B(11)-C(2)-B(6)	61.79(16)	B(8)-B(4)-B(3)	59.78(16)
B(7)-C(2)-B(6)	112.28(19)	C(1)-B(5)-B(9)	104.8(2)
C(1)-C(2)-B(3)	60.90(15)	C(1)-B(5)-B(10)	104.3(2)
B(11)-C(2)-B(3)	112.37(19)	B(9)-B(5)-B(10)	60.96(17)
B(7)-C(2)-B(3)	61.30(16)	C(1)-B(5)-B(4)	58.96(15)
B(6)-C(2)-B(3)	112.49(19)	B(9)-B(5)-B(4)	60.08(16)
C(1)-C(2)-Sn	113.26(14)	B(10)-B(5)-B(4)	108.9(2)
B(11)-C(2)-Sn	133.20(17)	C(1)-B(5)-B(6)	58.01(15)
B(7)-C(2)-Sn	119.99(16)	B(9)-B(5)-B(6)	108.6(2)
B(6)-C(2)-Sn	125.30(15)	B(10)-B(5)-B(6)	59.98(16)
B(3)-C(2)-Sn	105.83(16)	B(4)-B(5)-B(6)	108.1(2)
N(1)-C(3)-N(2)	129.7(2)	C(1)-B(6)-C(2)	57.67(15)
N(1)-C(3)-C(1)	117.2(2)	C(1)-B(6)-B(11)	104.07(19)
N(2)-C(3)-C(1)	113.0(2)	C(2)-B(6)-B(11)	58.52(15)
N(1)-C(4)-C(6)	110.8(2)	C(1)-B(6)-B(10)	104.73(19)
N(1)-C(4)-C(5)	108.63(19)	C(2)-B(6)-B(10)	105.90(19)
C(6)-C(4)-C(5)	109.4(2)	B(11)-B(6)-B(10)	60.27(16)
N(2)-C(7)-C(9)	111.1(2)	C(1)-B(6)-B(5)	58.88(16)
N(2)-C(7)-C(8)	107.1(2)	C(2)-B(6)-B(5)	105.84(19)
C(9)-C(7)-C(8)	111.0(2)	B(11)-B(6)-B(5)	107.47(19)
C(1)-B(3)-C(2)	57.17(14)	B(10)-B(6)-B(5)	59.63(16)
C(1)-B(3)-B(7)	103.7(2)	C(2)-B(7)-B(3)	59.84(15)
C(2)-B(3)-B(7)	58.86(15)	C(2)-B(7)-B(11)	58.78(15)
C(1)-B(3)-B(8)	104.3(2)	B(3)-B(7)-B(11)	108.6(2)
C(2)-B(3)-B(8)	105.9(2)	C(2)-B(7)-B(12)	106.2(2)
B(7)-B(3)-B(8)	60.16(17)	B(3)-B(7)-B(12)	108.7(2)
C(1)-B(3)-B(4)	58.55(15)	B(11)-B(7)-B(12)	60.44(18)
C(2)-B(3)-B(4)	105.5(2)	C(2)-B(7)-B(8)	106.9(2)
B(7)-B(3)-B(4)	107.5(2)	B(3)-B(7)-B(8)	60.43(17)
B(8)-B(3)-B(4)	59.81(16)	B(11)-B(7)-B(8)	108.8(2)
C(1)-B(4)-B(9)	104.2(2)	B(12)-B(7)-B(8)	60.26(18)
C(1)-B(4)-B(5)	58.61(15)	B(7)-B(8)-B(3)	59.41(16)
B(9)-B(4)-B(5)	59.68(16)	B(7)-B(8)-B(4)	107.42(18)
C(1)-B(4)-B(8)	104.3(2)	B(3)-B(8)-B(4)	60.41(15)
B(9)-B(4)-B(8)	60.19(17)	B(7)-B(8)-B(12)	59.82(18)
B(5)-B(4)-B(8)	107.9(2)	B(3)-B(8)-B(12)	107.5(2)
C(1)-B(4)-B(3)	58.64(14)	B(4)-B(8)-B(12)	107.4(2)
B(9)-B(4)-B(3)	107.9(2)	B(7)-B(8)-B(9)	107.4(2)

B(3)-B(8)-B(9)	108.04(19)	B(7)-B(12)-B(10)	107.8(2)
B(4)-B(8)-B(9)	59.74(17)	B(9)-B(12)-B(10)	60.62(17)
B(12)-B(8)-B(9)	59.67(18)	B(8)-B(12)-B(10)	108.8(2)
B(5)-B(9)-B(12)	107.6(2)	B(11)-B(12)-B(10)	59.90(17)
B(5)-B(9)-B(4)	60.24(16)		
B(12)-B(9)-B(4)	108.0(2)		
B(5)-B(9)-B(8)	108.21(19)		
B(12)-B(9)-B(8)	60.12(18)		
B(4)-B(9)-B(8)	60.07(17)		
B(5)-B(9)-B(10)	59.58(16)		
B(12)-B(9)-B(10)	59.94(18)		
B(4)-B(9)-B(10)	107.91(19)		
B(8)-B(9)-B(10)	108.2(2)		
B(5)-B(10)-B(6)	60.39(16)		
B(5)-B(10)-B(11)	107.6(2)		
B(6)-B(10)-B(11)	59.64(16)		
B(5)-B(10)-B(12)	107.1(2)		
B(6)-B(10)-B(12)	107.7(2)		
B(11)-B(10)-B(12)	60.04(18)		
B(5)-B(10)-B(9)	59.46(17)		
B(6)-B(10)-B(9)	107.8(2)		
B(11)-B(10)-B(9)	107.4(2)		
B(12)-B(10)-B(9)	59.44(18)		
C(2)-B(11)-B(7)	59.22(16)		
C(2)-B(11)-B(6)	59.69(15)		
B(7)-B(11)-B(6)	108.3(2)		
C(2)-B(11)-B(10)	106.7(2)		
B(7)-B(11)-B(10)	108.2(2)		
B(6)-B(11)-B(10)	60.09(16)		
C(2)-B(11)-B(12)	106.2(2)		
B(7)-B(11)-B(12)	59.96(17)		
B(6)-B(11)-B(12)	108.1(2)		
B(10)-B(11)-B(12)	60.06(17)		
B(7)-B(12)-B(9)	107.9(2)		
B(7)-B(12)-B(8)	59.93(18)		
B(9)-B(12)-B(8)	60.21(18)		
B(7)-B(12)-B(11)	59.60(17)		
B(9)-B(12)-B(11)	108.2(2)		
B(8)-B(12)-B(11)	107.9(2)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

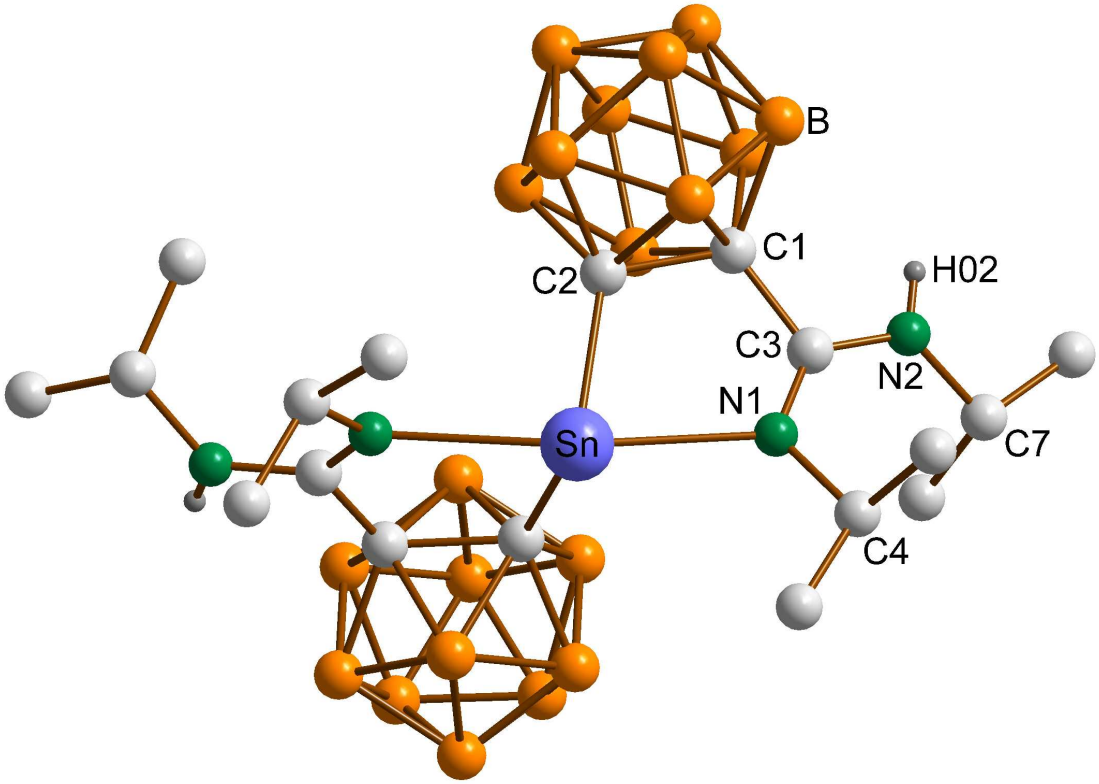

Figure 5. Molecular structure of **4**.

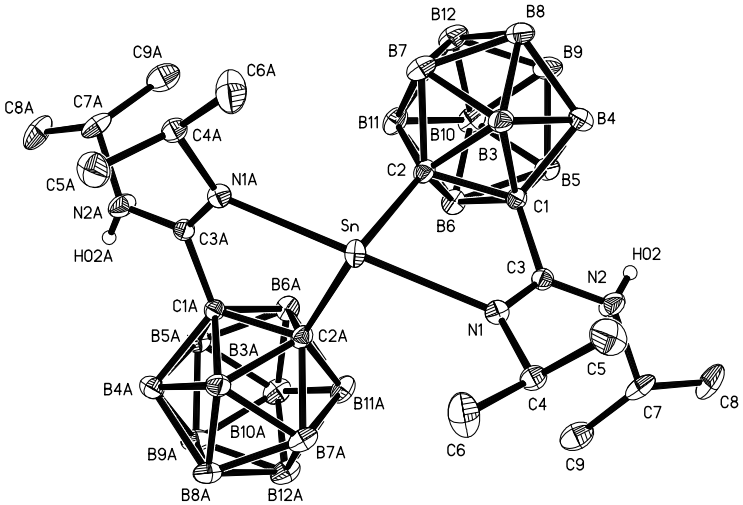

Figure 6. ORTEP drawing of the molecular structure of **4**.

Table 7. Crystallographic Data for **5**

Identification code	ip109	
Empirical formula	$C_{18}H_{50}B_{20}CrN_4$	
Formula weight	590.82	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2/n	
Unit cell dimensions	a = 13.749(3) Å	α= 90°
	b = 8.1504(16) Å	β= 103.10(3)°
	c = 15.296(3) Å	γ = 90°
Volume	1669.4(6) $Å^3$	
Z	2	
Density (calculated)	1.175 Mg/m^3	
Absorption coefficient	0.363 mm^{-1}	
F(000)	620	
Crystal size	0.40 x 0.27 x 0.20 mm^3	
Theta range for data collection	2.26 to 28.28°	
Index ranges	-18<=h<=18, -10<=k<=9, -20<=l<=15	
Reflections collected	9177	
Independent reflections	4036 [R(int) = 0.0859]	
Completeness to theta = 28.00°	97.1 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4036 / 0 / 203	
Goodness-of-fit on F^2	1.104	
Final R indices [I>2sigma(I)]	R1 = 0.0621, wR2 = 0.1280	
R indices (all data)	R1 = 0.0820, wR2 = 0.1360	
Largest diff. peak and hole	0.486 and -0.324 $e.Å^{-3}$	

Table 8. Bond lengths [A] and angles [deg] for **5**

Cr-N(1)#1	2.0852(19)	B(3)-B(7)	1.761(4)
Cr-N(1)	2.0852(19)	B(3)-B(8)	1.782(4)
Cr-C(2)#1	2.157(2)	B(3)-B(4)	1.796(4)
Cr-C(2)	2.157(2)	B(4)-B(9)	1.772(4)
N(1)-C(3)	1.303(3)	B(4)-B(8)	1.773(4)
N(1)-C(4)	1.490(3)	B(4)-B(5)	1.774(4)
N(2)-C(3)	1.347(3)	B(5)-B(9)	1.764(4)
N(2)-C(7)	1.471(3)	B(5)-B(10)	1.767(4)
C(1)-C(3)	1.510(3)	B(5)-B(6)	1.786(4)
C(1)-C(2)	1.664(3)	B(6)-B(11)	1.763(4)
C(1)-B(6)	1.702(3)	B(6)-B(10)	1.766(4)
C(1)-B(3)	1.704(3)	B(7)-B(11)	1.762(4)
C(1)-B(5)	1.713(3)	B(7)-B(12)	1.777(4)
C(1)-B(4)	1.713(3)	B(7)-B(8)	1.785(4)
C(2)-B(7)	1.708(4)	B(8)-B(9)	1.787(4)
C(2)-B(11)	1.714(3)	B(8)-B(12)	1.788(4)
C(2)-B(3)	1.717(3)	B(9)-B(12)	1.784(4)
C(2)-B(6)	1.744(3)	B(9)-B(10)	1.792(4)
C(4)-C(6)	1.523(3)	B(10)-B(12)	1.789(4)
C(4)-C(5)	1.527(3)	B(10)-B(11)	1.790(4)
C(7)-C(8)	1.521(3)	B(11)-B(12)	1.780(4)
C(7)-C(9)	1.524(3)		
N(1)#1-Cr-N(1)	161.45(10)	C(2)-C(1)-B(3)	61.29(14)
N(1)#1-Cr-C(2)#1	82.06(8)	B(6)-C(1)-B(3)	114.74(18)
N(1)-Cr-C(2)#1	105.72(8)	C(3)-C(1)-B(5)	123.20(19)
N(1)#1-Cr-C(2)	105.72(8)	C(2)-C(1)-B(5)	113.24(17)
N(1)-Cr-C(2)	82.06(8)	B(6)-C(1)-B(5)	63.08(14)
C(2)#1-Cr-C(2)	131.30(12)	B(3)-C(1)-B(5)	114.98(18)
C(3)-N(1)-C(4)	122.09(18)	C(3)-C(1)-B(4)	122.31(18)
C(3)-N(1)-Cr	118.09(15)	C(2)-C(1)-B(4)	112.87(18)
C(4)-N(1)-Cr	119.81(13)	B(6)-C(1)-B(4)	114.93(18)
C(3)-N(2)-C(7)	127.5(2)	B(3)-C(1)-B(4)	63.42(15)
C(3)-C(1)-C(2)	113.52(17)	B(5)-C(1)-B(4)	62.35(14)
C(3)-C(1)-B(6)	115.92(18)	C(1)-C(2)-B(7)	108.49(17)
C(2)-C(1)-B(6)	62.43(14)	C(1)-C(2)-B(11)	108.07(16)
C(3)-C(1)-B(3)	114.75(18)	B(7)-C(2)-B(11)	61.98(16)

C(1)-C(2)-B(3)	60.50(14)	B(8)-B(4)-B(3)	59.89(15)
B(7)-C(2)-B(3)	61.90(15)	B(5)-B(4)-B(3)	107.65(17)
B(11)-C(2)-B(3)	112.58(18)	C(1)-B(5)-B(9)	104.73(18)
C(1)-C(2)-B(6)	59.84(13)	C(1)-B(5)-B(10)	104.28(17)
B(7)-C(2)-B(6)	111.79(17)	B(9)-B(5)-B(10)	60.99(16)
B(11)-C(2)-B(6)	61.30(15)	C(1)-B(5)-B(4)	58.83(14)
B(3)-C(2)-B(6)	111.90(16)	B(9)-B(5)-B(4)	60.13(15)
C(1)-C(2)-Cr	105.14(14)	B(10)-B(5)-B(4)	108.89(19)
B(7)-C(2)-Cr	139.98(15)	C(1)-B(5)-B(6)	58.15(13)
B(11)-C(2)-Cr	125.67(15)	B(9)-B(5)-B(6)	108.29(19)
B(3)-C(2)-Cr	121.03(15)	B(10)-B(5)-B(6)	59.61(15)
B(6)-C(2)-Cr	103.52(14)	B(4)-B(5)-B(6)	107.93(17)
N(1)-C(3)-N(2)	128.8(2)	C(1)-B(6)-C(2)	57.73(13)
N(1)-C(3)-C(1)	116.74(19)	C(1)-B(6)-B(11)	104.19(18)
N(2)-C(3)-C(1)	114.38(19)	C(2)-B(6)-B(11)	58.49(14)
N(1)-C(4)-C(6)	108.41(18)	C(1)-B(6)-B(10)	104.78(18)
N(1)-C(4)-C(5)	109.64(19)	C(2)-B(6)-B(10)	106.42(19)
C(6)-C(4)-C(5)	109.53(19)	B(11)-B(6)-B(10)	60.96(16)
N(2)-C(7)-C(8)	111.2(2)	C(1)-B(6)-B(5)	58.77(14)
N(2)-C(7)-C(9)	106.7(2)	C(2)-B(6)-B(5)	106.02(17)
C(8)-C(7)-C(9)	111.3(2)	B(11)-B(6)-B(5)	108.04(19)
C(1)-B(3)-C(2)	58.20(13)	B(10)-B(6)-B(5)	59.64(15)
C(1)-B(3)-B(7)	104.29(18)	C(2)-B(7)-B(3)	59.32(14)
C(2)-B(3)-B(7)	58.79(15)	C(2)-B(7)-B(11)	59.18(15)
C(1)-B(3)-B(8)	104.20(18)	B(3)-B(7)-B(11)	108.21(19)
C(2)-B(3)-B(8)	106.39(19)	C(2)-B(7)-B(12)	106.61(19)
B(7)-B(3)-B(8)	60.48(16)	B(3)-B(7)-B(12)	108.55(19)
C(1)-B(3)-B(4)	58.53(14)	B(11)-B(7)-B(12)	60.42(16)
C(2)-B(3)-B(4)	106.42(18)	C(2)-B(7)-B(8)	106.69(19)
B(7)-B(3)-B(4)	107.68(19)	B(3)-B(7)-B(8)	60.33(16)
B(8)-B(3)-B(4)	59.40(15)	B(11)-B(7)-B(8)	108.68(19)
C(1)-B(4)-B(9)	104.37(17)	B(12)-B(7)-B(8)	60.28(16)
C(1)-B(4)-B(8)	104.21(17)	B(4)-B(8)-B(3)	60.71(16)
B(9)-B(4)-B(8)	60.54(16)	B(4)-B(8)-B(7)	107.69(19)
C(1)-B(4)-B(5)	58.82(14)	B(3)-B(8)-B(7)	59.19(15)
B(9)-B(4)-B(5)	59.66(15)	B(4)-B(8)-B(9)	59.71(15)
B(8)-B(4)-B(5)	108.13(19)	B(3)-B(8)-B(9)	108.03(19)
C(1)-B(4)-B(3)	58.04(14)	B(7)-B(8)-B(9)	107.48(19)
B(9)-B(4)-B(3)	108.03(19)	B(4)-B(8)-B(12)	107.52(19)

B(3)-B(8)-B(12)	107.13(19)	B(7)-B(12)-B(10)	107.76(19)
B(7)-B(8)-B(12)	59.64(15)	B(11)-B(12)-B(10)	60.21(16)
B(9)-B(8)-B(12)	59.85(16)	B(9)-B(12)-B(10)	60.20(15)
B(5)-B(9)-B(4)	60.21(15)	B(8)-B(12)-B(10)	108.2(2)
B(5)-B(9)-B(12)	107.63(18)		
B(4)-B(9)-B(12)	107.76(18)		
B(5)-B(9)-B(8)	107.94(18)		
B(4)-B(9)-B(8)	59.75(15)		
B(12)-B(9)-B(8)	60.11(16)		
B(5)-B(9)-B(10)	59.58(15)		
B(4)-B(9)-B(10)	107.83(18)		
B(12)-B(9)-B(10)	60.05(16)		
B(8)-B(9)-B(10)	108.12(18)		
B(6)-B(10)-B(5)	60.75(15)		
B(6)-B(10)-B(12)	107.38(18)		
B(5)-B(10)-B(12)	107.28(19)		
B(6)-B(10)-B(11)	59.44(15)		
B(5)-B(10)-B(11)	107.71(18)		
B(12)-B(10)-B(11)	59.66(15)		
B(6)-B(10)-B(9)	107.95(18)		
B(5)-B(10)-B(9)	59.43(15)		
B(12)-B(10)-B(9)	59.75(16)		
B(11)-B(10)-B(9)	107.35(19)		
C(2)-B(11)-B(7)	58.84(15)		
C(2)-B(11)-B(6)	60.21(14)		
B(7)-B(11)-B(6)	108.38(18)		
C(2)-B(11)-B(12)	106.18(18)		
B(7)-B(11)-B(12)	60.21(15)		
B(6)-B(11)-B(12)	107.89(18)		
C(2)-B(11)-B(10)	106.69(18)		
B(7)-B(11)-B(10)	108.36(18)		
B(6)-B(11)-B(10)	59.60(15)		
B(12)-B(11)-B(10)	60.13(15)		
B(7)-B(12)-B(11)	59.37(15)		
B(7)-B(12)-B(9)	107.98(19)		
B(11)-B(12)-B(9)	108.1(2)		
B(7)-B(12)-B(8)	60.08(15)		
B(11)-B(12)-B(8)	107.69(19)		
B(9)-B(12)-B(8)	60.04(16)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,y,-z+1/2

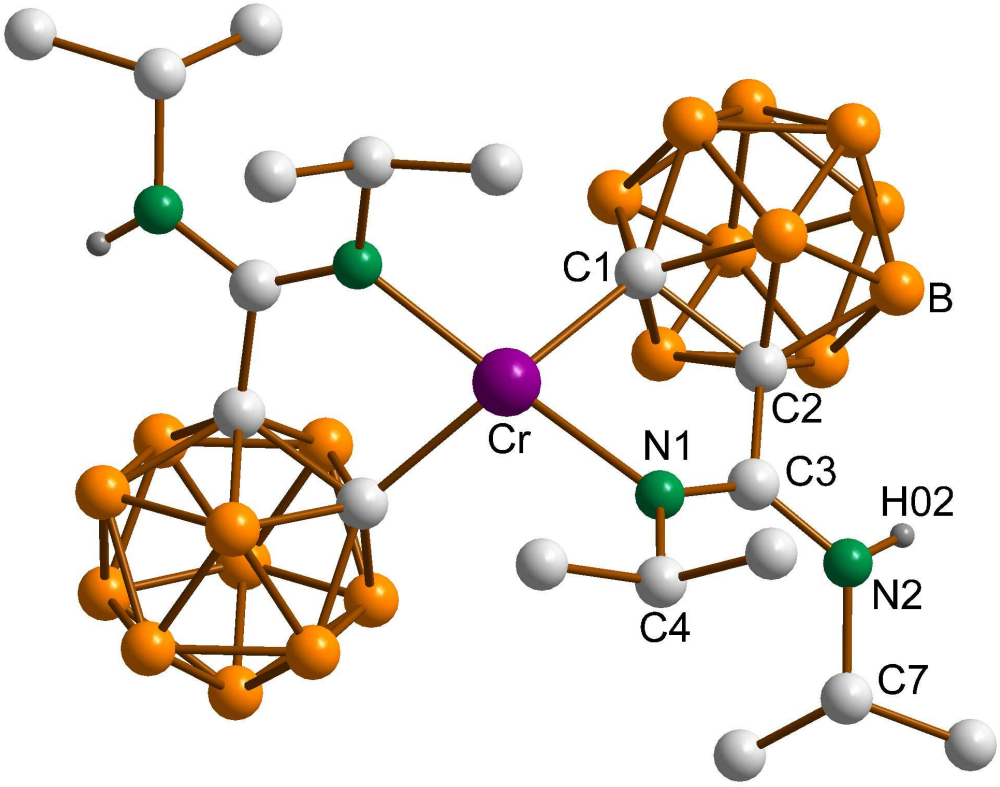

Figure 7. Molecular structure of **5**.

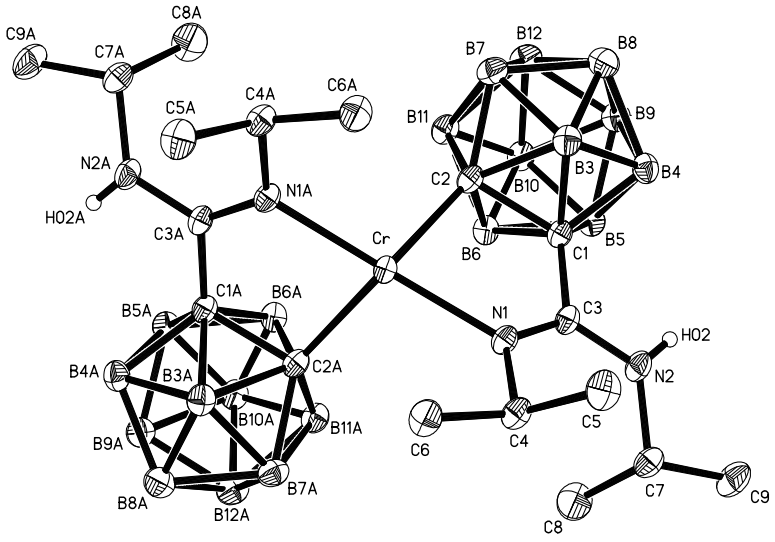

Figure 8. ORTEP drawing of the molecular structure of **5**.

Table 9. Crystallographic Data for **6**

Identification code	ip89	
Empirical formula	$C_{18}H_{50}B_{20}Cl_2Cr_2N_4$	
Formula weight	713.72	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.378(2) Å	α= 90°
	b = 11.887(2) Å	β= 103.29(3)°
	c = 15.418(3) Å	γ = 90°
Volume	1851.0(6) $Å^3$	
Z	2	
Density (calculated)	1.281 Mg/m^3	
Absorption coefficient	0.753 mm^{-1}	
F(000)	736	
Crystal size	0.41 x 0.34 x 0.23 mm^3	
Theta range for data collection	2.19 to 28.27°	
Index ranges	-13<=h<=13, -15<=k<=15, -20<=l<=20	
Reflections collected	19700	
Independent reflections	4584 [R(int) = 0.0651]	
Completeness to theta = 28.00°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4584 / 1 / 256	
Goodness-of-fit on F^2	1.208	
Final R indices [I>2sigma(I)]	R1 = 0.0414, wR2 = 0.0896	
R indices (all data)	R1 = 0.0490, wR2 = 0.0924	
Largest diff. peak and hole	0.456 and -0.406 $e.Å^{-3}$	

Table 10. Bond lengths [A] and angles [deg] for **6**

Cr-C(2)	2.0854(18)	C(7)-C(8)	1.517(3)
Cr-N(1)	2.1160(15)	B(3)-B(7)	1.758(3)
Cr-Cl#1	2.3789(7)	B(3)-B(8)	1.768(3)
Cr-Cl	2.4000(6)	B(3)-B(4)	1.786(3)
Cl-Cr#1	2.3789(7)	B(4)-B(9)	1.769(3)
N(1)-C(3)	1.304(2)	B(4)-B(8)	1.771(3)
N(1)-C(4)	1.487(2)	B(4)-B(5)	1.778(3)
N(2)-C(3)	1.349(2)	B(5)-B(10)	1.777(3)
N(2)-C(7)	1.481(2)	B(5)-B(9)	1.783(3)
C(1)-C(3)	1.512(2)	B(5)-B(6)	1.795(3)
C(1)-C(2)	1.644(2)	B(6)-B(11)	1.761(3)
C(1)-B(3)	1.696(3)	B(6)-B(10)	1.775(3)
C(1)-B(5)	1.706(3)	B(7)-B(11)	1.767(3)
C(1)-B(6)	1.709(3)	B(7)-B(12)	1.775(3)
C(1)-B(4)	1.712(3)	B(7)-B(8)	1.780(3)
C(2)-B(7)	1.712(3)	B(8)-B(12)	1.785(3)
C(2)-B(11)	1.715(3)	B(8)-B(9)	1.793(3)
C(2)-B(6)	1.718(3)	B(9)-B(12)	1.778(3)
C(2)-B(3)	1.730(3)	B(9)-B(10)	1.793(3)
C(4)-C(6)	1.518(2)	B(10)-B(11)	1.781(3)
C(4)-C(5)	1.521(3)	B(10)-B(12)	1.788(3)
C(7)-C(9)	1.512(3)	B(11)-B(12)	1.783(3)
C(2)-Cr-N(1)	81.92(6)	C(3)-C(1)-B(5)	123.56(14)
C(2)-Cr-Cl#1	91.47(5)	C(2)-C(1)-B(5)	113.24(13)
N(1)-Cr-Cl#1	169.34(4)	B(3)-C(1)-B(5)	115.43(14)
C(2)-Cr-Cl	166.11(5)	C(3)-C(1)-B(6)	115.97(14)
N(1)-Cr-Cl	103.86(5)	C(2)-C(1)-B(6)	61.63(11)
Cl#1-Cr-Cl	84.47(2)	B(3)-C(1)-B(6)	115.13(14)
Cr#1-Cl-Cr	95.53(2)	B(5)-C(1)-B(6)	63.41(12)
C(3)-N(1)-C(4)	118.88(15)	C(3)-C(1)-B(4)	122.32(14)
C(3)-N(1)-Cr	118.96(12)	C(2)-C(1)-B(4)	113.42(14)
C(4)-N(1)-Cr	122.05(11)	B(3)-C(1)-B(4)	63.19(12)
C(3)-N(2)-C(7)	132.39(16)	B(5)-C(1)-B(4)	62.70(12)
C(3)-C(1)-C(2)	112.81(14)	B(6)-C(1)-B(4)	115.36(14)
C(3)-C(1)-B(3)	113.83(14)	C(1)-C(2)-B(7)	108.37(13)
C(2)-C(1)-B(3)	62.36(11)	C(1)-C(2)-B(11)	108.94(14)

B(7)-C(2)-B(11)	62.08(12)	B(9)-B(4)-B(3)	108.13(15)
C(1)-C(2)-B(6)	61.02(11)	B(8)-B(4)-B(3)	59.61(12)
B(7)-C(2)-B(6)	112.61(14)	B(5)-B(4)-B(3)	107.62(14)
B(11)-C(2)-B(6)	61.70(12)	C(1)-B(5)-B(10)	103.93(14)
C(1)-C(2)-B(3)	60.29(11)	C(1)-B(5)-B(4)	58.81(11)
B(7)-C(2)-B(3)	61.41(12)	B(10)-B(5)-B(4)	108.02(15)
B(11)-C(2)-B(3)	112.42(14)	C(1)-B(5)-B(9)	104.11(14)
B(6)-C(2)-B(3)	112.87(13)	B(10)-B(5)-B(9)	60.47(12)
C(1)-C(2)-Cr	109.23(11)	B(4)-B(5)-B(9)	59.58(12)
B(7)-C(2)-Cr	127.39(12)	C(1)-B(5)-B(6)	58.35(11)
B(11)-C(2)-Cr	132.70(12)	B(10)-B(5)-B(6)	59.58(12)
B(6)-C(2)-Cr	117.34(12)	B(4)-B(5)-B(6)	108.00(14)
B(3)-C(2)-Cr	110.25(11)	B(9)-B(5)-B(6)	107.91(14)
N(1)-C(3)-N(2)	130.49(17)	C(1)-B(6)-C(2)	57.34(10)
N(1)-C(3)-C(1)	116.51(15)	C(1)-B(6)-B(11)	104.02(14)
N(2)-C(3)-C(1)	112.97(15)	C(2)-B(6)-B(11)	59.07(12)
N(1)-C(4)-C(6)	109.27(15)	C(1)-B(6)-B(10)	103.95(14)
N(1)-C(4)-C(5)	110.50(15)	C(2)-B(6)-B(10)	106.13(14)
C(6)-C(4)-C(5)	112.41(16)	B(11)-B(6)-B(10)	60.49(12)
N(2)-C(7)-C(9)	109.62(17)	C(1)-B(6)-B(5)	58.24(11)
N(2)-C(7)-C(8)	108.37(17)	C(2)-B(6)-B(5)	105.57(14)
C(9)-C(7)-C(8)	111.89(18)	B(11)-B(6)-B(5)	107.94(14)
C(1)-B(3)-C(2)	57.35(10)	B(10)-B(6)-B(5)	59.72(12)
C(1)-B(3)-B(7)	104.02(14)	C(2)-B(7)-B(3)	59.79(11)
C(2)-B(3)-B(7)	58.80(11)	C(2)-B(7)-B(11)	59.04(11)
C(1)-B(3)-B(8)	104.77(14)	B(3)-B(7)-B(11)	108.64(15)
C(2)-B(3)-B(8)	106.40(14)	C(2)-B(7)-B(12)	106.23(15)
B(7)-B(3)-B(8)	60.63(12)	B(3)-B(7)-B(12)	108.25(15)
C(1)-B(3)-B(4)	58.84(11)	B(11)-B(7)-B(12)	60.44(13)
C(2)-B(3)-B(4)	105.88(14)	C(2)-B(7)-B(8)	106.65(15)
B(7)-B(3)-B(4)	107.91(15)	B(3)-B(7)-B(8)	59.97(12)
B(8)-B(3)-B(4)	59.79(12)	B(11)-B(7)-B(8)	108.93(15)
C(1)-B(4)-B(9)	104.45(14)	B(12)-B(7)-B(8)	60.28(13)
C(1)-B(4)-B(8)	103.96(14)	B(3)-B(8)-B(4)	60.60(12)
B(9)-B(4)-B(8)	60.84(13)	B(3)-B(8)-B(7)	59.40(12)
C(1)-B(4)-B(5)	58.50(11)	B(4)-B(8)-B(7)	107.58(14)
B(9)-B(4)-B(5)	60.34(12)	B(3)-B(8)-B(12)	107.36(15)
B(8)-B(4)-B(5)	108.82(15)	B(4)-B(8)-B(12)	107.22(15)
C(1)-B(4)-B(3)	57.97(11)	B(7)-B(8)-B(12)	59.73(12)

B(3)-B(8)-B(9)	107.87(15)	B(11)-B(12)-B(8)	108.02(15)
B(4)-B(8)-B(9)	59.53(12)	B(7)-B(12)-B(10)	107.51(15)
B(7)-B(8)-B(9)	107.27(15)	B(9)-B(12)-B(10)	60.35(12)
B(12)-B(8)-B(9)	59.61(12)	B(11)-B(12)-B(10)	59.82(12)
B(4)-B(9)-B(12)	107.59(15)	B(8)-B(12)-B(10)	108.51(15)
B(4)-B(9)-B(5)	60.08(12)		
B(12)-B(9)-B(5)	107.60(15)		
B(4)-B(9)-B(8)	59.63(12)		
B(12)-B(9)-B(8)	59.96(13)		
B(5)-B(9)-B(8)	107.66(14)		
B(4)-B(9)-B(10)	107.73(15)		
B(12)-B(9)-B(10)	60.10(12)		
B(5)-B(9)-B(10)	59.60(12)		
B(8)-B(9)-B(10)	107.95(15)		
B(6)-B(10)-B(5)	60.70(12)		
B(6)-B(10)-B(11)	59.37(12)		
B(5)-B(10)-B(11)	107.84(14)		
B(6)-B(10)-B(12)	107.46(15)		
B(5)-B(10)-B(12)	107.41(15)		
B(11)-B(10)-B(12)	59.94(12)		
B(6)-B(10)-B(9)	108.36(14)		
B(5)-B(10)-B(9)	59.92(12)		
B(11)-B(10)-B(9)	107.70(15)		
B(12)-B(10)-B(9)	59.55(12)		
C(2)-B(11)-B(6)	59.24(11)		
C(2)-B(11)-B(7)	58.88(12)		
B(6)-B(11)-B(7)	108.00(14)		
C(2)-B(11)-B(10)	105.99(14)		
B(6)-B(11)-B(10)	60.14(12)		
B(7)-B(11)-B(10)	108.15(15)		
C(2)-B(11)-B(12)	105.74(14)		
B(6)-B(11)-B(12)	108.30(15)		
B(7)-B(11)-B(12)	59.98(12)		
B(10)-B(11)-B(12)	60.24(12)		
B(7)-B(12)-B(9)	108.13(15)		
B(7)-B(12)-B(11)	59.58(12)		
B(9)-B(12)-B(11)	108.25(15)		
B(7)-B(12)-B(8)	60.00(12)		
B(9)-B(12)-B(8)	60.42(12)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z

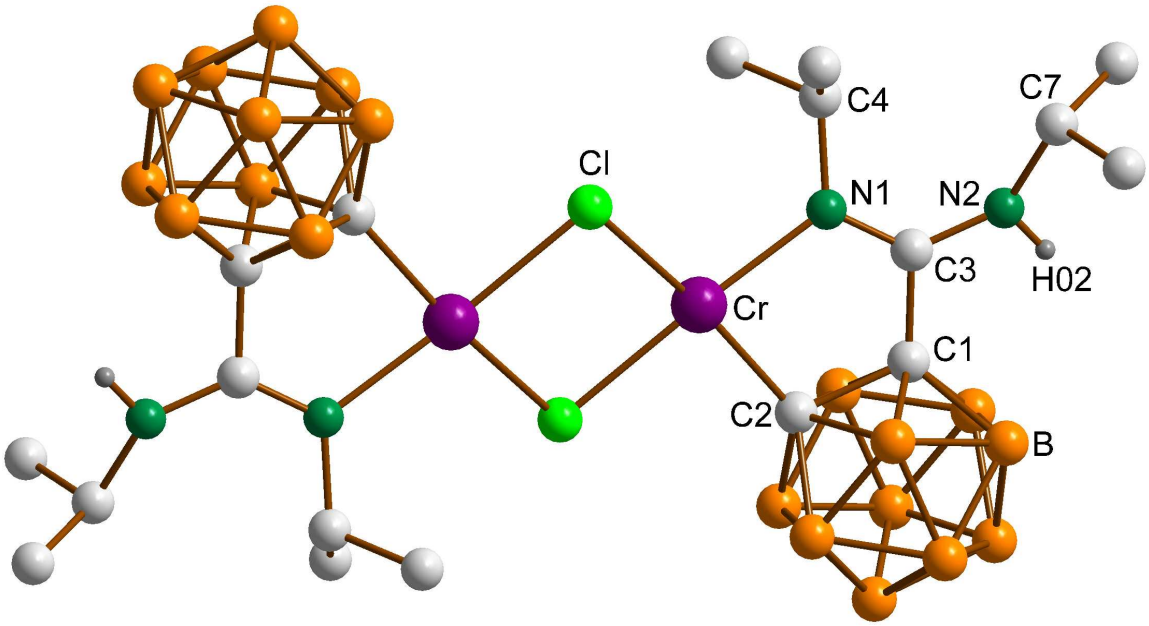

Figure 9. Molecular structure of **6**.

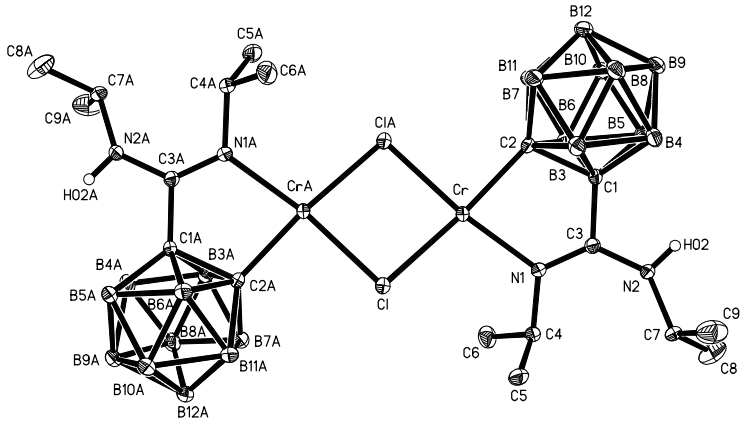

Figure 10. ORTEP drawing of the molecular structure of **6**.