Supporting Information

Isolation of a Planar 1,2-Dilithio-disilene and Its Conversion to Si–B Hybrid 2π-Electron System and a Planar Tetraboryldisilene

Miao Tian, Jianying Zhang, Lulu Guo, and Chunming Cui*

State Key Laboratory of Elemento-Organic Chemistry and College of Chemistry, Nankai University, Tianjin 300071, People's Republic of China

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Experiment Section

General Information. All operations were carried out under atmosphere of Argon using standard Schlenk line and glovebox techniques. All solvents were purified with M-Braun Solvent Purification System. ^{1}H, ^{13}C, ^{11}B, ^{29}Si NMR and ^{7}Li NMR spectra were recorded on a Bruker 400 MHz spectrometers at ambient temperature, usually in C_6D_6 with Me_4Si (^{1}H, ^{13}C, ^{7}Li and ^{29}Si) and $BF_3{\cdot}Et_2O$ (^{11}B) as internal standards, and the chemical shift (δ) are reported in parts per million (ppm). Elemental analysis was carried out on an Elemental Vario EL analyzer. All commercially available chemicals were employed as received if not stated otherwise. The starting materials, (boryl)$SiBr_3$ (**1**, boryl = $(HCNAr)_2B$, Ar = 2,6-*i*$Pr_2C_6H_3$), 1,1-dichloro-N,N-diphenylboranamine (Ph_2NBCl_2), dibromo(mesityl)borane ($MesBBr_2$) and dibromo(2,4,6-triisopropylphenyl)borane ($TipBBr_2$) were synthesized following the literature procedures.[S1,S2,S3,S4]

Preparation of 2. To lithium powder (28 mg, 4.00 mmol) in a flask was added a solution of (boryl)tribromosilane **1** (655 mg, 1.00 mmol) in dry Et_2O (60 mL). The mixture was stirred at –40 °C for 48 h. The mixture was allowed to settle at –40 °C, and then it was filtered. The red residuals were extracted with dry benzene. It was filtered and the filtrate was evaporated to dryness to give 1,2-dilithio-disilene **2** as red powder (310 mg, 73%). ^{1}H NMR (400 MHz, C_6D_6): δ 6.91-6.89 (m, 8H, Ar-H), 6.80-6.76 (m, 4H, Ar-H), 6.42 (s, 4H, N-CH), 3.57 (sept, *J* = 8.0 Hz, 8H, *i*Pr-CH), 1.29 (d, *J* = 8.0 Hz, 24H, *i*Pr-CH_3), 1.21 (d, *J* = 8.0 Hz, 24H, *i*Pr-CH_3); ^{13}C NMR (101 MHz, C_6D_6): δ 149.9 (4°), 145.8 (N-Ar), 125.1 (CH), 122.8 (CH), 119.7 (N-CH), 28.7 (*i*Pr-CH), 24.8 (*i*Pr-CH_3), 24.5 (*i*Pr-CH_3); ^{29}Si NMR (79.49 MHz, C_6D_6): δ 296.7 (s); ^{11}B NMR (128 MHz, C_6D_6): δ 35.1 (brs). ^{7}Li NMR (156 MHz, C_6D_6): δ –4.2. Elemental analysis calcd (%) for $C_{52}H_{72}B_2Li_2N_4Si_2$: C, 73.93; H, 8.59; N, 6.63. Found: C, 73.87; H, 8.43; N, 6.51.

Preparation of 3a. To a mixture of 1,2-dilithio-disilene **2** (120 mg, 0.14 mmol) and Ph_2NBCl_2 (36 mg, 0.14 mmol) in a Schlenk tube was added dry benzene (10 mL). The mixture was stirred at room temperature for 6 h. After removal of all volatiles in vacuo, *n*-pentane (20 mL) was added to the residuals. It was filtered off. Concentration of the solution to ~5 mL and then storage at 0 °C overnight yielded disilaborirene **3a** as yellow crystals (76 mg, 53%). Mp: 185-186 °C (dec). ^{1}H NMR (400 MHz, C_6D_6): δ 7.17-7.16 (m, 4H, Ar-H), 7.08-7.06 (m, 8H, Ar-H), 6.97-6.94 (m, 10H, Ar-H), 6.17 (s, 4H, N-CH), 3.13 (sept, *J* = 8.0 Hz, 8H, *i*Pr-*CH)*, 1.15 (d, *J* = 8.0 Hz, 24H, *i*Pr-CH_3), 1.03 (d, *J* = 8.0 Hz, 24H, *i*Pr-CH_3); ^{13}C NMR (101 MHz, C_6D_6): δ 151.5 (4°), 145.6 (N-Ar), 139.1 (Ph), 129.0 (Ph), 127.9 (Ph), 124.5 (CH), 123.9 (Ph), 122.9 (CH), 122.7 (N-CH), 28.6 (*i*Pr-CH), 25.1 (*i*Pr-CH_3), 24.3 (*i*Pr-CH_3); ^{29}Si NMR (79.49 MHz, C_6D_6): δ 112.2 (s); ^{11}B NMR (128 MHz, C_6D_6): δ 50.1 (brs), 24.2

(brs). Elemental analysis calcd (%) for $C_{64}H_{82}B_3N_5Si_2$: C, 76.11; H, 8.18; N, 6.93. Found: C, 76.49; H, 8.52; N, 6.62.

Preparation of 3b. A mixture of **2** (87 mg, 0.10 mmol) and $MesBBr_2$ (30 mg, 0.10 mmol) in dry benzene (10 mL) was stirred at room temperature for 6 h. The volatiles were removed under vacuum and *n*-pentane (16 mL) was added. It was filtered off. Evaporation of the solvents gave disilaborirene **3b** as orange yellow solid (83 mg, 86%). Mp: 192-194 °C (dec). ^{1}H NMR (400 MHz, C_6D_6): δ 7.23-7.19 (m, 4H, Ar-H), 7.07-7.05 (m, 8H, Ar-H), 6.75 (s, 2H, Mes-H), 6.17 (s, 4H, N-CH), 3.03 (sept, *J* = 8.0 Hz, 8H, *i*Pr-CH), 2.29 (s, 3H, Mes-CH_3), 1.58 (s, 6H, Mes-CH_3), 1.14 (d, *J* = 8.0 Hz, 24H, *i*Pr-CH_3), 1.07 (d, *J* = 8.0 Hz, 24H, *i*Pr-CH_3); ^{13}C NMR (101 MHz, C_6D_6): δ 145.8 (4°, N-Ar), 138.9 (Mes-C), 136.1 (Mes-C), 133.9 (Mes-C), 126.2 (CH), 123.7 (CH, Mes-C), 122.0 (N-CH), 28.8 (*i*Pr-CH), 24.6 (*i*Pr-CH_3), 24.5 (*i*Pr-CH_3), 23.6 (Mes-CH_3), 21.6 (Mes-CH_3); ^{29}Si NMR (79.49 MHz, C_6D_6): δ 142.0 (s); ^{11}B NMR (128 MHz, C_6D_6): δ 72.9 (brs), 23.5 (brs). Elemental analysis calcd (%) for $C_{61}H_{83}B_3N_4Si_2$: C, 76.24; H, 8.71; N, 5.83. Found: C, 76.51; H, 8.93; N, 5.62.

Preparation of 3c. A mixture of 1,2-dilithio-disilene **2** (87 mg, 0.10 mmol) and $TipBBr_2$ (38 mg, 0.10 mmol) in 10 mL of dry benzene was stirred at room temperature for 6 h. After removal of all volatiles under vacuum, the residual was extracted with *n*-pentane (16 mL). It was filtered off. Concentration of the filtrate to ~5 mL and storage at 0 °C for 12 h yielded disilaborirene **3c** as orange yellow solid (72 mg, 68%). Mp: 208-210 °C (dec). ^{1}H NMR (400 MHz, C_6D_6): δ 7.18-7.14 (m, 4H, Ar-H), 7.05-7.03 (m, 8H, Ar-H), 6.97 (brs, 2H, Tip-H), 6.13 (s, 4H, N-CH), 3.04 (sept, *J* = 8.0 Hz, 8H, *i*Pr-CH), 2.88 (sept, *J* = 8.0 Hz, 1H, Tip-*i*Pr-CH), 2.66 (sept, *J* = 8.0 Hz, 2H, Tip-*i*Pr-CH), 1.33 (d, *J* = 8.0 Hz, 6H, Tip-*i*Pr-CH_3), 1.15 (d, *J* = 8.0 Hz, 24H, *i*Pr-CH_3), 1.06 (d, *J* = 8.0 Hz, 24H, *i*Pr-CH_3), 0.95 (d, *J* = 8.0 Hz, 12H, Tip-*i*Pr-CH_3); ^{13}C NMR (101 MHz, C_6D_6): δ 147.4 (4°), 146.2 (Tip-C), 145.6 (N-Ar, Tip-C), 139.0 (Tip-C), 123.8 (CH, Tip-C), 122.4 (CH), 118.6 (N-CH), 35.0 (Tip-*i*Pr-CH), 34.5 (Tip-*i*Pr-CH), 28.8 (*i*Pr-CH), 24.7 (Tip-*i*Pr-CH_3), 24.69 (*i*Pr-CH_3), 24.6 (*i*Pr-CH_3), 23.9 (Tip-*i*Pr-CH_3); ^{29}Si NMR (79.49 MHz, C_6D_6): δ 141.1 (s); ^{11}B NMR (128 MHz, C_6D_6): δ 73.3 (brs), 23.4 (brs). Elemental analysis calcd (%) for $C_{67}H_{95}B_3N_4Si_2$: C, 77.00; H, 9.16; N, 5.36. Found: C, 76.71; H, 9.53; N, 5.17.

Preparation of 4. A mixture of 1,2-dilithio-disilene **2** (87 mg, 0.10 mmol) and (cat)BBr (40 mg, 0.20 mmol) in 6 mL of dry benzene was stirred at room temperature for 2 h. After removal of all volatiles under vacuum, the residuals were extracted with 16 mL of *n*-hexane. It was filtered off. Concentration of the filtrate to ~5 mL and storage at –20 °C for 12 h yielded tetraboryldisilene **4** as yellow solid (92 mg, 86%). Mp: 256-257 °C (dec). ^{1}H NMR (400 MHz, C_6D_6, 298 K): δ 7.12-7.05 (m, 8H, Ar-H), 7.01-6.99 (m, 8H, Ar-H), 6.84-6.80 (m, 4H, Ar-H), 6.44 (s, 4H, N-CH), 3.51 (sept, *J* = 8.0 Hz, 8H, *i*Pr-CH), 1.18 (d, *J* = 8.0 Hz, 24H, *i*Pr-CH_3), 0.92 (d, *J* = 8.0 Hz, 24H, *i*Pr-CH_3); ^{13}C NMR (101 MHz, C_6D_6, 298 K): δ 148.8 (O-

C), 146.4 (4°), 139.9 (N-Ar), 127.7 (Ar-C), 123.5 (Ar-C), 123.1 (Ar-C), 122.9 (Ar-C), 112.5 (N-CH), 28.4 (*i*Pr-CH), 26.4 (*i*Pr-CH_3), 23.1 (*i*Pr-CH_3); ^{29}Si NMR (79.49 MHz, C_6D_6, 298 K): δ 105.6 (s); ^{11}B NMR (128 MHz, C_6D_6, 298 K): δ 37.3 (brs), 26.2 (brs). Elemental analysis calcd (%) for $C_{64}H_{80}B_4N_4O_4Si_2$: C, 71.92; H, 7.55; N, 5.24. Found: C, 72.16; H, 7.92; N, 5.06.

X-ray Crystallographic Analysis. All intensity data of **2**, **3a**, **3b**, **3c** and **4** were collected with a Rigaku Saturn 724 CCD diffractometer using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) at 113 K. The structures were resolved by direct methods and refined by full-matrix least-squares on F^2.[S5,S6] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were considered in calculated positions. Crystallographic data for **2**, **3a**, **3b**, **3c** and **4** and their CCDC numbers were listed in Table S1.

Computational Details. All calculations on compound **2**, **3a**, **3c** and **4** were performed with the Gaussian 09 suite of programs, revision E.01.[S7] The structures of **2**, **3a**, **3c** and **4** were optimized with Density Functional Theory (DFT) with B3LYP functional and the 6-31G(d,p) basis set. The optimized structures of **2**, **3a**, **3c** and **4** are given in Figures S4, S9, S10 and S14, respectively. The UV-vis spectra of **2** and **4** was calculated using TD-PBE1PBE method at 6-311G (d) basis set. The IEFPCM solvation model with toluene was used for these calculations. The ^{29}Si NMR chemical shifts for **2** and Nucleus independent chemical shifts (NICS) for **3a** and **3c** were calculated by the GIAO methods at B3LYP/6-311+G(2d,p) level and were referenced to TMS and BF_3•Et_2O. NICS(1)zz values were averaged by two positions (above and below the plane) of all the equivalent rings.[S8] The Wiberg bond indices (WBI) of **2**, **3a** and **3c** were obtained with NBO 6.0 program at B3LYP/6-31G(d) level and the selected results are given in Table S2-4.[S9]

Table S1. Crystallographic Data and CCDC Numbers for Compounds 2, 3a-c and 4.

	2	**3a**	**3b**	**3c**	**4**
formula	$C_{52}H_{72}B_2Li_2N_4Si_2$	$C_{64}H_{82}B_3N_5Si_2$	$C_{122}H_{166}B_6N_8Si_4$	$C_{67}H_{95}B_3N_4Si_2$	$C_{64}H_{80}B_4N_4O_4Si_2 \cdot C_6H_{14}$
CCDC	2088661	2081430	2088665	2081431	2104803
fw	844.81	1009.95	1921.84	1045.07	1154.91
T (K)	113.15	113.15	113.15	113.15	113.15
space	P-1	P-1	$P2_12_12_1$	$P2_1/n$	$P2_1/n$

group					
a (Å)	10.6321(5)	13.3902(5)	17.3657(5)	14.0914(5)	14.9942(10)
b (Å)	12.6541(8)	13.4787(5)	17.4514(5)	24.4943(7)	11.7473(8)
c (Å)	19.8364(10)	18.5010(5)	39.6637(11)	20.4237(7)	19.3646(11)
α (deg.)	88.291(4)	90.572(3)	90	90	90
β (deg.)	89.058(4)	92.148(3)	90	90.338(3)	93.326(5)
γ (deg.)	82.021(4)	114.215(4)	90	90	90
V (Å^3)	2641.6(2)	3042.0(2)	12020.3(6)	7049.3(4)	3405.2(4)
Z, D (g/cm^3)	2, 1.062	2, 1.103	4, 1.062	4, 0.985	2, 1.126
F(000)	912.0	1088.0	4160.0	2272.0	1244.0
GOF	1.102	1.107	1.039	1.041	1.011
R_1	0.1167	0.0773	0.0668	0.0672	0.0824
wR_2 (all data)	0.3053	0.2253	0.1348	0.1780	0.1858

Table S2. Selected WBI values of 2 (NBO6.0, B3lyp/6-31G(d))

Atom	127	128	129	130	131	132	133	134
Si1	0.0000	0.0000	0.0000	**1.7732**	1.0500	0.0401	0.2640	0.0199
Si1'	0.0000	0.0000	**1.7732**	0.0000	0.0401	1.0500	0.0199	0.2640
Li1	0.0000	0.0000	**0.2640**	0.0199	0.0028	0.0006	0.0000	0.0058
Li1'	0.0000	0.0000	0.0199	**0.2640**	0.0006	0.0028	0.0058	0.0000

Table S3. Selected WBI values of 3a (NBO6.0, B3lyp/6-31G(d))

Atom	1	2	3	4	5	6	7	8	9
Si1	0.0000	**1.5131**	0.0120	0.0102	0.0410	0.0060	0.0061	0.0026	0.0007
Si2	**1.5131**	0.0000	0.0061	0.0060	0.0419	0.0101	0.0117	0.0102	0.0022
B1	**1.2461**	**1.2456**	0.0066	0.0087	0.8972	0.0087	0.0066	0.0153	0.0003

Table S4. Selected WBI values of 3c (NBO6.0, B3lyp/6-31G(d))

Atom	1	2	3	4	5	6	7	8	9
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Si1	0.0000	**1.4562**	0.0077	0.0104	0.0075	0.0133	0.0024	0.0004	0.0003
Si2	**1.4562**	0.0000	0.0104	0.0076	0.0133	0.0076	0.0008	0.0004	0.0003
B1	**1.2828**	**1.2845**	0.0103	0.0103	0.0075	0.0075	0.0003	0.0099	0.0003

Table S5. Selected data of Natural Bond Orbital Analysis for compound 3a

```
(1.95601) 3C (1) Si1–Si2–B82
              (38.08%)   0.6171*Si1   s(0.00%) p 1.00(99.55%) d 0.00(0.45%)
                                        0.0000   0.0000   0.0017 -0.0009 -0.0001
                                        0.0000   0.1537   0.0032   0.0000   0.0626
                                        0.0015   0.0000   0.9836 -0.0219   0.0049
                                        0.0611   0.0187   0.0088 -0.0178
              (38.14%)   0.6176*Si2   s(0.00%) p 1.00(99.55%) d 0.00(0.45%)
                                        0.0000   0.0000   0.0013   0.0025   0.0000
                                        0.0000   0.1437   0.0011   0.0000   0.0635
                                       -0.0040   0.0000   0.9851 -0.0212 -0.0034
                                       -0.0616   0.0198 -0.0109   0.0134
               ( 23.78%)   0.4876* B82   s(0.00%) p 1.00(99.82%) d 0.00(0.18%)
                                        0.0000   0.0004   0.0007   0.0001   0.0841
                                       -0.0130   0.0539   0.0003   0.9940 -0.0011
                                       -0.0030   0.0005 -0.0418   0.0024   0.0043
```

Table S6. Selected data of Natural Bond Orbital Analysis for compound 3c

```
(Occupancy)    Bond orbital / Coefficients / Hybrids
-------------------------------------------------------------------------------------------
(1.94971) 3C (1) Si1–Si2–B95
               (36.81%)    0.6067*Si1   s(0.00%) p1.00 (99.52%) d0.00(0.47%)
```

```
                              0.0000    0.0000    0.0064 -0.0029    0.0001
                              0.0000    0.0764    0.0033    0.0000    0.1837
                             -0.0009    0.0000 -0.9774    0.0182 -0.0108
                               0.0333    0.0544    0.0087    0.0214
(36.79%)      0.6066*Si2       s(0.00%) p1.00 (99.52%) d0.00(0.47%)
                               0.0000    0.0000 -0.0055    0.0027 -0.0001
                               0.0000    0.0739 -0.0047    0.0000    0.1853
                               0.0017    0.0000 -0.9773    0.0187    0.0046
                               0.0064 -0.0642 -0.0134 -0.0191
(26.40%)      0.5138* B95     s(0.00%) p1.00 (99.86%) d 0.00 (0.14%)
                              0.0000    0.0004 -0.0003    0.0000    0.0714
                             -0.0011    0.1689 -0.0011 -0.9819    0.0307
                              0.0054 -0.0352    0.0086    0.0041 -0.0019
```

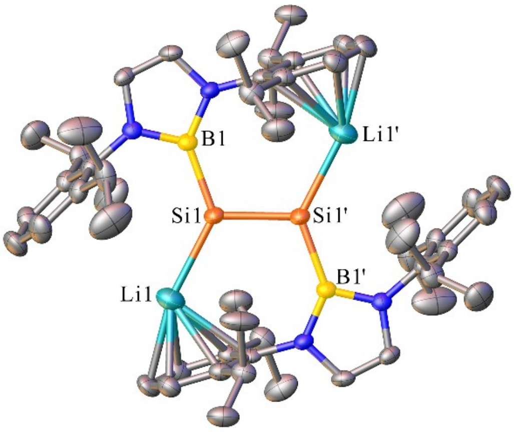


Figure S1. OLEX2 drawing of **2** with 50% ellipsoid probability. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Si1–Si1′ 2.223(3), Si1–B1 2.022(6), Si1–Li1 2.474(10); Si1'–Si1–Li1 117.3(3), B1–Si1–Si1' 109.6(2), B1–Si1–Li1 132.6(3).

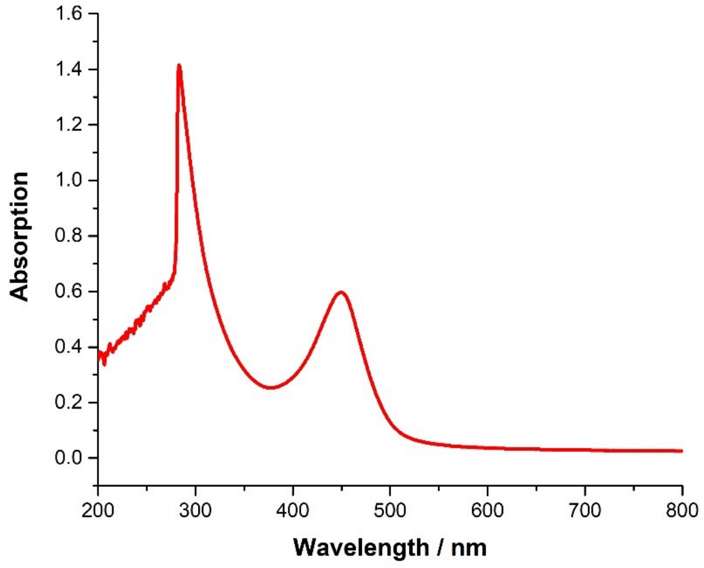
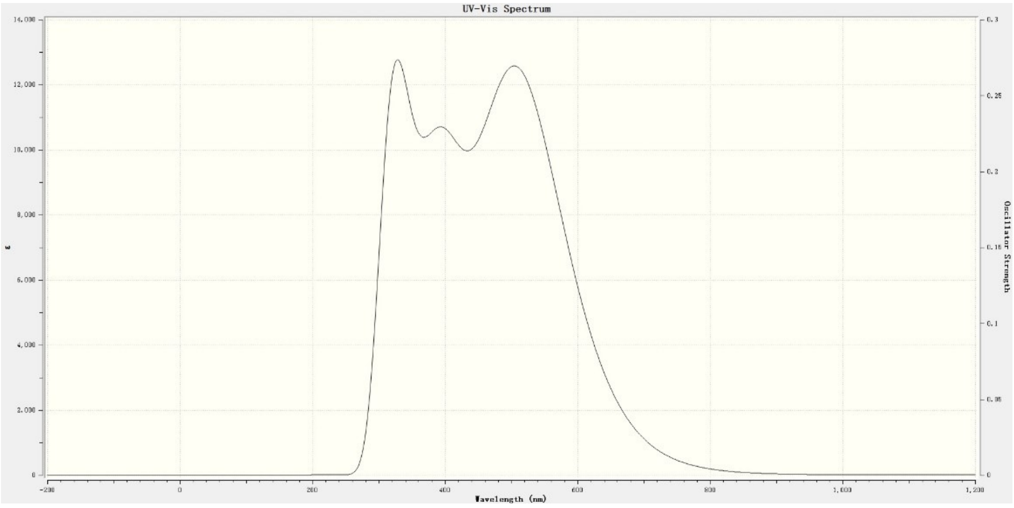


Figure S2. UV-vis spectrum of **2** in toluene (1x10^{-4} mol/L) at room temperature.



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                                   <S**2>=0.000
                              227 -> 233                0.69434
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Figure S3. Calculated UV-vis spectrum of **2** at TD-PBE1PBE/6-311G (d) and the IEFPCM solvation model with toluene was used for calculation.

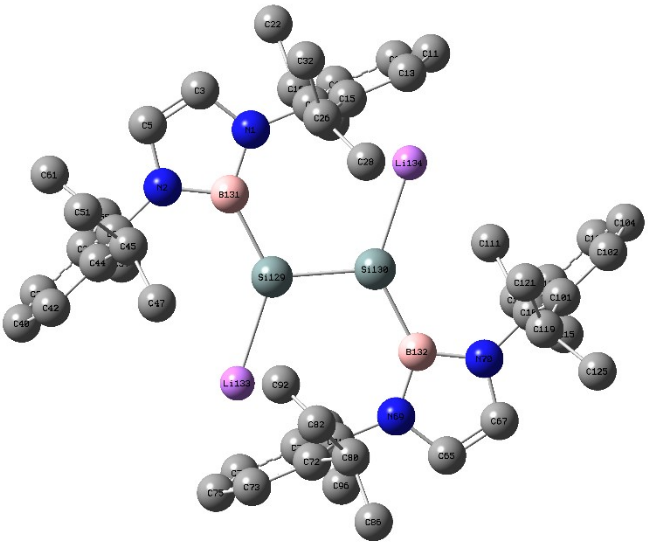


Figure S4. Optimized geometry of **2**. Selected computed bond lengths (Å) and angles (deg): Si129−Si130 2.24575, Si130−Li134 2.42208, B131−Si129 2.03014; B131−Si129−Li133 135.06510, Li133−Si129−Si130 111.60643, B131−Si129−Si130 113.32846.

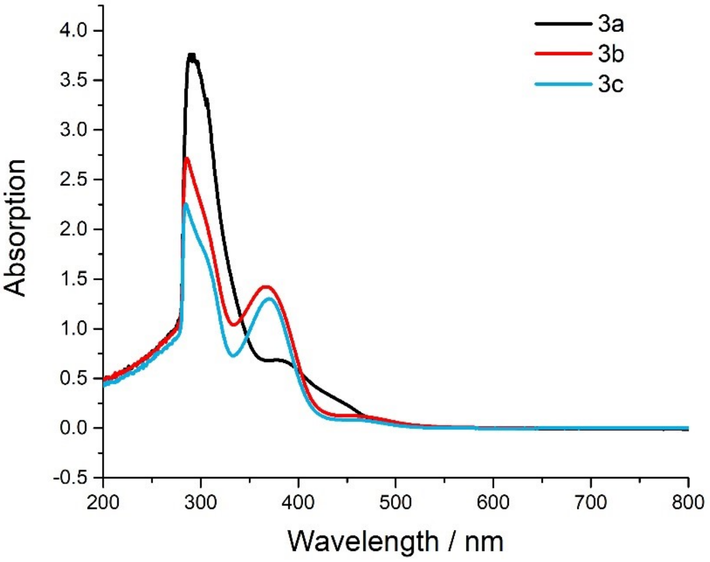


Figure S5. UV-vis spectrum of **3a-c** in toluene (1x10^{-4} mol/L) at room temperature.

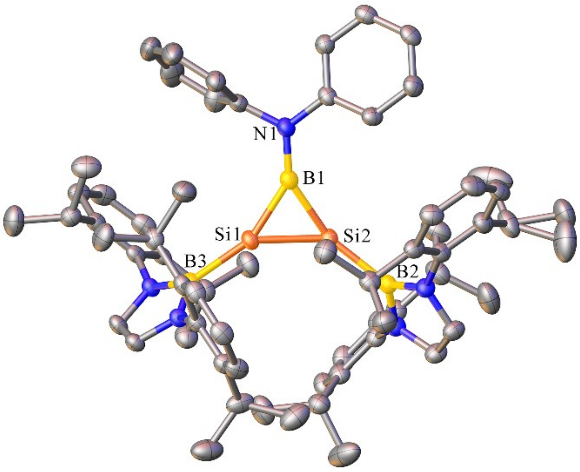


Figure S6. OLEX2 drawing of **3a** with 50% ellipsoid probability. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Si1–Si2 2.1469(11), Si1–B1 1.926(3), Si1–B3 1.985(3), Si2–B3 1.952(3), Si2–B2 1.998(3); B1–Si1–B3 156.07(14), B1–Si1–Si2 56.96(10), B3–Si1–Si2 146.72(10), B1–Si2–B2 158.01(14), B1–Si2–Si1 55.82(10), B2–Si2–Si1 139.45(10).

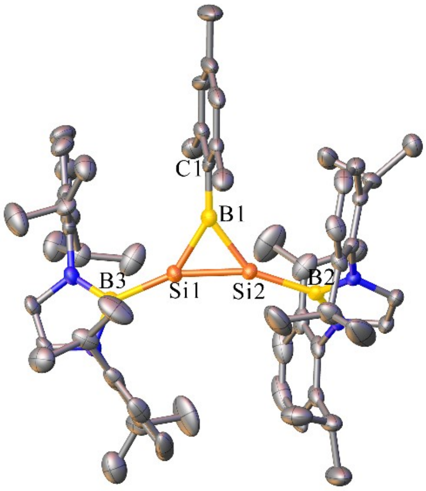


Figure S7. OLEX2 drawing of **3b** with 50% ellipsoid probability. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Si1–Si2 2.133(2), Si1–B1 1.911(7), Si1–B3 1.985(7), Si2–B1 1.925(7), Si2–B2 1.986(7); B1–Si1–B3 145.6(3), B1–Si1–Si2 56.5(2), B3–Si1–Si2 157.8(2), B1–Si2–B2 144.9(3), B1–Si2–Si1 55.9(2), B2–Si2–Si1 158.6(2).

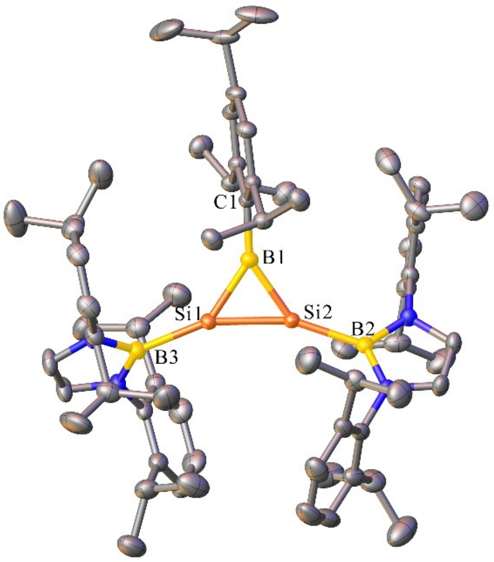


Figure S8. OLEX2 drawing of **3c** with 50% ellipsoid probability. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Si1–Si2 2.1452(6), Si1–B1 1.9248(17), Si1–B3 1.9949(18), Si2–B1 1.9266(18), Si2–B2 1.9918(18); B1–Si1–B3 145.82(8), B1–Si1–Si2 56.19(5), B3–Si1–Si2 157.92(6), B1–Si2–B2 142.32(7), B1–Si2–Si1 56.11(5), B2–Si2–Si1 160.63(6).

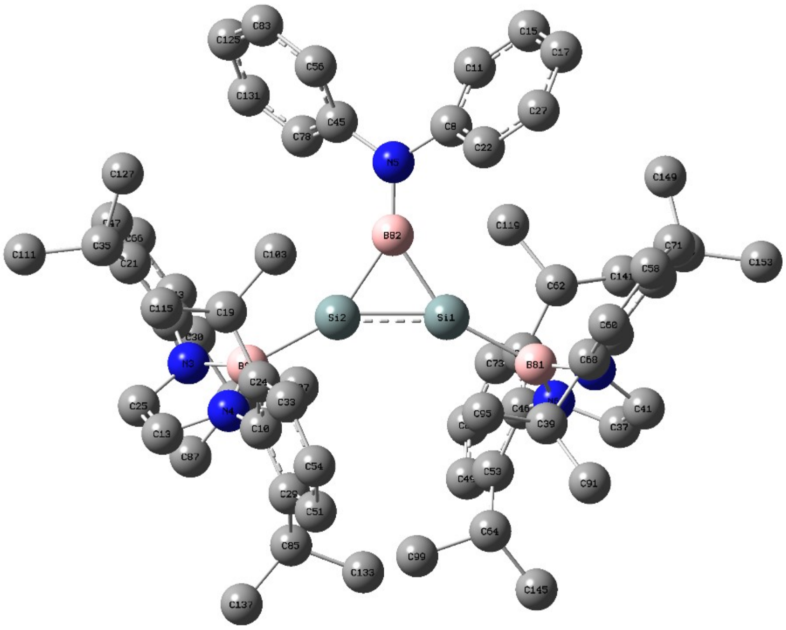


Figure S9. Optimized geometry of **3a**. Selected computed bond lengths (Å) and angles (deg): Si1−Si2 2.17371, Si2−B82 1.95424, Si1−B82 1.95292, B81−Si1 2.02479, B83−Si2 2.02443; B82−Si2−Si1 56.16789, B82−Si1−Si2 56.22609, Si1− B82−Si2 67.60602, B83−Si2−Si1 151.96661, B81−Si1−Si2 152.40336.

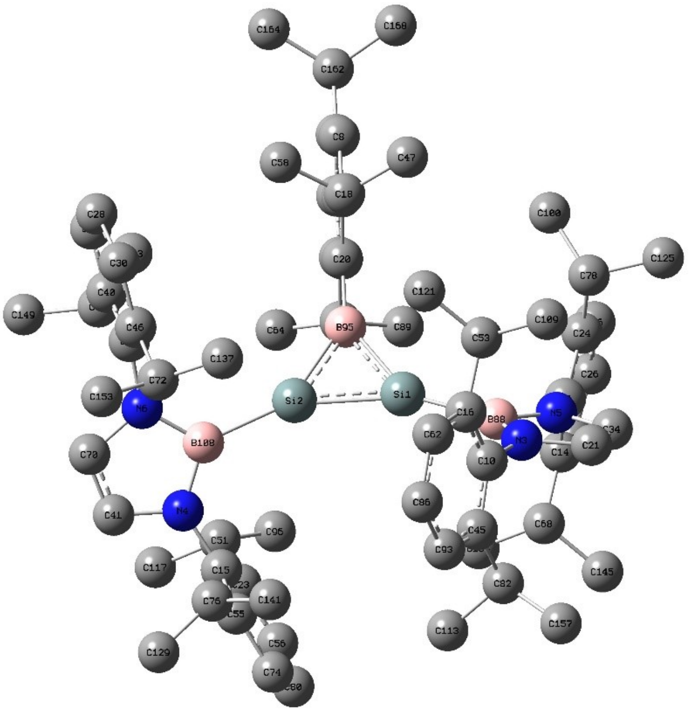


Figure S10. Optimized geometry of **3c**. Selected computed bond lengths (Å) and angles (deg): Si1−Si2 2.16784, Si1−B95 1.94802, Si2−B95 1.94802; B95−Si2−Si1 56.19135, B95−Si1−Si2 56.19127, Si1−B82−Si2 67.61737.

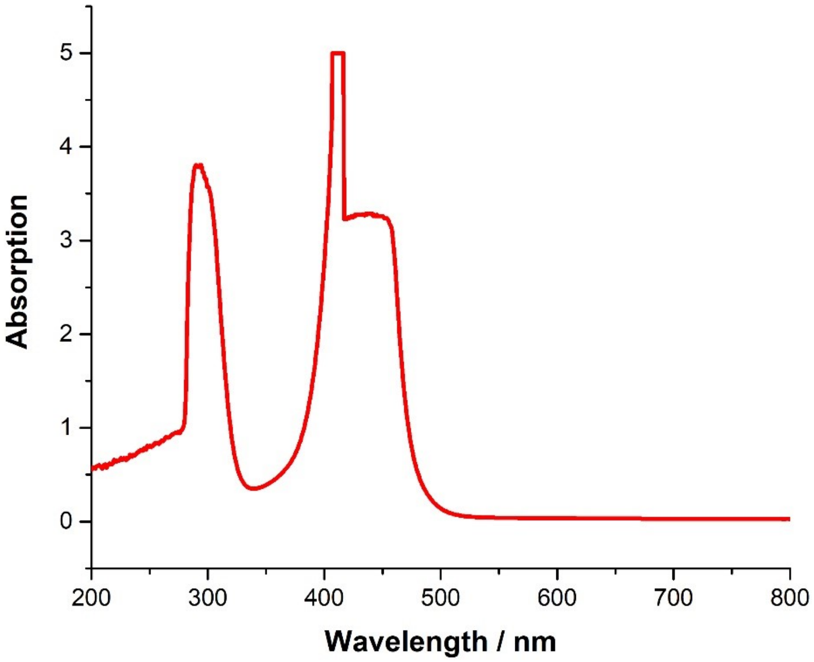
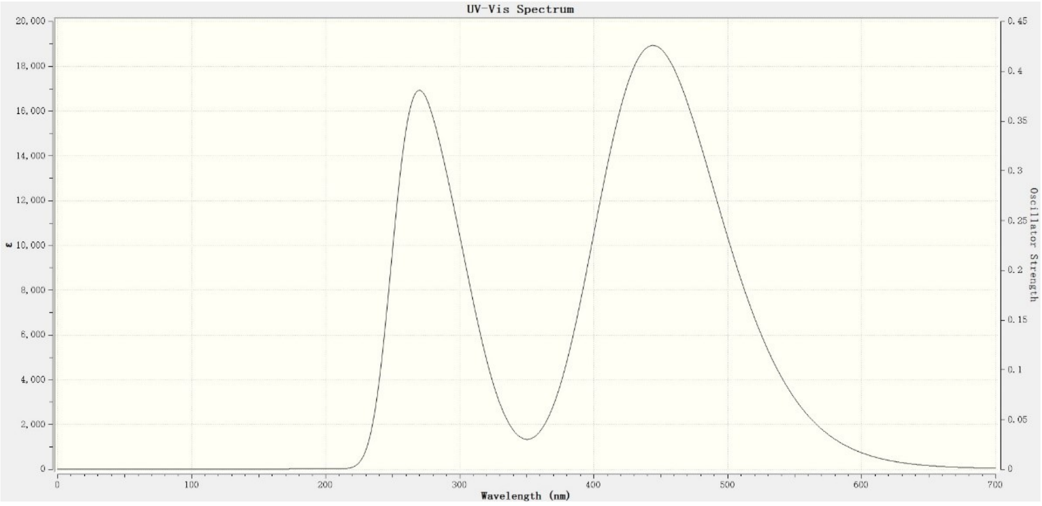


Figure S11. UV-vis spectrum of **4** in toluene (1x10^{-3} mol/L) at room temperature.



Excited State 1: Singlet-A 2.7864 eV 444.96 nm f=0.4433
<S**2>=0.000
285 -> 287 -0.13747
286 -> 287 0.69042

Figure S12. Calculated UV-vis spectrum of **4** at TD-PBE1PBE/6-311G (d) and the IEFPCM solvation model with toluene was used for calculation.

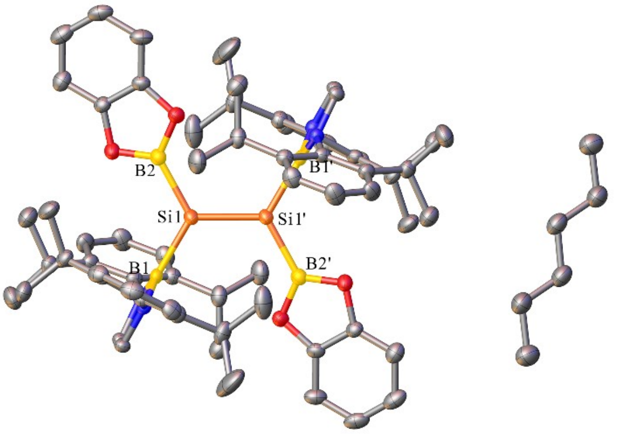


Figure S13. OLEX2 drawing of **4** with 50% ellipsoid probability. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Si1–Si1' 2.1654(12), Si1–B1 1.991(3), Si1–B2 1.983(3); B1–Si1–B3 145.82(8), B1–Si1–Si1' 120.49(8), B2–Si1–Si1' 118.70(9), B2–Si1–B1 120.78(10).

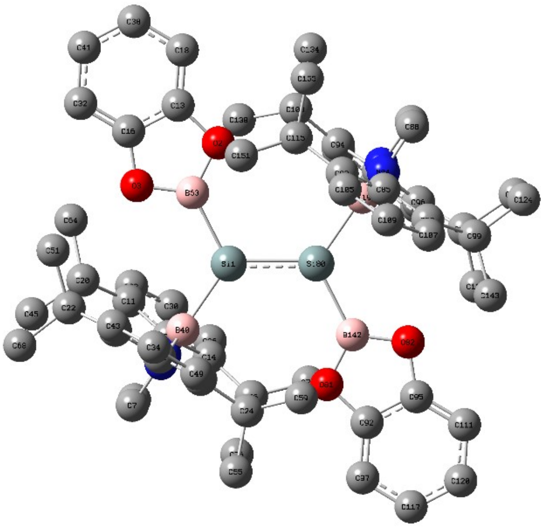


Figure S14. Optimized geometry of **4**. Selected computed bond lengths (Å) and angles (deg): Si1−Si80 2.18498, Si1−B40 2.01272, Si1–B63 1.99421; B40–Si1–B60 118.56756, B63−Si1−Si80 116.68074, B40−Si1−Si80 124.75170.

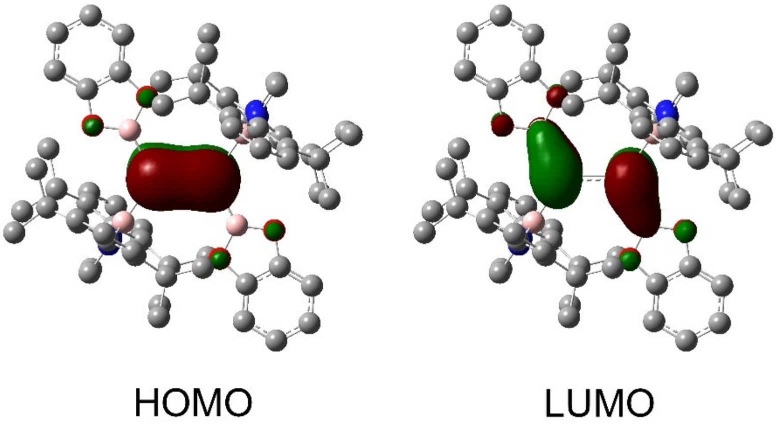


Figure S15. Frontier orbitals of **4**.

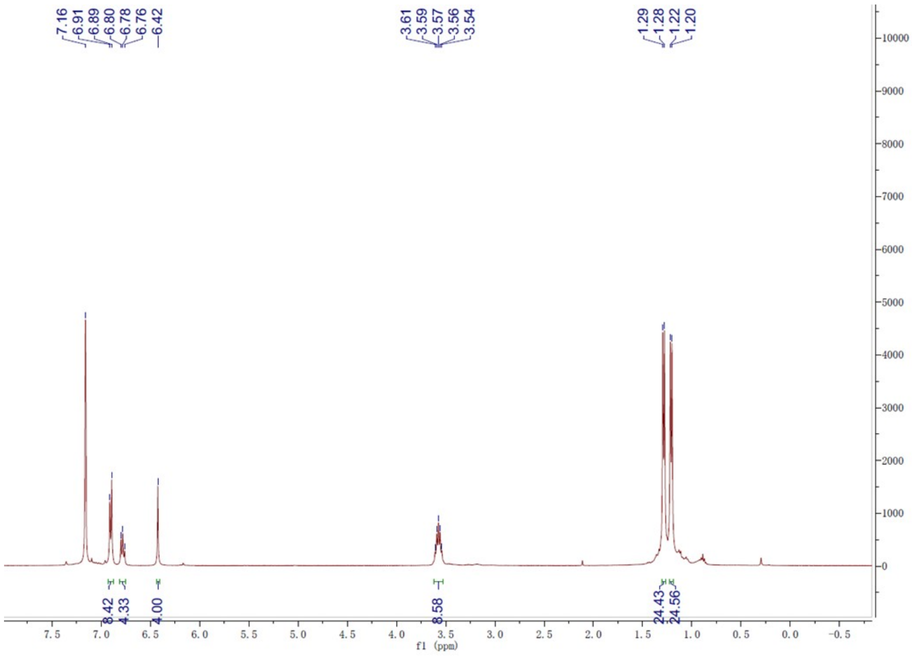


Figure S16. ^{1}H NMR spectrum of **2** in C_6D_6.

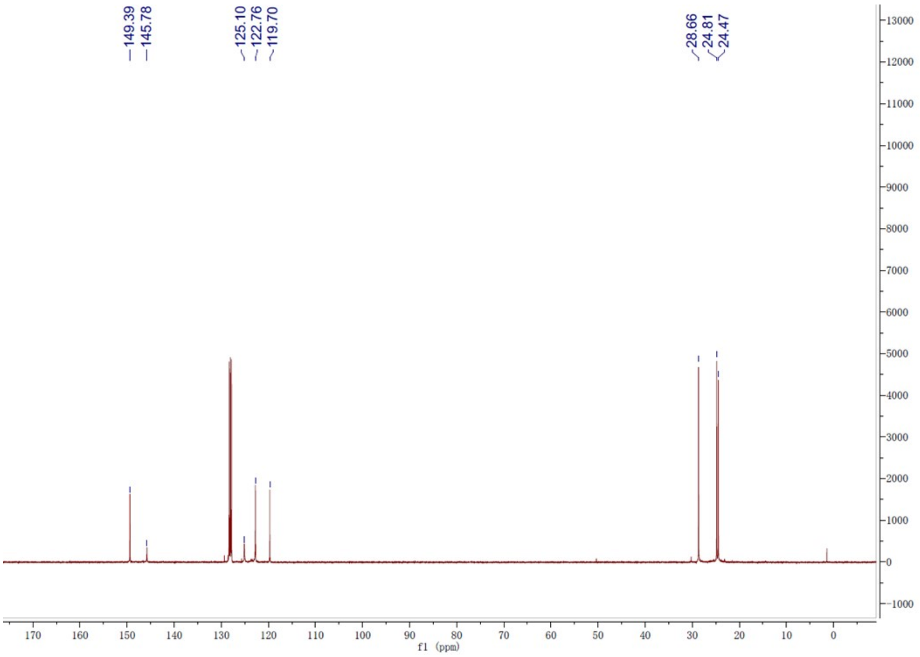


Figure S17. ^{13}C NMR spectrum of **2** in C_6D_6.

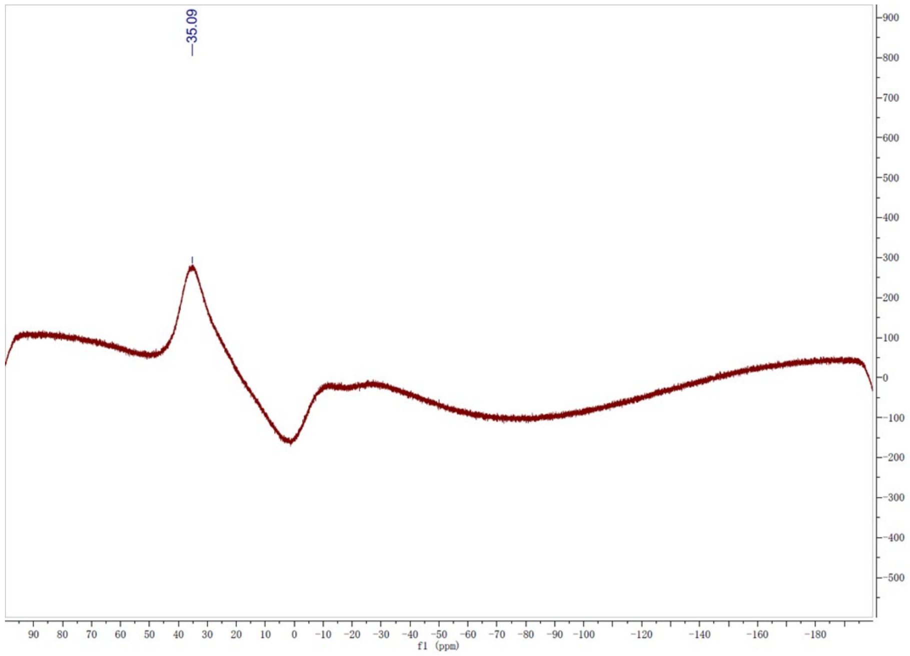


Figure S18. ^{11}B NMR spectrum of **2** in C_6D_6.

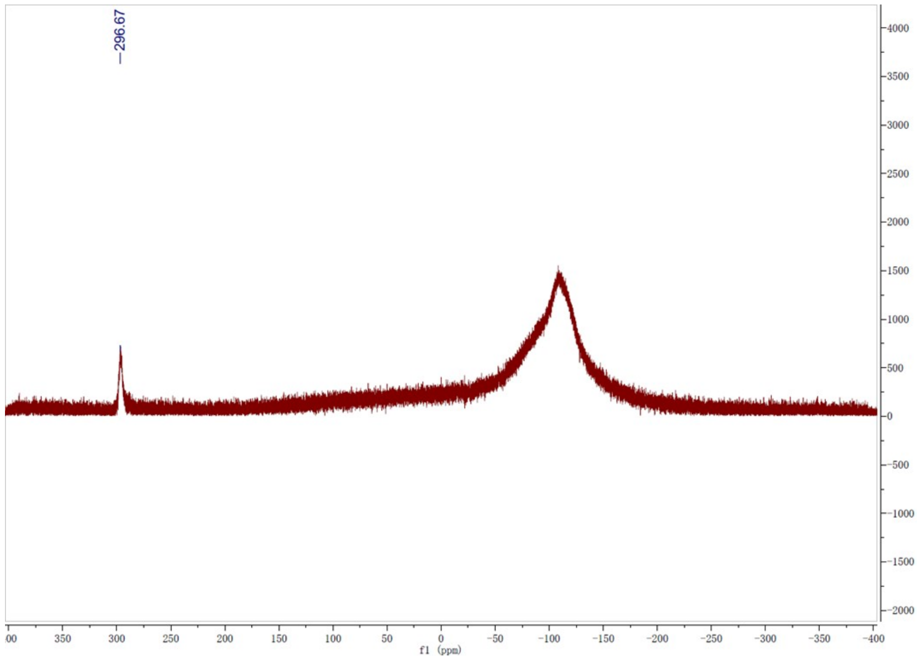


Figure S19. ^{29}Si NMR spectrum of **2** in C_6D_6.

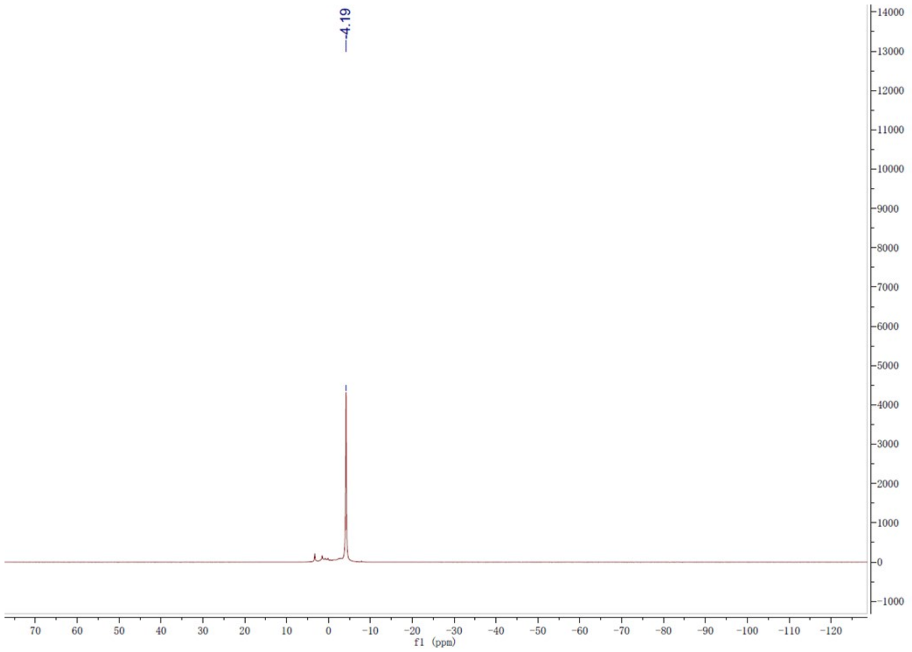


Figure S20. ^{7}Li NMR spectrum of **2** in C_6D_6.

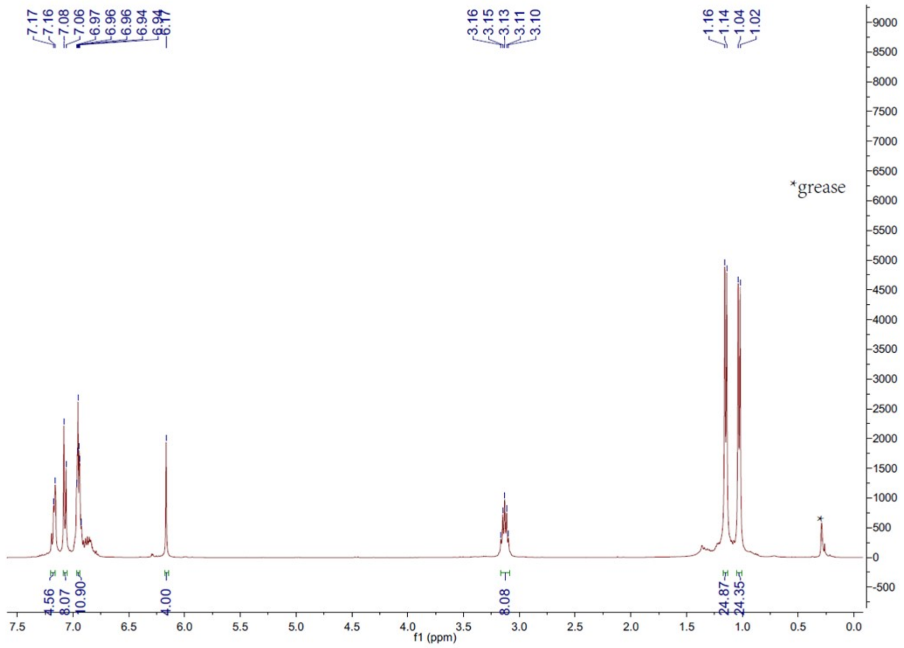


Figure S21. ^{1}H NMR spectrum of **3a** in C_6D_6.

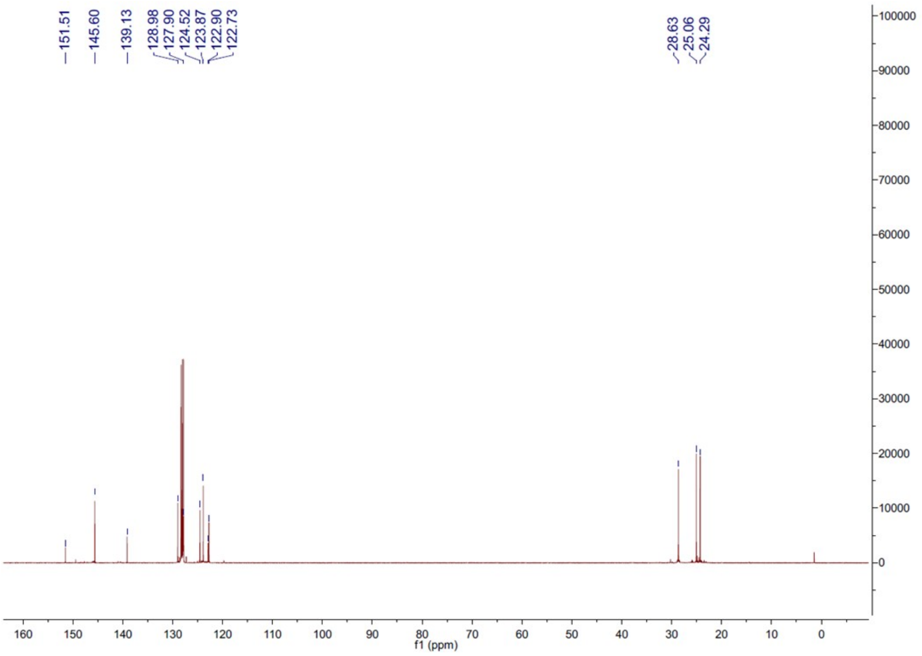


Figure S22. ^{13}C NMR spectrum of **3a** in C_6D_6.

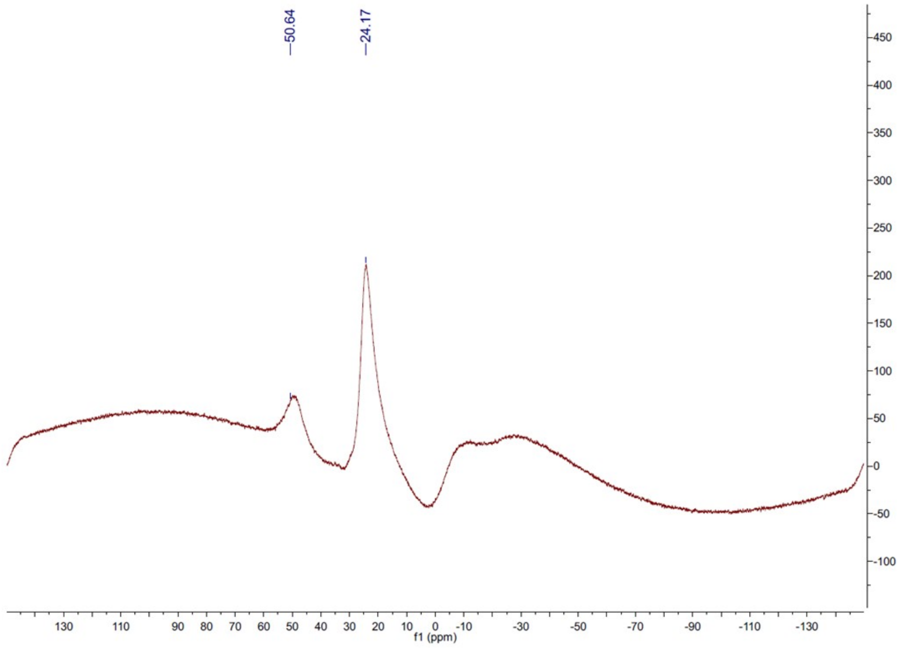


Figure S23. ^{11}B NMR spectrum of **3a** in C_6D_6.

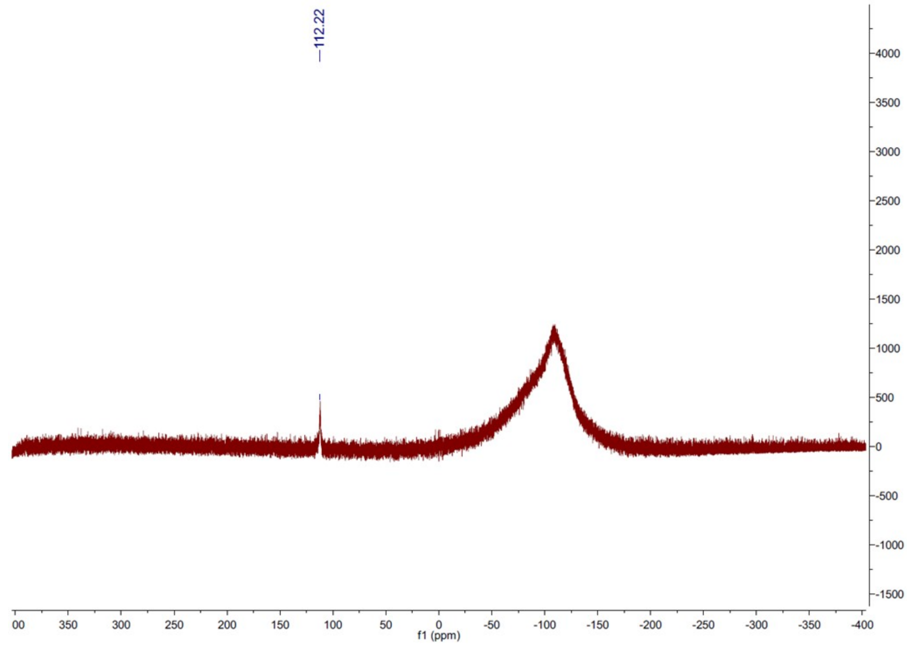


Figure S24. ^{29}Si NMR spectrum of **3a** in C_6D_6.

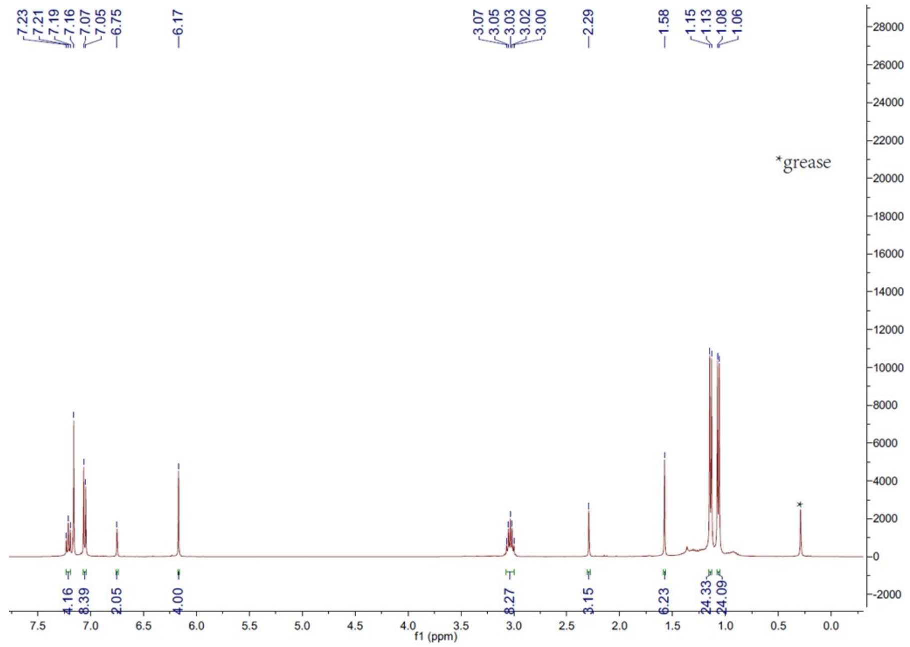


Figure S25. ^{1}H NMR spectrum of **3b** in C_6D_6.

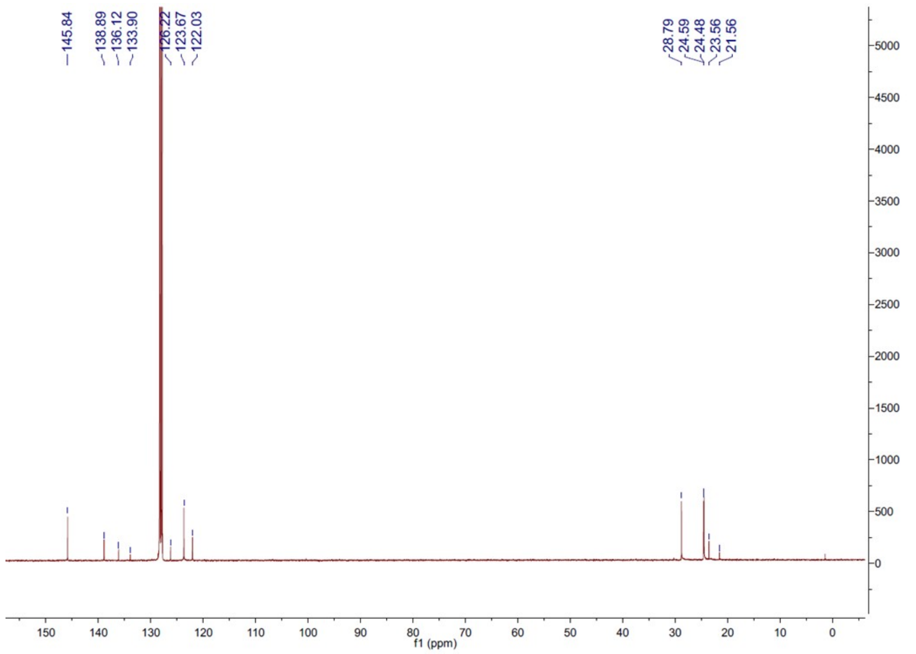


Figure S26. ^{13}C NMR spectrum of **3b** in C_6D_6.

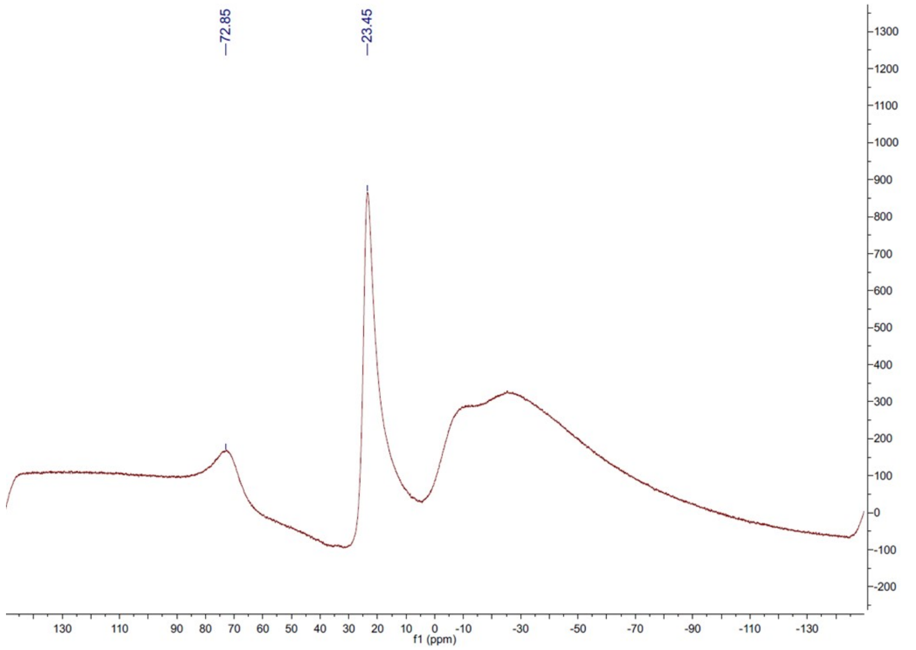


Figure S27. ^{11}B NMR spectrum of **3b** in C_6D_6.

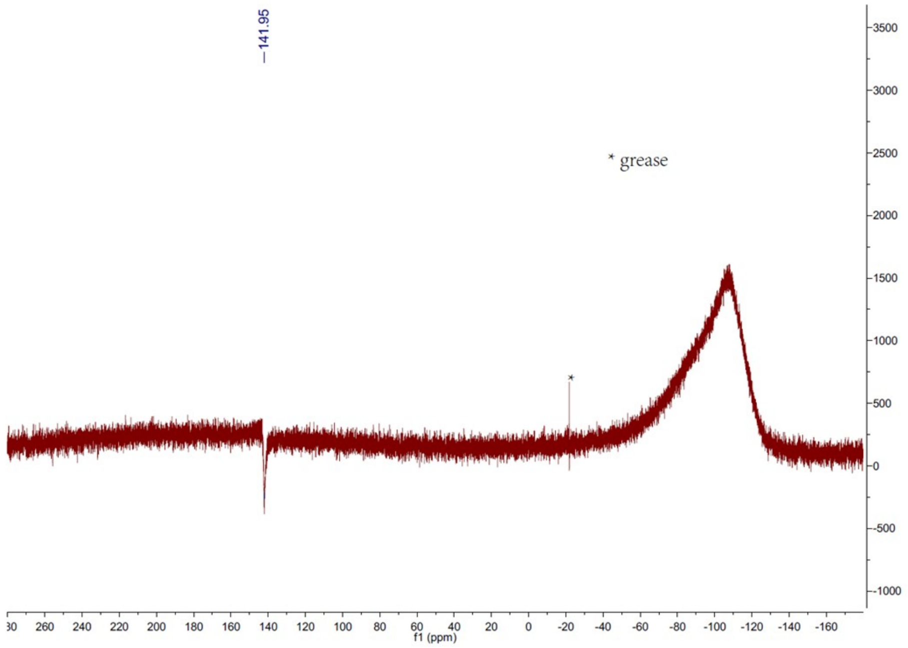


Figure S28. ^{29}Si NMR spectrum of **3b** in C_6D_6.

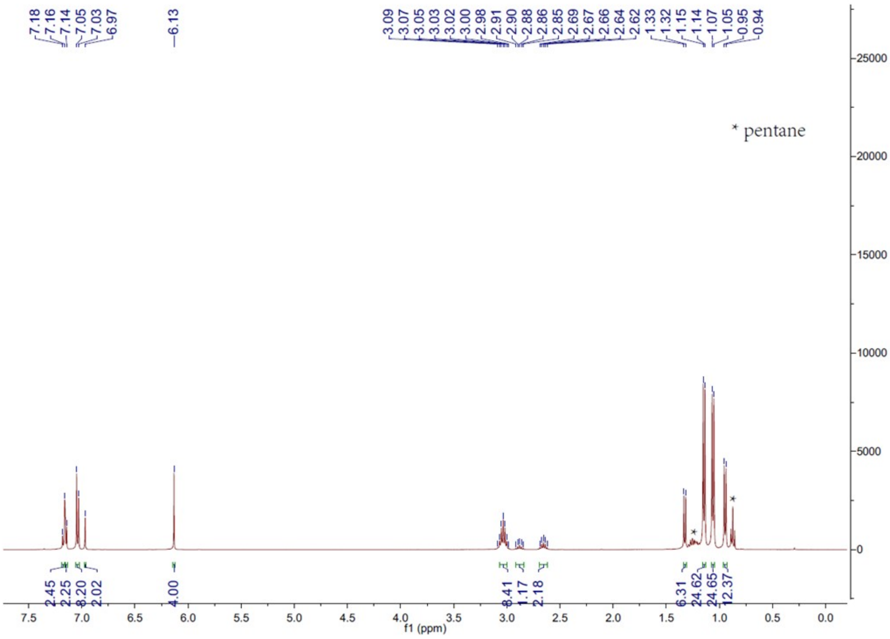


Figure S29. ^{1}H NMR spectrum of **3c** in C_6D_6.

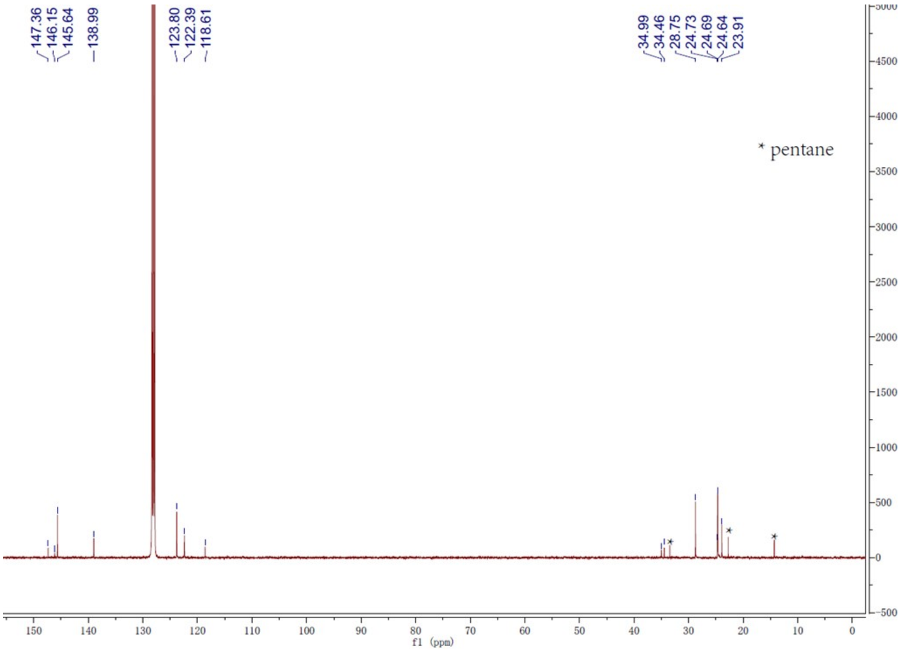


Figure S30. ^{13}C NMR spectrum of **3c** in C_6D_6.

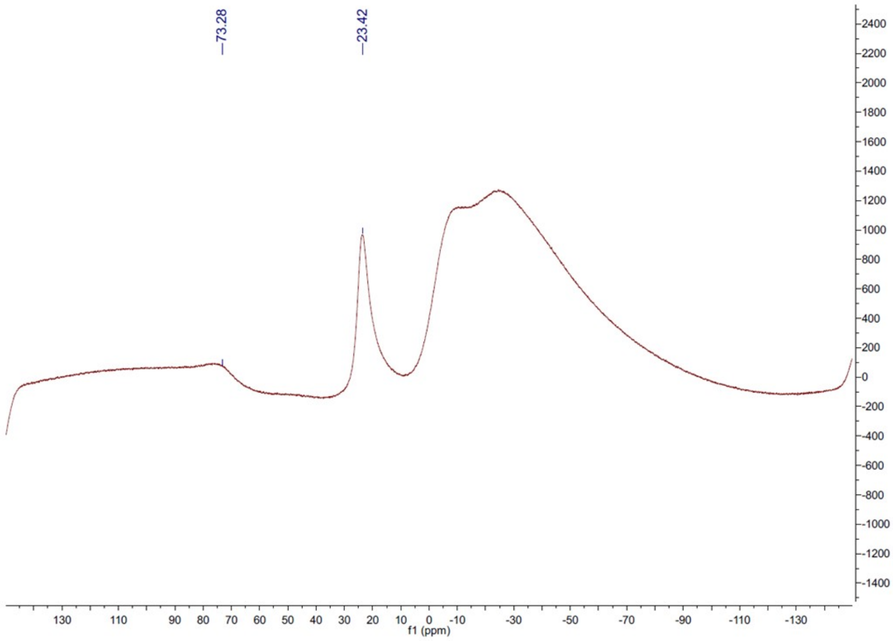


Figure S31. ^{11}B NMR spectrum of **3c** in C_6D_6.

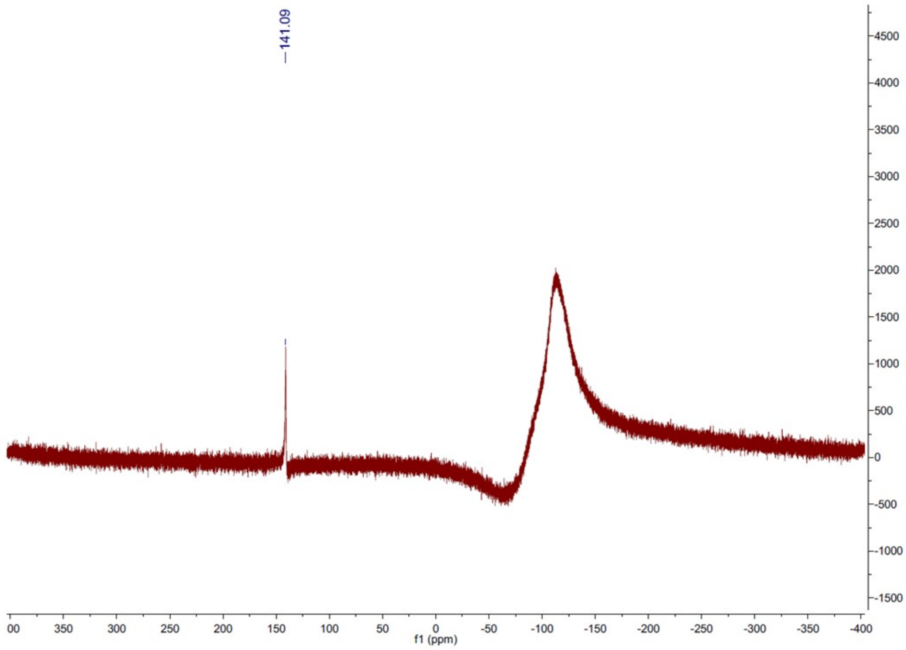


Figure S32. ^{29}Si NMR spectrum of **3c** in C_6D_6.

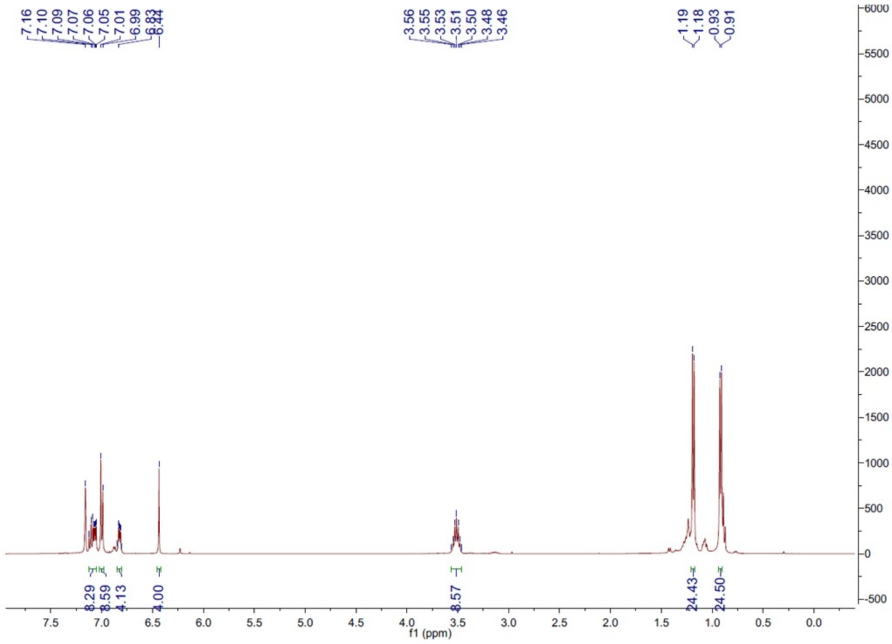


Figure S33. ^{1}H NMR spectrum of **4** in C_6D_6.

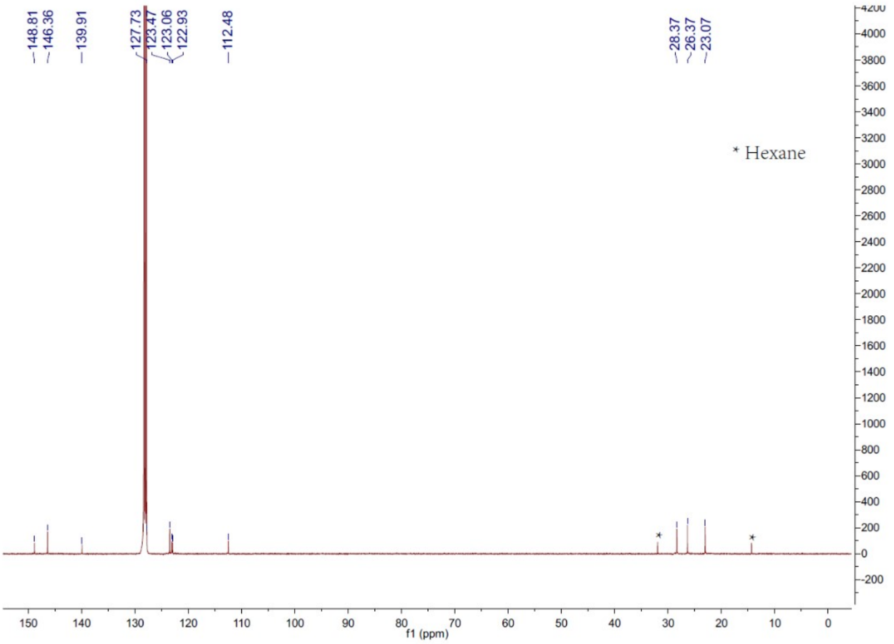


Figure S34. ^{13}C NMR spectrum of **4** in C_6D_6.

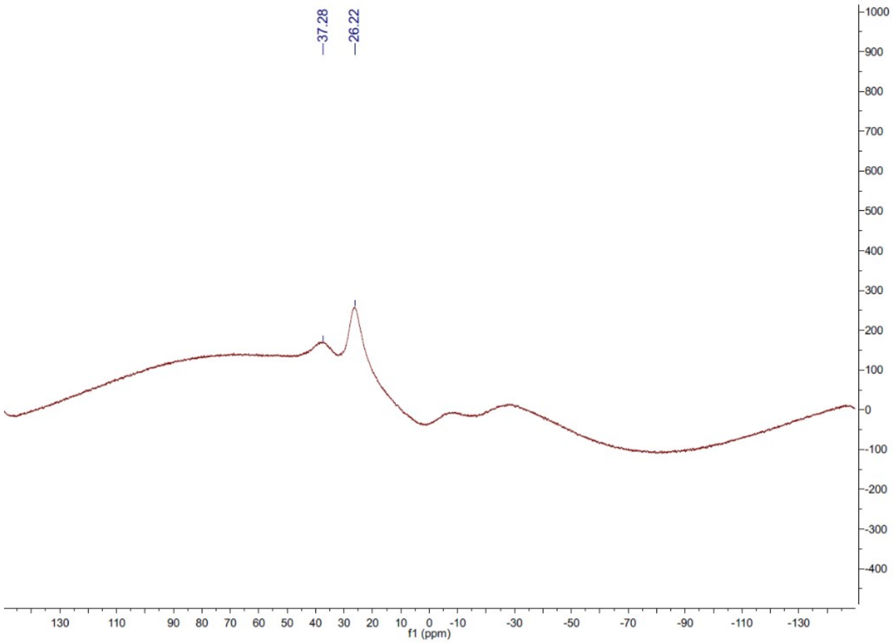


Figure S35. ^{11}B NMR spectrum of **4** in C_6D_6.

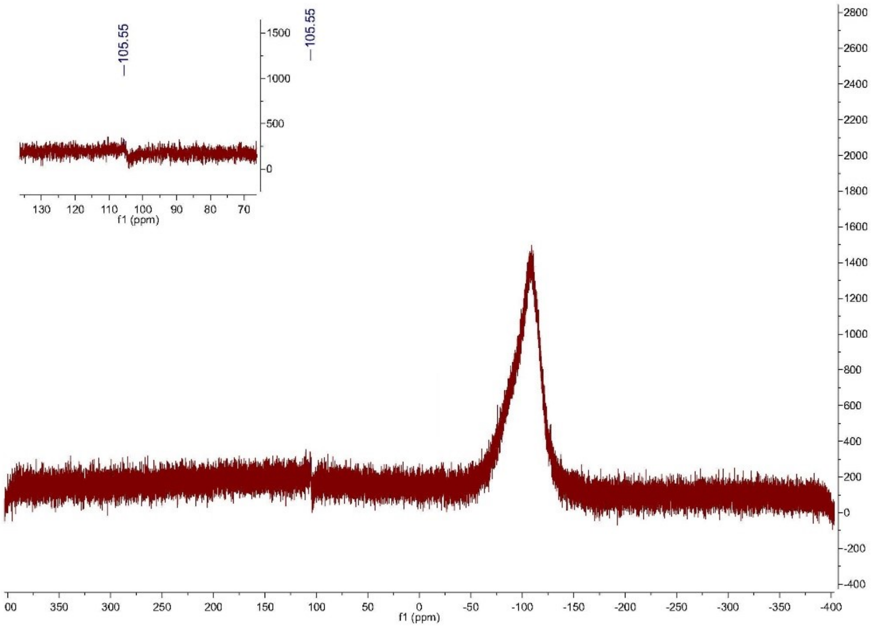


Figure S36. ^{29}Si NMR spectrum of **4** in C_6D_6.

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