Supporting Information for:

"Synthesis of 9-Borafluorene Analogues Featuring a Three-Dimensional 1,1'-Bis(*o*-carborane) Backbone"

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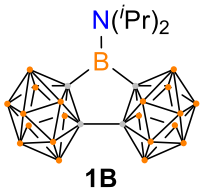
Experimental section

General Considerations. All manipulations were performed under an inert atmosphere in a nitrogen-filled MBraun Unilab glovebox. Solvents were purchased from commercial sources as anhydrous grade, dried further using a JC Meyer Solvent System with dual columns packed with solvent-appropriate drying agents and stored over molecular sieves. *O*-carborane and triethylphosphine oxide were purchased from Health Consumer Research and Alfa Aesar and used as received. Dichloro(diisopropylamino)borane and potassium bis(trimethylsilyl)amide [(K(HMDS)] were purchased from Sigma-Aldrich Chemicals and used as received. 1,1′-bis(*o*-carborane, **B**) and 9,9′,10,10′,11,11′,12,12′-octamethyl-bis(*o*-carborane, **BMe$_8$**) were synthesized according to published procedures.[1-2] $CDCl_3$ and C_6D_6 for NMR spectroscopy were purchased from Cambridge Isotope Laboratories and dried by stirring for 3 days over CaH_2, distilled, and stored over 4 Å molecular sieves. Multinuclear NMR spectra were recorded on Bruker 400 or 600 MHz spectrometers. FT-IR spectra were recorded on a Bruker Alpha ATR FT-IR spectrometer on solid samples. High resolution mass spectra (HRMS) were obtained at the University of Texas at Austin Mass Spectrometry Center on a Micromass Autospec Ultima spectrometer using CI. Melting points were measured with a Thomas Hoover Uni-melt capilliary melting point apparatus and are uncorrected. UV-Vis spectra were recorded using an Agilent 8453 UV-Vis spectrophotometer. Solutions were prepared in a nitrogen filled glovebox and measured in screw capped quartz cuvettes for UV-Vis spectroscopy. For the Gutmann−Beckett studies, samples were prepared in a 1:2 stoichiometric ratio of Lewis acid:Et_3PO. Subsequent ^{31}P NMR spectroscopy was done in C_6D_6. Samples were prepared in a glovebox under a N_2 atmosphere. Cyclic voltammetry experiments were performed in an argon filled glovebox using a CH Instruments Model 1140 electrochemical analyzer with a platinum working electrode and a platinum wire auxiliary electrode. The reference electrode was AgCl coated silver wire and was referenced by the standard ferrocene/ferrocinium redox couple (0.56 V in THF) as an internal standard. Single crystal X-ray diffraction data were collected on a Bruker Apex II-CCD detector using Mo-K_α radiation (λ = 0.71073 Å). Crystals were selected under paratone oil, mounted on MiTeGen micromounts, and immediately placed in a cold stream of N_2. Structures were solved and refined using SHELXTL and figures were produced using OLEX2.[3,4]

Computational Details. Density functional theory calculations were performed with ADF 2014 Suite version 2014.04[5] using Slater-type orbitals. Geometry optimizations were performed using PBE-D3(BJ)[6, 7] with TZP (double-ζ core, triple-ζ valence + 1 polarization function) basis sets and single point calculations were performed using B3LYP-D3(BJ)[6,8] with TZ2P (double-ζ core, triple-ζ valence + 2 polarization functions) basis sets. All calculations were performed in the gas phase.



1B

1B: To a solution of K(HMDS) (345.0 mg, 1.730 mmol) in tetrahydrofuran (2 mL) was added a solution of **B** (248.0 mg, 0.860 mmol) in tetrahydrofuran (2 mL) at room temperature. Upon completion of the addition, the clear solution became orange and the mixture was stirred for an additional 45 min. Dichloro(diisopropylamino)borane (166.0 µL, 0.946 mmol) was added dropwise and stirred for 5 min before removing the solvent *in vacuo*. The residue was extracted with CH_2Cl_2 (2 mL), filtered, and the solvent removed *in vacuo* resulting in a tan residue. The product was purified *via* recrystallization by dissolving the residue in a minimal amount of Et_2O (~2 mL) and storing at -35 °C overnight. The supernatant was decanted to produce white crystals.

Yield (304.0 mg, 89%)

Crystals of **1B** for X-ray diffraction studies were grown by the slow evaporation of a concentrated CH_2Cl_2 solution into hexanes at ambient temperature.

mp (231 – 232 °C)

^{1}H NMR (600 MHz, $CDCl_3$) δ 4.44 (sept, *J* = 6.0 Hz, 2H), 2.92 – 1.74 (m, 20H), 1.38 (d, *J* = 6.0 Hz, 12H) ppm

^{1}H{^{11}B} NMR (600 MHz, $CDCl_3$) δ 4.44 (sept, *J* = 6.0 Hz, 2H), 3.21 (s, 3H), 2.59-2.02 (m, 17H), 1.38 (d, *J* = 6.0 Hz, 12H) ppm

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 75.34, 52.01, 24.78 ppm

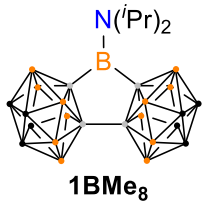
^{11}B NMR (128 MHz, $CDCl_3$) δ 32.9 (s, 1B), 2.78 (d, 2B), -1.8 to -12.0 (m, 18B) ppm

^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$) δ 32.9 (s, 1B), 1.7 (s, 2B), -3.1 to -11.2 (m, 18B) ppm

FT-IR (ranked intensity, cm^{-1}) 2972 (12), 2577 (1), 1519 (13), 1491 (4), 1463 (10), 1370 (6), 1177 (3), 1112 (5), 1065 (8), 981 (15), 912 (14), 813 (7), 732 (2), 714 (11), 647 (9)

HRMS (CI) for $C_{10}H_{33}B_{21}N$ $(M\text{-}H)^+$, calcd: 394.4712; found: 394.4709

UV-Vis (CH_2Cl_2) λ_{max} (233 nm): ε = 12,600 $Lmol^{-1}cm^{-1}$



1BMe$_8$

1BMe$_8$: To a solution of K(HMDS) (351.0 mg, 1.760 mmol) in tetrahydrofuran (2 mL) was added a solution of **BMe$_8$** (351.0 mg, 0.880 mmol) in tetrahydrofuran (2 mL) at room temperature. Upon completion of the addition, the clear solution became orange and the mixture was stirred for an additional 45 min. Dichloro(diisopropylamino)borane (155.0 µL, 0.882 mmol) was added dropwise and stirred for 5 min before removing the solvent *in vacuo*. The residue was extracted with CH_2Cl_2 (2 mL), filtered, and the solvent removed *in vacuo* resulting in a tan powder. The product was purified *via* recrystallization by dissolving the tan residue in a minimal amount of *n*-pentane (~1 mL) and storing at -35 °C overnight. The supernatant was decanted to produce white crystals.

Yield (300.0 mg, 67%)

Crystals of **1BMe$_8$** for X-ray diffraction studies were grown by the slow evaporation of a concentrated diethyl ether solution into hexanes at -35 °C.

mp (189 – 192 °C)

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.44 (sept, *J* = 4.0 Hz, 2H), 3.48 – 1.54 (m, 12H), 1.36 (d, *J* = 4.0 Hz, 12H), 0.20 – 0.17 (m, 11H), 0.10 – 0.05 (m, 3H), 0.00 – -0.05 (m, 10H) ppm

^{1}H{^{11}B} NMR (600 MHz, $CDCl_3$) δ 4.44 (sept, *J* = 6.0 Hz, 2H), 3.03 (s, 3H), 2.37 – 1.88 (m, 9H), 1.36 (d, *J* = 6.0 Hz, 12H) 0.19 – 0.17 (m, 11H), 0.10 – 0.05 (m, 3H), 0.00 – -0.05 (m, 10H) ppm

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 77.36, 67.50, 51.66, 24.88, -2.66 ppm

^{11}B NMR (128 MHz, $CDCl_3$) δ 33.7 (s, 1B), 11.3 (s, 2B), 5.9 (s, 2B), 1.4 (s, 4B), -5.2 to -13.1 (m, 12B) ppm

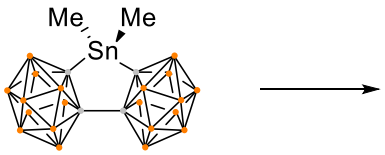
$^{11}B\{^{1}H\}$ NMR (128 MHz, $CDCl_3$) δ 33.7 (s, 1B), 11.3 (s, 2B), 6.0 (s, 2B), 1.1 (s, 4B), -6.8 to -13.7 (m, 12B) ppm

FT-IR (ranked intensity, cm^{-1}) 2905 (9), 2700 (15), 2584 (4), 1516 (11), 1489 (2), 1465 (12), 1386 (14), 1369 (7), 1309 (3), 1182 (5), 1114 (1), 1025 (6), 958 (10), 783 (13), 750 (8)

HRMS (CI) for $C_{18}H_{50}B_{21}N$ (M^+), calcd: 509.5970; found: 509.5973

UV-Vis (CH_2Cl_2) λ_{max} (233 nm): ε = 13,300 $Lmol^{-1}cm^{-1}$

Table S-1: Attempted transmetallation reaction of **$Me_2Sn(B)$** with boranes.



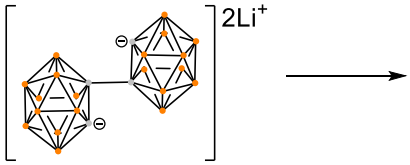
$Me_2Sn[B]$

● = BH ● = C

$RBCl_2$	Solvent	Temp	Time	Result
Ph	CH_2Cl_2, PhMe	23 °C	72 h	NR
Ph	PhMe	100 °C	72 h	NR
p-Tolyl	CH_2Cl_2, PhMe	23 °C	72 h	NR
p-Tolyl	PhMe	100 °C	72 h	NR
Mes	CH_2Cl_2, PhMe	23 °C	72 h	NR
Mes	PhMe	100 °C	72 h	NR
$^{i}Pr_2N$	CH_2Cl_2, PhMe	23 °C	72 h	NR
$^{i}Pr_2N$	PhMe	100 °C	72 h	NR
NPh_3	CH_2Cl_2, PhMe	23 °C	72 h	NR
NPh_3	PhMe	100 °C	72 h	NR
Trip	CH_2Cl_2, PhMe	23 °C	72 h	NR
Trip	PhMe	100 °C	72 h	NR

BR_3	Solvent	Temp	Time	Result
Cl	CH_2Cl_2, PhMe	23 °C	72 h	NR
Cl	PhMe	100 °C	72 h	NR
Br	CH_2Cl_2, PhMe	23 °C	72 h	NR
Br	PhMe	100 °C	72 h	NR
I	CH_2Cl_2, PhMe	23 °C	72 h	NR
I	PhMe	100 °C	72 h	NR

Table S-2: Attempted transmetallation reaction of **Li_2[B]** with boranes.



Li_2[B]

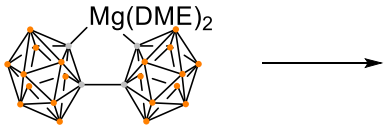
● = BH ● = C

$RBCl_2$	Solvent	Temp	Time	Result
Ph	THF, PhMe	23 °C	48 h	Decomp
Ph	PhMe	100 °C	72 h	NR
Ph	THF	-78 °C	72 h	Decomp
p-Tolyl	THF, PhMe	23 °C	48 h	NR
p-Tolyl	PhMe	100 °C	72 h	NR
p-Tolyl	THF	-78 °C	72 h	Decomp
Mes	THF, PhMe	23 °C	48 h	NR
Mes	PhMe	100 °C	72 h	Decomp
Mes	THF	-78 °C	72 h	Decomp
$^{i}Pr_2N$	THF, PhMe	23 °C	48 h	NR
$^{i}Pr_2N$	PhMe	100 °C	72 h	Decomp
$^{i}Pr_2N$	THF	-78 °C	72 h	NR
NPh_3	THF, PhMe	23 °C	48 h	NR
NPh_3	PhMe	100 °C	72 h	Decomp
NPh_3	THF	-78 °C	72 h	NR
Trip	THF, PhMe	23 °C	48 h	NR
Trip	PhMe	100 °C	72 h	Decomp
Trip	THF	-78 °C	72 h	NR

BR_3	Solvent	Temp	Time	Result
Cl	THF, PhMe	23 °C	48 h	NR
Cl	PhMe	100 °C	72 h	Decomp
Cl	THF	-78 °C	72 h	NR
Br	THF, PhMe	23 °C	48 h	NR
Br	PhMe	100 °C	72 h	Decomp
Br	THF	-78 °C	72 h	NR
I	THF, PhMe	23 °C	48 h	NR
I	PhMe	100 °C	72 h	Decomp
I	THF	-78 °C	72 h	NR
F	THF, PhMe	23 °C	48 h	NR
F	PhMe	100 °C	72 h	Multiple products
F	THF	-78 °C	72 h	NR

Decomposition was identified as the **nido-B compound.*

Table S-3: Attempted transmetallation reaction of **$(DME)_2Mg(B)$** with boranes.



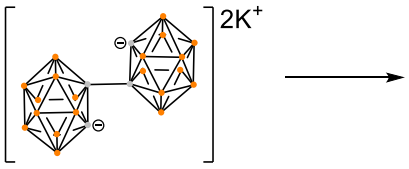
$(DME)_2Mg[B]$

● = BH ● = C

$RBCl_2$	Solvent	Temp	Time	Result
Ph	CH_2Cl_2, PhMe	23 °C	72 h	NR
Ph	PhMe	100 °C	72 h	NR
p-Tolyl	CH_2Cl_2, PhMe	23 °C	72 h	NR
p-Tolyl	PhMe	100 °C	72 h	NR
Mes	CH_2Cl_2, PhMe	23 °C	72 h	NR
Mes	PhMe	100 °C	72 h	NR
$^{i}Pr_2N$	CH_2Cl_2, PhMe	23 °C	72 h	NR
$^{i}Pr_2N$	PhMe	100 °C	72 h	NR
NPh_3	CH_2Cl_2, PhMe	23 °C	72 h	NR
NPh_3	PhMe	100 °C	72 h	NR
Trip	CH_2Cl_2, PhMe	23 °C	72 h	NR
Trip	PhMe	100 °C	72 h	NR

BR_3	Solvent	Temp	Time	Result
Cl	CH_2Cl_2, PhMe	23 °C	72 h	NR
Cl	PhMe	100 °C	72 h	NR
Br	CH_2Cl_2, PhMe	23 °C	72 h	NR
Br	PhMe	100 °C	72 h	NR
I	CH_2Cl_2, PhMe	23 °C	72 h	NR
I	PhMe	100 °C	72 h	NR

Table S-4: Attempted transmetallation reaction of **K_2[B]** with boranes.



K_2[B]

● = BH ● = C

$RBCl_2$	Solvent	Temp	Time	Result
Ph	THF, PhMe	23 °C	48 h	Decomp
Ph	PhMe	100 °C	72 h	NR
Ph	THF	-78 °C	72 h	Decomp
p-Tolyl	THF, PhMe	23 °C	48 h	NR
p-Tolyl	PhMe	100 °C	72 h	NR
p-Tolyl	THF	-78 °C	72 h	Decomp
Mes	THF, PhMe	23 °C	48 h	NR
Mes	PhMe	100 °C	72 h	Decomp
Mes	THF	-78 °C	72 h	Decomp
$^{i}Pr_2N$	THF, PhMe	23 °C	48 h	**$^{11}B\{^1H\}$ 32.9 ppm**
$^{i}Pr_2N$	PhMe	100 °C	72 h	NR
$^{i}Pr_2N$	THF	-78 °C	72 h	**$^{11}B\{^1H\}$ 32.9 ppm**
NPh_3	THF, PhMe	23 °C	48 h	NR
NPh_3	PhMe	100 °C	72 h	Decomp
NPh_3	THF	-78 °C	72 h	NR
Trip	THF, PhMe	23 °C	48 h	NR
Trip	PhMe	100 °C	72 h	Decomp
Trip	THF	-78 °C	72 h	NR

BR_3	Solvent	Temp	Time	Result
Cl	THF, PhMe	23 °C	48 h	NR
Cl	PhMe	100 °C	72 h	Decomp
Cl	THF	-78 °C	72 h	NR
Br	THF, PhMe	23 °C	48 h	NR
Br	PhMe	100 °C	72 h	Decomp
Br	THF	-78 °C	72 h	NR
I	THF, PhMe	23 °C	48 h	NR
I	PhMe	100 °C	72 h	Decomp
I	THF	-78 °C	72 h	NR
F	THF, PhMe	23 °C	48 h	NR
F	PhMe	100 °C	72 h	Multiple products
F	THF	-78 °C	72 h	NR

Figure S-1: ^{1}H NMR spectrum of **1B** in $CDCl_3$.

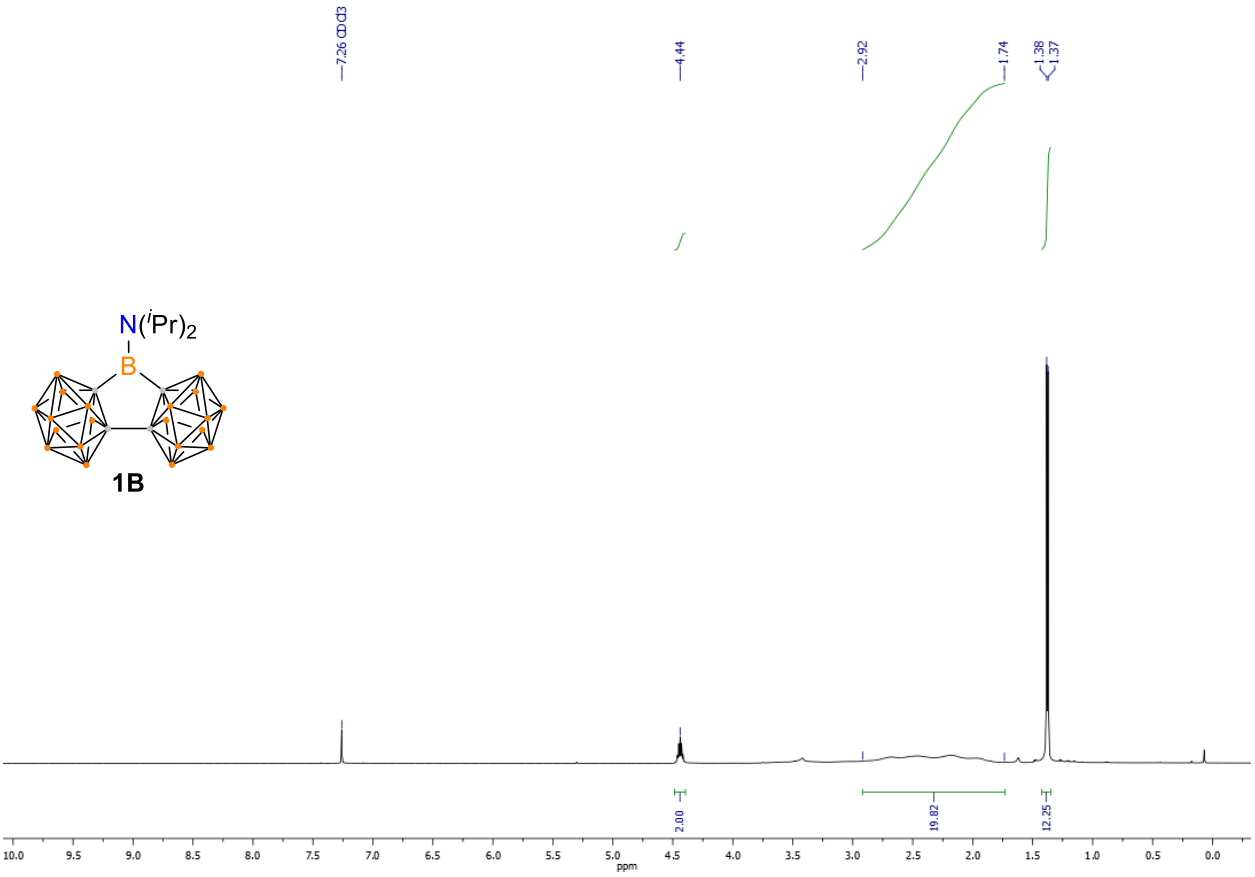


Figure S-2: Expansion of the ^{1}H NMR spectrum of **1B** in $CDCl_3$.

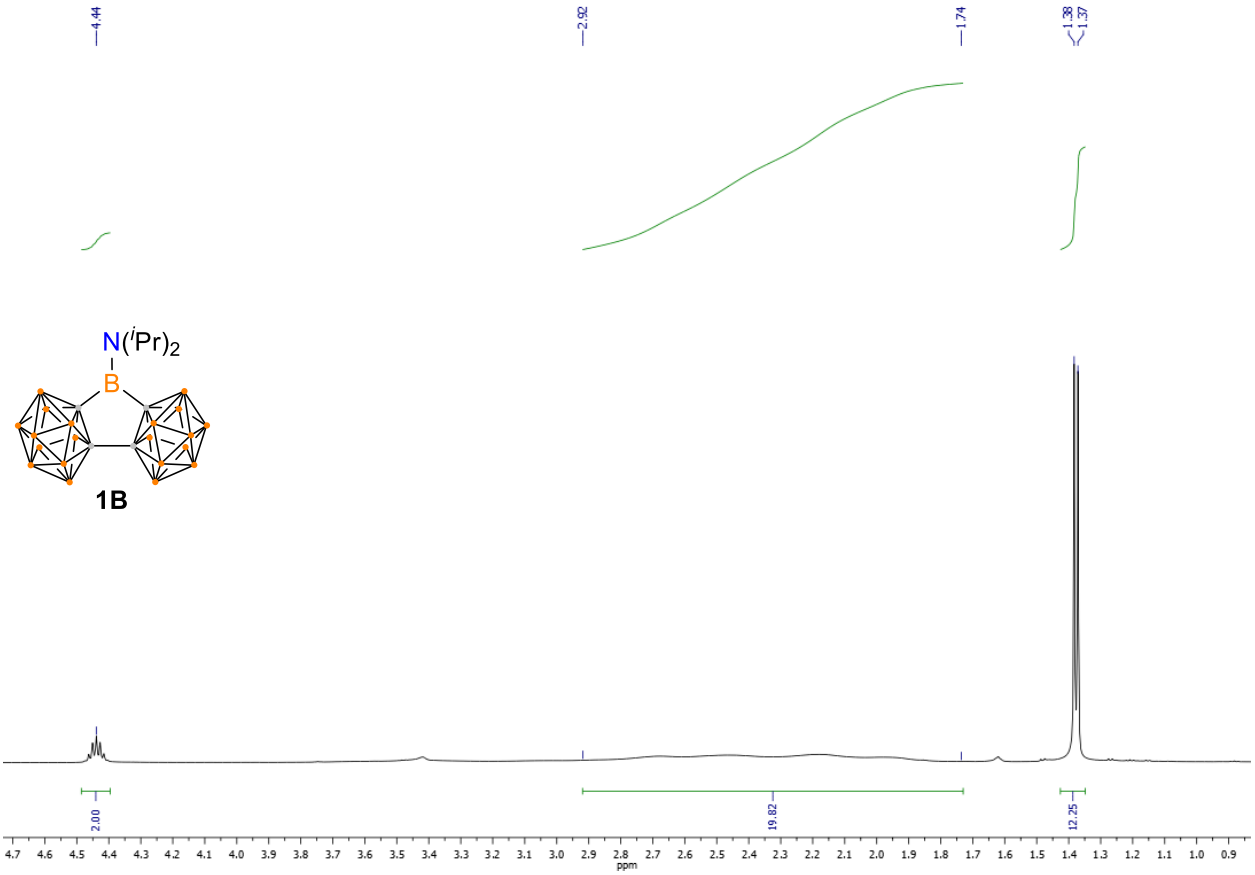


Figure S-3: $^{1}H\{^{11}B\}$ NMR spectrum of **1B** in $CDCl_3$.

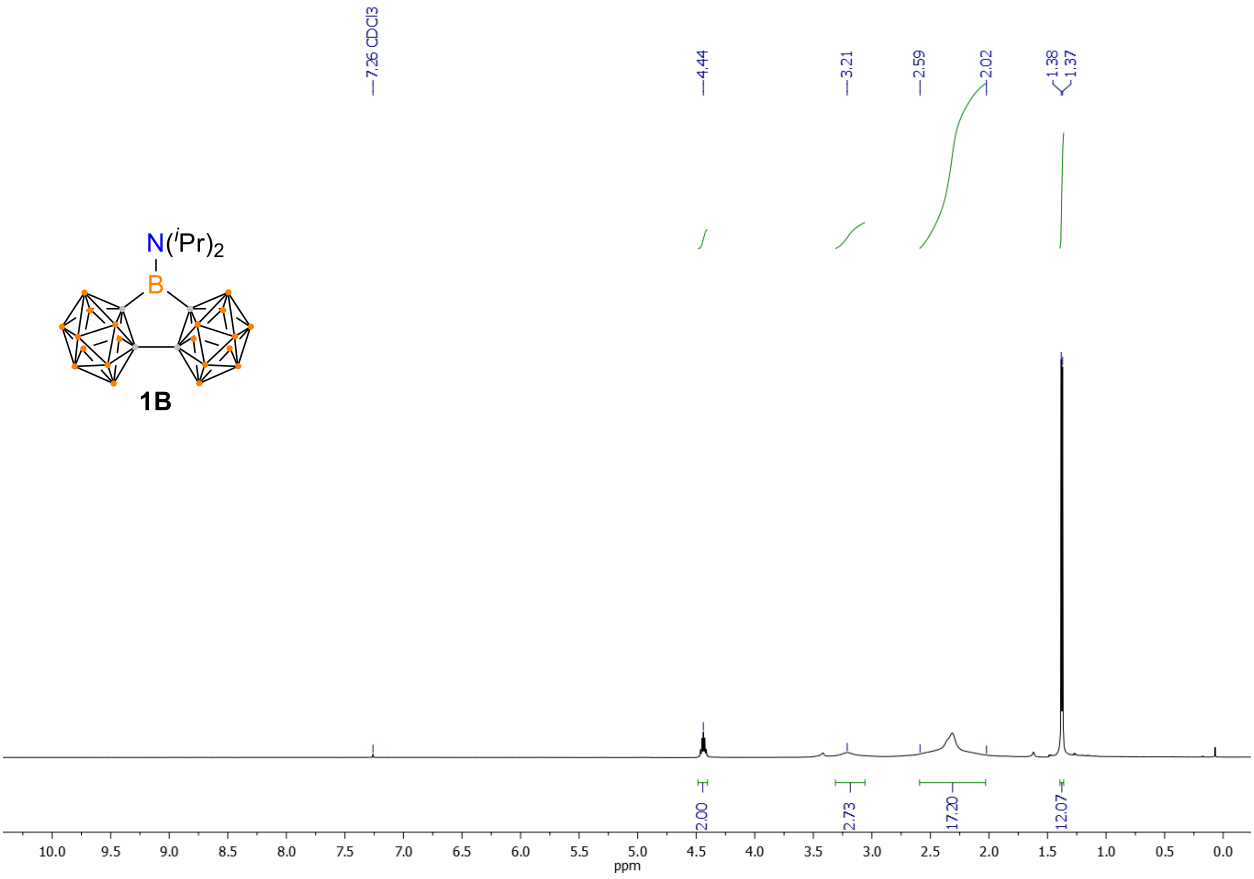


Figure S-4: Expansion of the $^{1}H\{^{11}B\}$ NMR spectrum of **1B** in $CDCl_3$.

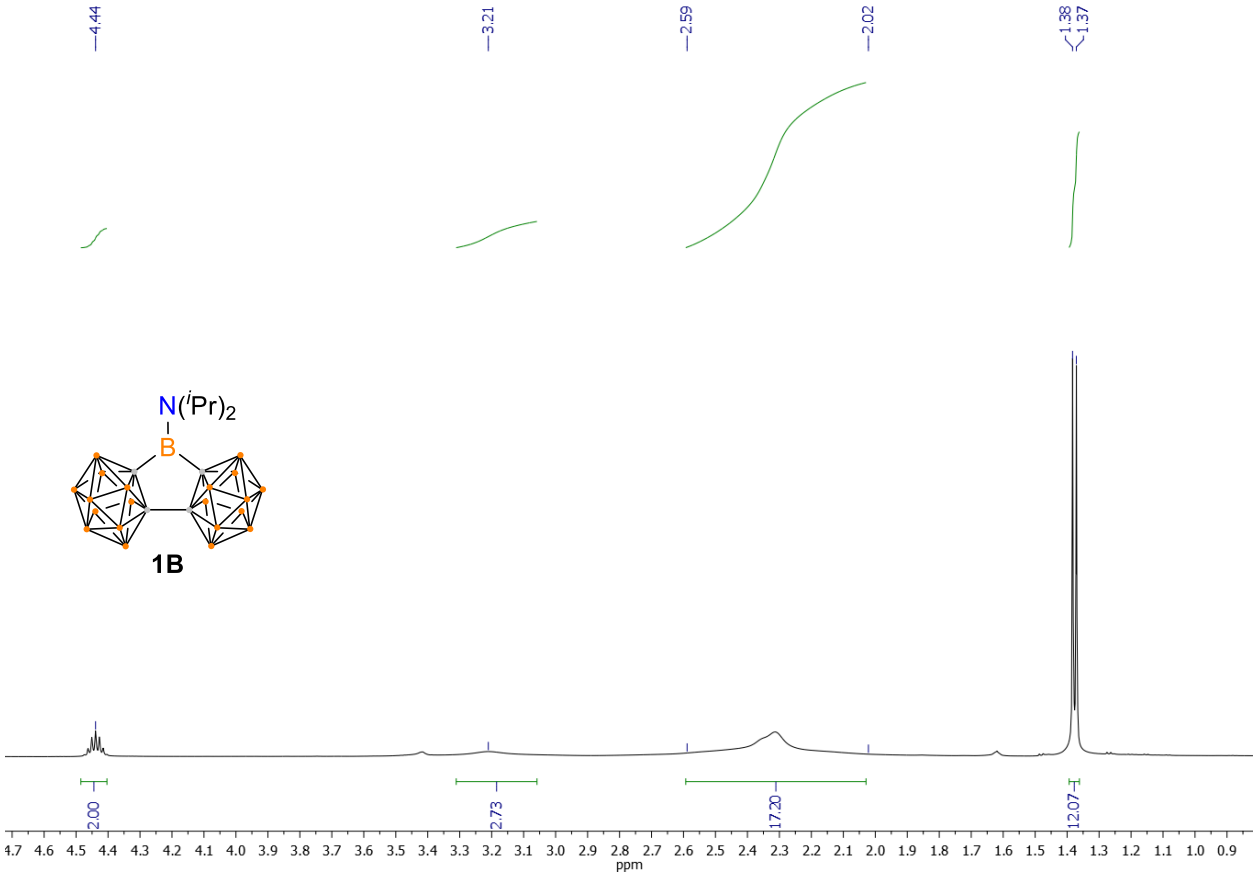


Figure S-5: $^{13}C\{^{1}H\}$ NMR spectrum of **1B** in $CDCl_3$.

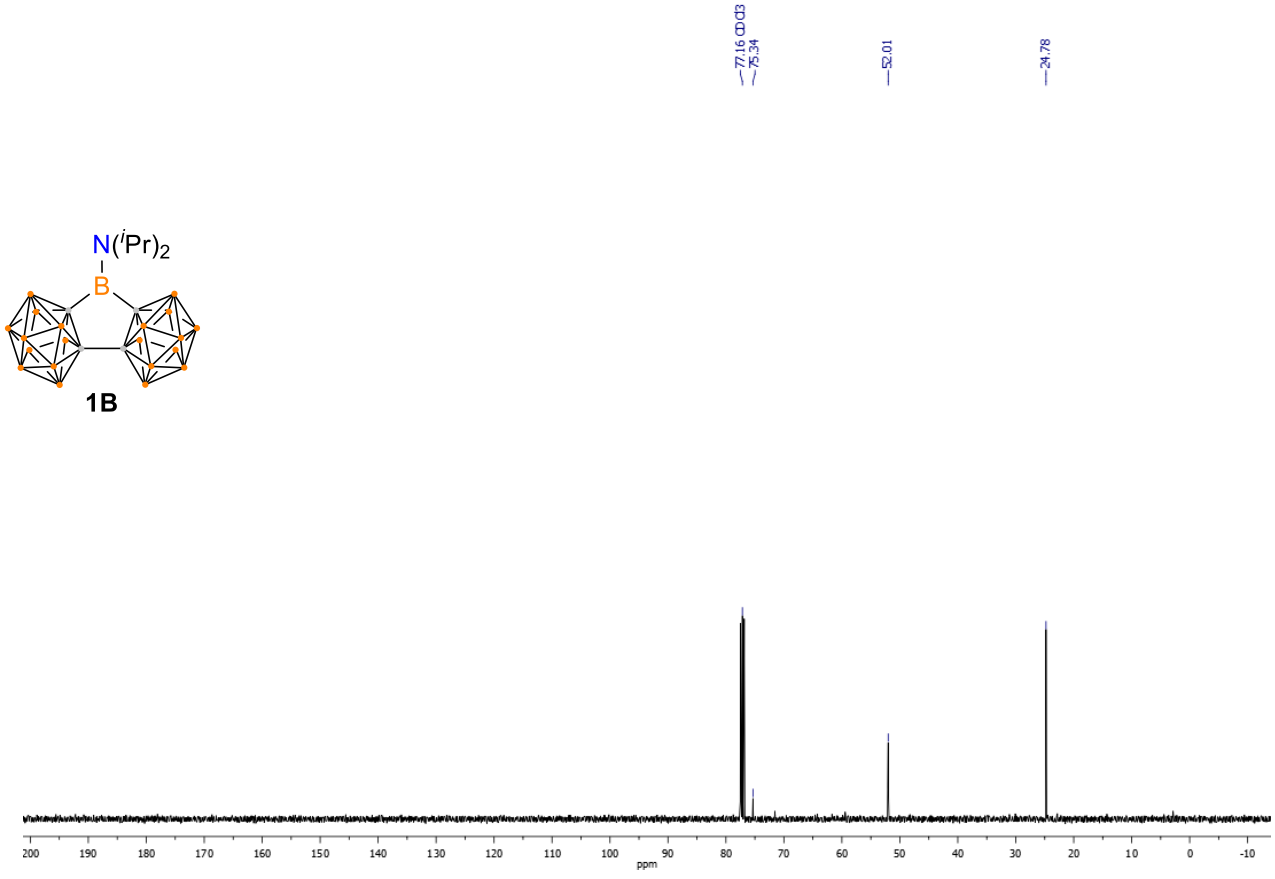


Figure S-6: Expansion of $^{13}C\{^{1}H\}$ NMR spectrum of **1B** in $CDCl_3$ (aryl region).

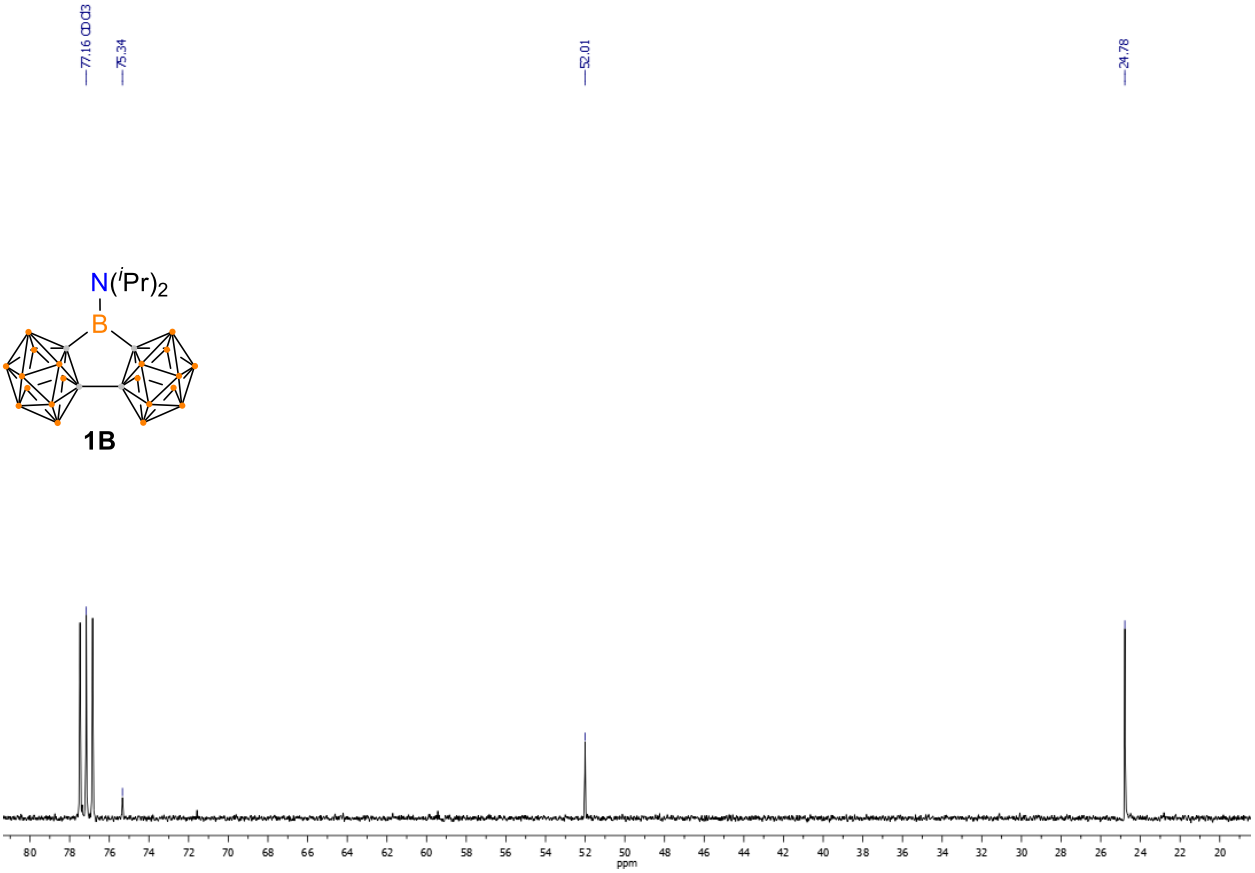


Figure S-7: ^{11}B NMR spectrum of **1B** in $CDCl_3$.

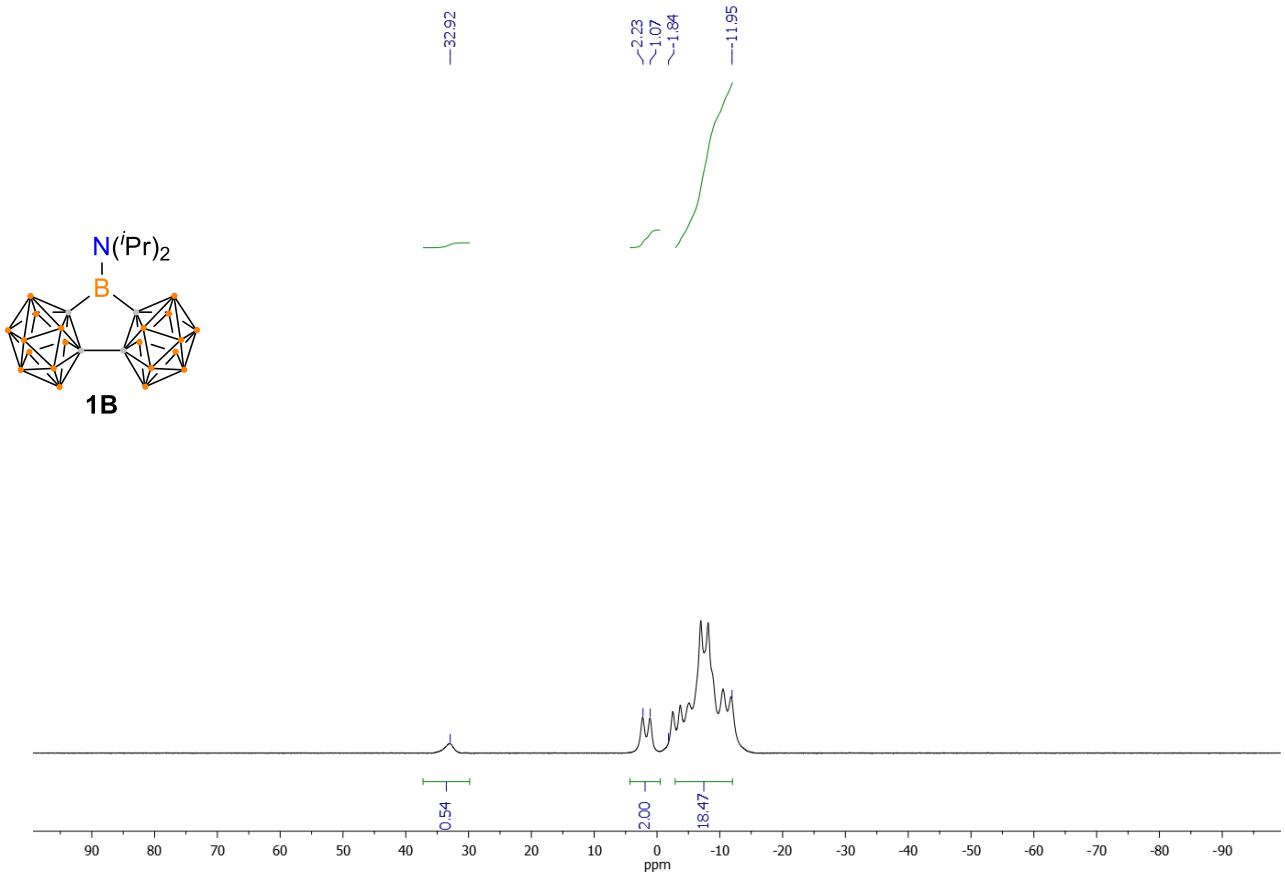


Figure S-8: $^{11}B\{^{1}H\}$ NMR spectrum of **1B** in $CDCl_3$.

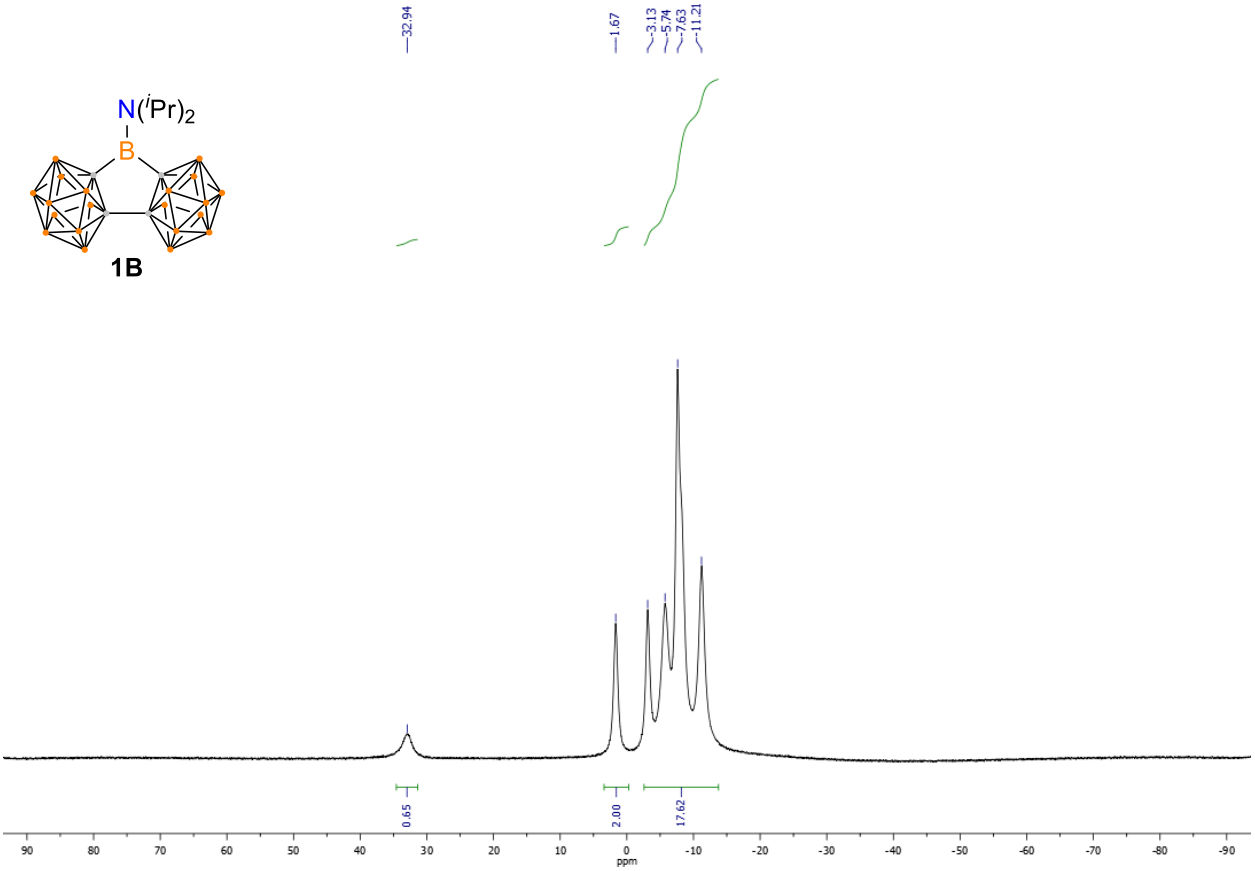


Figure S-9: FT-IR spectrum of **1B**.

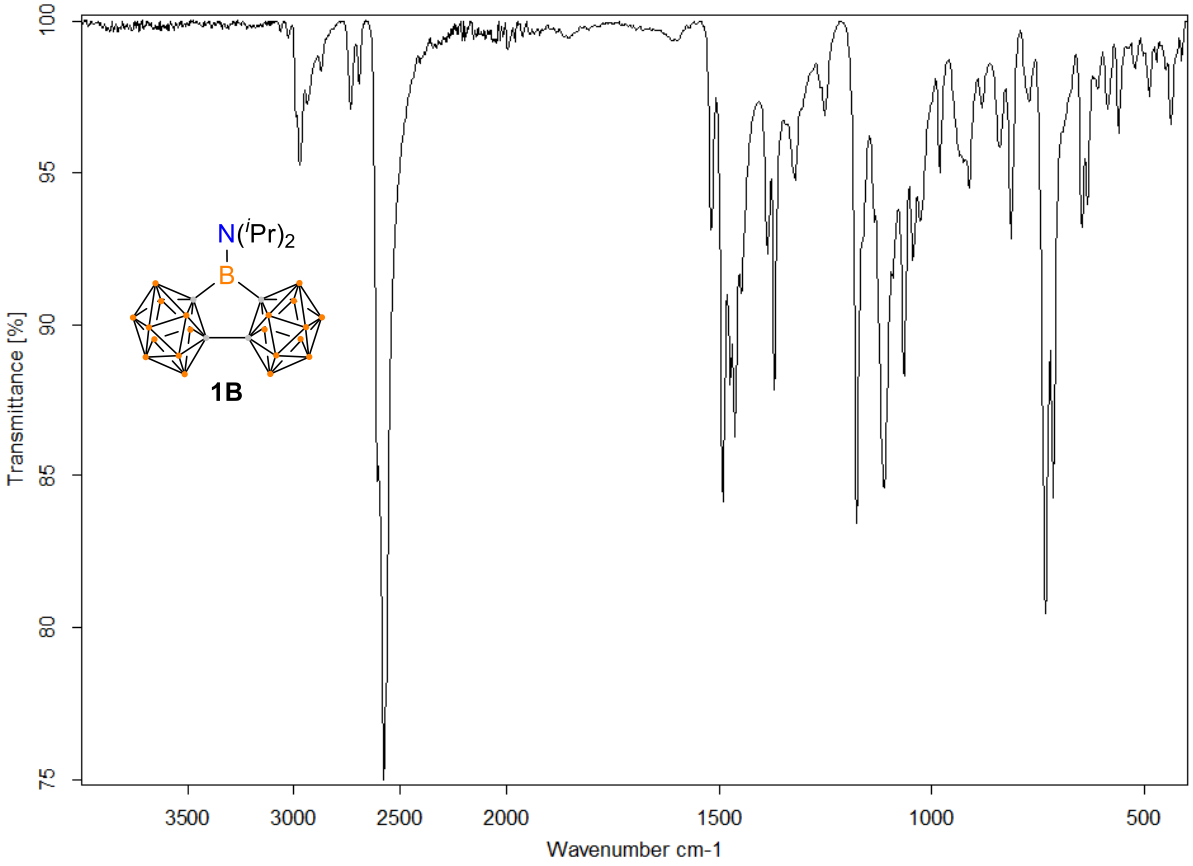


Figure S-10: ^{1}H NMR spectrum of **1BMe$_8$** in $CDCl_3$.

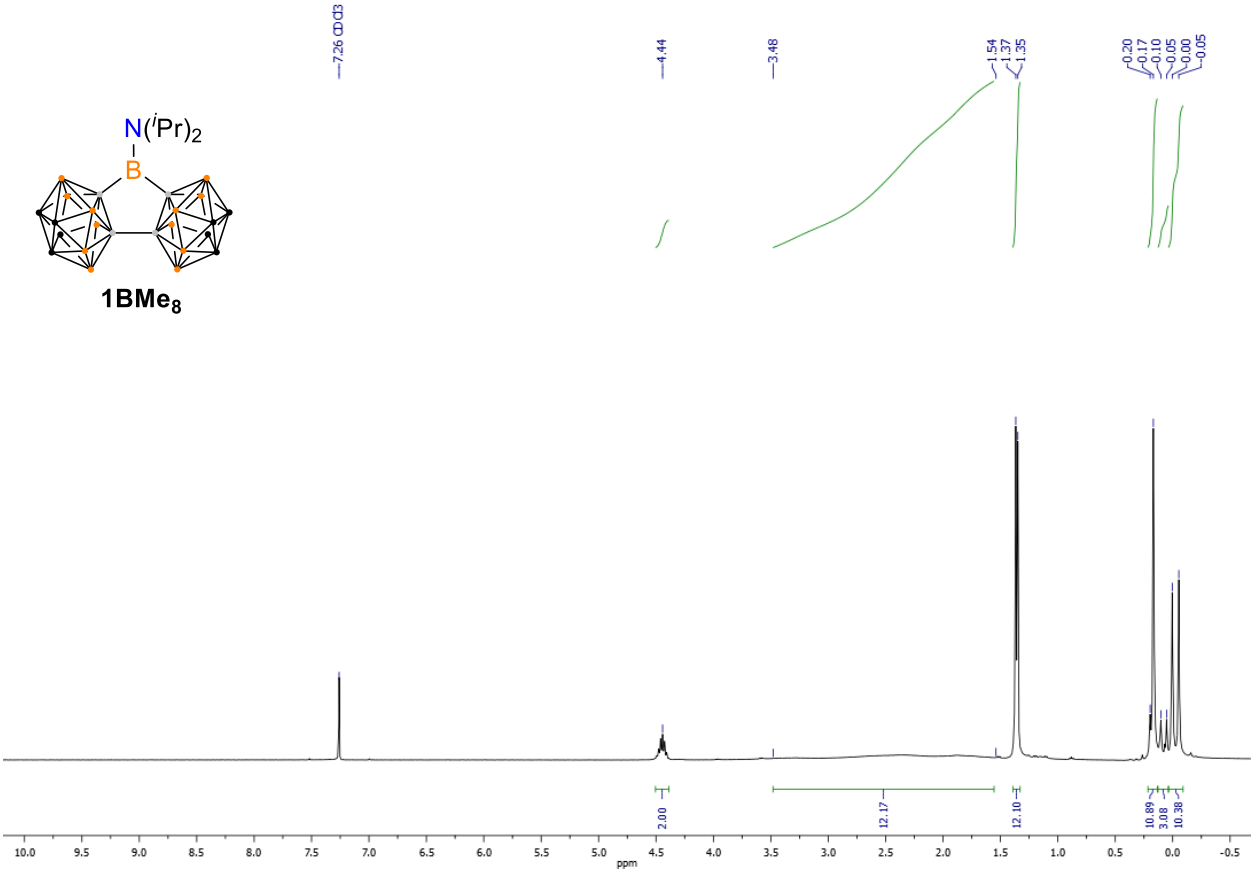


Figure S-11: Expansion of the ^{1}H NMR spectrum of **1BMe$_8$** in $CDCl_3$.

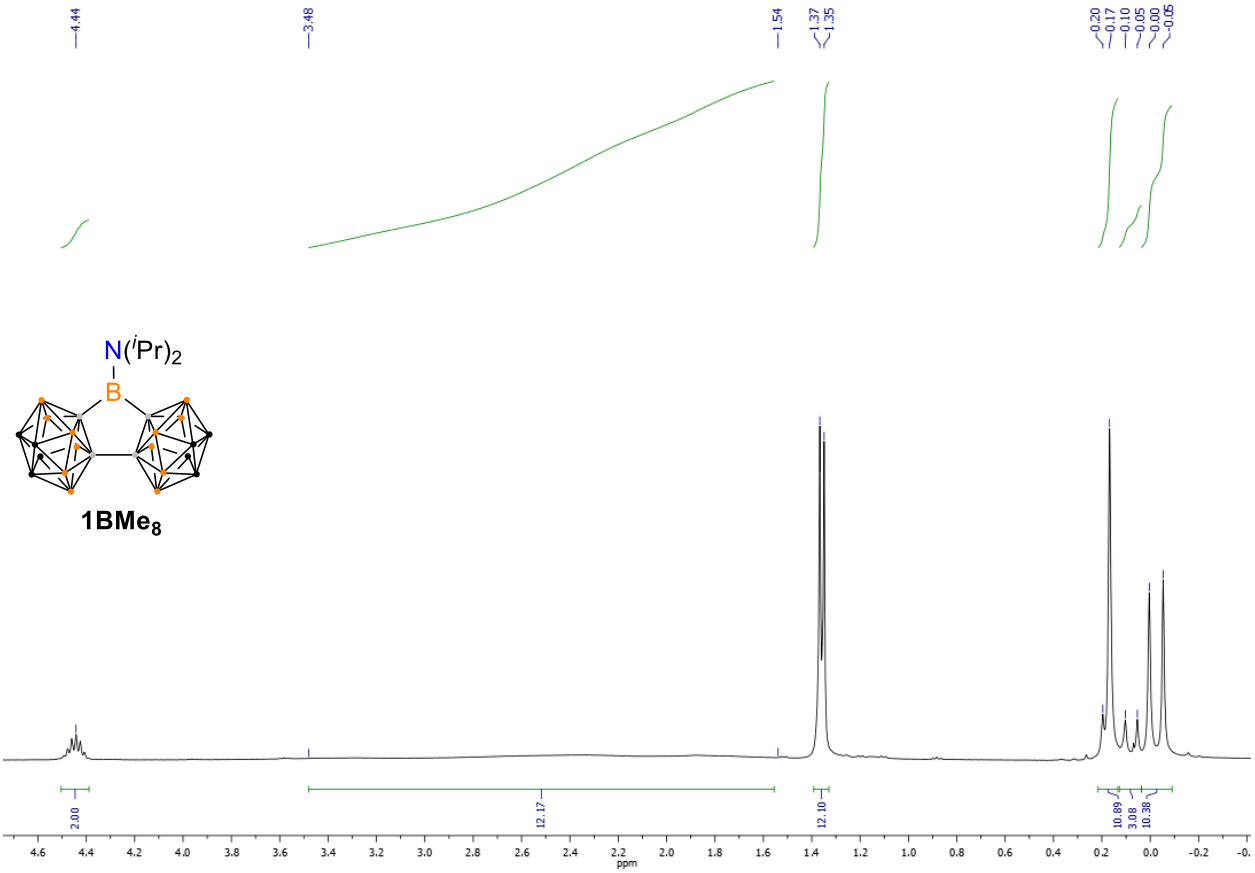


Figure S-12: $^{1}H\{^{11}B\}$ NMR spectrum of **1BMe$_8$** in $CDCl_3$.

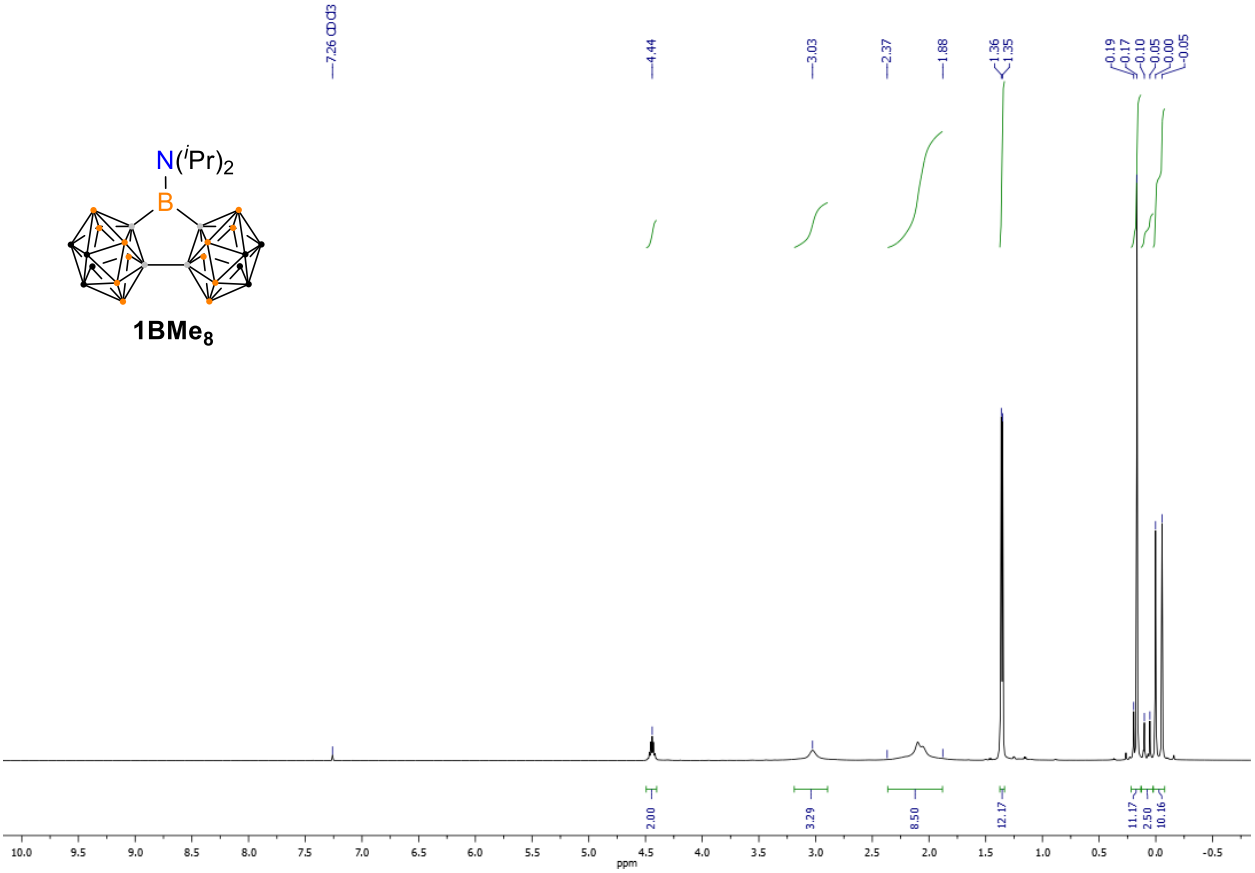


Figure S-13: Expansion of the $^{1}H\{^{11}B\}$ NMR spectrum of **1BMe$_8$** in $CDCl_3$.

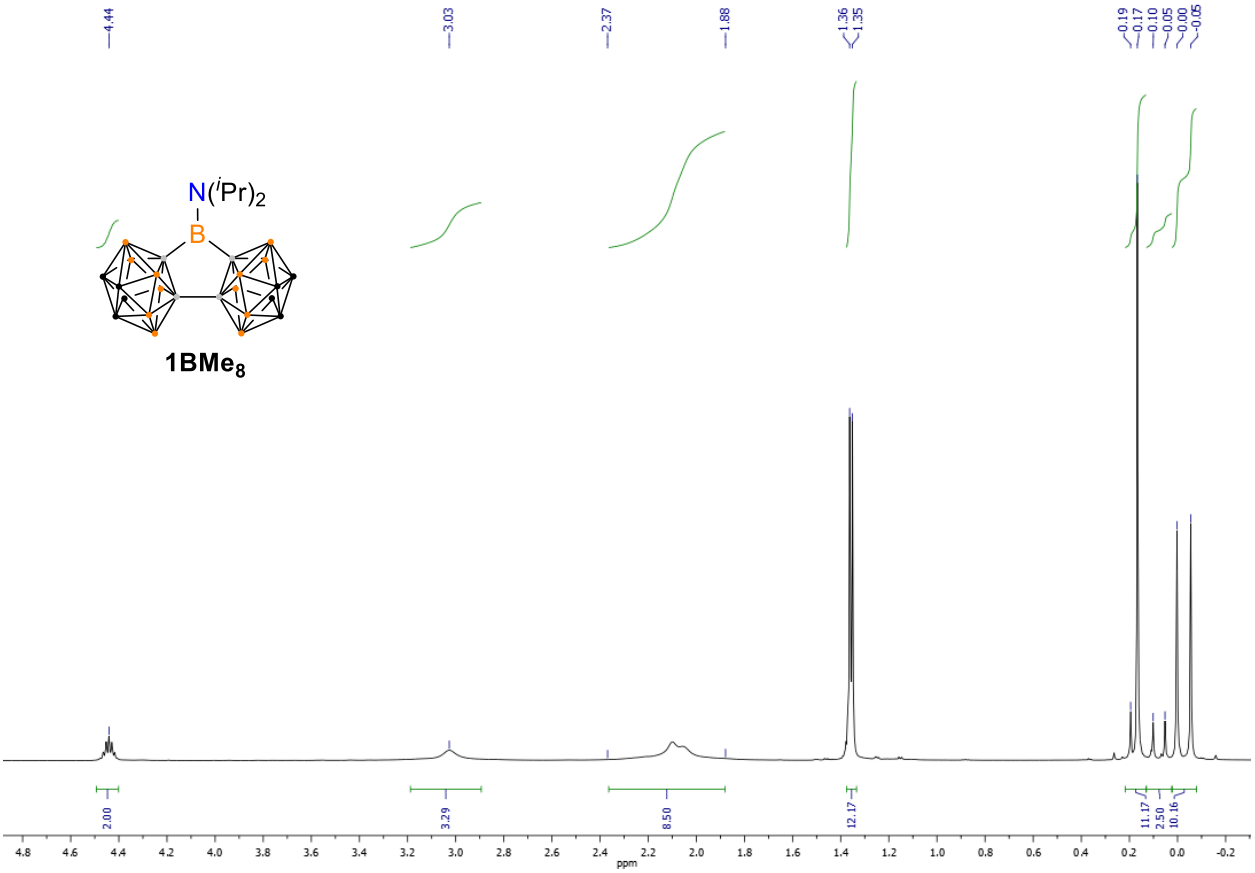


Figure S-14: $^{13}C\{^{1}H\}$ NMR spectrum of **1BMe$_8$** in $CDCl_3$.

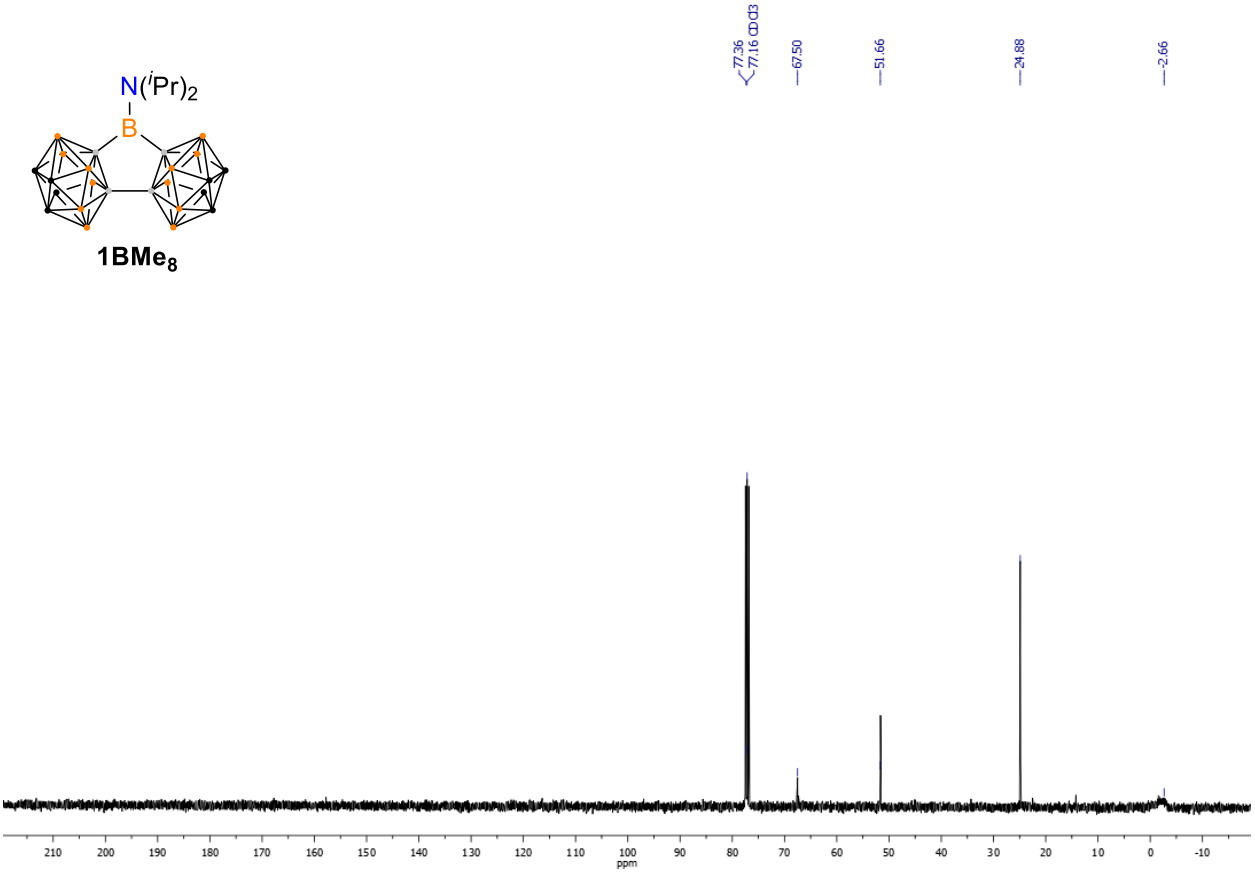


Figure S-15: Expansion of $^{13}C\{^{1}H\}$ NMR spectrum of **1BMe$_8$** in $CDCl_3$ (aryl region).

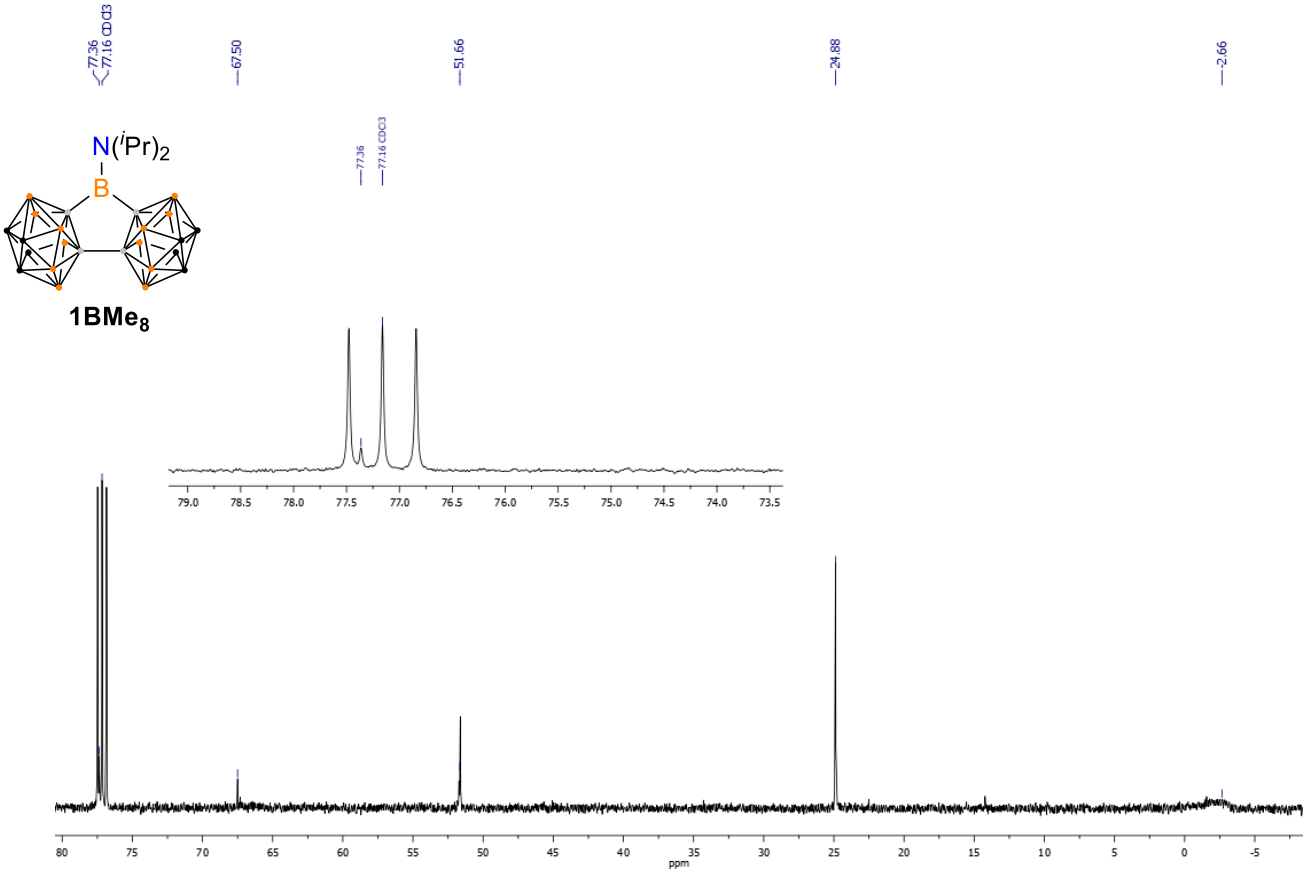


Figure S-16: ^{11}B NMR spectrum of **1BMe$_8$** in $CDCl_3$.

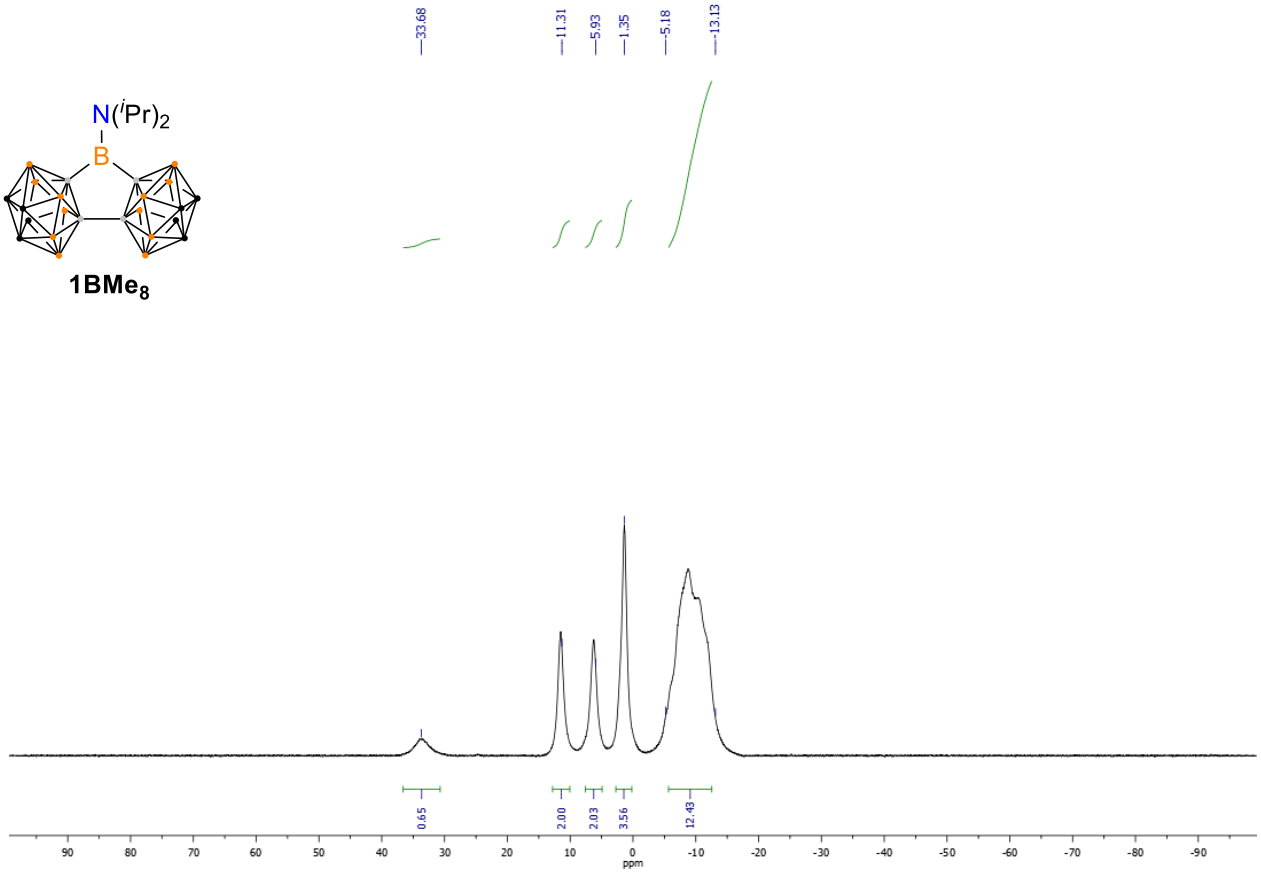


Figure S-17: $^{11}B\{^{1}H\}$ NMR spectrum of **1BMe$_8$** in $CDCl_3$.

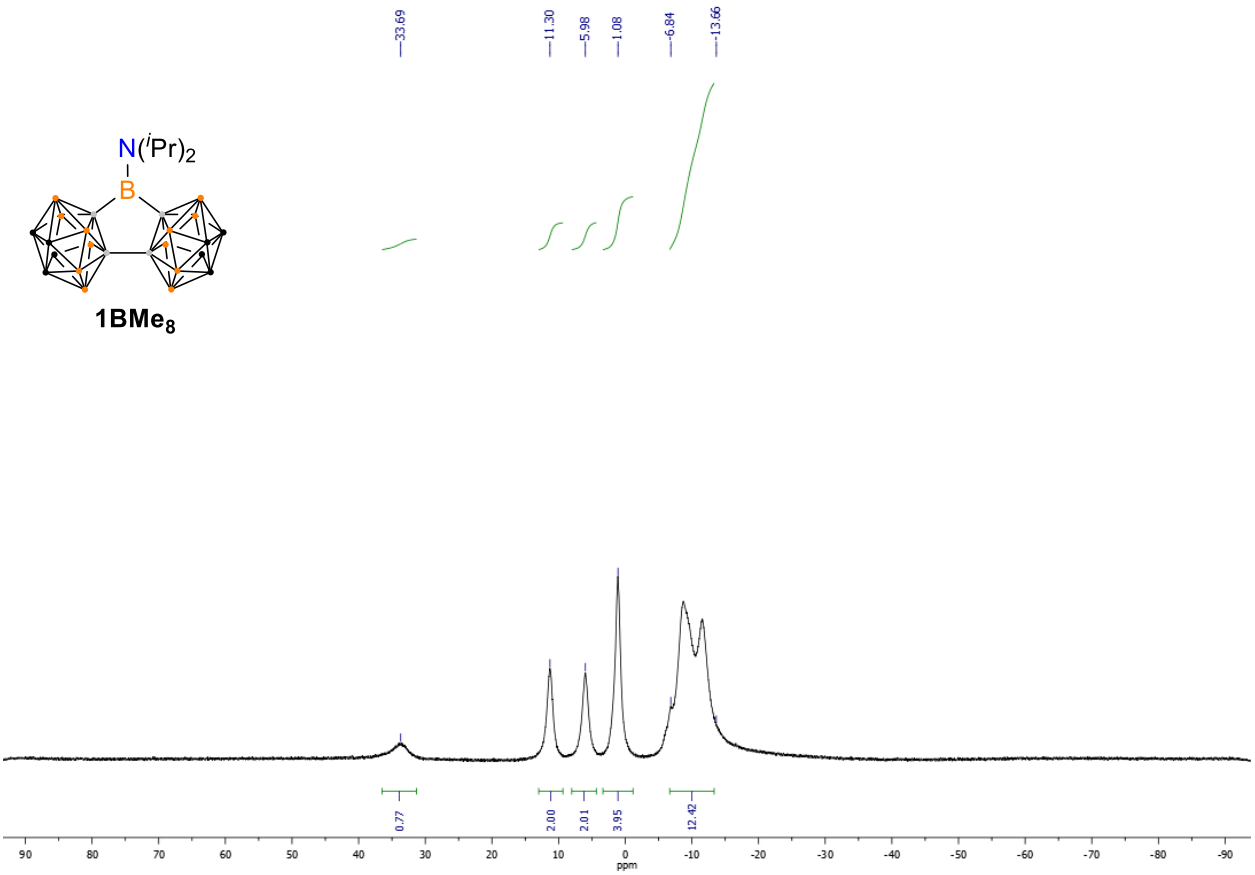
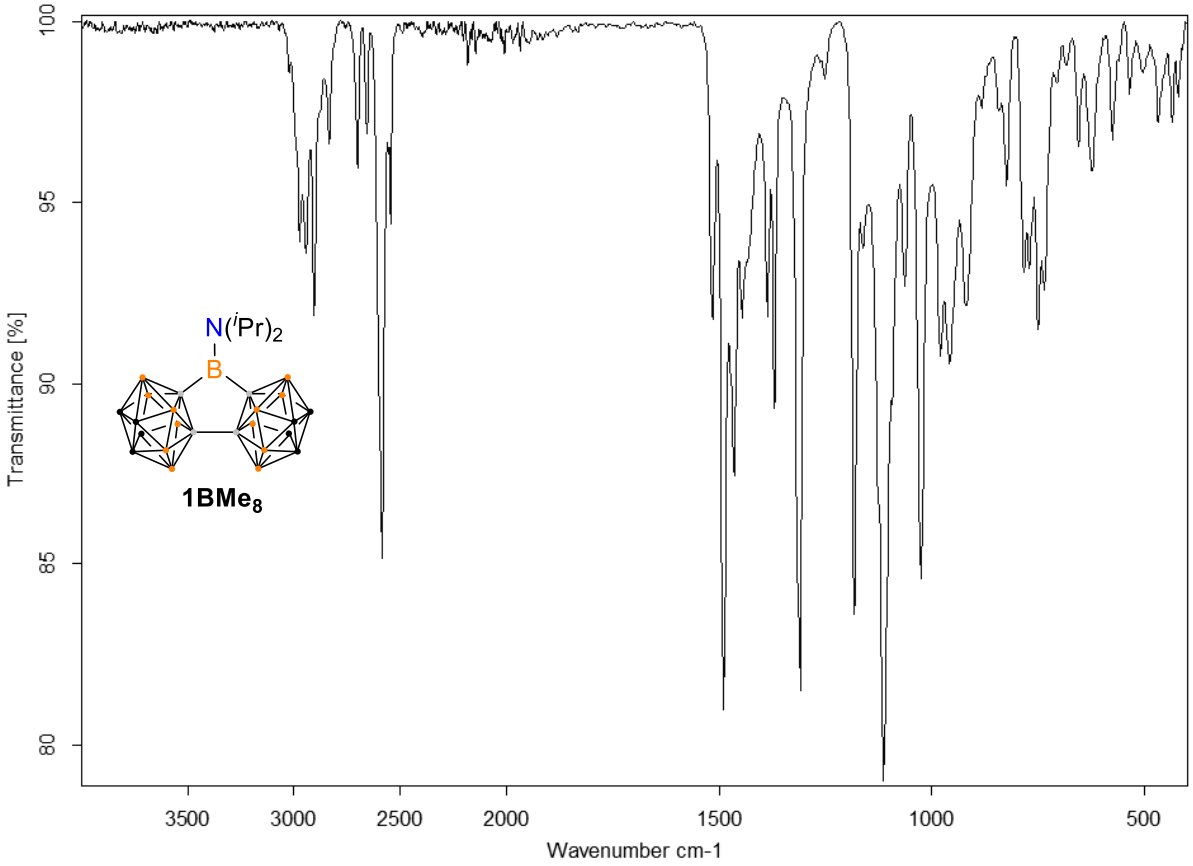


Figure S-18: FT-IR spectrum of **1BMe$_8$**.



X-ray crystallographic details

Table S-5: Crystallographic data for **1B** and **1BMe$_8$**.

	1B	**1BMe$_8$**
CCDC	1884761	1884762
Empirical formula	$C_{10}H_{34}B_{21}N$	$C_{18}H_{36}B_{21}N$
FW (g/mol)	395.39	493.49
Crystal system	Triclinic	Monoclinic
Space group	P-*1*	P 21/n
a (Å)	10.5847(11)	11.7390(7)
b (Å)	10.7181(11)	16.5577(11)
c (Å)	12.7511(13)	19.2181(13)
α (deg)	93.570(6)	90
β (deg)	109.312(5)	96.680(2)
γ (deg)	116.930(6)	90
V (Å^3)	1177.9(2)	3710.1(4)
Z	2	4
D_c (mg m^{-3})	1.115	0.883
radiation, λ (Å)	0.71073	0.71073
temp (K)	150(2)	150(2)
$R1[I>2\sigma I]^a$	0.0546	0.0988
$wR2(F^2)^a$	0.1399	0.2898
GOF (S)^a	1.055	1.048

^{a} $R1(F[\mathrm{I} > 2(\mathrm{I})]) = \sum\|\|F_o| - |F_c\|\|/ \sum |F_o|$; $wR2(F^2$ [all data]) = $[w(F_o^2 - F_c^2)^2]^{1/2}$; S(all data) = $[w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = no. of data; p = no. of parameters varied; $w = 1/[^2(F_o^2) + (aP)^2 + bP]$ where $P = (F_o^2 + 2F_c^2)/3$ and a and b are constants suggested by the refinement program.

Coordinates for geometry optimized structures of 1A, 1B, and $1BMe_8$

1A

N	-3.15442387	9.96704909	3.51892173
C	-4.66959764	11.49289484	2.20047046
H	-4.05728387	12.40166500	2.16391970
H	-5.72402248	11.79735301	2.12541361
H	-4.42709274	10.87580411	1.32575656
C	-4.45130418	10.69376783	3.49500131
H	-5.19903505	9.89283350	3.51062950
H	-0.28285940	8.50749397	4.40053722
C	-1.70343919	10.66055216	5.46245407
H	-2.36477922	11.37952211	5.96038679
H	-0.66640406	10.94106178	5.69996069
H	-1.89503190	9.66483075	5.88279547
C	-1.89970213	10.64523864	3.93825661
H	-1.10871781	10.01499179	3.51656644
C	-1.68358763	12.03084312	3.31718306
H	-1.76825976	11.99202667	2.22396841
H	-0.66904668	12.37240121	3.56626518
H	-2.38419766	12.78483337	3.69730239
C	-4.24564551	7.76634151	2.39727186
H	-3.99565604	4.49614567	1.31594564
C	-2.33916157	6.35237326	2.71610788
C	-4.73702629	11.53425415	4.74578463
H	-4.64171652	10.93152680	5.65763616
H	-5.77043694	11.90427210	4.69047495
H	-4.08118014	12.40937914	4.83328068
B	-3.11219846	8.61280649	3.12740904
C	-1.90974755	7.58287793	3.28965339
H	1.14322008	6.50974744	4.40864525
C	-1.53047539	5.21563193	2.72971871
C	-0.26840266	5.27951327	3.33277827
C	0.16555294	6.46797661	3.92511610
C	-0.65230045	7.60775466	3.90717322
H	0.37232744	4.39604815	3.34922981
H	-1.87459760	4.27979171	2.28469703
C	-3.70621868	6.46850351	2.16662363
H	-7.25320043	7.27822861	0.83299220
C	-5.52496736	8.03525336	1.89243278
C	-6.25611712	7.04920628	1.21291845
C	-5.71058864	5.77849416	1.01432804
C	-4.42574995	5.48499719	1.48693636
H	-6.28309881	5.01652713	0.48215902
H	-5.98174128	9.01895941	2.00583399

1B

N	-3.09410817	9.87831787	3.52897163
C	-3.96573152	11.60024356	1.91469165
H	-3.25782676	12.41988166	2.08546121
H	-4.91137537	12.03936405	1.56488383
H	-3.57341013	10.96111115	1.11185173
C	-4.23975472	10.77376897	3.17853963
H	-5.05239586	10.08863605	2.92074446
C	-1.85838527	7.52130179	3.18373204
C	-2.18256904	10.42304743	5.81170124
H	-2.85179991	11.23637798	6.11646680
H	-1.22516762	10.56184170	6.33469397
H	-2.61478888	9.46999108	6.14624616
C	-1.92191337	10.39660222	4.29963195
H	-1.14022161	9.64798157	4.14236127
C	-1.34685370	11.71524006	3.78124685

H	-1.11394140	11.65550752	2.71001685
H	-0.40974802	11.91812035	4.31912013
H	-2.01373321	12.57042404	3.95145969
C	-4.40418471	7.76947071	2.51294378
C	-3.91111904	6.21323127	2.27054557
C	-2.40375563	6.11243450	2.51643022
C	-4.76702994	11.62750501	4.33220983
H	-5.01208002	11.01140981	5.20712079
H	-5.69102598	12.12143109	3.99954496
H	-4.06725789	12.41598399	4.63810993
B	-3.11632236	8.54841725	3.12515463
B	-1.40214875	7.17582377	1.55448123
H	-1.86225194	7.85617459	0.71183452
B	-1.24161592	5.41480358	1.46928513
H	-1.63538767	4.85428385	0.49843056
B	0.11413482	4.97576239	2.53571366
H	0.80092076	4.03413829	2.28876912
B	-5.70945629	8.13948754	1.42803014
H	-5.78477559	9.24438389	0.99282938
B	-4.37031579	7.14641420	0.88159980
H	-3.56534177	7.53052337	0.11615316
B	-5.10328403	5.08409876	2.75616646
H	-4.73690888	4.06262083	3.23965301
B	-4.79163158	5.43294238	1.03996737
H	-4.21363807	4.64757593	0.36141332
B	-5.99246125	6.64208957	0.49838301
H	-6.33813403	6.68616102	-0.64104299
B	-7.03550446	7.03975138	1.87266116
H	-8.17129767	7.37163950	1.73087408
B	-6.03037860	7.78801569	3.12250360
H	-6.31927279	8.64634771	3.89519162
B	-4.88782272	6.58187428	3.67405759
H	-4.41371725	6.65669358	4.74840377
B	-6.50163839	6.07632634	3.26697193
H	-7.21697633	5.71153172	4.14710972
B	-6.46322007	5.36219415	1.64161251
H	-7.18203728	4.46653106	1.32412901
B	-0.22687057	7.82719247	2.67367950
H	0.09546307	8.96152158	2.51135917
B	0.19176238	6.47548322	1.59022631
H	0.90406203	6.64286975	0.65000451
B	0.74306190	6.47373367	3.27781008
H	1.88728817	6.63329988	3.57006745
B	-1.55986222	4.74866356	3.08905090
H	-2.16882039	3.73675501	3.21689112
B	-1.92843084	6.09332877	4.18310100
H	-2.72700318	6.00821962	5.04098291
B	-0.55190947	7.17639727	4.27676970
H	-0.44708903	7.84313407	5.25704110
B	-0.32720558	5.40782072	4.20299034
H	0.00817974	4.79474662	5.16802831

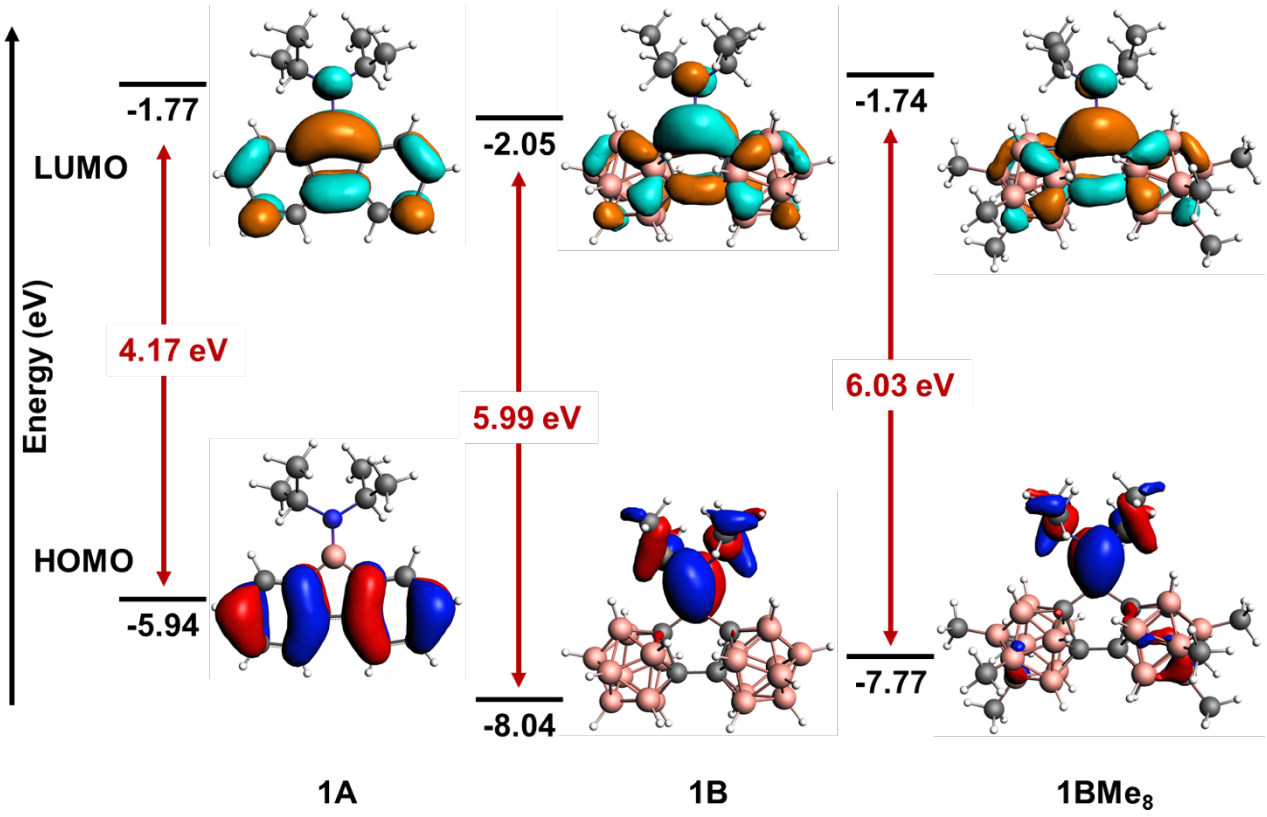
1BMe$_8$

C	6.09095469	11.53162286	6.08272552
H	5.98560440	10.71504617	6.81280457
H	5.53554744	11.22968664	5.18226660
H	5.57981736	12.41030273	6.50354531
C	9.55272085	12.74482404	3.92748528
B	10.32197462	13.09624643	2.54466266
C	11.91932554	13.12135162	2.81675292
C	15.88988002	14.11278773	1.67284181
H	15.92481090	13.49744698	0.76131789
H	16.85268141	13.97677311	2.18787036
H	15.83763324	15.16456315	1.35386409

C	15.54142478	10.89932746	2.99805188	B	14.66420358	13.71176358	2.60330076
H	15.22395227	9.93943153	3.43089082	B	14.49076562	12.06172856	3.27181544
H	16.52259911	11.14467737	3.43144077	B	14.80496298	13.44301983	4.38198800
H	15.69607534	10.73977321	1.92074225	B	13.24872801	13.90697480	5.12333057
C	12.09414801	12.85657342	4.43891106	H	13.06306823	14.30695641	6.22850554
C	10.74526781	12.46503623	5.03646309	B	13.91482687	14.86832165	3.75719599
C	8.70752649	10.92889381	8.38566397	B	13.03166623	14.33770919	2.29562039
H	9.00536457	11.64116976	9.16963393	H	12.68360536	15.07143030	1.42270878
H	9.27799903	10.00343970	8.55422148	B	12.78012476	11.69830038	3.35218874
H	7.64556846	10.69213467	8.55136201	H	12.30632462	10.62805517	3.23196091
C	8.39926618	8.96750641	5.48790848	B	13.60944284	12.19999011	4.82779241
H	7.72672238	8.70098950	4.65918606	H	13.66751215	11.42796386	5.73109634
H	7.87805644	8.71293755	6.42292284	B	12.20910421	14.49076441	3.82443472
H	9.28111509	8.31371909	5.41944953	H	11.32249535	15.25672565	3.95070055
C	7.82569527	14.21555833	7.52326889	B	9.66051003	13.78223868	5.32713314
H	7.33368324	13.67643816	8.34657082	H	10.02146984	14.89707162	5.22165606
H	7.05752462	14.83402692	7.03545617	B	8.49950973	13.20187973	6.49983101
H	8.55973386	14.89976381	7.97347730	B	10.22627883	12.72972998	6.62740825
N	9.71035578	13.32993777	1.31719788	H	11.01189919	13.16959403	7.40512865
C	14.41324791	16.36560372	3.95357059	B	8.95531541	11.51744067	6.93076672
H	14.52177573	16.61838556	5.01863838	B	10.40758434	11.08814129	5.98657876
H	13.72014454	17.09684161	3.51216019	H	11.31764333	10.39962600	6.32370584
H	15.39579431	16.52122359	3.48356592	B	9.94602354	11.10465877	4.28435608
C	16.17183024	13.59076585	5.17970473	H	10.46924739	10.48311423	3.43107585
H	16.08681494	14.32478849	5.99485502	B	8.79203094	10.50784975	5.45572686
H	16.99106790	13.92801558	4.52703815	B	8.10784132	13.22204124	4.75256303
H	16.48670576	12.63884110	5.63255864	H	7.39221374	14.02288381	4.23511894
B	7.61915939	11.83059768	5.75957310	C	10.54275904	13.35118706	0.07585189
B	8.28072166	11.59146033	4.13088606	C	10.25890149	14.51578732	-0.87354280
H	7.69823886	11.22549604	3.15716260	C	10.54256138	11.99574226	-0.64426849
B	13.36673514	12.64233047	2.00201391	C	7.50517910	12.69832858	0.21138749
H	13.28358033	12.16289836	0.91395896	C	7.85628964	15.02707842	1.18373320

C	8.23268377	13.54090260	1.25970747	H	7.74702290	11.63291918	0.31986900
H	11.56477257	13.50288150	0.43523999	H	7.72774684	13.00890176	-0.81785875
H	9.28255514	14.43718847	-1.36936444	H	6.78520421	15.13525918	1.40888930
H	11.02719689	14.51318671	-1.66003393	H	8.03694273	15.46422400	0.19460007
H	10.31533720	15.47969890	-0.35137269	H	8.41823854	15.60512770	1.93011656
H	10.74242519	11.18218336	0.06659331	H	7.87030805	13.18989069	2.23040274
H	11.34384606	11.99077779	-1.39770468				
H	9.59626143	11.78593400	-1.15745679				
H	6.42279248	12.81597476	0.36279734				

Figure S-19: HOMO and LUMO diagrams for **1A**, **1B**, and **1BMe$_8$**.



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