Supporting Information for:

Hydroboration without a B-H Bond: Reactions of The Borenium Cation, $[(i\mathrm{Pr}_2\mathrm{N})_2\mathrm{B}]^+$ with Alkyne, Nitrile, Ketone and Diazomethane

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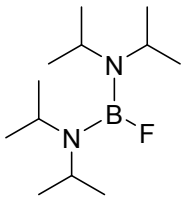
Materials and Methods

General Considerations
All reactions and work-up procedures were performed under an inert atmosphere of dry, oxygen-free nitrogen using standard Schlenk techniques or a glovebox (Vac, equipped with a -35 °C freezer) unless otherwise specified. Pentane, diethyl ether, dichloromethane, and toluene (Aldrich) were dried using a Grubbs-type Innovative Technologies solvent purification system. Chloroform-*d1* ($CDCl_3$) was purchased from Cambridge Isotope Laboratories, Inc. and stored over activated 4Å molecular sieves prior to use, unless otherwise specified. BCl_3 (1M in hexane) was purchased from Acros Organics. $[CPh_3][B(C_6F_5)_4]$ was purchased from Boulder Scientific Company. Phenylacetylene, phenylacetylene-*d1*, benzophenone, *n*-BuLi (2.5 M in hexane), boron trifluoride diethyl etherate, triethylsilane, diisopropylamine and benzonitrile were purchased from Sigma-Aldrich. Lithium diisopropylamide (LDA) was freshly prepared from an equimolar mixture of *n*-BuLi and diisopropylamine in hexanes. $[SiEt_3][B(C_6F_5)_4]$ was freshly prepared as a toluene adduct by a literature procedure.[1]

NMR spectra were obtained on a Bruker Avance III 400 MHz, Agilent DD2 500 MHz, or Agilent DD2 600 MHz spectrometer and spectra were referenced to residual solvent of $CDCl_3$ (^1H = 7.26; ^{13}C = 77.2), or externally (^{11}B, $(Et_2O)BF_3$; ^{19}F, $CFCl_3$). Chemical shifts (δ) are reported in ppm and coupling constants are listed in Hz. Complete assignment of the ^1H and $^{13}C\{^1H\}$ NMR spectra for compounds **2**, **2-d$_1$**, **3**, **4**, and **5** was accomplished using 2D NMR techniques (COSY, HSQC, HMBC) and by comparison of the experimentally observed chemical shifts with computed values. High-resolution mass spectra (HRMS) were obtained on an Agilent 6538 Q-TOF (ESI). Elemental analysis was unavailable.

Synthesis and Characterization

$((i\text{-}Pr)_2N)_2BF$



A cold (-35oC) solution of lithium diisopropylamine (283.0 mg, 2.64 mmol) in 5 mL Et2O was added to a cold (308K) solution of BF3OEt2 (0.31 mL, 2.6 mmol in 10 mL pentane). This was stirred overnight before filtering to remove eliminated LiF. The solvent was removed from the filtrate in vacuo and the product was recrystalized from cold pentane. Yield: 266.9 mg (1.16 mmol, 88%).

1H NMR (400 MHz, C6D6): δ 2.98 (hept, 3JH-H = 6 Hz, 4H, NCH(CH3)2), 0.96 (d, 3JH-H = 7 Hz, 24H, NCH(CH3)2). 11B NMR (128 MHz, C6D6) δ 25 (br, FBN2). 13C{1H} NMR (101 MHz, C6D6): δ 45.2 (s, 8C, NCH(CH3)2), 23.7 (s, 8C, NCH(CH3)2). 19F{1H} NMR (377 MHz, C6D6): δ -109.1 (br, FBN2).

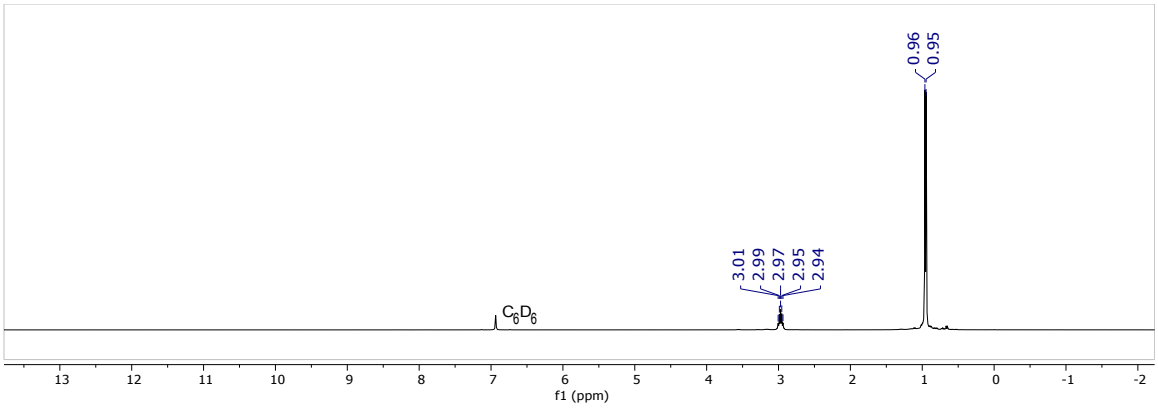


Figure S1. ^{1}H NMR (400 MHz) spectrum of $((i\text{-Pr})_2\text{N})_2\text{BF}$ in $CDCl_3$ at 298 K.

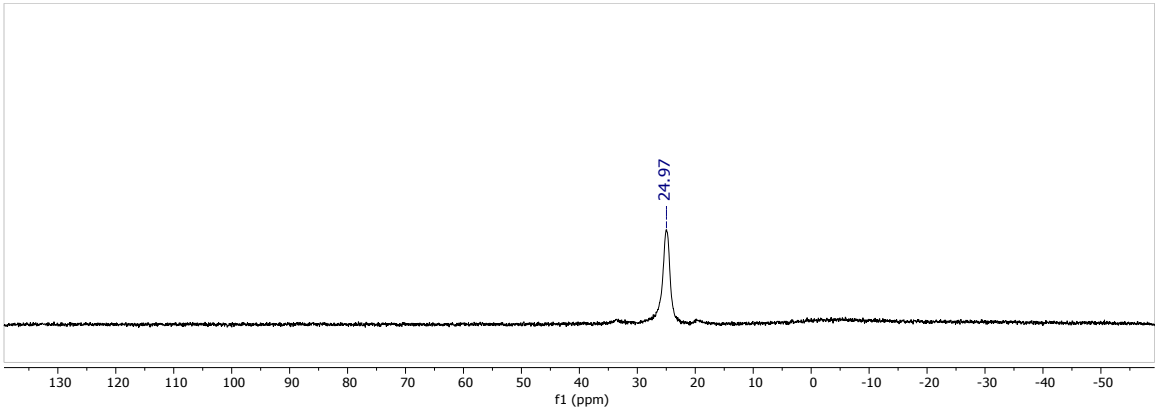


Figure S2. ^{11}B NMR (128 MHz) spectrum of $((i\text{-Pr})_2\text{N})_2\text{BF}$ in $CDCl_3$ at 298 K.

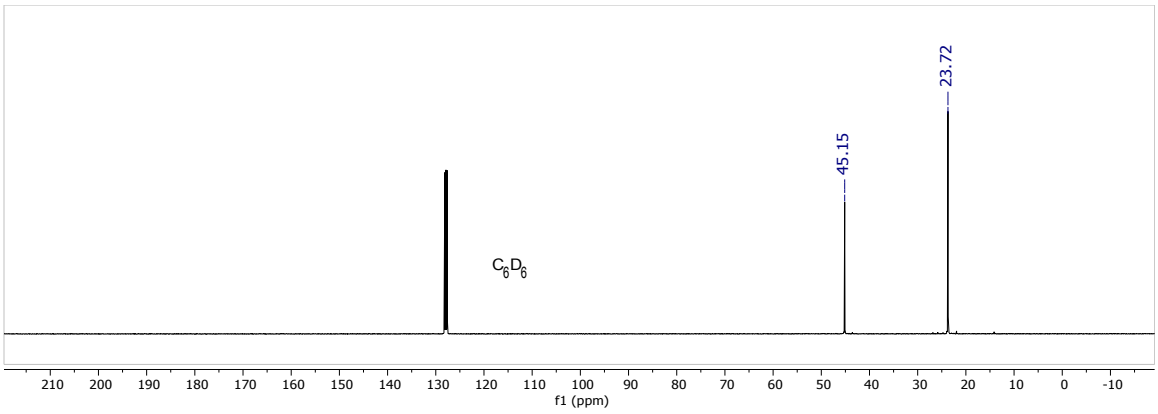


Figure S3. ^{13}C{^{1}H} NMR (101 MHz) spectrum of $((i\text{-Pr})_2\text{N})_2\text{BF}$ in $CDCl_3$ at 298 K.

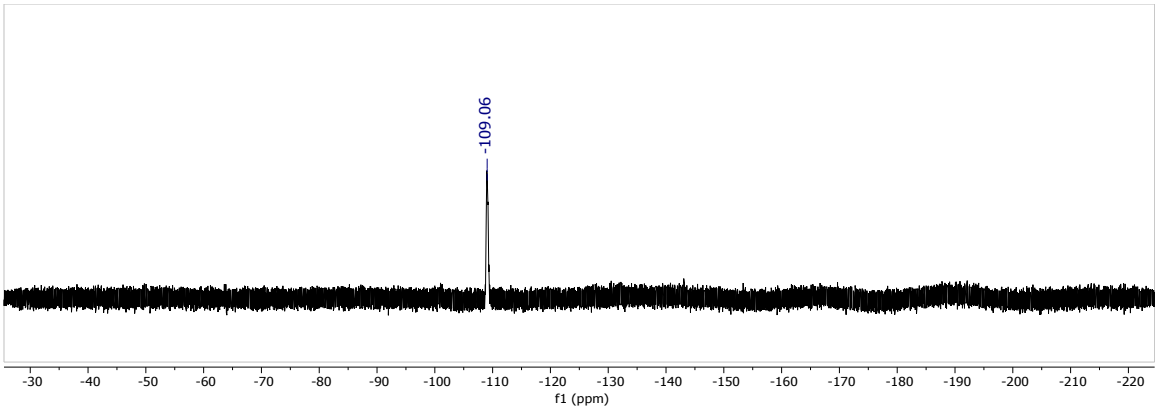
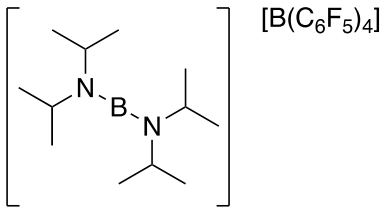


Figure S4. $^{19}F\{^{1}H\}$ NMR (377 MHz) spectrum of $((i\text{-Pr})_2N)_2BF$ in $CDCl_3$ at 298 K.

Compound 1: $[((i\text{-Pr})_2N)_2B][B(C_6F_5)_4]$
To a solution of $(i\text{-Pr})_2BF$ (90.5 mg, 0.393 mmol) in 5 mL toluene was added to a solution of $[Et_3Si(tol)][B(C_6F_5)_4]\bullet tol$ (344.8 mg, 0.389 mmol) in 1 mL 1,2-difluorobenzene. After stirring 1 hour, 10 mL of pentane was added to the vial. The resultant beige powder was washed with 3 x 3 mL aliquots of pentane. Yield: 318.3 mg (0.3576 mmol, 92%). ^{1}H and ^{11}B NMR data match previously reported values.[2]



^{1}H NMR (500 MHz, 298 K, $CDCl_3$) δ 3.54 (sept, $^{3}J_{H\text{-}H}$ = 7 Hz, 4H, methine-H), 1.39 (d, $^{3}J_{H\text{-}H}$ = 7 Hz, 24H, methyl-H). ^{11}B NMR (128 MHz, 298 K, $CDCl_3$) δ 37.32 (s, br, $[(R_2N)_2B]^{+}$), -16.65 (s, $[B(C_6F_5)_4]^{-}$). $^{13}C\{^{1}H\}$ NMR (126 MHz, 298 K, $CDCl_3$) δ 148.1 (d, $^{1}J_{C\text{-}F}$ = 241 Hz), 138.1 (d, $^{1}J_{C\text{-}F}$ = 245 Hz), 136.2 (d, $^{1}J_{C\text{-}F}$ = 241), 51.7 (s, methine-C), 23.1 (s, methyl-C). $^{19}F\{^{1}H\}$ NMR (377 MHz, $CDCl_3$) δ -132.6 (m, br, *o*-(C_6F_5)), -163.1 (m, br, 1F, *p*-(C_6F_5)), -166.9 (m, br, 2F, *m*-(C_6F_5)). ^{15}N NMR (51 MHz, $CDCl_3$) δ 132.8.

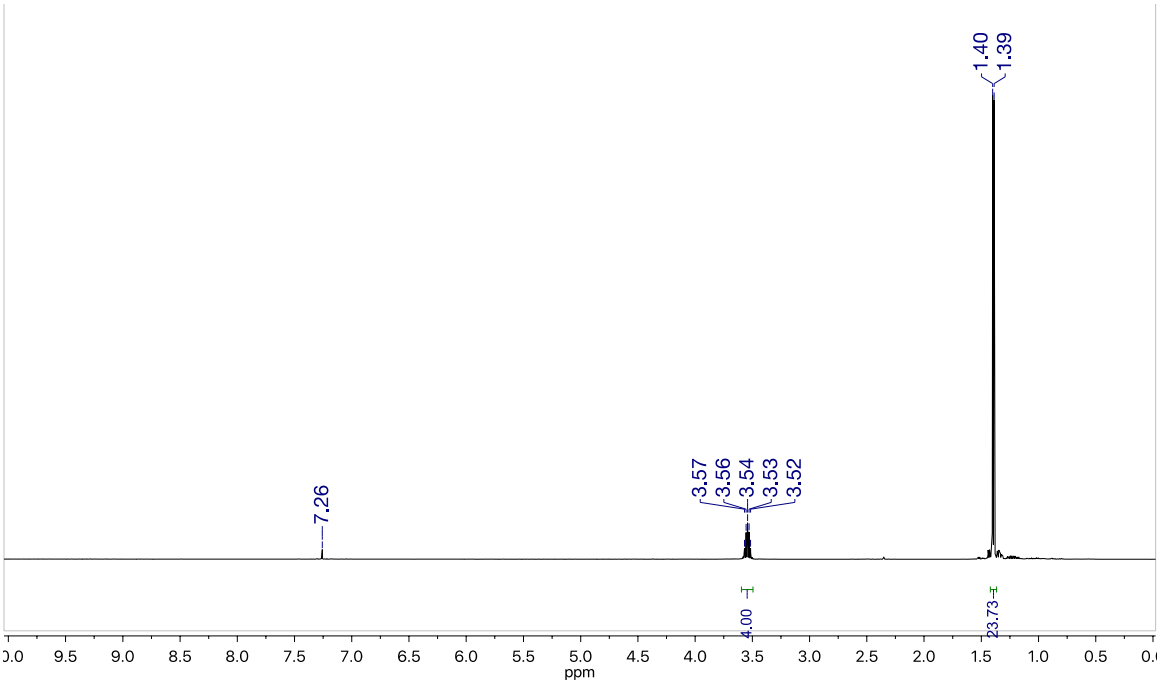


Figure S5. ^{1}H NMR (500 MHz) spectrum of **1** in $CDCl_3$ at 298 K.

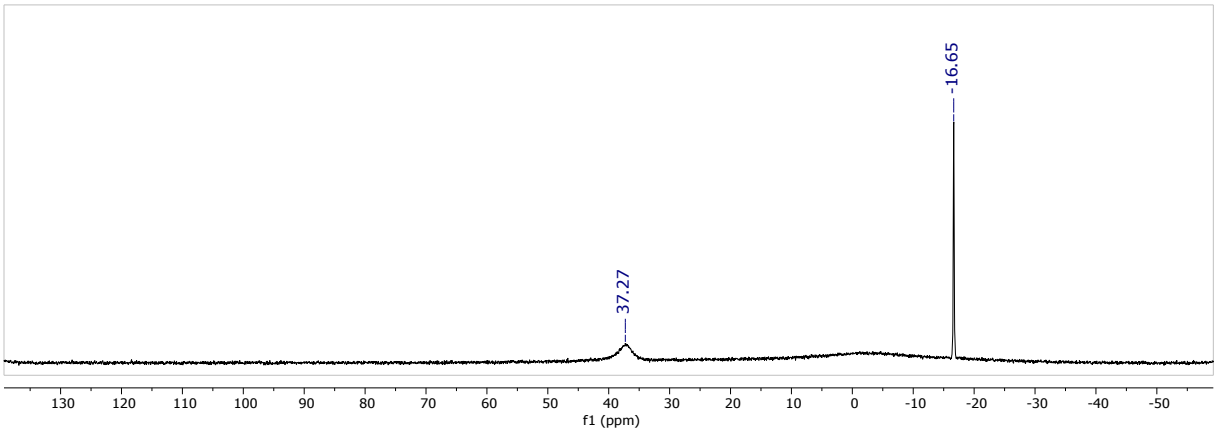


Figure S6. ^{11}B NMR (128 MHz) of **1** in $CDCl_3$ at 298 K.

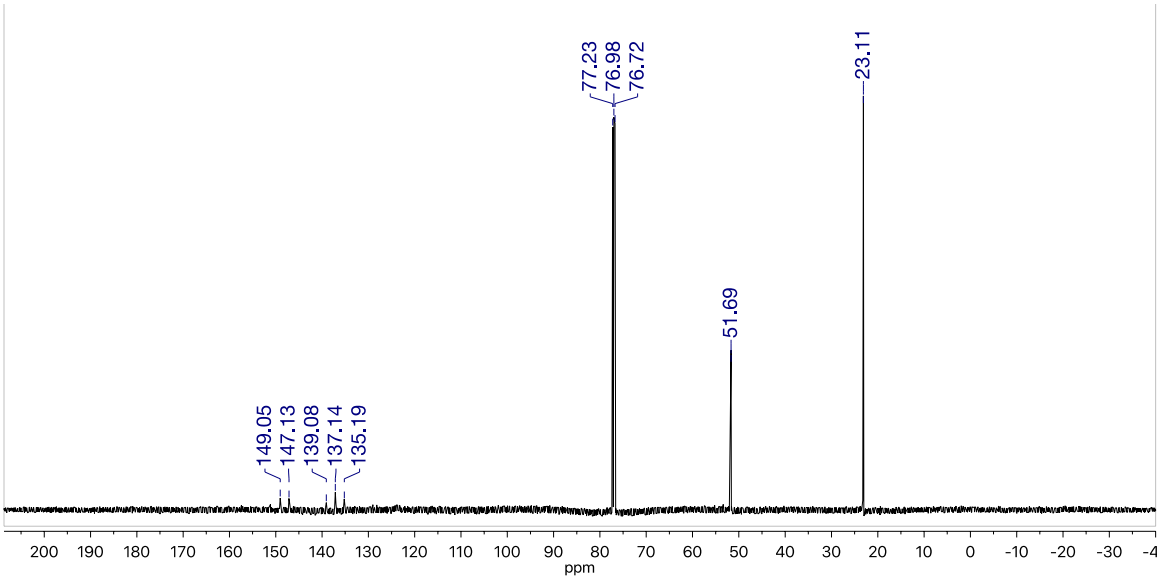


Figure S7. $^{13}C\{^{1}H\}$ NMR (126 MHz) spectrum of **1** in $CDCl_3$ at 298 K.

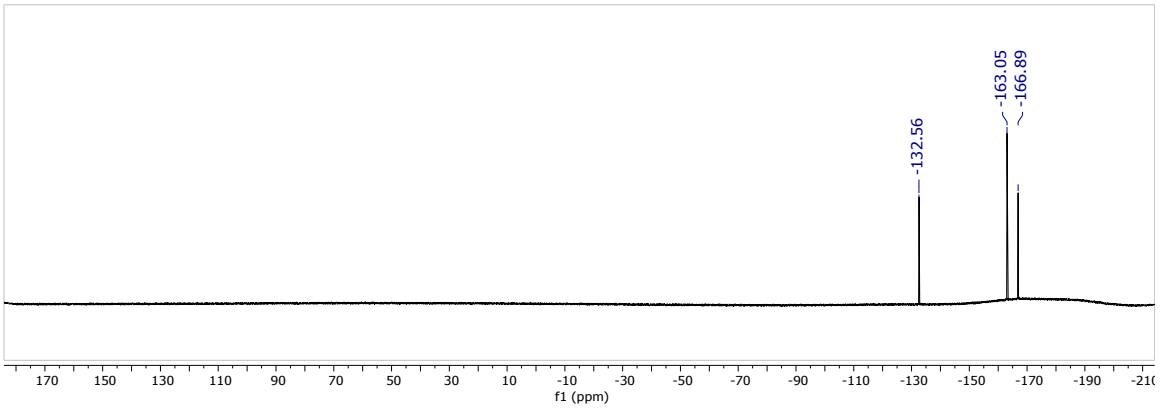


Figure S8. $^{19}F\{^{1}H\}$ NMR (377 MHz) spectrum of **1** in $CDCl_3$ at 298 K.

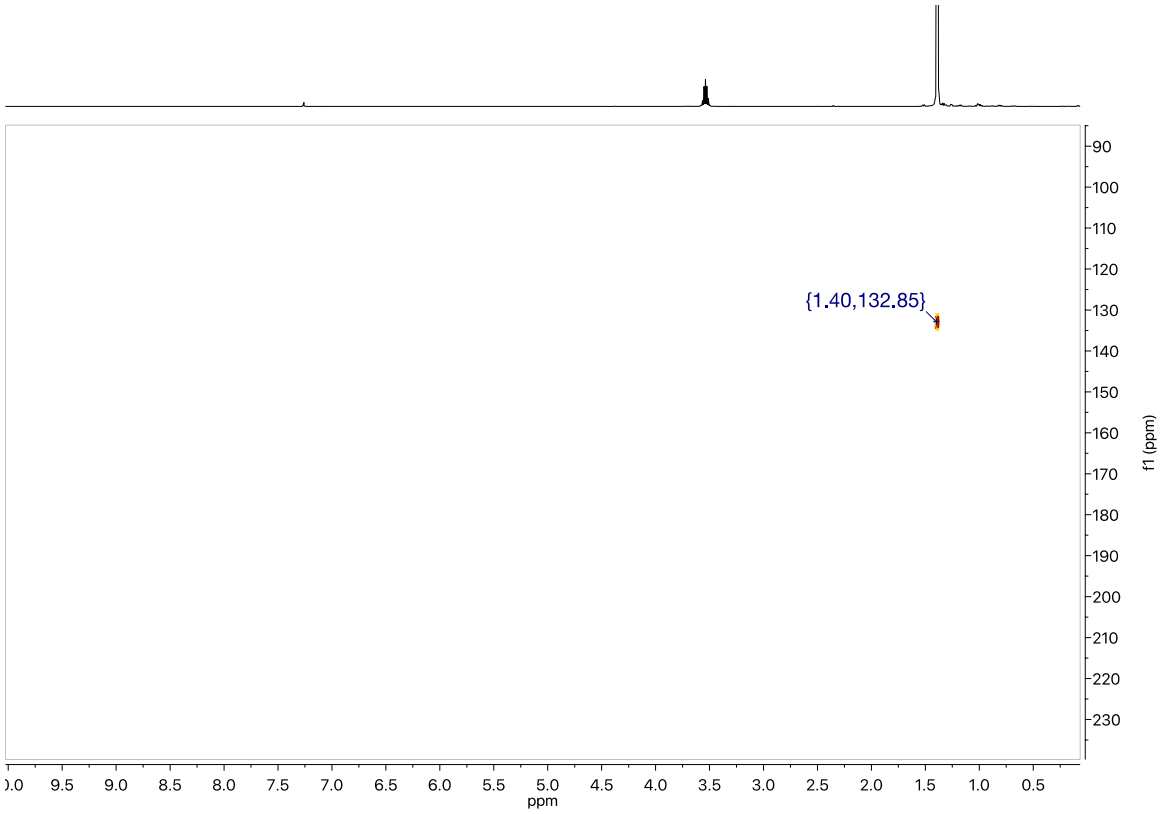
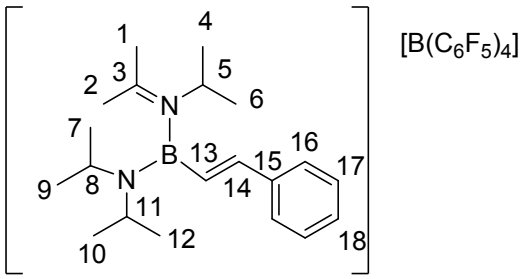


Figure S9. ^{1}H-^{15}N HSQC (500 MHz) of **1** in $CDCl_3$ at 298K.

Reactions of 1:
Compounds **2-5** were prepared in analogous fashion and thus only one preparation is detailed.

Compound 2: $[C_{20}H_{34}BN_2][B(C_6F_5)_4]$, Hydroboration of phenylacetylene
Under inert atmosphere, **1** was dissolved in 0.15 mL chloroform and added to a stirred solution of phenylacetylene in 0.15 mL chloroform. After 1 h, multinuclear NMR spectroscopy was performed on the sample. There is some remaining unconsumed phenylacetylene, as evident in the ^{1}H NMR data, which accounts for the unusually high integration in the aromatic region. The multiplet from 1.54 – 1.48 ppm corresponds to three overlapping methyl-^{1}H signals. This prevented the assignment of ^{13}C NMR shifts for *iso*-propyl-methyl groups by conventional 2D heteronuclear NMR techniques.



^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ 7.57 – 7.32 (m, 5H, $H_{16, 17, 18}$), 6.85 (d, $^{3}J_{H\text{-}H}$ = 18 Hz, 1H, H_{13}), 6.51 (d, $^{3}J_{H\text{-}H}$ = 18 Hz, 1H, H_{14}), 4.37 (hept, $^{3}J_{H\text{-}H}$ = 7 Hz, 1H, H_5), 3.64 (hept, $^{3}J_{H\text{-}H}$ = 7 Hz, 1H, H_{11}), 3.43 (hept, $^{3}J_{H\text{-}H}$ = 7 Hz, 1H, H_8), 2.66 (s, 3H, H_2), 2.52 (s, 3H, H_1), 1.57 (d, $^{3}J_{H\text{-}H}$ = 7 Hz, 3H, H_{12}), 1.54 – 1.48 (m, 9H, $H_{4,6,10}$), 1.26 (d, J = 7 Hz, 3H, H_9), 1.16 (d, $^{3}J_{H\text{-}H}$ =

7 Hz, 3H, H_7). ^{11}B NMR (128 MHz, $CDCl_3$) δ 32.3 (s, br, $[B]^+$), -16.7 (s, $[B(C_6F_5)_4]^-$). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 190.3 (s, 1C, C_3), 150.0 (s, 1C, C_{14}), 148.3 (d, br, $^1J_{C\text{-}F}$ = 242 Hz, 2C, aryl-CF), 137.4 (m, br, 3C, aryl-CF), 135.6 (s, 1C, C_{15}), 130.8 (s, 1C, C_{18}), 129.3 (s, 2C, C_{17}), 129.0 (s, 1C, C_{13}), 127.4 (s, 2C, C_{16}), 56.8 (s, 1C, C_5), 51.7 (s, 1C, C_8), 46.3 (s, 1C, C_{11}), 28.9 (s, 1C, C_2), 25.0 (s, 1C, C_{10}), 24.6 (s, 1C, C_{12}), 23.3 (s, 1C, C_1) 21.9 (s, 1C, C_4) 20.9 (s, 1C, $C_{6,9}$), 20.9 (s, 1C, C_7).$^{19}F\{^1H\}$ NMR (377 MHz, $CDCl_3$) δ -132.6 (m, br, *o*-(C_6F_5)), -162.8 (m, br, 1F, *p*-(C_6F_5)), -166.8 (m, br, 2F, *m*-(C_6F_5)).

MS (TOF, ESI+) *m/z* 312.2849 (high res., calc. for $[C_{20}H_{34}BN_2]^+$: 312.2846), 214.18 ($[C_{14}H_{21}BN]^+$, loss of $(Me)_2CN(i\text{-}Pr)$ fragment)

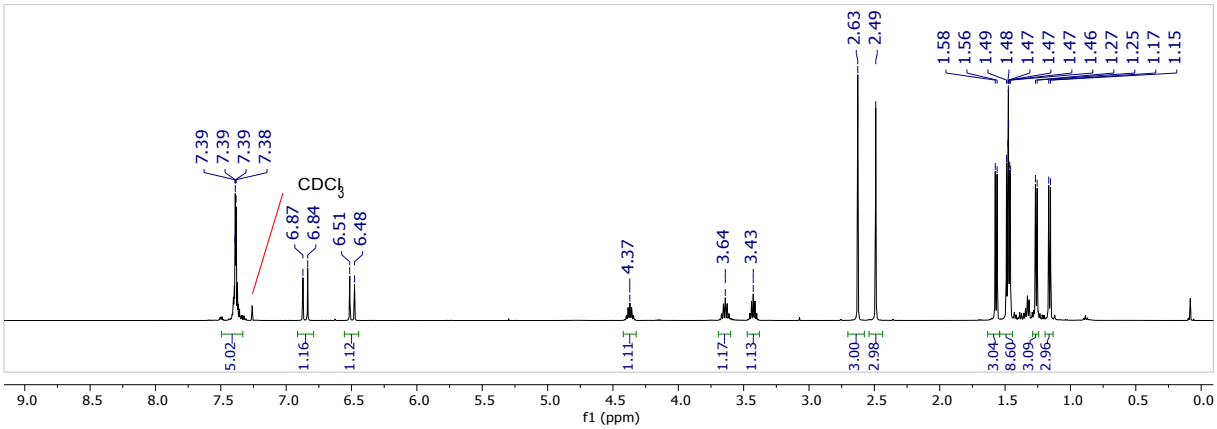


Figure S10. ^1H NMR (400 MHz) of compound **2** in $CDCl_3$ at 298 K.

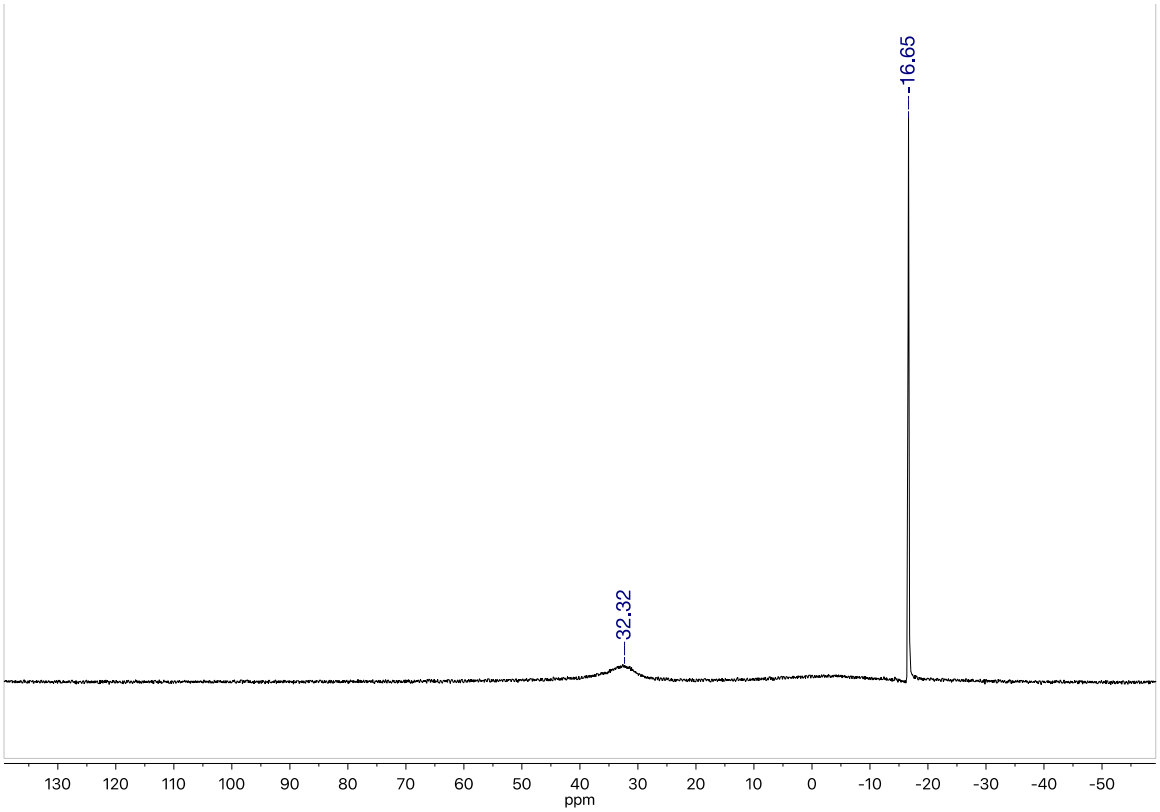


Figure S11. ^{11}B NMR (128 MHz) spectrum of **2** in $CDCl_3$ at 298 K.

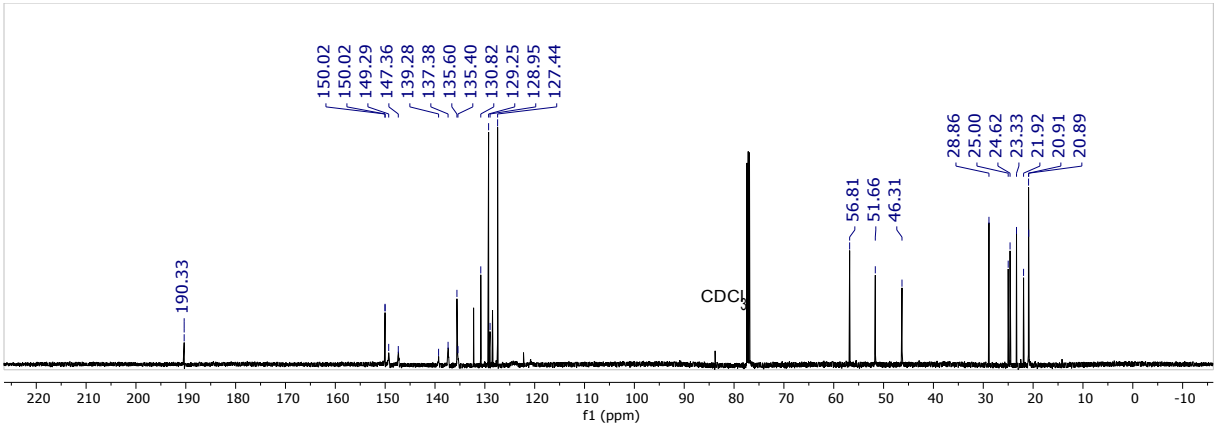


Figure S12. $^{13}C\{^{1}H\}$ NMR (126 MHz) spectrum of **2** in $CDCl_3$ at 298 K

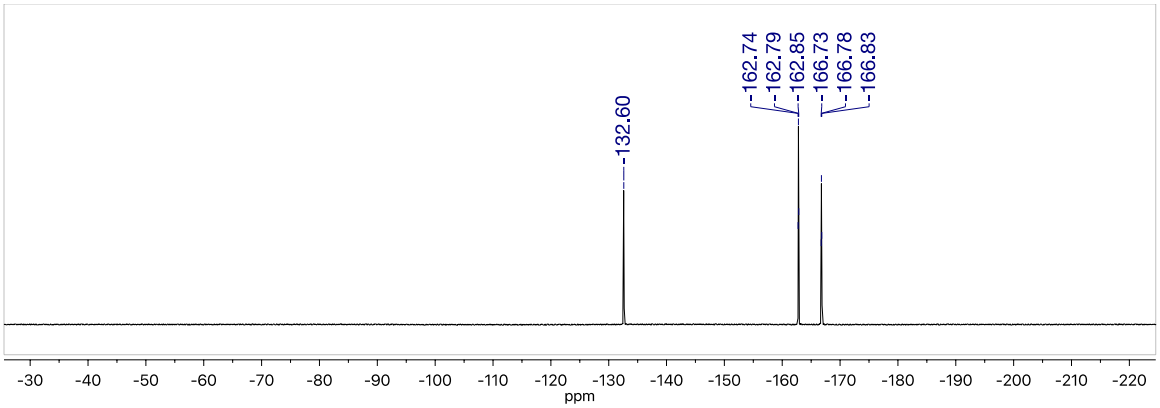
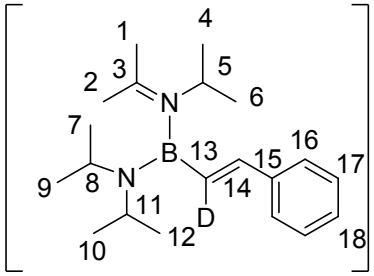


Figure S13. $^{19}F\{^{1}H\}$ NMR (377 MHz) spectrum of **2** in $CDCl_3$ at 298 K.

Compound 2-d_1: $[C_{20}H_{33}DBN_2][B(C_6F_5)_4]$ Hydroboration of PhCCD
Under inert atmosphere, **1** was dissolved in 0.5 mL chloroform and added to a stirred solution of PhCCD in 0.5 mL chloroform. After 1 h, ^{1}H, ^{11}B, ^{13}C and ^{19}F NMR spectroscopy was performed on the sample. The multiplet from 1.51 – 1.41 ppm corresponds to three overlapping methyl-H signals. The ^{2}H NMR signal for **2-*d*$_1$** was obscured by the $CDCl_3$ resonance Thus for ^{2}H NMR spectroscopic characterization, under inert atmosphere, **1** was dissolved in 0.15 mL dichloromethane and added to a stirred solution of PhCCD in 0.15 mL dichloromethane. After 1 h, ^{2}H NMR spectroscopy was performed on the sample, using a capillary of dilute CD_3CN in CH_3CN.



$[B(C_6F_5)_4]$

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.29 (m, 5H, $H_{16, 17, 18}$), 6.47 (s, 1H, H_{14}), 4.35 (hept, $^{3}J_{H\text{-}H}$ = 14, 7 Hz, 1H, H_5), 3.62 (hept, $^{3}J_{H\text{-}H}$ = 7 Hz, 1H, H_{11}), 3.41 (hept, $^{3}J_{H\text{-}H}$ = 7 Hz, 1H, H_8), 2.61 (s, 3H, H_2), 2.47 (s, 3H, H_1), 1.55 (d, $^{3}J_{H\text{-}H}$ = 7.1 Hz, 3H, H_{12}), 1.51 – 1.41 (m, 9H, $H_{4, 6,}$

$_{10}$), 1.24 (d, $^{3}J_{H\text{-}H}$ = 6.5 Hz, 3H, H_9), 1.14 (d, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 3H, H_7). ^{2}H NMR (77 MHz, CH_2Cl_2, CD_3CN external standard) δ 6.02 (br, BC<u>D</u>CHPh). ^{11}B NMR (128 MHz, $CDCl_3$) δ 32.5 (s, br, $[B]^+$), -16.7 (s, $[B(C_6F_5)_4]^-$). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 190.4 (s, 1C, C_3), 150.0 (s, 1C, C_{14}), 148.3 (d, $^{1}J_{C\text{-}F}$ = 241.2 Hz, 2C aryl-<u>C</u>F), 140.0– 134.9 (m, 3C, aryl-<u>C</u>F), 135.6 (s, 1C, C_{15}), 130.8 (s, 1C, C_{18}), 129.2 (s, 2C, C_{17}), 129.0 (s, 1C, C_{13}), 127.4 (s, 2C, C_{16}), 56.8 (s, 1C, C_5), 51.6 (s, 1C, C_8), 46.3 (s, 1C, C_{11}), 28.8 (s, 1C, C_2), 25.0 (s, 1C, C_{10}), 24.6 (s, 1C, C_{12}), 23.3 (s, 1C, C_1), 21.9 (s, 1C, C_4), 20.9 (s, 2C, C_9), 20.9 (s, 2C, C_7), 20.9 (s, 1C, C_6). $^{19}F\{^1H\}$ NMR (377 MHz, $CDCl_3$) δ -132.6 (m, br, *o*-(C_6F_5)), -162.8 (m, br, 1F, *p*-(C_6F_5)), -166.8 (m, br, 2F, *m*-(C_6F_5)).

MS (TOF, ESI+) *m/z* 313.2910 (high res., calc. for $[C_{20}H_{33}DBN_2]^+$: 313.2909), 215.18 ($[C_{14}H_{20}DBN]^+$, loss of $(Me)_2CN(i\text{-}Pr)$ fragment)

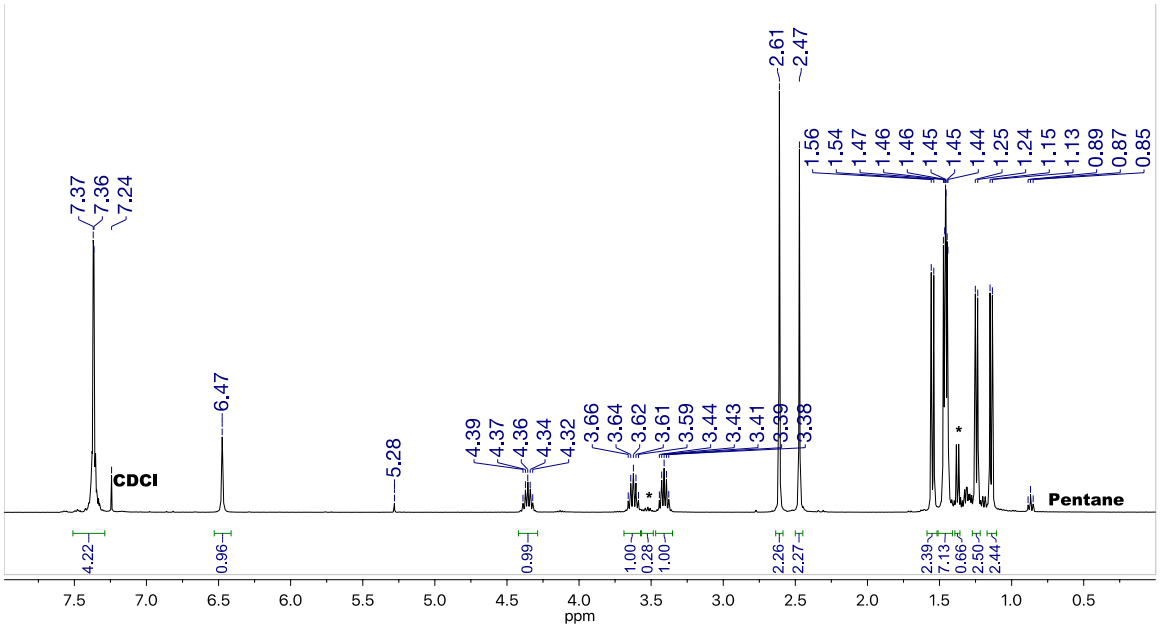


Figure S14. ^{1}H NMR (400 MHz) spectrum of **2-*d*$_1$** in $CDCl_3$ at 298 K.

The signals marked * are residual compound 1.

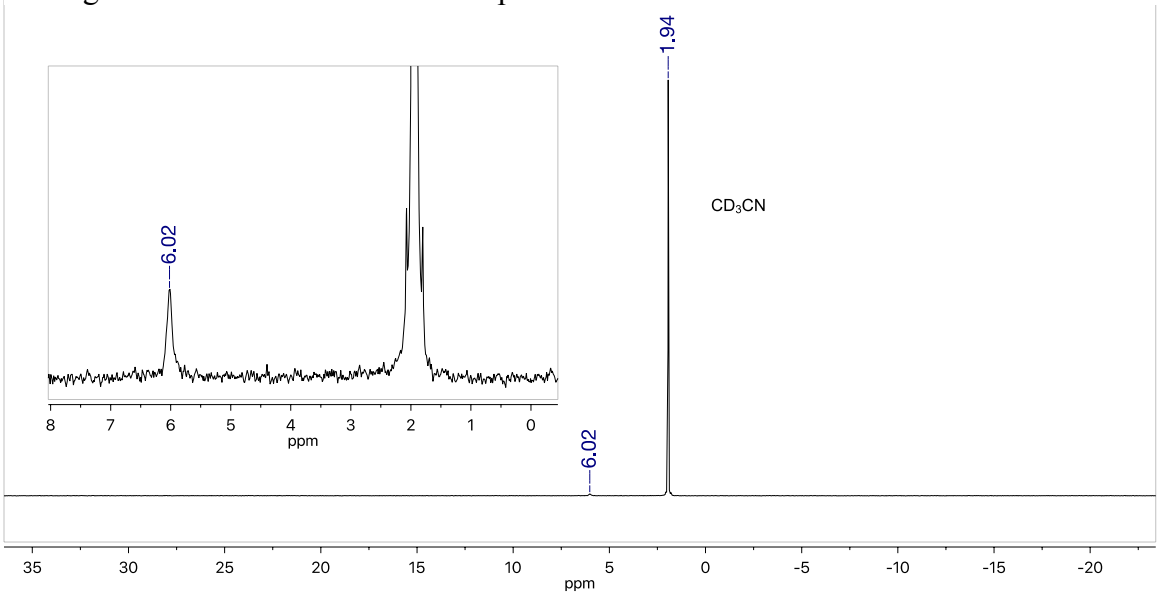


Figure S15. ^{2}H NMR (77 MHz) of **2-*d*$_1$** in $CHCl_2$ with CD_3CN external standard at 298K

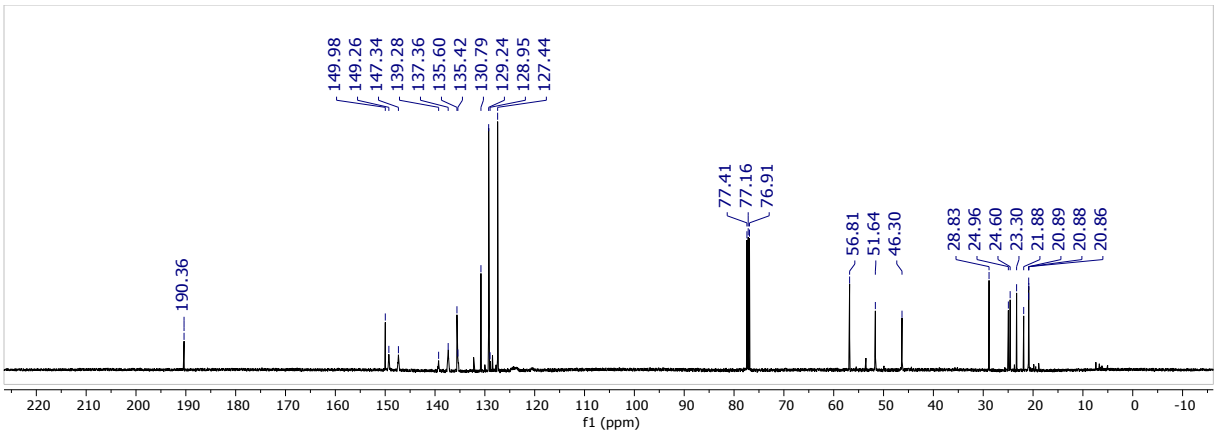


Figure S16. $^{13}C\{^{1}H\}$ NMR (126 MHz) of compound 2-d_1 in CDCl3 at 289K

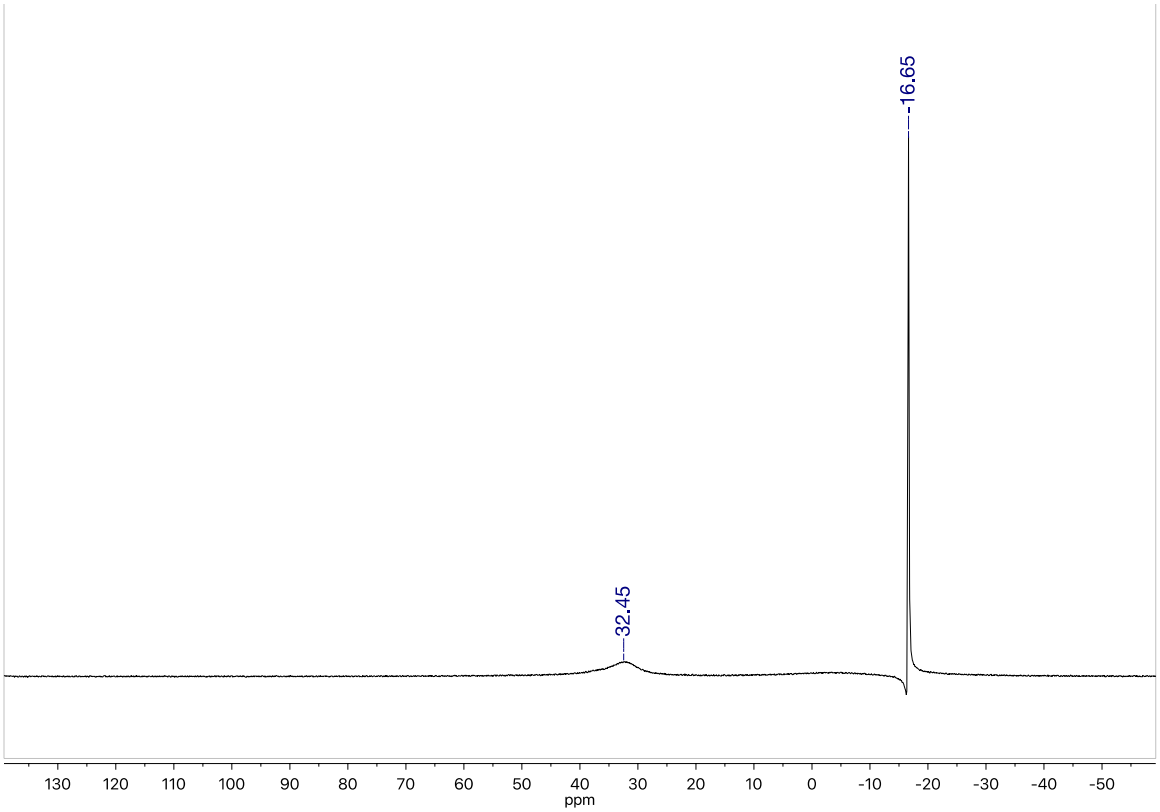
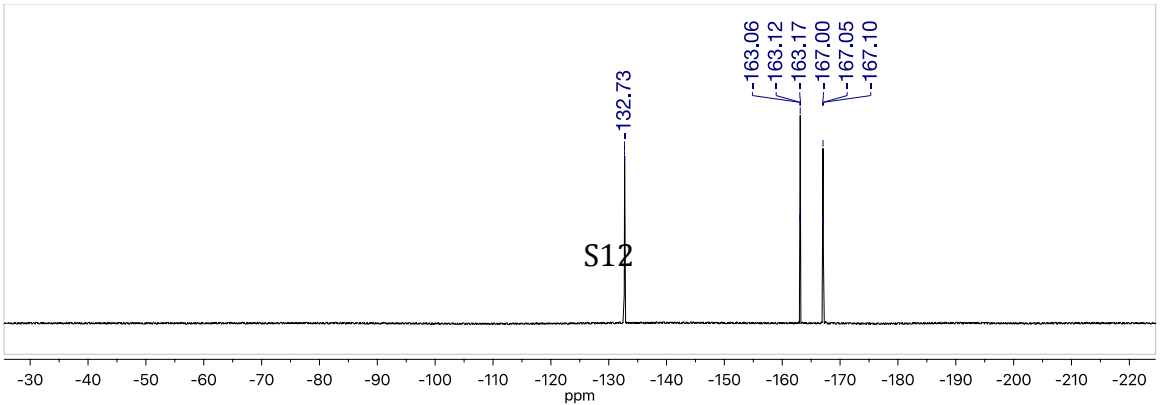
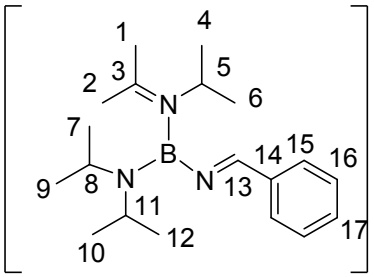


Figure S177. ^{11}B NMR (128 MHz) spectrum of **2-*d*$_1$** in $CDCl_3$ at 298 K.

Figure S18. $^{19}F\{^{1}H\}$ NMR (377 MHz) spectrum of **2-*d*$_1$** in $CDCl_3$ at 298K



Compound 3: $[C_{20}H_{33}BN_3][B(C_6F_5)_4]$ Hydroboration of benzonitrile



Prepared by analogous procedure to compound 2.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.75 (s, 1H, H_{13}), 7.73 – 7.66 (m, 2H, H_{15}), 7.65 – 7.55 (m, 1H, H_{17}), 7.50 (m, 2H, H_{16}), 4.33 (hept, $^3J_{H\text{-}H}$ = 6.7 Hz, 1H, H_5), 3.45 (hept, $^3J_{H\text{-}H}$ = 6.8 Hz, 1H, H_{11}), 3.25 (hept, $^3J_{H\text{-}H}$ = 6.6 Hz, 1H, H_8), 2.66 (s, 3H, H_2), 2.48 (s, 3H, H_1), 1.60 (d, $^3J_{H\text{-}H}$ = 6.7 Hz, 3H, H_6), 1.34 (d, $^3J_{H\text{-}H}$ = 6.6 Hz, 3H, H_4), 1.24 (d, $^3J_{H\text{-}H}$ = 6.7 Hz, 6H, $H_{9,10}$), 1.21 (d, $^3J_{H\text{-}H}$ = 6.9 Hz, 3H, H_7), 1.17 (d, $^3J_{H\text{-}H}$ = 6.6 Hz, 3H, H_{12}). ^{11}B NMR (128 MHz, $CDCl_3$) δ 25.8 (br, $[B]^+$), -16.6 (s, $[B]^-$). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 190.0 (s, 1C, C_3), 162.4 (s, 1C, C_{13}), 148.3 (d, $^1J_{C\text{-}F}$ = 240.7 Hz, Hz, 2C, aryl-CF), 139.8–135.1 (m, br, 3C, aryl-CF) 135.8 (s, 1C, C_{14}), 133.8 (s, 1C, C_{17}), 129.4 (s, 2C, C_{16}), 129.3 (s, 2C, C_{15}), 56.7 (s, 1C, C_5), 49.9 (s, 1C, C_8), 45.1 (s, 1C, C_{11}), 28.6 (s, 1C, C_2), 24.3 (s, 1C, C_{10}), 23.1 (s, 1C, C_4), 22.9 (s, 1C, C_1), 22.1 (s, 1C, C_9), 21.4 (s, 1C, C_7), 21.1 (s, 1C, C_{12}), 20.4 (s, 1C, C_6). ^{19}F{^{1}H} NMR (377 MHz, $CDCl_3$) δ -132.6 (m, br, 2F, *o*-(C_6F_5)), -162.9 (m, br, 1F, *p*-(C_6F_5)) -166.7 (m, br, 2F, *m*-(C_6F_5)).

MS (TOF, ESI+) *m/z* 314.28 (calc. for $[C_{19}H_{33}BN_3]^+$: 314.30)

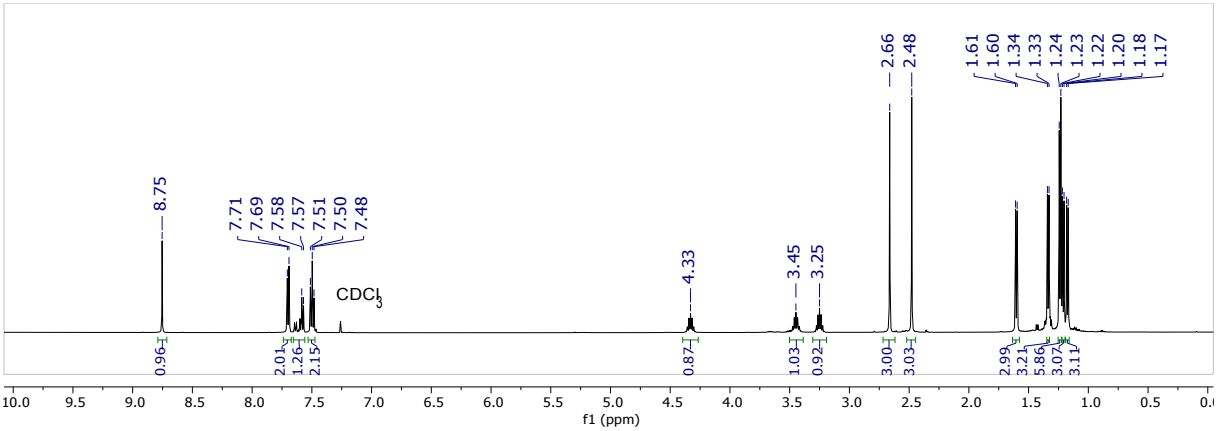


Figure S19. ^{1}H NMR (500 MHz) of **3** in $CDCl_3$ at 298K

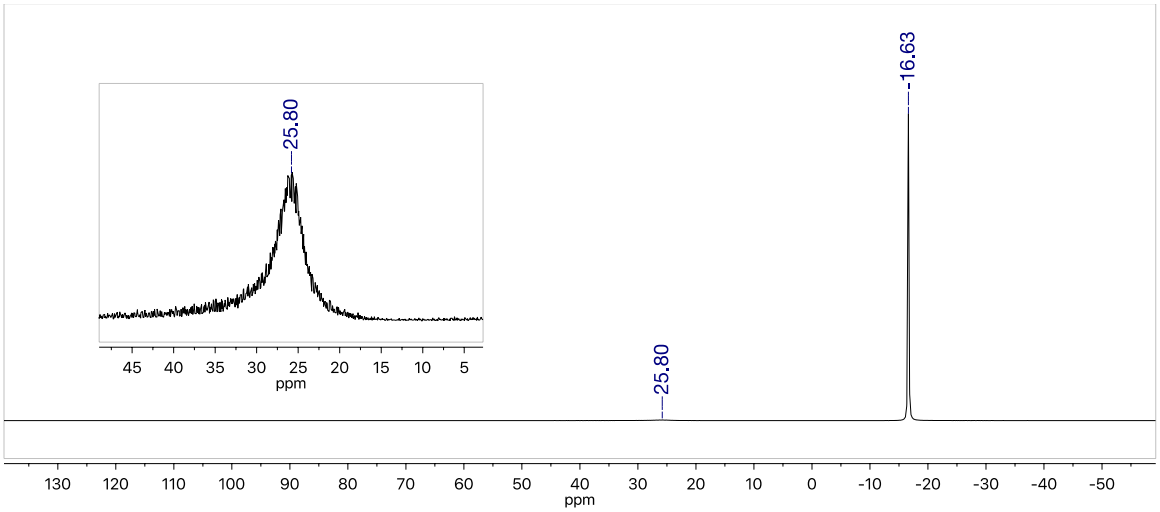


Figure S20. ^{11}B NMR (128 MHz) of **3** in $CDCl_3$ at 298K

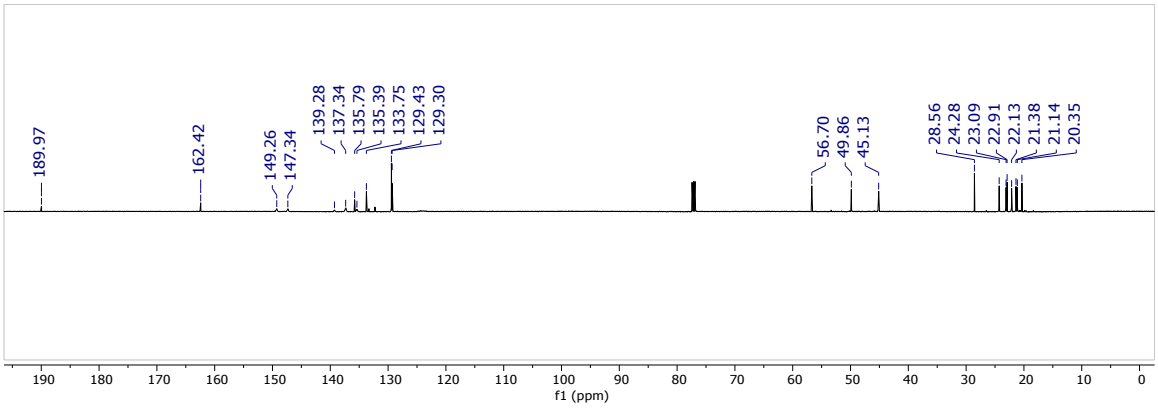


Figure S21. $^{13}C\{^1H\}$ NMR (126 MHz) of **3** in $CDCl_3$ at 298K

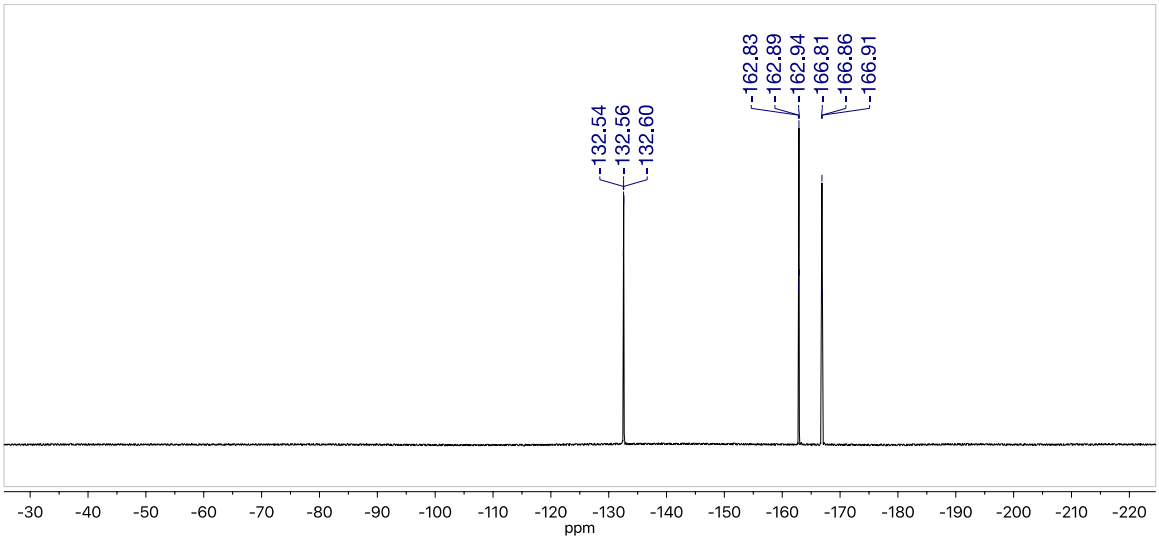
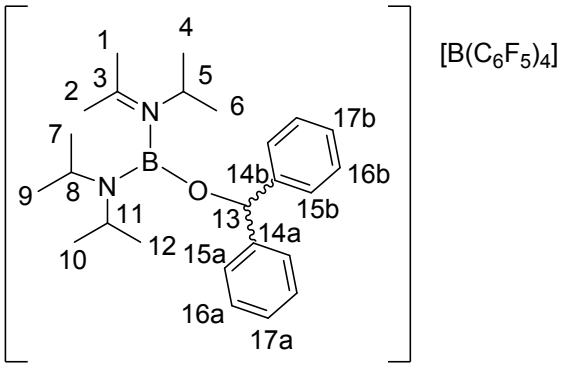


Figure S22. $^{19}F(^1H\}$ NMR (377 MHz) of **3** in $CDCl_3$ at 298K

Compound 4: $[C_{25}H_{38}BN_2O][B(C_6F_5)_4]$ Hydroboration of Benzophenone



Prepared by procedure analogous to compound **2**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 – 7.27 (m, 10H, aryl-C<u>H</u>), 5.51 (s, 1H, H_{13}), 4.36 (hept, $^3J_{H\text{-}H}$ = 6.7 Hz, 1H, H_5), 3.44 (hept, $^3J_{H\text{-}H}$ = 6.7 Hz, 1H, H_8), 3.08 (hept, $^3J_{H\text{-}H}$ = 6.6 Hz, 1H, H_{11}), 2.43 (s, 3H, H_1), 1.69 (s, 3H, H_2), 1.56 (d, $^3J_{H\text{-}H}$ = 6.9 Hz, 3H, H_7), 1.52 (d, $^3J_{H\text{-}H}$ = 6.6 Hz, 3H, H_4), 1.48 (d, $^3J_{H\text{-}H}$ = 6.9 Hz, 3H, H_9), 1.45 (d, $^3J_{H\text{-}H}$ = 6.6 Hz, 3H, H_6), 1.20 (d, $^3J_{H\text{-}H}$ = 6.6 Hz, 3H, H_{10}), 1.06 (d, $^3J_{H\text{-}H}$ = 6.6 Hz, 3H, H_{12}). ^{11}B NMR (128 MHz, $CDCl_3$) δ 22.9 (s, br, $[B]^+$), -16.6 (s, $[B(C_6F_5)_4]^-$). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 194.8 (s, 1C, C_3), 148.2 (d, br, $^1J_{C\text{-}F}$ = 241.3 Hz, 2C, aryl-<u>C</u>F), 141.4 (s, 1C,C_{14a} or C_{14b}), 140.2 (s, 1C, C_{14b} or C_{14a}), 139.5–134.9 (m, br, 3C, aryl-<u>C</u>F), 129.7 (s, 1C, C_{16b}129.4 (s, 1C, C_{17a}), 129.1 (s, 1C, C_{16a}), 128.4 (s, 1C, C_{17b}), 126.2 (s, 1C, C_{15b}), 125.3 (s, 1C, C_{15a}), 81.8 (s, 1C, C_{13}), 56.1 (s, 1C, C_5), 49.1 (s, 1C, C_{11}), 45.0 (s, 1C, C_8), 28.3 (s, 1C, C_2), 23.2 (s, 1C, C_7), 23.1 (s,1C, C_1), 23.0 (s, 1C, C_9), 21.8 (s, 1C, C_6), 21.2 (s, 1C, C_{10}), 21.1 (s, 1C, C_{12}), 19.9 (s, 1C, C_4). ^{19}F{^{1}H} NMR (377 MHz, $CDCl_3$) δ -132.5 (m, br, 2F, *o*-(C_6F_5)), -162.8 (m, br, 1F, *p*-(C_6F_5)), -166.7 (m, br, 2F, *m*-(C_6F_5)).

MS (TOF, ESI+) *m/z* 392.3112 (high res., calc. for $[C_{25}H_{38}BN_2O]^+$: 392.3108)

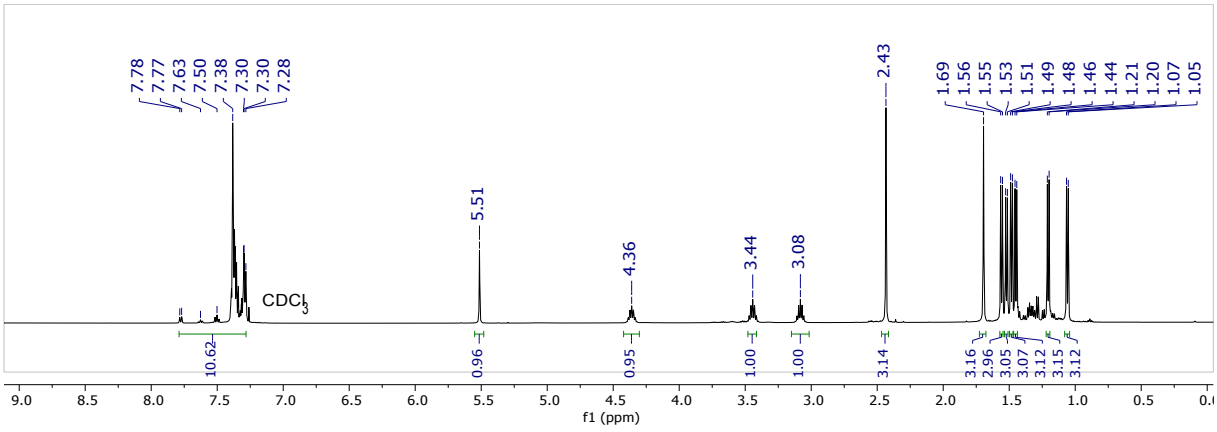


Figure S23. ^{1}H NMR (500 MHz) of **4** in $CDCl_3$ at 298K

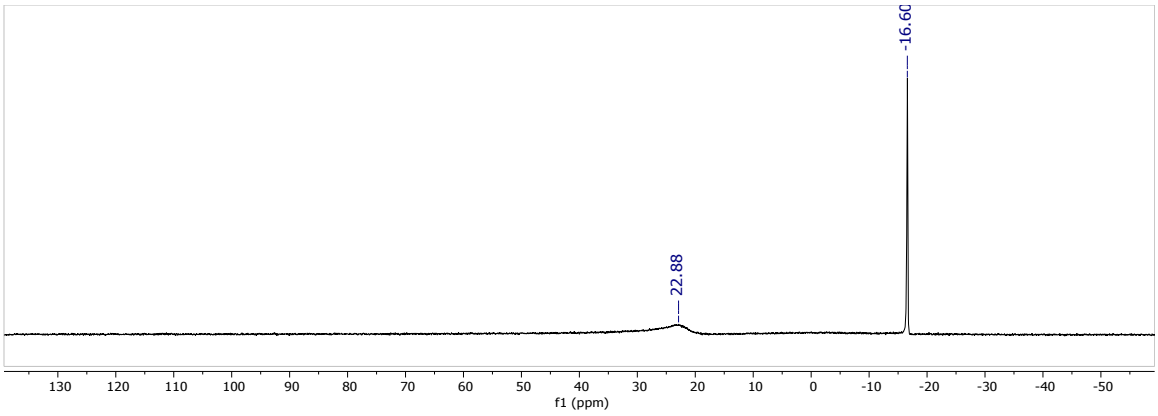


Figure S24. ^{11}B NMR (128 MHz) of **4** in $CDCl_3$ at 298K

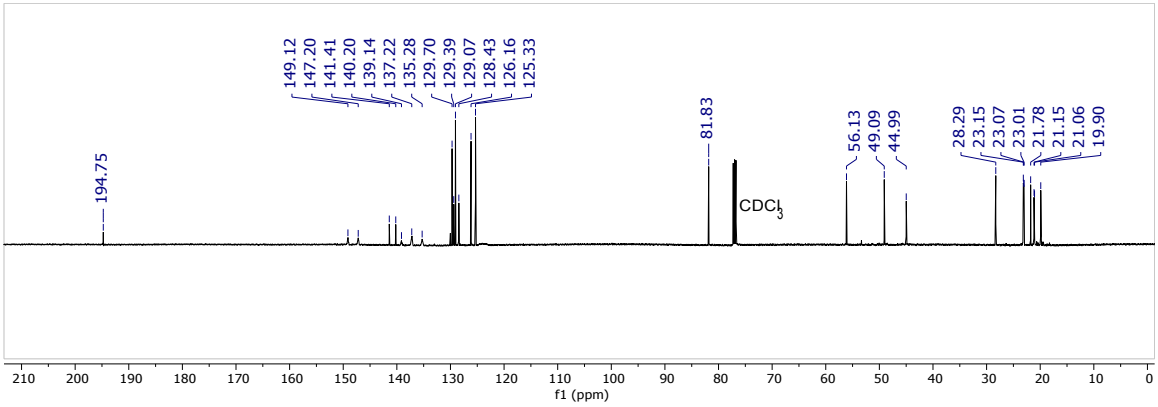


Figure S25. $^{13}C\{^1H\}$ NMR (126 MHz) of **4** in $CDCl_3$ at 298K

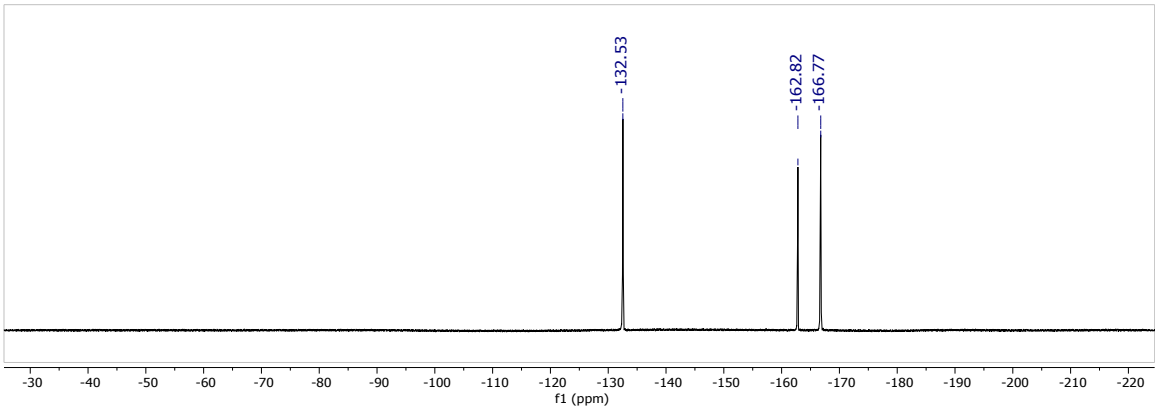
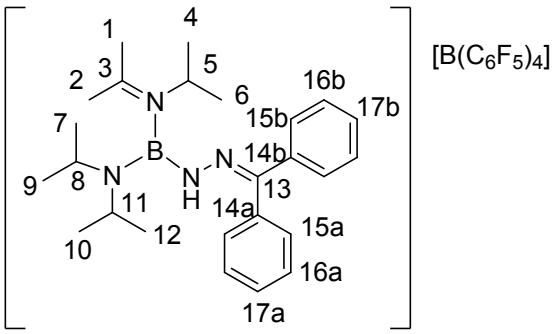


Figure S26. $^{19}F\{^1H\}$ NMR (377 MHz) of **4** in $CDCl_3$ at 298K

Compound 5: $[C_{25}H_{38}BN_4][B(C_6F_5)_4]$ 1,1-Hydroboration of Diazodiphenylmethane



Prepared by analogous procedure to compound **2**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 – 7.24 (m, 10H, aryl C-H), 6.78 (s, 1H, N-H), 4.47 (hept, J = 6.7 Hz, 3H, H_5), 3.37 (hept, J = 7.1 Hz, 3H, H_{11}), 3.31 (hept, J = 6.5 Hz, 3H, H_8), 2.69 (s, 3H, H_2), 2.55 (s, 3H, H_1), 1.58 (d, J = 6.6 Hz, 3H, H_9), 1.53 (d, J = 6.7 Hz, 3H, H_6), 1.19 (d, J = 6.3 Hz, 5H, H_{10}), 1.09 (d, J = 6.5 Hz, 5H, H_7), 0.97 – 0.91 (m, 6H, $H_{4,12}$). ^{11}B NMR (160 MHz, $CDCl_3$) δ 24.1 (s, br, $[B]^+$), -16.6 (s, $[B(C_6F_5)_4]^-$). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 192.5 (s, 1C, C_3), 153.9 (s, 1C, C_{13}), 148.31 (d, J = 240.9 Hz, 2C, aryl-CF), 139.7 – 135.2 (m, br, 3C, aryl-CF), 136.5 (s, 1C, C_{14b}), 132.2 (s, 1C, , C_{14a}), 130.4 (s, 1C, C_{17a}), 130.3 (s, 2C, C_{15a}), 129.9 (s, 1C,C_{17b}), 128.7 (s, 2C, C_{15b}), 128.5 (s, 2C, C_{16a}), 126.7 (s, 2C, C_{16b}),, 56.8 (s, 1C, C_5), 49.9 (s, 1C, C_8), 43.4 (s, 1C, C_{11}), 28.3 (s, 1C, C_2), 23.4 (s, 1C, C_1), 22.8 (s, 1C, C_4), 22.5 (s, 1C, C_{12}), 21.5 (s, 1C, C_{10}), 21.3 (s, 1C, C_9), 21.0 (s, 1C, C_7), 20.7 (s, 1C, C_6). ^{19}F{^{1}H} NMR (377 MHz, $CDCl_3$) δ -132.6(m, br, *o*-(C_6F_5)), -163.1 (m, br, 1F, *p*-(C_6F_5)), -167.0 (m, br, 2F, *m*-(C_6F_5)). ^{15}N NMR (51 MHz, $CDCl_3$) δ 226.9 (N-C_3), 137.7 (N-H), 106.6 (N-C_8).

MS (TOF, ESI+) *m/z* 404.3214 (high res., calc. for $[C_{25}H_{38}BN_4]^+$: 404.3220)

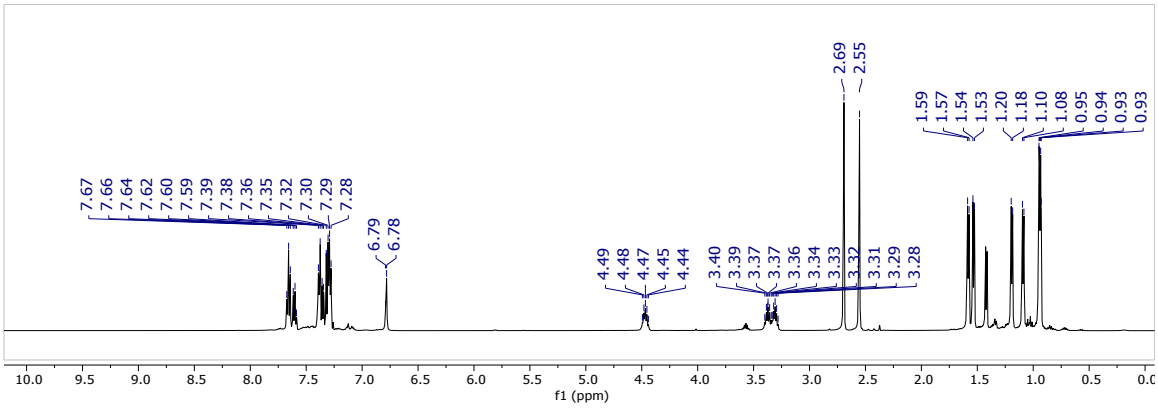


Figure S27. ^{1}H NMR (500 MHz) spectrum of **5** in $CDCl_3$ at 298K

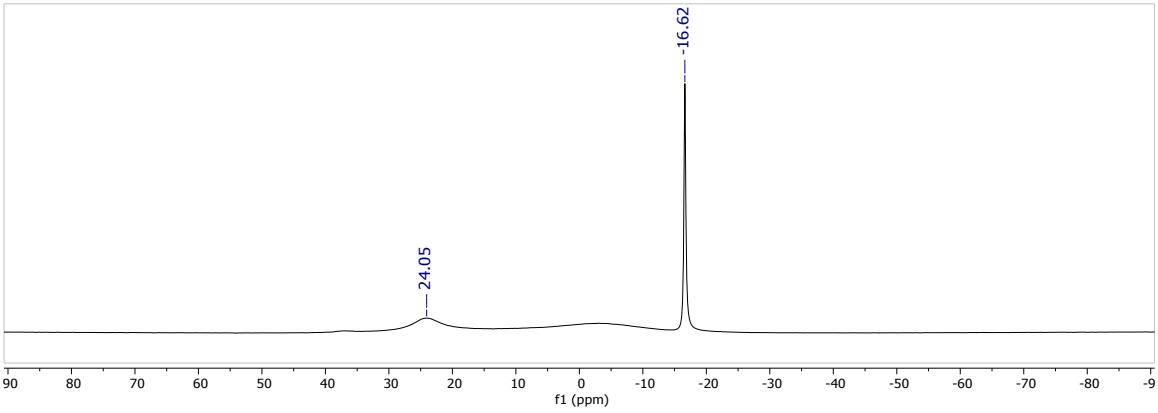


Figure S28 ^{11}B NMR (160 MHz) spectrum of **5** in $CDCl_3$ at 298K

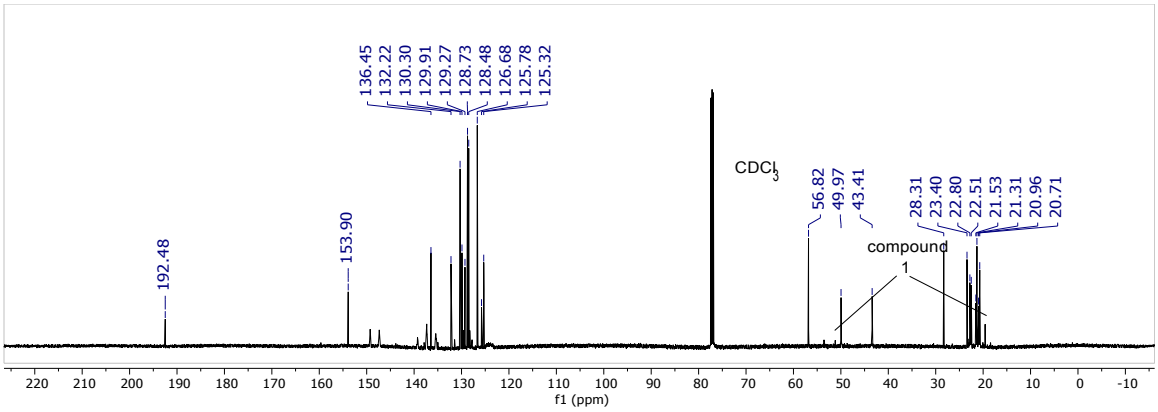


Figure S29. $^{13}C\{^{1}H\}$ NMR (126 MHz) of **5** in $CDCl_3$ at 298K

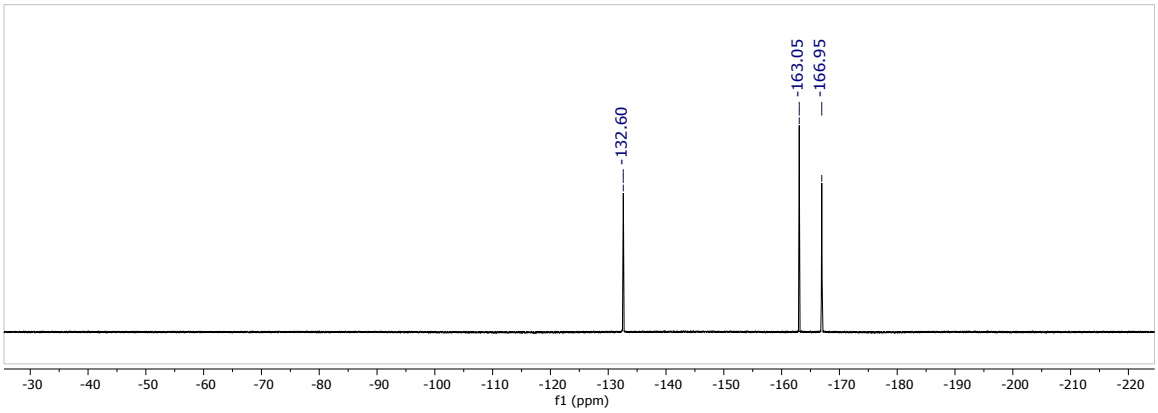


Figure S30. $^{19}F\{^{1}H\}$ NMR (337 MHz) spectrum of **5** in $CDCl_3$ at 298K

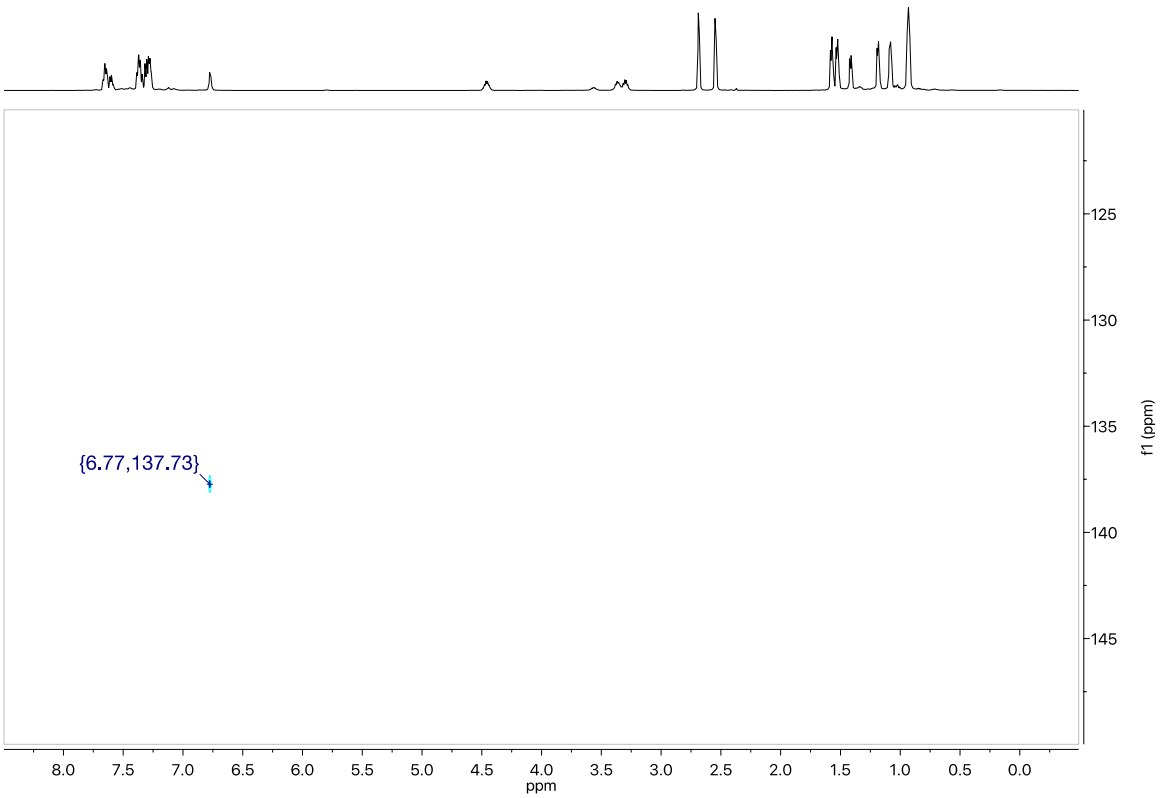


Figure S31. ^{1}H-^{15}N (500MHz) HSQC spectrum of **5** in $CDCl_3$ at 298K.

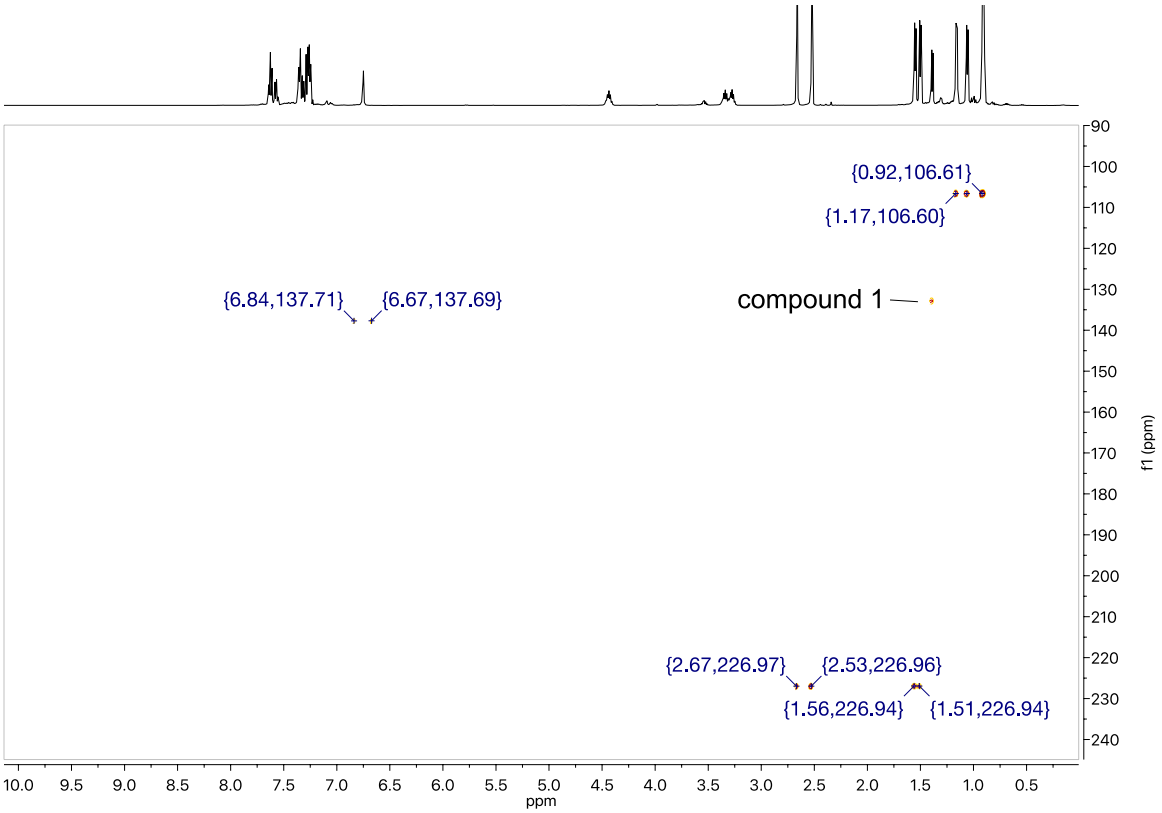


Figure S32. ^{1}H-^{15}N (500MHz) HMBC spectrum of **5** in $CDCl_3$ at 298K.

Synthetic References

(1) Connelly, S. J.; Kaminsky, W.; Heinekey, D. M. Structure and Solution Reactivity of

(Triethylsilylium)Triethylsilane Cations. *Organometallics.* **2013**, 32 (24), 7478–7481.

(2) Higashi, J.; Eastman, A. D.; Parry, R. W. Synthesis and Characterization of Salts of the Bis(Diisopropylamido)Boron(III) Cation and Attempted Reactions To Make the Corresponding Bis(Dimethylamido)Boron(III) Cation. *Inorg. Chem.* **1982**, *21* (2), 716–720.

Computational details

The quantum chemical DFT calculations have been performed with the TURBOMOLE 7.3 suite of programs[1] The structures are fully optimized at the TPSS-D3/def2-TZVP + COSMO($CHCl_3$) level of theory, which combines the TPSS meta-GGA density functional[2] with the BJ-damped DFT-D3 dispersion correction[3, 4] and the def2-TZVP basis set,[5, 6] using the Conductor-like Screening Model (COSMO) continuum solvation model[7] for $CHCl_3$ solvent (dielectric constant ε = 4.8 and solvent diameter R_{solv} = 3.17 Å). The density-fitting RI-J approach[5, 8, 9] is used to accelerate the geometry optimization and numerical harmonic frequency calculations[10] in solution. The optimized structures are characterized by frequency analysis to identify the nature of located stationary points (no imaginary frequency for true minima and only one imaginary frequency for transition state) and to provide thermal corrections (at 298.15 K and 1 atm) according to the modified ideal gas–rigid rotor–harmonic oscillator model.[11]

The final solvation free energies in $CHCl_3$ are computed with the COSMO-RS solvation model[12] (parameter file: BP_TZVP_C30_1601.ctd) using the COSMOtherm program package[13] on the above TPSS-D3 optimized structures, and corrected by +1.90 kcal/mol to account for higher reference solute concentration of 1 mol/L usually used in solution. To check the effects of the chosen DFT functional on the reaction energies and barriers, single-point calculations at the TPSS-D3[2] and hybrid PW6B95-D3[14] levels are performed using a larger def2-QZVP basis set.[6, 15] The final reaction Gibbs free energies (ΔG) are determined from the electronic single-point energies plus TPSS-D3 thermal corrections and COSMO-RS solvation free energies. As expected, the results from both DFT functionals are in good mutual agreement despite in average 1.8 ± 2.5 kcal/mol higher reaction barriers are found at the hybrid PW6B95-D3 level as expected (see Table S1 below). In our discussion, the higher-level PW6B95-D3 Gibbs free energies (in kcal/mol, at 298.15 K and 1 mol/L standard state concentration) will be used in our discussion unless specified otherwise.

To help the atomic assignment of experimental ^{1}H, ^{13}C, ^{11}B, ^{15}N and ^{19}F NMR spectra, NMR shieldings σ (in ppm) are also computed[16] at the TPSS-D3/def2-TZVP level based on the above TPSS-D3 + COSMO optimized geometries after careful conformation search. NMR shifts δ (in ppm) are then obtained by comparing nuclear shieldings σ of the test substrates with a reference molecule ($\delta_{subst} = \delta_{ref} + \sigma_{ref} - \sigma_{subst}$). The silane $Si(CH_3)_4$ (known $\delta_{ref}(^{1}H) = 0.0$ and computed $\sigma_{ref}(^{1}H) = 31.86$; known $\delta_{ref}(^{13}C) = 0.0$ and computed $\sigma_{ref}(^{13}C) = 185.40$), diborane $(HB(C_6F_5)_2)_2$ (known $\delta_{ref}(^{11}B) = 18.0$ and computed $\sigma_{ref}(^{11}B) = 89.0$), cation **1**$^{+}$ (iPr$_2$N)$_2$B^{+} (known $\delta_{ref}(^{15}N) = 132.8$ and computed $\sigma_{ref}(^{15}N) = 98.22$), and C_6H_5F (known $\delta_{ref}(^{19}F) = -113.11$ and computed $\sigma_{ref}(^{19}F) = 270.82$) are chosen as reference molecules to compute the ^{1}H, ^{13}C, ^{11}B, ^{15}N and ^{19}F chemical shifts as shown in Table S3 for comparison with experiment.

Figure S33. Reaction free energy paths (in kcal/mol) for borenium cation 1+ (labeled R in figure). NB: conformation changes, and hydride migration within **R**, and reactivity of different conformers toward nucleophile PhCCH addition, computed at the PW6B95-D3/def2-QZVP + COSMO-RS // TPSS-D3/def2-TZVP + COSMO level of theory in $CHCl_3$ solution.

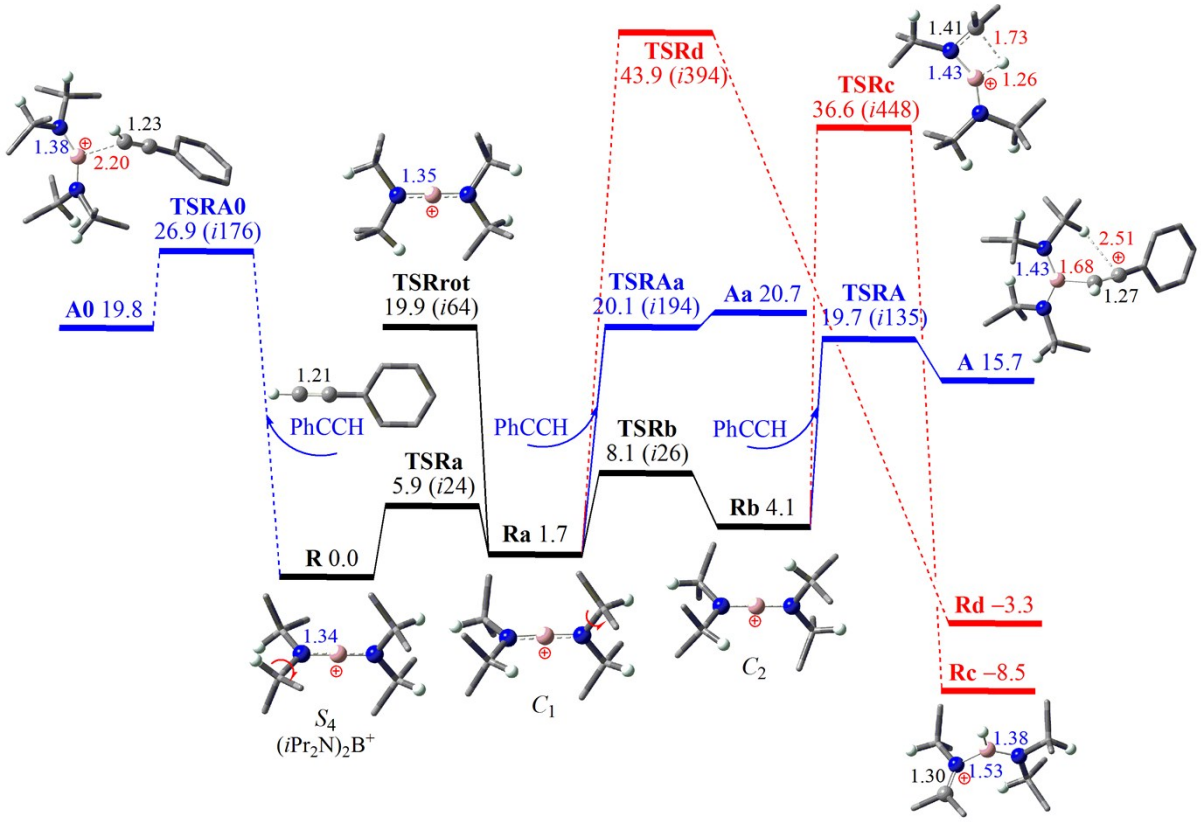


Figure S34. Reaction free energy paths (in kcal/mol, at 298K and 1 M) for possible reactions of borenium cation 1+ (labeled R in figure) and nucleophile PhCCH. NB computed at the PW6B95-D3/def2-QZVP + COSMO-RS // TPSS-D3/def2-TZVP + COSMO level of theory in CHCl3

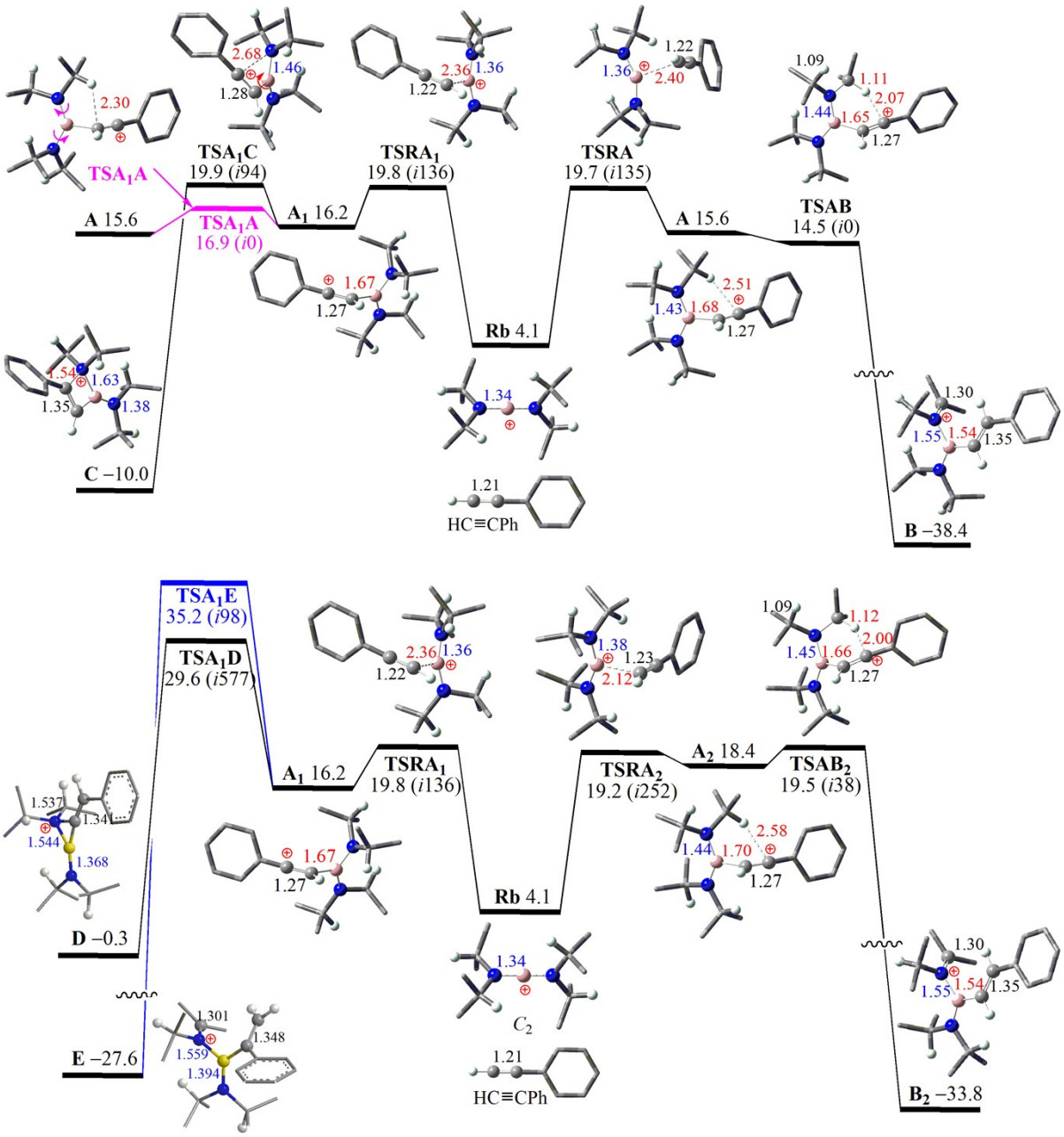


Table S1. Results of computations

TPSS-D3/def2-TZVP + COSMO computed imaginary frequency (ImF), zero-point energies (ZPE), gas-phase enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections in $CHCl_3$ solution; TPSS-D3/def2-QZVP and PW6B95-D3/def2-QZVP single-point energies (TPSS-D3 and PW6B95-D3); the relative electronic energies (ΔET and ΔEP) and Gibbs free-energies (ΔGT and ΔGP) at the TPSS-D3 and PW6B95-D3 levels. Each structure is labeled either by its molecular formula or a specific name in bold. Each transition structure (with only one imaginary frequency) are indicated by the "TS" prefix (See also Figures S1 and S2).

Reactions	ImF	ZPE	Hc	Gc	Hsol	Gsol	TPSS-D3	PW6B95-D3	ΔET	ΔEP	ΔGP	ΔGT
	cm^{-1}	kcal /mol	kcal /mol	kcal /mol	kcal /mol	kcal /mol	E_h	E_h	kcal /mol	kcal /mol	kcal /mol	kcal /mol
Borenium **R** conformation changes and hydride migration												
R (or **1**$^+$)	0	245.58	258.54	218.52	-47.50	-42.19	-608.764093	-609.402162	0.0	0.0	0.0	0.0
TSR0	-34	244.99	257.74	217.19	-47.43	-42.13	-608.758439	-609.395686	3.6	4.1	2.8	2.3
R0	0	245.09	258.25	218.19	-47.42	-42.09	-608.763193	-609.400690	0.6	0.9	0.7	0.3
TSRa	-24	245.15	257.78	217.97	-47.45	-42.13	-608.754941	-609.392044	5.7	6.4	5.9	5.3
Ra	0	245.24	258.40	217.45	-47.04	-41.78	-608.760724	-609.398333	2.1	2.4	1.7	1.4
TSRrot	-64	244.67	257.44	217.32	-47.66	-42.23	-608.731210	-609.368418	20.6	21.2	19.9	19.4
TSRb	-26	245.43	257.96	218.33	-47.33	-41.99	-608.752080	-609.389250	7.5	8.1	8.1	7.5
Rb	0	245.31	258.50	217.88	-47.23	-41.89	-608.757795	-609.395060	4.0	4.5	4.1	3.6
TSRd	-394	242.36	255.21	214.91	-48.16	-42.82	-608.693404	-609.325485	44.4	48.1	43.9	40.1
Rd	0	244.35	257.39	216.78	-48.17	-42.87	-608.768188	-609.403512	-2.6	-0.9	-3.3	-5.0
TSRc	-448	242.65	255.33	215.43	-48.29	-42.94	-608.703122	-609.337720	38.3	40.4	36.6	34.4
Rc	0	244.24	257.37	216.51	-48.78	-43.41	-608.774881	-609.410533	-6.8	-5.3	-8.5	-10.0
Reactivity of three borenium conformers towards nucleophile PhCCH												
R/PhCCH	0	313.51	331.02	267.95	-57.20	-48.61	-917.361780	-918.341929	0.0	0.0	0.0	0.0
TSRA$_0$	-176	313.64	331.29	281.19	-48.79	-42.35	-917.355201	-918.327188	4.1	9.3	26.9	21.7
A$_0$	0	314.84	332.18	282.96	-48.84	-42.45	-917.370892	-918.341164	-5.7	0.5	19.8	13.6
TSAB$_0$	-30	313.54	330.81	281.51	-48.53	-42.22	-917.369897	-918.339644	-5.1	1.4	19.5	13.0
B$_0$	0	316.23	333.47	284.25	-51.42	-44.64	-917.445179	-918.421852	-52.3	-50.2	-31.8	-34.0
TSRAa	-194	313.67	331.35	281.26	-48.79	-42.51	-917.364676	-918.337770	-1.8	2.6	20.1	15.7
Aa	0	315.22	332.59	283.23	-48.63	-42.30	-917.370132	-918.340383	-5.2	1.0	20.7	14.5
TSRA	-135	314.13	331.76	281.78	-49.11	-42.71	-917.364357	-918.338939	-1.6	1.9	19.7	16.2
A	0	315.46	332.75	283.55	-48.95	-42.55	-917.377799	-918.348490	-10.1	-4.1	15.7	9.7
TSAB	0	313.48	331.42	280.45	-48.44	-42.10	-917.376985	-918.346659	-9.5	-3.0	14.2	7.6
B (or **2**$^+$)	0	315.98	333.38	283.79	-51.78	-44.96	-917.454183	-918.431204	-58.0	-56.0	-38.4	-40.4
Low-lying conformers of hydroboration product **B**												
B (or **2**$^+$)	0	315.98	333.38	283.79	-51.78	-44.96	-917.454183	-918.431204	0.0	0.0	0.0	0.0
Ba	0	315.89	333.34	283.64	-52.05	-45.15	-917.454183	-918.430681	0.0	0.3	0.0	-0.3
Bb	0	315.76	333.38	283.24	-51.46	-44.62	-917.452469	-918.428493	1.1	1.7	1.5	0.9
Bc	0	315.63	333.14	283.27	-52.58	-45.63	-917.447036	-918.423549	4.5	4.8	3.6	3.3
B$_2$	0	316.31	333.55	284.31	-51.48	-44.67	-917.447958	-918.425178	3.9	3.8	4.6	4.7

B_3	0	316.18	333.57	284.01	-51.17	-44.37	-917.446732	-918.423179	4.7	5.0	5.8	5.5
Potential side-reactions of borenium **R** with PhCCH												
R/PhCCH	0	313.51	331.02	267.95	-57.20	-48.61	-917.361780	-918.341929	0.0	0.0	0.0	0.0
$TSRA_2$	-252	313.29	331.11	280.59	-48.88	-42.51	-917.364707	-918.338209	-1.8	2.3	19.2	15.0
A_2	0	314.98	332.45	282.88	-49.00	-42.60	-917.373696	-918.342873	-7.5	-0.6	18.5	11.6
$TSAB_2$	-38	313.81	331.01	281.85	-48.60	-42.19	-917.373170	-918.340155	-7.2	1.1	19.6	11.3
B_2	0	316.31	333.55	284.31	-51.48	-44.67	-917.447958	-918.425178	-54.1	-52.2	-33.8	-35.7
$TSRA_1$	-136	313.77	331.56	281.13	-49.04	-42.61	-917.363367	-918.337943	-1.0	2.5	19.8	16.3
A_1	0	315.05	332.46	282.96	-48.75	-42.33	-917.377244	-918.347080	-9.7	-3.2	16.2	9.7
TSA_1A	0	314.07	331.97	281.16	-48.79	-42.42	-917.373778	-918.342951	-7.5	-0.6	16.9	10.0
TSA_1C	-94	314.49	331.51	282.89	-49.25	-42.97	-917.367666	-918.339998	-3.7	1.2	19.9	15.0
C	0	317.39	334.10	286.28	-50.26	-43.80	-917.413548	-918.391643	-32.5	-31.2	-10.0	-11.2
TSA_1D	-577	311.96	329.62	279.39	-49.84	-43.19	-917.344628	-918.318543	10.8	14.7	29.7	25.7
D	0	316.31	333.49	284.49	-49.99	-43.42	-917.398492	-918.373971	-23.0	-20.1	-0.3	-3.2
TSA_1E	-98	312.73	330.08	280.93	-48.86	-42.62	-917.345124	-918.312798	10.5	18.3	35.4	27.5
E	0	315.67	333.05	283.76	-51.70	-45.19	-917.439226	-918.416644	-48.6	-46.9	-29.6	-31.3

Table S2. The TPSS-D3/def2-TZVP + COSMO optimized atomic Cartesian coordinates (in Å) in $CHCl_3$ solution.

Each structure is labelled by the specific name (See Figures S1 and S3 and Table S1), followed by the number of atoms, the total energy, and the detailed atomic coordinates (in double-column text list).

A_0
57
Energy = -917.3531954935

B	1.0495149	-0.3701937	-0.0823921
N	1.6949220	0.9199633	0.0259983
N	1.2681082	-1.5572397	0.5985115
C	-0.0855327	1.4996970	1.6630067
C	3.4040561	-2.7289090	1.1224020
C	1.6989114	3.1726169	1.0981129
C	2.9428953	-0.5377153	2.2647405
C	2.7237605	1.3228661	-0.9685286
C	0.4302926	-2.7965725	0.4450314
C	0.8496822	2.0154354	0.5634411
C	2.3156704	-1.7856783	1.6540535
C	3.4965710	0.1029681	-1.4668061
C	-0.9260450	-2.6114602	1.1296051
C	2.1421781	2.1169082	-2.1507750
C	0.3198154	-3.3165856	-0.9902029
H	-0.6504785	0.6136273	1.3540163
H	4.0711509	-3.0106463	1.9428799
H	2.3823827	2.8149599	1.8748794
H	2.1909262	0.1419027	2.6671753
H	3.4282048	1.9734285	-0.4362860
H	0.9705892	-3.5612177	1.0079991
H	-0.8082072	2.2801091	1.9186681
H	3.9994999	-2.2352884	0.3495018
H	2.2835241	3.6604543	0.3142490
H	3.5835293	-0.8660651	3.0904012
H	4.2655002	0.4233013	-2.1751834
H	-0.7946300	-2.3014561	2.1709824
H	1.6105743	3.0134839	-1.8203999
H	-0.3772268	-2.7344672	-1.5966234
H	0.4723317	1.2423009	2.5673679
H	2.9862908	-3.6463761	0.6988541
H	1.0377275	3.9253527	1.5384938
H	3.5607545	0.0109601	1.5516782
H	0.2206867	2.3952779	-0.2598548
H	1.7756660	-2.3024777	2.4582288
H	2.8420922	-0.6079786	-1.9857617
H	-1.4826971	-3.5540373	1.1182336
H	2.9587630	2.4340668	-2.8067288
H	1.2984711	-3.3194689	-1.4798645
H	3.9867999	-0.4196733	-0.6432214
H	-1.5242992	-1.8534954	0.6179648
H	1.4510735	1.5045830	-2.7388024
H	-0.0506646	-4.3463739	-0.9611929
C	-0.1067581	-0.3358998	-1.3144623
C	-1.3010158	0.0638826	-1.1803789
H	0.3444792	-0.6037825	-2.2691000
C	-2.5935746	0.4928449	-0.9351295
C	-2.8922337	1.8825674	-0.8686172
C	-3.6388261	-0.4592023	-0.7706065
C	-4.1930199	2.2963612	-0.6469372
H	-2.0891626	2.6007898	-0.9930218
C	-4.9322070	-0.0256594	-0.5358742
H	-3.4081602	-1.5165580	-0.8395221
C	-5.2098402	1.3462026	-0.4743515
H	-4.4257812	3.3548428	-0.5980160
H	-5.7315875	-0.7475697	-0.4065332
H	-6.2269945	1.6787558	-0.2916446

A_1
57
Energy = -917.3594712052

B	0.0450989	-0.2569122	0.5907929
N	-0.1584923	1.1166525	0.6444723
N	-0.2435576	-1.2200421	1.6260147
C	1.5872583	2.0910362	-0.9069823
C	-2.6687692	-1.0158190	2.1605653
C	-0.8838462	2.0181766	-1.5639678
C	-1.8934656	-2.6669599	0.4218059
C	-0.6106862	1.7268778	1.9371917
C	0.9292631	-1.8073634	2.3215898
C	0.1330116	2.1191123	-0.4248058
C	-1.5304083	-1.9454302	1.7286693
C	0.5303301	2.5152148	2.5883530
C	0.7755482	-1.6567873	3.8415877
C	-1.8735132	2.5755079	1.7702049
C	1.2068233	-3.2640404	1.9217551
H	1.8068402	1.2120867	-1.5164866
H	-2.8299919	-0.2299983	1.4151644
H	-0.8207235	1.0484067	-2.0629068
H	-2.0755217	-1.9423486	-0.3805544
H	-0.8437788	0.8753417	2.5772527
H	1.7901086	-1.1977368	2.0166540
H	2.2763649	2.1084764	-0.0573675
H	-2.4542841	-0.5476650	3.1249935
H	-1.9026294	2.1392368	-1.1862755
H	-1.0924985	-3.3423881	0.1108367
H	1.4071180	1.8774661	2.7372279
H	0.6368559	-0.6070832	4.1151889
H	-2.6748497	2.0072153	1.2899819
H	1.3354536	-3.3622707	0.8395423
H	1.7744463	2.9798531	-1.5181275
H	-3.5970863	-1.5887073	2.2521843
H	-0.6937419	2.8001000	-2.3063103
H	-2.8094217	-3.2499074	0.5600649
H	-0.0133904	3.0900403	0.0538615
H	-1.3910228	-2.6993251	2.5090034
H	0.2030163	2.8890964	3.5635594
H	1.6703076	-2.0357296	4.3455035
H	-2.2215106	2.8893282	2.7593034
H	2.1224651	-3.6102405	2.4111491
H	0.8271793	3.3789814	1.9839657
H	-0.0847309	-2.2280674	4.2060034
H	-1.6887591	3.4812292	1.1838215
H	0.3908054	-3.9232214	2.2347412
C	0.8858743	-0.9427842	-0.6784384
C	0.4024971	-1.2421740	-1.8114791
H	1.9104278	-1.1799862	-0.3845745
C	-0.2184809	-1.5603012	-3.0035889
C	-0.9135626	-2.7961224	-3.1386955
C	-0.1464132	-0.6677701	-4.1116326
C	-1.5204706	-3.1133040	-4.3410372
H	-0.9509059	-3.4770934	-2.2963922
C	-0.7694958	-0.9994254	-5.3007239

H	0.4008577	0.2625608	-4.0078127
C	-1.4550452	-2.2172571	-5.4164585
H	-2.0467477	-4.0555195	-4.4513929
H	-0.7216587	-0.3216129	-6.1463826
H	-1.9366315	-2.4723883	-6.3553699

A_2

57

Energy = -917.3559223665

B	0.2354440	0.0173969	0.3892404
N	0.0763218	1.2700351	-0.1981936
N	0.2632106	-1.3207324	-0.1373746
C	1.1754893	0.7273410	-2.3974974
C	-2.2204025	-1.3655114	0.0470425
C	-1.2655207	1.4028138	-2.3372160
C	-1.0935678	-2.4115184	-1.9676200
C	0.0079189	2.5113075	0.6350536
C	1.4922673	-2.0984552	0.1828093
C	0.1066832	1.5434170	-1.6720006
C	-0.9708727	-2.0828774	-0.4713640
C	1.3303240	3.2839977	0.5696477
C	1.2728550	-3.1806127	1.2504399
C	-1.1895934	3.3997551	0.2878295
C	2.1705733	-2.6954801	-1.0596246
H	0.9084826	-0.3297494	-2.4406429
H	-2.3362842	-0.3768493	-0.4061527
H	-1.5911386	0.3612956	-2.3547130
H	-1.2176670	-1.5079993	-2.5686312
H	-0.1304305	2.1727115	1.6632848
H	2.1888410	-1.3557909	0.5918739
H	2.1451812	0.8245619	-1.8992148
H	-2.1864651	-1.2490112	1.1351307
H	-2.0278415	1.9919290	-1.8240327
H	-0.2188863	-2.9486230	-2.3379044
H	2.1722753	2.6324662	0.8219695
H	0.7634312	-2.7782041	2.1304866
H	-2.1289406	2.8447258	0.3643722
H	2.3099089	-1.9438420	-1.8394160
H	1.2739215	1.0987254	-3.4223666
H	-3.1081782	-1.9548239	-0.1996901
H	-1.2003757	1.7524356	-3.3728139
H	-1.9732153	-3.0456445	-2.1210239
H	0.3996354	2.5947188	-1.7464731
H	-0.8968189	-3.0343507	0.0653598
H	1.3051071	4.1174472	1.2788421
H	2.2451558	-3.5782619	1.5598364
H	-1.2244746	4.2325308	0.9971451
H	3.1530316	-3.0858313	-0.7746784
H	1.5099323	3.7017366	-0.4260372
H	0.6925190	-4.0226912	0.8628157
H	-1.1103405	3.8250998	-0.7173283
H	1.5894099	-3.5267513	-1.4675922
C	0.4085617	0.0328187	2.0784119
C	1.5566165	0.1262327	2.6013528
H	-0.5368423	-0.0734000	2.6069163
C	2.8587547	0.2409446	3.0582293
C	3.6621257	-0.9188292	3.2418422
C	3.3905698	1.5230815	3.3715415
C	4.9550337	-0.7895719	3.7169974
H	3.2441197	-1.8934888	3.0165865
C	4.6902512	1.6320702	3.8346780
H	2.7650128	2.3998733	3.2474219
C	5.4707539	0.4812144	4.0069513
H	5.5706551	-1.6707702	3.8628990
H	5.1025568	2.6074789	4.0700164
H	6.4875049	0.5744270	4.3757306

Aa

57

Energy = -917.3521648108

B	0.9083476	-0.1323052	-0.3236320
N	1.3704673	1.1980782	-0.0660182
N	1.3554730	-1.3798310	0.1154430
C	0.9380291	2.9891921	1.6015679
C	3.4129221	-2.0716057	1.4394569
C	-0.0099921	3.2094559	-0.7332698
C	1.7007899	-0.5274048	2.4771831
C	2.6280218	1.7148304	-0.6824940
C	1.1021216	-2.6777089	-0.5902352
C	0.4009919	2.2330408	0.3772417
C	1.9392035	-1.6491788	1.4742714
C	3.8869903	1.0765887	-0.1025064
C	-0.2815099	-3.2607123	-0.2834033
C	2.5991062	1.5528291	-2.2097327
C	1.3880085	-2.6145586	-2.0913498
H	1.1602355	2.3047647	2.4226141
H	3.6700161	-2.5403800	2.3947950
H	0.8385572	3.8124660	-1.0707016
H	0.6445610	-0.2390466	2.5056504
H	2.6487727	2.7825091	-0.4475376
H	1.8427007	-3.3587059	-0.1604184
H	0.1872616	3.7097500	1.9407319
H	4.0705566	-1.2129667	1.2962227
H	-0.4276575	2.6817370	-1.5948428
H	1.9862742	-0.8829146	3.4721189
H	4.7676021	1.5679917	-0.5284573
H	-0.4989450	-3.2220910	0.7887995
H	1.7099224	2.0150624	-2.6464439
H	0.5997190	-2.0969281	-2.6440921
H	1.8472098	3.5465972	1.3542890
H	3.6119644	-2.7991838	0.6470923
H	-0.7672521	3.8996326	-0.3464988
H	2.2971719	0.3562352	2.2458700
H	-0.4871506	1.6784557	0.7001058
H	1.3591135	-2.5148807	1.8211406
H	3.9343061	0.0159675	-0.3616552
H	-0.3176460	-4.3076042	-0.6008361
H	3.4839920	2.0203089	-2.6530326
H	2.3437742	-2.1182366	-2.2852975
H	3.9263733	1.1817962	0.9846578
H	-1.0578911	-2.7148995	-0.8232574
H	2.6105188	0.4896943	-2.4793215
H	1.4448893	-3.6334424	-2.4870753
C	-0.3960552	-0.1032914	-1.4204473
C	-1.5696812	-0.0668525	-0.9523399
H	-0.0952665	-0.0400764	-2.4619793
C	-2.7857442	0.0110020	-0.2923748
C	-3.3074456	1.2814286	0.0813073
C	-3.5300137	-1.1659573	-0.0040940
C	-4.5285980	1.3608650	0.7264205
H	-2.7439637	2.1760854	-0.1593928
C	-4.7436911	-1.0663495	0.6544199
H	-3.1369899	-2.1305002	-0.3036132
C	-5.2429514	0.1908259	1.0186956
H	-4.9328608	2.3278198	1.0065867
H	-5.3115189	-1.9622752	0.8818446
H	-6.1982127	0.2604569	1.5296922

A

57

Energy = -917.3601025521

B	0.1550668	-0.3272928	0.7409152
N	0.0855136	1.0989081	0.6282332
N	1.2601668	-1.1392469	1.0054339

C	2.1468478	2.4725705	0.0347824
C	0.4406138	-3.4523940	1.6763856
C	0.9649330	1.0595738	-1.7028066
C	1.2244135	-2.9734971	-0.6971243
C	-1.0072711	1.8169179	1.3301268
C	2.4759337	-0.5339318	1.6309686
C	0.8026726	1.8799979	-0.4203687
C	1.3655365	-2.6132360	0.7846252
C	-0.4649324	2.9975933	2.1471294
C	2.6849881	-1.0757393	3.0494235
C	-2.1416977	2.2571472	0.3937478
C	3.7292102	-0.7124046	0.7678330
H	2.9323212	1.7148743	0.0666089
H	-0.5896903	-3.4422601	1.3146850
H	1.5894490	0.1778491	-1.5263759
H	0.2126438	-2.7803230	-1.0665744
H	-1.4154393	1.0971971	2.0471153
H	2.2496437	0.5301368	1.7089797
H	2.0694443	2.9403675	1.0186757
H	0.4588158	-3.0897949	2.7082209
H	-0.0071854	0.7290419	-2.0821304
H	1.9302630	-2.4010655	-1.3055057
H	0.3254082	2.6716640	2.8293728
H	1.7985442	-0.9002782	3.6667433
H	-2.5291857	1.4097403	-0.1787254
H	3.5575798	-0.3818459	-0.2604368
H	2.4538591	3.2384613	-0.6854956
H	0.7877960	-4.4907033	1.6706155
H	1.4488941	1.6662488	-2.4741663
H	1.4305381	-4.0393167	-0.8391821
H	0.1429720	2.7229356	-0.6461464
H	2.3876799	-2.8633676	1.0770142
H	-1.2769118	3.4356139	2.7360245
H	3.5360677	-0.5653325	3.5113957
H	-2.9579795	2.6827093	0.9874558
H	4.5458232	-0.1177240	1.1896507
H	-0.0660175	3.7800131	1.4939988
H	2.9031423	-2.1488874	3.0474095
H	-1.8155720	3.0306603	-0.3077252
H	4.0622483	-1.7549180	0.7419152
C	-1.3151923	-1.0881520	0.4612456
C	-2.1713201	-1.1985625	1.3867105
H	-1.4397178	-1.4413977	-0.5607786
C	-3.0159455	-1.2622346	2.4791264
C	-2.9441667	-2.3699582	3.3702655
C	-3.9672245	-0.2283871	2.7099345
C	-3.7895861	-2.4224992	4.4643012
H	-2.2238084	-3.1576320	3.1807659
C	-4.8124220	-0.3079242	3.8017087
H	-4.0249181	0.6025503	2.0156623
C	-4.7208168	-1.3974638	4.6794478
H	-3.7365892	-3.2602509	5.1513345
H	-5.5446613	0.4722316	3.9803854
H	-5.3839875	-1.4493435	5.5373986

B_0

57

Energy = -917.4307199921

B	0.9253808	0.2153198	0.0085422
N	1.9943916	1.1026890	0.1942865
N	1.1543647	-1.3147879	-0.0637569
C	1.2444417	3.2500745	-0.9402690
C	1.3579720	-3.5261037	0.9733136
C	0.8709368	2.8851896	1.5778057
C	0.9430694	-1.4221160	2.3514293
C	3.4630635	0.8438399	0.3446688
C	1.2461566	-1.9570324	-1.4299514
C	1.7347087	2.5817474	0.3491882
C	1.1428497	-2.0459230	1.0105224
C	3.9020904	-0.5991216	0.5853518
C	-0.1242575	-2.4849358	-1.8734652
C	4.2492099	1.4376207	-0.8359691
C	1.7915695	-0.9699563	-2.4564086
H	1.8992336	2.9959457	-1.7784151
H	1.1930288	-3.9561750	1.9611607
H	-0.1490433	2.5076202	1.4757219
H	0.8634480	-0.3350646	2.3127570
H	3.7450186	1.4057332	1.2449598
H	1.9455368	-2.7899268	-1.3210535
H	1.2630626	4.3365563	-0.8071598
H	2.3953501	-3.7300605	0.6759742
H	1.3150540	2.4383986	2.4733861
H	0.0303103	-1.8392092	2.7947812
H	4.9843186	-0.5834400	0.7445454
H	-0.5917183	-3.1262816	-1.1219491
H	4.0262138	2.4960578	-0.9885740
H	1.1374892	-0.0968128	-2.5506947
H	0.2257065	2.9650431	-1.2096376
H	0.7097312	-4.0250227	0.2497636
H	0.8218917	3.9685977	1.7265387
H	1.7666573	-1.7112173	3.0143646
H	2.7187675	3.0090061	0.5593268
H	-1.3772077	-1.2761141	0.3705564
H	3.7109825	-1.2537532	-0.2685669
H	0.0128686	-3.0731260	-2.7850275
H	5.3207747	1.3472244	-0.6338800
H	2.7979271	-0.6331571	-2.2064538
H	3.4488181	-1.0256477	1.4822380
H	-0.7995873	-1.6546990	-2.0927584
H	4.0291998	0.9044550	-1.7649012
H	1.8301829	-1.4699516	-3.4277727
C	-0.5639974	0.6115450	-0.1084239
C	-1.5942473	-0.2379003	0.1172092
H	-0.8280923	1.6376158	-0.3450378
C	-3.0214818	0.0641652	0.0790449
C	-3.5300364	1.3429992	-0.2207962
C	-3.9346369	-0.9714866	0.3517786
C	-4.9005315	1.5711234	-0.2464331
H	-2.8502409	2.1621436	-0.4363470
C	-5.3083412	-0.7434070	0.3261078
H	-3.5539570	-1.9634209	0.5845379
C	-5.7954558	0.5298675	0.0266920
H	-5.2776060	2.5626844	-0.4789381
H	-5.9971874	-1.5555795	0.5384950
H	-6.8655226	0.7135965	0.0056686

B_2

57

Energy = -917.4332728775

B	-0.4926255	0.6670570	-0.1735988
N	-0.7298099	0.9165885	-1.5319509
N	-1.6568779	0.1853234	0.7261181
C	-2.4344804	-0.7076156	-2.4746164
C	-1.9880387	0.9954568	3.0775621
C	-3.1597560	1.6184302	-1.8157523
C	-1.9005705	2.6463805	1.2060430
C	0.4085808	1.3828438	-2.3843443
C	-1.9595201	-1.0761182	0.8221605
C	-2.0002869	0.7531395	-2.3110146
C	-2.3285265	1.2340179	1.6022753
C	0.7221965	0.3913007	-3.5107283
C	-3.1150288	-1.5920665	1.6144392
C	0.1703947	2.8054366	-2.9009437
C	-1.1076161	-2.1074364	0.1530111

H	-2.9152013	-1.0906896	-1.5700081
H	-0.9293359	1.2003372	3.2563827
H	-2.8819059	2.6747093	-1.7760417
H	-2.4866228	3.3518322	1.8014700
H	1.2805301	1.4060309	-1.7314893
H	0.4081539	-0.4457864	2.1710559
H	-1.5905575	-1.3523821	-2.7305479
H	-2.2136050	-0.0189587	3.4109575
H	-3.9946096	1.5153850	-2.5163325
H	-0.8427503	2.8091989	1.4315726
H	1.6188777	0.7262673	-4.0410396
H	-3.6594527	-2.3106202	0.9926409
H	-0.0145676	3.4925536	-2.0696435
H	-1.7234574	-2.8067419	-0.4180692
H	-3.1710363	-0.7698934	-3.2817261
H	-2.5772551	1.6900406	3.6828503
H	-3.5188016	1.3049542	-0.8318615
H	-2.0768721	2.8628700	0.1532954
H	-1.7522653	1.1161715	-3.3101179
H	-3.4037540	1.1193049	1.4379720
H	-0.0884455	0.3237255	-4.2429694
H	-3.7983418	-0.8184908	1.9583087
H	1.0567980	3.1486566	-3.4435014
H	-0.3419949	-1.6737126	-0.4912567
H	0.9148398	-0.6077229	-3.1075387
H	-2.7447001	-2.1547721	2.4797420
H	-0.6787122	2.8555145	-3.5903964
H	-0.6149220	-2.6910105	0.9417605
C	0.8547115	0.8403433	0.5619580
C	1.1539377	0.2136791	1.7250491
H	1.6252004	1.4844487	0.1403003
C	2.3928246	0.2922749	2.4928730
C	2.4845618	-0.4326549	3.6956380
C	3.4991066	1.0656014	2.0911500
C	3.6372654	-0.3863189	4.4760407
H	1.6372619	-1.0350445	4.0155651
C	4.6495314	1.1118246	2.8692116
H	3.4588036	1.6316565	1.1651737
C	4.7237455	0.3872139	4.0646844
H	3.6885343	-0.9512681	5.4020280
H	5.4948122	1.7124006	2.5463160
H	5.6252687	0.4265838	4.6688219

B_3

57

Energy = -917.4317702541

B	0.6350465	-0.4323412	0.3753201
N	0.1722063	0.8915254	-0.2870741
N	-0.0755121	-1.6247406	0.1874802
C	1.6301668	0.3895878	-2.1511632
C	-2.5678712	-1.3147063	0.2438937
C	0.4334463	2.6168361	-2.0413895
C	-1.3501369	-1.3424211	-1.9923089
C	-0.7561309	1.7150525	0.5854047
C	0.4883176	-2.8950863	0.7446281
C	0.7004024	1.2909169	-1.4045601
C	-1.3622386	-1.8387160	-0.5434113
C	0.0050941	2.7857546	1.3726439
C	-0.4567478	-3.5596680	1.7492162
C	-1.9685513	2.2775077	-0.1664035
C	0.9101627	-3.8472616	-0.3819113
H	1.2745540	0.2872295	-3.1829408
H	-2.5882083	-0.2241173	0.2797116
H	-0.4387934	2.5226850	-2.7008744
H	-1.3857648	-0.2525489	-2.0613964
H	-1.1173553	0.9748910	1.3046908
H	1.3963694	-2.6138005	1.2764677
H	1.7297531	-0.5970033	-1.6974333
H	-2.5611406	-1.6937771	1.2685540
H	0.2341596	3.4099721	-1.3239510
H	-0.4664596	-1.7048655	-2.5240417
H	0.7818822	2.3389780	1.9953093
H	-0.7169113	-2.8684663	2.5565471
H	-2.3514146	1.5761414	-0.9119360
H	1.6090911	-3.3541539	-1.0646352
H	2.6163747	0.8648836	-2.2057760
H	-3.4906155	-1.6473507	-0.2424389
H	1.2834838	2.8939293	-2.6680786
H	-2.2366512	-1.7295846	-2.5038700
H	2.5677843	1.5559198	0.4395557
H	-1.4714155	-2.9240397	-0.5967759
H	-0.7089435	3.2977958	2.0241339
H	0.0411338	-4.4302598	2.1871474
H	-2.7613714	2.4585626	0.5646987
H	1.4097317	-4.7185327	0.0524676
H	0.4597266	3.5332419	0.7172834
H	-1.3798557	-3.9106939	1.2766822
H	-1.7496328	3.2265428	-0.6580302
H	0.0547063	-4.2108336	-0.9601721
C	1.9008782	-0.2749554	1.2489216
C	2.7676185	0.7624246	1.1617992
H	2.1320966	-1.0391901	1.9895585
C	3.9883078	0.9766118	1.9315575
C	4.4517283	0.0719630	2.9066579
C	4.7376338	2.1436313	1.6910302
C	5.6203509	0.3308113	3.6123807
H	3.8947149	-0.8372594	3.1124289
C	5.9085053	2.4038625	2.3988756
H	4.3898140	2.8494809	0.9400711
C	6.3537179	1.4968218	3.3618699
H	5.9659818	-0.3762190	4.3607730
H	6.4720179	3.3107438	2.2009105
H	7.2673206	1.6932059	3.9150476

Ba

57

Energy = -917.4396484032

B	0.3540735	-0.3564632	1.2472200
N	0.2529851	1.1843388	1.0695431
N	1.6208581	-0.9460017	1.2602927
C	1.4370955	2.3355189	-0.8124433
C	1.3551629	-2.9411138	2.7696685
C	-0.4191659	0.6953407	-1.2943906
C	1.2734360	-3.2030789	0.2178809
C	0.1388449	1.9579496	2.1091500
C	2.8831309	-0.1618808	1.1758364
C	0.1055521	1.7517757	-0.3247773
C	1.8345639	-2.4203543	1.4098185
C	0.2804594	1.4022671	3.4856340
C	3.7085530	-0.2771737	2.4636642
C	-0.1568051	3.4208961	1.9937490
C	3.7072344	-0.5436167	-0.0596236
H	2.1448412	1.5407833	-1.0582072
H	1.6415361	-3.9920596	2.8774425
H	0.2621542	-0.1604577	-1.3536740
H	1.5415725	-4.2596225	0.3166809
H	-2.1953215	0.6722604	1.5696054
H	2.5820385	0.8816459	1.0706810
H	1.8965413	2.9990208	-0.0748935
H	0.2705543	-2.8714065	2.8810499
H	-1.4098553	0.3351319	-1.0134710
H	0.1849171	-3.1338365	0.1520600
H	1.1268816	1.8983946	3.9766503
H	4.0757651	-1.2961820	2.6204320

H	-1.1854570	3.5615126	1.6365667
H	4.1102970	-1.5579755	0.0196971
H	1.2485436	2.9133001	-1.7212801
H	1.8192215	-2.3745113	3.5822319
H	-0.4797517	1.1471621	-2.2882233
H	1.6960872	-2.8276142	-0.7187678
H	-0.6308684	2.5544338	-0.2420650
H	2.9187509	-2.5544306	1.3897342
H	0.4287825	0.3219926	3.5018465
H	3.1203882	0.0175443	3.3374843
H	-0.0653391	3.8999612	2.9684974
H	3.1050752	-0.4853865	-0.9713748
H	-0.6109177	1.6595846	4.0693461
H	4.5791642	0.3821552	2.3943274
H	0.5049121	3.9209627	1.2828725
H	4.5539175	0.1426182	-0.1579701
C	-1.0025225	-1.0641168	1.4315643
C	-2.1823888	-0.4190072	1.5949737
H	-1.0331647	-2.1499306	1.4594824
C	-3.4985922	-1.0102609	1.8114417
C	-3.7162956	-2.4005322	1.8745819
C	-4.6042252	-0.1526834	1.9635301
C	-4.9931634	-2.9078319	2.0817283
H	-2.8829799	-3.0875203	1.7601530
C	-5.8842963	-0.6607343	2.1707130
H	-4.4486752	0.9228104	1.9169815
C	-6.0824333	-2.0410727	2.2302278
H	-5.1451616	-3.9821234	2.1288570
H	-6.7249926	0.0170492	2.2850051
H	-7.0784244	-2.4428185	2.3909487

Bb

57

Energy = -917.4376043186

B	0.3765233	-0.5509364	1.3328675
N	0.6339367	0.9664826	1.5184967
N	1.4927258	-1.3831621	1.2087720
C	-0.4521623	2.4003254	-0.2495336
C	0.7039946	-3.6184278	2.0427255
C	2.0773766	2.5493195	0.1362160
C	0.7992489	-3.1154338	-0.4705020
C	0.5890001	1.5319186	2.6854504
C	2.8862142	-0.8873096	1.3738274
C	0.8218873	1.6743466	0.1895224
C	1.3978295	-2.8471381	0.9145670
C	0.4312930	0.6812203	3.9050704
C	3.5911816	-1.5586247	2.5591274
C	0.7144594	3.0011578	2.9239109
C	3.6910240	-1.0182159	0.0754964
H	-1.2987815	1.7119468	-0.2920008
H	1.2006064	-3.4286296	2.9987719
H	2.2943757	2.7548554	-0.9156244
H	0.8543553	-4.1863960	-0.6897747
H	-1.9165972	0.8905917	1.8911976
H	2.8011318	0.1754148	1.6087601
H	-0.2868963	2.8029807	-1.2527798
H	0.7552286	-4.6920454	1.8358429
H	1.9473512	3.5071508	0.6419779
H	-0.2479508	-2.8099331	-0.5352691
H	1.2336558	0.9223115	4.6121403
H	3.0127943	-1.4366646	3.4798090
H	1.7596793	3.2276354	3.1706908
H	3.1865978	-0.5111024	-0.7525903
H	-0.7034132	3.2331803	0.4116924
H	-0.3481810	-3.3411346	2.1440939
H	2.9435137	2.0384928	0.5646113
H	1.3595409	-2.5768878	-1.2403293
H	0.9755933	0.8363449	-0.4977041
H	2.4319115	-3.1989969	0.8819950
H	0.4459982	-0.3871839	3.6837652
H	4.5728013	-1.0970902	2.7032613
H	0.4197958	3.6103996	2.0732747
H	4.6778765	-0.5648962	0.2107676
H	-0.5118305	0.9336807	4.4028458
H	3.7493670	-2.6277714	2.3876043
H	0.1163402	3.2744717	3.7967128
H	3.8418991	-2.0660380	-0.2021858
C	-1.1076957	-0.9511803	1.2530854
C	-2.1365508	-0.1310091	1.5777969
H	-1.3659300	-1.9623637	0.9498522
C	-3.5615010	-0.4430961	1.5733408
C	-4.0721905	-1.7030489	1.2046729
C	-4.4703012	0.5627648	1.9522511
C	-5.4409451	-1.9416930	1.2154971
H	-3.3954363	-2.4988404	0.9077057
C	-5.8422426	0.3239337	1.9631834
H	-4.0876571	1.5397738	2.2387517
C	-6.3315673	-0.9301887	1.5944120
H	-5.8201702	-2.9179786	0.9284404
H	-6.5279650	1.1126851	2.2578266
H	-7.4003879	-1.1220323	1.6009174

Bc

57

Energy = -917.4329914950

B	0.3879775	-0.2333591	1.5703625
N	0.7433929	1.2240647	1.9975192
N	1.4233412	-1.0664769	1.1559993
C	0.6484961	1.8432794	-0.4165419
C	0.6697281	-3.2281807	2.1740305
C	-1.0019570	2.8234110	1.2328838
C	0.5133707	-2.8983596	-0.3415810
C	1.1351060	1.5053554	3.2051280
C	2.8226571	-0.5813034	0.9641858
C	0.4326377	2.3270522	1.0141295
C	1.2680564	-2.5435176	0.9429270
C	1.2985467	0.4273624	4.2223917
C	3.7876233	-1.1685754	2.0018917
C	1.4229105	2.9068607	3.6471187
C	3.3164696	-0.8429989	-0.4637325
H	0.4117591	2.6634653	-1.0992556
H	1.2630850	-3.0100909	3.0677972
H	-1.1766615	3.1248701	2.2690052
H	0.8747448	-2.3117914	-1.1904825
H	-1.6225214	-0.9585104	-0.2657078
H	2.7880944	0.5006112	1.1132832
H	-0.0136521	1.0052085	-0.6574782
H	0.6655204	-4.3122759	2.0227630
H	-1.1739033	3.6901801	0.5887483
H	0.6671753	-3.9588120	-0.5661655
H	1.0940092	-0.5708446	3.8336855
H	4.7705512	-0.7024238	1.8832034
H	1.7182188	2.9157139	4.6962117
H	2.6297956	-0.4270955	-1.2060134
H	1.6829341	1.5425273	-0.5928700
H	-0.3603048	-2.9028809	2.3451703
H	-1.7193669	2.0421242	0.9721638
H	-0.5592053	-2.7323482	-0.2262579
H	1.1378500	3.1329893	1.2282846
H	2.2888666	-2.9154914	0.8290378
H	0.6198434	0.6409105	5.0575680
H	3.9158101	-2.2474522	1.8710920
H	2.2366363	3.3342404	3.0492727
H	4.2968662	-0.3752562	-0.5962716

H	2.3132162	0.4633073	4.6345807
H	3.4410448	-0.9850301	3.0218478
H	0.5502460	3.5541829	3.5189286
H	3.4305419	-1.9135465	-0.6597455
C	-1.1280454	-0.5200163	1.7307787
C	-2.0016802	-0.8221390	0.7467384
H	-1.5453308	-0.3223706	2.7231517
C	-3.4536330	-0.9626290	0.8588360
C	-4.1547517	-0.7693866	2.0637566
C	-4.1846866	-1.3094251	-0.2917095
C	-5.5352864	-0.9241939	2.1129039
H	-3.6173464	-0.4932552	2.9664371
C	-5.5684573	-1.4655490	-0.2431938
H	-3.6547270	-1.4589394	-1.2296118
C	-6.2483600	-1.2740005	0.9603490
H	-6.0619113	-0.7713681	3.0505015
H	-6.1148972	-1.7358248	-1.1419876
H	-7.3269454	-1.3931734	1.0033200

B (or **2**$^{+}$)

57

Energy = -917.4398539979

B	0.4057765	-0.3028946	1.2046130
N	0.3022339	1.2271619	0.9594017
N	1.6830337	-0.8667323	1.2957804
C	0.7652080	0.7736191	-1.4542285
C	1.3059114	-2.7172716	2.9560307
C	-1.4135354	1.8315719	-0.7550510
C	1.4865899	-3.2255696	0.4482912
C	0.3000059	2.0706808	1.9490948
C	2.9413325	-0.0805081	1.1592121
C	0.0853679	1.7070702	-0.4580547
C	1.9090988	-2.3144620	1.6058981
C	0.4126313	1.5908838	3.3565482
C	3.6902461	0.0196336	2.4947704
C	0.1860774	3.5490665	1.7408490
C	3.8561666	-0.6374194	0.0599811
H	0.3596378	-0.2413571	-1.3887902
H	0.2146813	-2.6608706	2.9550781
H	-1.8821846	0.8453854	-0.7896153
H	0.4069790	-3.2082398	0.2804750
H	-2.1150220	0.6656415	1.7644135
H	2.6401264	0.9272459	0.8628505
H	1.8451867	0.7378620	-1.3053579
H	1.6819980	-2.0671873	3.7520045
H	-1.9345376	2.4422181	-0.0125110
H	1.9801459	-2.9219015	-0.4790733
H	0.5018541	0.5070644	3.4372906
H	3.0531971	0.4327154	3.2809053
H	-0.7131294	3.8086134	1.1749335
H	3.3241506	-0.7523787	-0.8878921
H	0.5728687	1.1491625	-2.4627467
H	1.5945094	-3.7468872	3.1898921
H	-1.5321116	2.3089671	-1.7316541
H	1.7777264	-4.2568057	0.6717521
H	0.5524314	2.6923992	-0.5155468
H	2.9919790	-2.4177930	1.7078769
H	-0.4748867	1.9255386	3.9075517
H	4.5611797	0.6714059	2.3761749
H	0.1620951	4.0627972	2.7016983
H	4.6902432	0.0540095	-0.0920106
H	1.2716091	2.0746486	3.8357251
H	4.0505127	-0.9603757	2.8237394
H	1.0466912	3.9163881	1.1688230
H	4.2790118	-1.6077655	0.3373292
C	-0.9404078	-1.0363654	1.3514099
C	-2.1088551	-0.4189637	1.6489204
H	-0.9679140	-2.1186559	1.2554431
C	-3.4147741	-1.0351029	1.8573432
C	-3.6331846	-2.4235196	1.7646121
C	-4.5090118	-0.2044444	2.1631017
C	-4.9005493	-2.9551926	1.9692758
H	-2.8081260	-3.0894329	1.5293883
C	-5.7795178	-0.7369089	2.3679241
H	-4.3524378	0.8692794	2.2376615
C	-5.9788783	-2.1149809	2.2710520
H	-5.0533879	-4.0279036	1.8960816
H	-6.6117435	-0.0799445	2.6024111
H	-6.9675026	-2.5355502	2.4291230

C

57

Energy = -917.3970842209

B	0.7817394	0.8759212	0.4683129
N	-0.3741310	1.6276477	0.4295553
N	1.1002778	-0.7250400	0.4257573
C	0.3750022	3.6700314	1.6738161
C	-0.7309180	-1.9073994	-0.9334081
C	0.4824279	3.5901504	-0.8746893
C	1.1580252	-0.7078417	-2.0767611
C	-1.7673368	1.1142196	0.3903532
C	0.9079426	-1.4981092	1.7646142
C	-0.2499923	3.1268835	0.3870321
C	0.7385564	-1.5061779	-0.8449705
C	-2.5989012	1.6260352	1.5727741
C	-0.4338168	-1.2155194	2.4284033
C	-2.4384245	1.4360824	-0.9496914
C	1.1960820	-2.9907094	1.6337348
H	1.4124841	3.3403022	1.7809791
H	-1.3697483	-1.0563711	-1.1732635
H	1.5272445	3.2671542	-0.8718317
H	0.6276497	0.2496558	-2.1232373
H	-1.6855739	0.0318399	0.4863653
H	1.6831087	-1.0544314	2.3961790
H	-0.1868618	3.3342782	2.5500960
H	-1.0996557	-2.3919231	-0.0287490
H	-0.0004978	3.1920293	-1.7719621
H	2.2318535	-0.5072167	-2.1032057
H	-2.1098073	1.4133686	2.5274076
H	-0.5893312	-0.1430443	2.5654359
H	-1.8463469	1.0627702	-1.7908256
H	2.1754117	-3.1840206	1.1905287
H	0.3654188	4.7642562	1.6542400
H	-0.8226221	-2.6268540	-1.7521920
H	0.4639867	4.6831300	-0.9289524
H	0.8959660	-1.2842037	-2.9678338
H	-1.2755884	3.4983254	0.3300449
H	1.3318724	-2.4192557	-0.7791267
H	-3.5726250	1.1273668	1.5652466
H	-0.4170725	-1.6761323	3.4205245
H	-3.4268829	0.9681180	-0.9850086
H	1.1983957	-3.4128191	2.6428155
H	-2.7776275	2.7034684	1.5082449
H	-1.2785062	-1.6377416	1.8800023
H	-2.5748815	2.5143075	-1.0788757
H	0.4299702	-3.5149502	1.0570021
C	2.2929650	1.1219109	0.4976410
C	2.5427224	-0.1992258	0.4066783
H	3.0158776	1.9249009	0.5396637
C	3.7594803	-1.0064393	0.4325774
C	4.7692795	-0.5934927	1.3239304
C	3.9982350	-2.1185372	-0.3949816
C	5.9749491	-1.2838222	1.3966985
H	4.5880686	0.2591640	1.9711639

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C     5.2088668   -2.8018764   -0.3203260
H     3.2616314   -2.4373901   -1.1222074
C     6.1970687   -2.3921472    0.5768478
H     6.7382015   -0.9599524    2.0974481
H     5.3821813   -3.6530369   -0.9713268
H     7.1367878   -2.9327184    0.6344645
```

D

```
57
Energy = -917.3812151339
B     0.0654682    0.3194987   -0.7808521
N     0.0443416    1.5401113   -1.3986034
N     0.0396160   -1.1848591   -1.1256183
C    -1.1701111    2.8680276    0.3156217
C    -2.4651006   -1.0945740   -1.0793223
C     1.3815269    2.9384486    0.1601981
C    -1.3022980   -2.0387272   -3.0952458
C    -0.0322740    1.6829293   -2.8803188
C     1.3848647   -1.8463281   -1.4789309
C     0.0579117    2.8034769   -0.5955818
C    -1.2480044   -1.8711488   -1.5794493
C    -1.3539013    2.3313682   -3.3028448
C     1.3200266   -3.3607881   -1.3111907
C     1.1813151    2.4398998   -3.4271902
C     1.9188688   -1.4001068   -2.8365488
H    -1.1774278    2.0339347    1.0240763
H    -2.4921286   -0.0863534   -1.5066327
H     1.5258824    2.0992480    0.8483918
H    -1.2468193   -1.0719294   -3.6045552
H    -0.0077560    0.6616191   -3.2699973
H     2.0531175   -1.4445353   -0.7115301
H    -2.0911928    2.8232095   -0.2725104
H    -2.4916385   -1.0146123    0.0086793
H     2.2255424    2.9539418   -0.5350181
H    -0.5139314   -2.6871180   -3.4787994
H    -2.2106887    1.7655876   -2.9259559
H     0.9559980   -3.6447210   -0.3198974
H     2.1171495    1.9642608   -3.1193643
H     2.0011017   -0.3115069   -2.8851213
H    -1.1652936    3.8034666    0.8830279
H    -3.3643742   -1.6225718   -1.4067822
H     1.3898409    3.8667197    0.7391753
H    -2.2620997   -2.4969673   -3.3504541
H    -0.0095315    3.6177048   -1.3209397
H    -1.2271868   -2.8550959   -1.1013744
H    -1.4097564    2.3575195   -4.3950830
H     2.3332737   -3.7576640   -1.4194036
H     1.1381334    2.4474186   -4.5201044
H     2.9254596   -1.8122995   -2.9562906
H    -1.4293653    3.3610286   -2.9394744
H     0.6917908   -3.8362915   -2.0687617
H     1.1925795    3.4799202   -3.0867737
H     1.3101894   -1.7487142   -3.6719848
C     0.0441731   -0.6586839    0.3188038
C    -0.0243601   -1.3823615    1.4457218
H    -0.1346348   -2.4622290    1.3474385
C     0.0144453   -0.8911141    2.8119775
C    -0.1525775   -1.8187256    3.8581067
C     0.2107845    0.4655319    3.1337959
C    -0.1354999   -1.4014154    5.1859000
H    -0.2965462   -2.8690592    3.6184720
C     0.2279589    0.8798371    4.4584275
H     0.3549027    1.1878992    2.3386425
C     0.0527766   -0.0517097    5.4891831
H    -0.2667382   -2.1266100    5.9830064
H     0.3807023    1.9282869    4.6958902
H     0.0681784    0.2761864    6.5241384
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E

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57
Energy = -917.4258270636
B    -0.1368550   -0.5898046    0.3403761
N    -0.2309290    0.7919222    0.4973778
N    -0.4925626   -1.4886492    1.5636843
C     1.7135779    1.5184209   -0.9201573
C    -2.9468582   -1.2012967    1.2227173
C    -0.6543086    2.0646094   -1.6712020
C    -1.7981449   -3.3893890    0.6077667
C    -0.7769072    1.4162418    1.7442364
C     0.3819916   -1.7551885    2.4895891
C     0.2787053    1.8141495   -0.4812434
C    -1.8308921   -2.1876425    1.5577456
C     0.2912310    2.1821322    2.5375052
C     1.7333832   -1.1232502    2.4818243
C    -1.9806708    2.3149981    1.4413026
C     0.1036582   -2.7136501    3.6078309
H     1.7700467    0.6222790   -1.5414477
H    -2.7736338   -0.7006046    0.2655042
H    -0.5923849    1.2656967   -2.4097350
H    -1.7171015   -3.0761926   -0.4349209
H    -1.1242254    0.5906159    2.3671629
H     1.7219166   -2.5877087    0.2602566
H     2.3690826    1.3872177   -0.0533929
H    -3.0558457   -0.4400062    1.9983124
H    -1.6939450    2.1614887   -1.3493641
H    -0.9588373   -4.0528761    0.8333301
H     1.1841623    1.5763245    2.7062426
H     1.8990726   -0.4593030    1.6332563
H    -2.7513821    1.7772582    0.8832613
H    -0.1813266   -3.6979533    3.2229306
H     2.0882866    2.3621528   -1.5081335
H    -3.8881010   -1.7520705    1.1506663
H    -0.3567642    3.0014529   -2.1538489
H    -2.7297080   -3.9484634    0.7330848
H     0.3089627    2.7408888    0.0956592
H    -1.9875138   -2.5478213    2.5741831
H    -0.1244679    2.4604127    3.5107209
H     2.4910109   -1.9155117    2.4850075
H    -2.4127897    2.6609595    2.3851976
H     0.9905737   -2.8224561    4.2320441
H     0.5926023    3.1052402    2.0335378
H     1.8690740   -0.5697883    3.4187322
H    -1.6868044    3.1988253    0.8670424
H    -0.7200416   -2.3514725    4.2331953
C     1.3059441   -2.3631690   -0.7173571
C     0.3653505   -1.4164944   -0.9075111
H     1.6980517   -2.9533765   -1.5424730
C    -0.1609654   -1.2060702   -2.2813891
C     0.7029456   -1.1725365   -3.3878285
C    -1.5391156   -1.0722909   -2.5098507
C     0.2038119   -1.0073282   -4.6786015
H     1.7748308   -1.2529160   -3.2285546
C    -2.0423489   -0.9221754   -3.7999327
H    -2.2268718   -1.0837707   -1.6698438
C    -1.1710181   -0.8840867   -4.8901493
H     0.8898950   -0.9679811   -5.5197735
H    -3.1133975   -0.8285544   -3.9536826
H    -1.5595781   -0.7532121   -5.8956508
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PhCCH
14
Energy = -308.5847705702
C    -3.2326550   -0.0000129   -0.0001901
C    -2.0212443   -0.0000642    0.0002219
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H	-4.2999793	-0.0000327	-0.0003936
C	-0.5951988	-0.0000294	0.0004688
C	0.1178432	-1.2146355	0.0003731
C	0.1177578	1.2146272	0.0003341
H	-0.4296854	-2.1518820	0.0004087
C	1.5100267	-1.2090142	-0.0000190
C	1.5099390	1.2090969	-0.0000139
H	-0.4298350	2.1518357	0.0002431
H	2.0504724	-2.1511843	-0.0001690
C	2.2101752	0.0000669	-0.0002789
H	2.0503182	2.1513044	0.0000195
H	3.2962731	0.0001134	-0.0004966

R0

43

Energy = -608.7660766786

B	0.0036966	0.0313713	0.0009441
N	-0.4622990	0.7906246	1.0018428
N	0.4699597	-0.7283729	-0.9994227
C	0.8739583	1.1790877	3.0519137
C	-0.9049507	-1.2190339	-3.0015288
C	1.5783728	2.2060017	0.8432044
C	-0.0206112	1.1209601	-2.5902777
C	-1.8898446	0.7015711	1.4714242
C	1.2562483	-1.9870507	-0.7459884
C	0.4103133	1.7815172	1.7252055
C	0.2406103	-0.3733808	-2.4443432
C	-2.6931268	1.8631407	0.8853720
C	2.7477988	-1.7002210	-0.9218481
C	-2.4855057	-0.6534937	1.1087418
C	0.9341101	-2.5479938	0.6339570
H	0.0319061	0.8287627	3.6552891
H	-1.8513933	-0.9408773	-2.5260074
H	1.2288027	2.6713617	-0.0825586
H	0.8243675	1.7100032	-2.2232184
H	-1.8412713	0.7972434	2.5604846
H	0.9225426	-2.6936359	-1.5119650
H	1.4099205	1.9390317	3.6277818
H	-0.7348563	-2.2877749	-2.8447958
H	2.1958017	2.9300603	1.3810405
H	-0.1761803	1.3614752	-3.6450608
H	-3.6979946	1.8632731	1.3173693
H	2.9625089	-1.2471968	-1.8937527
H	-1.9220760	-1.4709315	1.5670748
H	1.5085494	-3.4633918	0.7973542
H	1.5518295	0.3376981	2.8734147
H	-0.9939805	-1.0447975	-4.0776896
H	2.2175327	1.3496240	0.5935969
H	-0.9268046	1.4190934	-2.0477850
H	-0.2330990	2.6457447	1.9162001
H	1.1733258	-0.6307540	-2.9555640
H	-2.7828348	1.7559919	-0.2007777
H	3.3078194	-2.6373767	-0.8542583
H	-3.5176196	-0.7040661	1.4649172
H	1.2124381	-1.8392561	1.4241913
H	-2.2304417	2.8292781	1.1050571
H	3.1028693	-1.0268417	-0.1346701
H	-2.5052357	-0.7986392	0.0211821
H	-0.1288968	-2.7865960	0.7278381

Ra

43

Energy = -608.7635309948

B	-0.0115286	-0.1255624	0.0163565
N	0.0428924	1.1309463	0.4696394
N	-0.1208580	-1.3880564	-0.4171551
C	2.4544580	1.7158046	0.2680830
C	-2.0132563	-0.6480643	-1.8455770
C	0.7933739	2.3931323	-1.5331097
C	-0.0693494	-1.9467153	-2.8335620
C	-0.9469298	1.5512778	1.5345937
C	0.5647169	-2.5338387	0.2759612
C	1.0248633	2.1538087	-0.0422076
C	-0.9663028	-1.7326438	-1.6145327
C	-0.2102415	1.9473882	2.8127582
C	1.7640636	-2.0253944	1.0675165
C	-1.8658224	2.6482851	1.0001413
C	-0.4418145	-3.2720708	1.1593054
H	3.1532923	2.4991214	-0.0388347
H	-2.6498898	-0.9288172	-2.6884483
H	0.9980269	1.4797694	-2.1050719
H	-0.6765955	-2.2953417	-3.6739160
H	-1.5446640	0.6545994	1.7334965
H	0.9094215	-3.1936254	-0.5262035
H	2.7058797	0.8031743	-0.2844463
H	-1.5402368	0.3098310	-2.0939347
H	-0.2355104	2.7074725	-1.7285769
H	0.4152164	-1.0076704	-3.1206481
H	0.4104485	2.8354767	2.6586781
H	1.4503174	-1.3170838	1.8451109
H	-2.3855191	2.3213674	0.0952441
H	-1.3204329	-3.5937709	0.5933598
H	2.5882316	1.5274946	1.3366206
H	-2.6484549	-0.5155017	-0.9638150
H	1.4703229	3.1733662	-1.8923643
H	0.7038050	-2.6959019	-2.6414976
H	0.7978276	3.0672855	0.5115036
H	-1.4659228	-2.6701866	-1.3522418
H	0.4234186	1.1315547	3.1718163
H	2.4931114	-1.5370845	0.4145843
H	-2.6130986	2.8875746	1.7620936
H	0.0320399	-4.1627062	1.5820256
H	-0.9450582	2.1828967	3.5879176
H	2.2556891	-2.8643112	1.5665982
H	-1.3099206	3.5643597	0.7777544
H	-0.7703140	-2.6286629	1.9824089

Rb

43

Energy = -608.7602254489

B	-0.0000103	-0.0000092	0.0928482
N	-0.0319814	1.3360104	0.1181240
N	0.0319402	-1.3360262	0.1182034
C	2.2993136	1.6775064	-0.6483332
C	-2.2993150	-1.6779879	-0.6482575
C	0.3480067	2.1608859	-2.2026606
C	-0.3479026	-2.1602925	-2.2028150
C	-0.9716040	2.0289793	1.0797615
C	0.9715540	-2.0290313	1.0798196
C	0.8596636	2.1748393	-0.7626803
C	-0.8595190	-2.1748442	-0.7628270
C	-0.1709650	2.7627897	2.1547921
C	0.1709570	-2.7626839	2.1549907
C	-1.9409074	2.9367685	0.3261052
C	1.9407140	-2.9369502	0.3261296
H	2.3798102	0.6450721	-1.0125742
H	-2.3801505	-0.6454726	-1.0121933
H	0.4277439	1.1535387	-2.6264808
H	-0.4279304	-1.1528327	-2.6263156
H	-1.5391392	1.2191577	1.5517789
H	1.5392168	-1.2192356	1.5517302
H	2.6480434	1.7146536	0.3873762
H	-2.6479740	-1.7155398	0.3874616
H	-0.6943175	2.4829314	-2.2605661

H	0.6945156	-2.4820219	-2.2608258
H	0.5017375	2.0787177	2.6797770
H	-0.5016465	-2.0785132	2.6799752
H	-2.5091016	2.3767901	-0.4218372
H	2.5088768	-2.3770570	-0.4219020
H	2.9576684	2.2981519	-1.2622635
H	-2.9575119	-2.2986640	-1.2623262
H	0.9547810	2.8353375	-2.8138164
H	-0.9544902	-2.8347163	-2.8141866
H	0.7908899	3.1871653	-0.3580076
H	-0.7904220	-3.1872768	-0.3584767
H	-0.8645460	3.1944928	2.8820200
H	0.8645756	-3.1943664	2.8821944
H	-2.6449709	3.3715267	1.0412929
H	2.6448140	-3.3717334	1.0412669
H	0.4186512	3.5802411	1.7284709
H	-0.4187556	-3.5801367	1.7288066
H	-1.4156071	3.7594243	-0.1686771
H	1.4152949	-3.7595879	-0.1685609

Rc

43

Energy = -608.7801574779

B	-0.7572912	0.1764771	0.5235725
N	-0.0775757	1.5136686	0.1984660
N	-0.3419376	-1.0105875	-0.0397142
C	0.5465543	1.5653670	2.6029140
C	-0.8572127	-2.5904100	1.8232056
C	2.3327244	1.5275670	0.8044034
C	-2.5133723	-2.2473632	-0.0766790
C	-0.4311008	2.2330706	-0.8247871
C	0.7515353	-1.1442738	-1.0390950
C	0.9364388	2.0161150	1.1955103
C	-1.0398276	-2.2862983	0.3347090
C	0.1653996	3.5764172	-1.1041546
C	1.8824653	-2.0393417	-0.5207564
C	-1.4858128	1.7446194	-1.7576609
C	0.2155634	-1.6408173	-2.3871275
H	0.5709334	0.4732744	2.6919730
H	-1.3507003	-1.8297890	2.4368928
H	2.4072601	0.4421086	0.9100527
H	-3.0531000	-1.4771123	0.4833488
H	-1.6543304	0.2338774	1.2976537
H	1.1511132	-0.1362926	-1.1809454
H	-0.4480848	1.9221236	2.8807248
H	0.2036447	-2.6195300	2.0888299
H	2.5872500	1.8018676	-0.2230855
H	-2.6157668	-2.0397220	-1.1461297
H	-0.2111614	4.3062994	-0.3763094
H	2.2479982	-1.6969541	0.4514185
H	-1.9564097	0.8168633	-1.4267789
H	-0.5810806	-0.9930404	-2.7626499
H	1.2738033	1.9749048	3.3089058
H	-1.3008440	-3.5622384	2.0608456
H	3.0652692	1.9851568	1.4747260
H	-2.9819882	-3.2138862	0.1330068
H	0.8993646	3.1055037	1.1481762
H	-0.5462139	-3.0743814	-0.2388084
H	-0.1227809	3.9113879	-2.1009338
H	2.7141791	-2.0191389	-1.2311799
H	-2.2470770	2.5252227	-1.8686165
H	1.0288219	-1.6493097	-3.1186349
H	1.2555197	3.5637076	-1.0284367
H	1.5569695	-3.0791307	-0.4188115
H	-1.0447606	1.5946203	-2.7505972
H	-0.1743795	-2.6606025	-2.3110980

Rd

43

Energy = -608.7731585372

B	-0.1436244	0.1099985	-0.6986756
N	-1.2804409	-0.1721536	0.0300262
N	1.3056464	0.0033835	-0.2078914
C	-2.8570393	1.3660693	-1.1913364
C	3.4208384	-1.2386754	0.0235618
C	-2.6843381	-1.0938015	-1.8220633
C	1.2944294	-2.3438955	-0.8035539
C	-1.4692001	-0.5905012	1.4484933
C	1.9789632	1.3163086	0.1243759
C	-2.5987970	-0.0585887	-0.6992151
C	1.9710974	-1.1094107	-0.3034453
C	-0.2054399	-1.0642392	2.1606077
C	2.6988345	1.8335071	-1.1245981
C	-2.1443631	0.5315543	2.2508520
C	0.9545718	2.3188433	0.6475026
H	-2.7781644	2.0845656	-0.3700736
H	3.9857474	-1.2844856	-0.9165556
H	-1.9505576	-0.8803448	-2.6061865
H	0.2567935	-2.1729604	-1.0956548
H	-2.1611793	-1.4415312	1.4025661
H	2.7010774	1.1042673	0.9152087
H	-3.8648755	1.4319600	-1.6131313
H	3.5878372	-2.1905398	0.5354839
H	-2.5048380	-2.1027128	-1.4363005
H	1.8573497	-2.7282461	-1.6620023
H	-0.4904492	-1.4031711	3.1606718
H	1.9819782	2.0294177	-1.9272923
H	-3.0727821	0.8683700	1.7828051
H	0.1917916	2.5467053	-0.1049678
H	-2.1430080	1.6478458	-1.9711927
H	3.8179645	-0.4234935	0.6256461
H	-3.6816519	-1.0716322	-2.2724424
H	1.3273353	-3.1221760	-0.0330588
H	-3.3591784	-0.3066469	0.0465038
H	-0.2287249	0.4851929	-1.8243978
H	0.5271306	-0.2619641	2.2843593
H	3.4438903	1.1200073	-1.4855309
H	-2.3862993	0.1643425	3.2526547
H	0.4621256	1.9587059	1.5528212
H	0.2627881	-1.9072007	1.6481488
H	3.2084800	2.7690608	-0.8787283
H	-1.4770815	1.3926427	2.3509268
H	1.4751838	3.2490616	0.8893610

R (or **1**$^{+}$)

43

Energy = -608.7673463723

B	0.0197632	0.0211942	0.0079620
N	-0.8723248	0.5706152	0.8430181
N	0.9121290	-0.5278960	-0.8270137
C	0.9991699	1.0688849	2.3938169
C	0.7089012	-0.3455239	-3.2947690
C	-0.6330648	2.8851993	1.7090747
C	1.1889823	1.7025896	-1.8778312
C	-2.3528104	0.3866854	0.6480740
C	1.4730107	-1.9035137	-0.5895218
C	-0.4419598	1.4008472	2.0216205
C	1.4029808	0.2022310	-2.0474695
C	-2.6449650	0.0139556	-0.8015743
C	2.8846854	-1.7965511	-0.0121588
C	-2.8810189	-0.6563496	1.6332808
C	0.5367861	-2.6987146	0.3141995
H	1.1114859	0.0080844	2.6394489
H	1.1445243	0.1193199	-4.1840034

H	0.0477144	3.1992438	0.9113887
H	1.7148088	2.0811815	-0.9955018
H	-2.7970366	1.3622530	0.8685051
H	1.5116903	-2.3744963	-1.5766095
H	1.2970660	1.6565811	3.2658828
H	-0.3609015	-0.1145838	-3.2702250
H	-1.6590111	3.1073166	1.4027278
H	1.5703458	2.2289015	-2.7565682
H	-3.7234928	-0.0943866	-0.9417231
H	2.8565627	-1.3555165	0.9894566
H	-2.6314929	-0.4018220	2.6670448
H	0.4482812	-2.2275580	1.3011426
H	1.6849851	1.3206738	1.5752205
H	0.8322169	-1.4282236	-3.3861074
H	-0.4140227	3.4739603	2.6046016
H	0.1217145	1.9401172	-1.7872026
H	-1.1055199	1.1065444	2.8405950
H	2.4757479	-0.0080121	-2.0982898
H	-2.1794108	-0.9445229	-1.0631352
H	3.5376117	-1.1890410	-0.6448830
H	-3.9706723	-0.7096394	1.5530269
H	-0.4602770	-2.7889949	-0.1284382
H	-2.2846456	0.7849691	-1.4899861
H	3.3217027	-2.7966842	0.0608787
H	-2.4668177	-1.6435297	1.4046039
H	0.9382092	-3.7042175	0.4638642

TSA_1A

57

Energy = -917.3561868044

B	0.3288926	-0.0292919	0.8981976
N	-0.0442213	1.1587912	1.6175700
N	0.0381940	-1.3685399	1.1526835
C	0.0443400	3.3272634	0.2810198
C	-0.3665282	-1.8283939	3.6150832
C	-1.8498355	1.6798447	0.0085537
C	-2.2880591	-1.1631654	2.1112508
C	0.6725950	1.4197384	2.8978337
C	0.6612815	-2.4812840	0.3712431
C	-0.8149760	2.2554561	0.9809202
C	-0.9310831	-1.8585577	2.1907403
C	1.9235860	2.3085533	2.7666142
C	1.3862516	-3.4922008	1.2657565
C	-0.2695308	1.9638483	3.9772315
C	-0.3726372	-3.1522886	-0.5403520
H	0.6964353	2.8781739	-0.4729772
H	-0.3505548	-0.8134941	4.0170688
H	-1.3732412	1.1030357	-0.7912610
H	-2.2062367	-0.1071871	2.3789345
H	1.0237660	0.4337469	3.2159294
H	1.4164958	-2.0150342	-0.2619667
H	0.6663453	3.8802809	0.9853749
H	0.6442700	-2.2406911	3.6578755
H	-2.5594536	1.0282495	0.5201308
H	-2.7119491	-1.2441092	1.1063975
H	2.5418676	2.0163424	1.9129513
H	2.1351346	-2.9959593	1.8901147
H	-1.1562489	1.3332347	4.0898747
H	-0.8473834	-2.4169174	-1.1969948
H	-0.6178008	4.0441136	-0.2159577
H	-1.0104192	-2.4306511	4.2644238
H	-2.4064536	2.4964585	-0.4598903
H	-2.9751208	-1.6420080	2.8163169
H	-1.3615272	2.7481515	1.7921455
H	-1.0948195	-2.9078052	1.9325824
H	2.5266522	2.1998887	3.6739877
H	1.8980418	-4.2217798	0.6304793
H	0.2604108	1.9926446	4.9343881
H	0.1199133	-3.9091860	-1.1592042
H	1.6651620	3.3650281	2.6638204
H	0.6979068	-4.0435603	1.9138232
H	-0.5938672	2.9837672	3.7488477
H	-1.1578840	-3.6553005	0.0329411
C	1.4238536	0.2846668	-0.3551335
C	1.0386316	0.2506370	-1.5604528
H	2.4204293	0.5381049	-0.0002601
C	0.4702763	0.1892292	-2.8195029
C	0.5139696	-1.0250365	-3.5607178
C	-0.1447987	1.3412319	-3.3856192
C	-0.0603415	-1.0804190	-4.8181885
H	0.9991778	-1.8924347	-3.1275377
C	-0.7016544	1.2678158	-4.6499666
H	-0.1618190	2.2659123	-2.8195720
C	-0.6654863	0.0609906	-5.3620109
H	-0.0360282	-2.0042007	-5.3864074
H	-1.1678178	2.1430288	-5.0897048
H	-1.1089494	0.0108183	-6.3516303

TSA_1C

57

Energy = -917.3514337901

B	-0.8677009	0.1548171	0.4621253
N	-2.1846512	0.4279938	0.0458670
N	-0.0725946	-1.0476835	0.2059615
C	-3.0958823	2.4215857	1.3379050
C	-0.6972309	-2.9101133	-1.4637222
C	-2.0179597	2.7114764	-0.9476313
C	0.0219026	-0.6018391	-2.2279094
C	-3.1172279	-0.7038231	-0.2256807
C	0.4116976	-1.7906270	1.4042822
C	-2.8127806	1.7783867	-0.0291581
C	0.1344295	-1.6593838	-1.1285206
C	-4.2356797	-0.7563608	0.8233397
C	-0.7181182	-2.6016847	2.0625602
C	-3.7040949	-0.6880588	-1.6424031
C	1.6350658	-2.6705349	1.1367196
H	-2.1992417	2.8508959	1.7933136
H	-1.7509914	-2.6749094	-1.6299844
H	-1.0318044	2.9356281	-0.5278444
H	-0.9889466	-0.1970946	-2.3037908
H	-2.5088803	-1.6018940	-0.1086720
H	0.7035538	-1.0205255	2.1296008
H	-3.5292171	1.7002971	2.0344043
H	-0.6295360	-3.6623445	-0.6742253
H	-1.8799441	2.2598355	-1.9342519
H	0.7073590	0.2294412	-2.0365309
H	-3.8227273	-0.7999456	1.8355639
H	-1.5651844	-1.9509761	2.3034841
H	-2.9261080	-0.6580376	-2.4083527
H	2.4427247	-2.1164793	0.6494424
H	-3.8084283	3.2420180	1.2028008
H	-0.3064443	-3.3563167	-2.3847605
H	-2.5535411	3.6583911	-1.0694931
H	0.2851463	-1.0467332	-3.1920627
H	-3.7838361	1.6114623	-0.5020564
H	1.1819802	-1.9831935	-1.1198790
H	-4.8444549	-1.6509637	0.6577028
H	-0.3615651	-3.0555008	2.9939944
H	-4.2961204	-1.5966705	-1.7932157
H	2.0106282	-3.0459352	2.0934358
H	-4.8974936	0.1131418	0.7525927
H	-1.0742795	-3.4017075	1.4068938
H	-4.3713431	0.1665152	-1.7949964
H	1.3886694	-3.5371453	0.5155213

C	-0.0494610	1.2899680	1.2891896
C	1.1461163	1.2526380	0.8393780
H	-0.4305772	2.0249177	1.9925300
C	2.4212248	1.1979552	0.3196198
C	3.4365848	0.4746315	1.0066835
C	2.7242224	1.8850933	-0.8899545
C	4.7155258	0.4376556	0.4828533
H	3.1930242	-0.0261294	1.9365792
C	4.0062108	1.8223186	-1.4034230
H	1.9428083	2.4448151	-1.3922113
C	4.9963055	1.1010708	-0.7203999
H	5.5003617	-0.1043485	0.9991682
H	4.2483622	2.3347797	-2.3280638
H	6.0016107	1.0603573	-1.1282731

TSA_1D

57

Energy = -917.3270943496

B	-1.0056999	-0.0284707	-0.1948252
N	-1.0866947	1.4087034	-0.3140387
N	-2.0171741	-0.9872044	-0.0491908
C	-3.1733863	2.6679679	0.4619750
C	-1.0288455	-3.2236355	-0.6899947
C	-1.4834149	1.7551561	2.1153185
C	-1.1898229	-2.5075336	1.7551642
C	-0.2495326	2.0714266	-1.3515898
C	-3.4302277	-0.6326834	-0.3474448
C	-1.6971029	2.3091589	0.7039435
C	-1.8002643	-2.4064934	0.3536757
C	-1.1107888	2.9201844	-2.2960516
C	-3.9549507	-1.4399890	-1.5422092
C	0.9130646	2.8917405	-0.7738841
C	-4.3423833	-0.7781419	0.8750437
H	-3.8448523	1.8623302	0.7666399
H	0.0422300	-2.9904971	-0.7030310
H	-1.9761609	0.7845407	2.2337934
H	-0.1853720	-2.0734137	1.7887012
H	0.1752482	1.2543425	-1.9461476
H	-3.4000960	0.4162882	-0.6449471
H	-3.3627554	2.9069626	-0.5870745
H	-1.4275541	-3.0601941	-1.6939764
H	-0.4167380	1.6293387	2.3265365
H	-1.8115854	-1.9803498	2.4841957
H	-1.9219558	2.3249959	-2.7253005
H	-3.3102549	-1.3044959	-2.4158111
H	1.4804397	2.3133506	-0.0382014
H	-3.9584468	-0.2148536	1.7300927
H	-3.4228913	3.5485823	1.0635893
H	-1.1102036	-4.2881774	-0.4497412
H	-1.9070964	2.4404924	2.8556416
H	-1.1169533	-3.5575253	2.0557670
H	-1.1308013	3.2414676	0.6266129
H	-2.8004166	-2.8428559	0.4070202
H	-0.4904035	3.3064262	-3.1112207
H	-4.9613571	-1.0929115	-1.7963194
H	1.5879679	3.1843340	-1.5848121
H	-5.3402701	-0.3995105	0.6323721
H	-1.5433990	3.7767529	-1.7691751
H	-4.0210024	-2.5095203	-1.3166506
H	0.5690276	3.8108371	-0.2901107
H	-4.4512188	-1.8258002	1.1746107
C	0.5089332	-0.4173932	-0.1564429
C	1.7475231	-0.6165790	-0.0667467
H	1.1688945	-1.5304826	-0.6397336
C	3.1653656	-0.6254796	0.1353567
C	3.9460200	0.4092517	-0.4122664
C	3.7609483	-1.6590554	0.8814056
C	5.3187103	0.4112381	-0.1915419
H	3.4768888	1.1890651	-1.0014632
C	5.1346453	-1.6416461	1.0898789
H	3.1480745	-2.4527365	1.2962416
C	5.9117430	-0.6091201	0.5567063
H	5.9272801	1.2076815	-0.6071147
H	5.5999788	-2.4320656	1.6694671
H	6.9844365	-0.6014312	0.7227886

TSA_1E

57

Energy = -917.3288362198

B	0.1808232	-0.0285397	0.6274991
N	-0.0403445	1.2582755	1.0877700
N	-0.1779830	-1.3038093	1.1979915
C	2.0841893	2.5570764	1.2306867
C	-2.6008509	-1.4578243	0.7165293
C	0.5757428	2.9036784	-0.7792669
C	-0.9939158	-2.8858461	-0.6067116
C	-1.1086873	1.4394329	2.1333173
C	0.9922165	-1.8503714	1.8886447
C	0.6461039	2.5383688	0.7030816
C	-1.2687678	-2.2061966	0.7447160
C	-0.5996601	2.1534157	3.3892085
C	1.2693585	-1.1085941	3.2042780
C	-2.3197237	2.1574061	1.5318538
C	1.0010524	-3.3626933	2.0964462
H	2.7092073	1.8412204	0.6897295
H	-2.5799999	-0.6378144	-0.0089902
H	1.1971100	2.2549375	-1.3991974
H	-1.0922421	-2.1730416	-1.4288062
H	-1.3972970	0.4231163	2.4100063
H	1.8629506	-1.5897174	1.2076988
H	2.1176637	2.3180412	2.2968352
H	-2.8537179	-1.0523452	1.6992602
H	-0.4508486	2.8731085	-1.1519877
H	0.0070302	-3.3219491	-0.6487262
H	0.2676695	1.6487166	3.8207797
H	1.3579071	-0.0324609	3.0400499
H	-2.7001561	1.6254710	0.6554311
H	0.8597605	-3.9195862	1.1688144
H	2.5111236	3.5545351	1.0877143
H	-3.3954096	-2.1450786	0.4119672
H	0.9473839	3.9271562	-0.8907834
H	-1.7246755	-3.6862913	-0.7597256
H	0.0885958	3.3107074	1.2359905
H	-1.3353069	-2.9804405	1.5127092
H	-1.4020342	2.1433828	4.1332826
H	2.2082485	-1.4670061	3.6361282
H	-3.1195377	2.2110365	2.2764925
H	1.9703152	-3.6424568	2.5177743
H	-0.3412044	3.1993662	3.2003536
H	0.4595064	-1.2900029	3.9174854
H	-2.0691698	3.1814849	1.2358236
H	0.2287556	-3.6623725	2.8124233
C	2.3107232	-0.4891866	-0.3504036
C	1.1574711	-0.2490587	-0.7931231
H	3.3371884	-0.5725840	-0.0534753
C	0.4754300	-0.1341891	-2.0911902
C	1.1792142	-0.5127526	-3.2478910
C	-0.8457000	0.3145149	-2.2017559
C	0.5584729	-0.4390624	-4.4901830
H	2.2010696	-0.8682640	-3.1619121
C	-1.4612172	0.3868116	-3.4479206
H	-1.3865424	0.6210104	-1.3124898
C	-0.7614492	0.0087184	-4.5948208
H	1.1068161	-0.7342547	-5.3795819

H	-2.4852025	0.7386604	-3.5230030
H	-1.2413549	0.0622138	-5.5670317

$TSAB_0$

57

Energy = -917.3523489533

B	1.0859945	0.0341035	-0.1750511
N	0.9605650	1.4554329	0.0729446
N	2.0720425	-0.8676894	0.2000342
C	-0.4366541	0.8365562	2.0298941
C	4.5645335	-0.6903524	0.2266933
C	-0.1414328	3.2504721	1.4143384
C	3.2515617	0.7968309	1.7710513
C	1.3541431	2.4193277	-0.9891347
C	2.0591144	-2.3385455	-0.1229361
C	-0.2280605	1.8206410	0.8721916
C	3.2745899	-0.5443728	1.0463708
C	2.5446593	1.8874374	-1.7846671
C	0.8576730	-3.0678192	0.4894325
C	0.1947449	2.7710827	-1.9379629
C	2.2385069	-2.6367886	-1.6143016
H	-0.4009525	-0.2090552	1.7035281
H	5.4261568	-0.5546896	0.8875479
H	0.7535268	3.3638689	2.0346229
H	2.3560311	0.9147108	2.3820552
H	1.6700749	3.3351347	-0.4748659
H	2.9459197	-2.7272138	0.3832721
H	-1.4182209	1.0102352	2.4803105
H	4.6127381	0.0664750	-0.5611283
H	-0.1153514	4.0015847	0.6215125
H	4.1234447	0.8207664	2.4337974
H	2.8705862	2.6462030	-2.5013153
H	0.6762013	-2.7250813	1.5127937
H	-0.6366891	3.2509597	-1.4143010
H	1.3466318	-2.3991374	-2.1997073
H	0.3244513	0.9720911	2.8032208
H	4.6518027	-1.6760541	-0.2377733
H	-1.0198908	3.4493285	2.0354843
H	3.3195618	1.6452015	1.0880067
H	-1.1116016	1.7429263	0.2107691
H	3.2719651	-1.3251283	1.8184420
H	2.2789809	0.9853899	-2.3494036
H	1.0666877	-4.1417796	0.5193804
H	0.5537539	3.4654239	-2.7038162
H	3.0856652	-2.0823851	-2.0267894
H	3.3863782	1.6496843	-1.1316327
H	-0.0492425	-2.9174860	-0.0998028
H	-0.1830576	1.8737168	-2.4384879
H	2.4309606	-3.7069338	-1.7428893
C	-0.1918428	-0.5360099	-1.1112828
C	-1.4160644	-0.5890509	-0.7856239
H	0.1572291	-0.8264147	-2.1022577
C	-2.7306103	-0.7039022	-0.3678473
C	-3.6470035	0.3702495	-0.5428316
C	-3.1748997	-1.9186965	0.2248283
C	-4.9617555	0.2220039	-0.1423532
H	-3.3004108	1.2938715	-0.9942299
C	-4.4904213	-2.0392548	0.6401348
H	-2.4734493	-2.7365626	0.3478315
C	-5.3825015	-0.9758962	0.4549102
H	-5.6660520	1.0355336	-0.2807271
H	-4.8306546	-2.9603322	1.1014639
H	-6.4137997	-1.0791203	0.7777997

$TSAB_2$

57

Energy = -917.3553985088

B	-0.8926566	0.2961870	0.2906420
N	-1.4807198	1.4946273	-0.1159836
N	-1.2263883	-1.0919906	0.0375264
C	-2.4618729	0.7750967	-2.3331478
C	-2.8087825	-0.9379046	1.9673051
C	-3.9912595	1.4747962	-0.4456975
C	-3.3695067	-2.3608140	-0.0765368
C	-0.8965786	2.8103292	0.2949066
C	-0.1405820	-1.8708606	-0.5738042
C	-2.6131362	1.6480857	-1.0906241
C	-2.2637408	-1.8047492	0.8313830
C	-0.1381069	3.4561630	-0.8708367
C	-0.0090745	-3.3192509	-0.1019015
C	-1.9347201	3.7517109	0.9118614
C	-0.1422878	-1.7804050	-2.1079834
H	-2.5371463	-0.2863529	-2.0902150
H	-3.3177979	-0.0442017	1.6021047
H	-4.2013529	0.4255917	-0.2291967
H	-3.9501339	-1.5565139	-0.5351697
H	-0.1614578	2.5913536	1.0704717
H	0.7923473	-1.3506116	-0.2502681
H	-1.5022670	0.9581193	-2.8242604
H	-2.0024394	-0.6285606	2.6410456
H	-4.0810401	2.0473905	0.4802588
H	-2.9475159	-2.9743096	-0.8776985
H	0.6251208	2.7732264	-1.2570967
H	0.1123620	-3.3907054	0.9828921
H	-2.4413354	3.2771114	1.7573807
H	-0.1016817	-0.7410901	-2.4403898
H	-3.2612224	1.0234312	-3.0386705
H	-3.5274012	-1.5218989	2.5496513
H	-4.7559953	1.8296918	-1.1443174
H	-4.0491777	-2.9859936	0.5118751
H	-2.5427184	2.6867498	-1.4228610
H	-1.7651066	-2.6571987	1.3012133
H	0.3541824	4.3702644	-0.5246270
H	0.8830330	-3.7456758	-0.5701825
H	-1.4250209	4.6487777	1.2765377
H	0.7311667	-2.3052750	-2.5072240
H	-0.8062141	3.7293226	-1.6936690
H	-0.8639852	-3.9327114	-0.4013484
H	-2.6879643	4.0713918	0.1853963
H	-1.0445642	-2.2425725	-2.5200909
C	0.4576702	0.4469786	1.2476527
C	1.6171458	0.0016424	0.9668197
H	0.2656179	0.9709212	2.1859372
C	2.9344436	-0.3363505	0.6847690
C	3.4531241	-1.6090229	1.0489892
C	3.7762601	0.6095579	0.0383787
C	4.7770400	-1.9101378	0.7835852
H	2.8031921	-2.3258943	1.5392289
C	5.0936112	0.2811210	-0.2360522
H	3.3721725	1.5790063	-0.2330358
C	5.5947469	-0.9721080	0.1370044
H	5.1817564	-2.8751201	1.0700752
H	5.7378572	0.9980879	-0.7340034
H	6.6294035	-1.2211946	-0.0768215

TSAB

57

Energy = -917.3610210978

B	0.9292146	-0.1392681	-0.4039043
N	1.1391188	1.2650789	-0.1519420
N	1.7205695	-1.2103376	0.0069284
C	3.2415423	2.6094808	0.1193292
C	0.2498482	-3.2703279	-0.0744172
C	2.8108458	1.2725895	-1.9931152

C	1.9607600	-2.7998447	-1.9110101
C	0.0598273	1.9470497	0.5729560
C	2.7694336	-0.9811090	1.0496553
C	2.1791212	2.0627695	-0.8467405
C	1.5980564	-2.6332400	-0.4316081
C	0.2804532	1.8926585	2.0955326
C	2.4094203	-1.7085315	2.3498153
C	-0.2538485	3.3630775	0.0900340
C	4.1743409	-1.3523781	0.5660406
H	3.8134028	1.7988942	0.5804843
H	-0.5609528	-2.9011800	-0.7067969
H	3.3506627	0.3939971	-1.6311060
H	1.2279315	-2.3239402	-2.5700750
H	-0.8394831	1.3297850	0.3751175
H	2.7381481	0.0925417	1.2429994
H	2.7887913	3.2096724	0.9132277
H	-0.0056086	-3.0742317	0.9709505
H	2.0500759	0.9422815	-2.7086291
H	2.9420757	-2.3651718	-2.1204263
H	0.4466075	0.8629067	2.4253737
H	1.4151385	-1.4142672	2.6991764
H	-0.4152290	3.3947546	-0.9918545
H	4.4358388	-0.8230255	-0.3539476
H	3.9381133	3.2484143	-0.4334668
H	0.3188398	-4.3536620	-0.2158902
H	3.5222477	1.9116690	-2.5235847
H	1.9918019	-3.8641106	-2.1652484
H	1.6644654	2.9205606	-1.2923787
H	2.3567536	-3.1697439	0.1427402
H	-0.5988387	2.2850598	2.6166300
H	3.1392864	-1.4512083	3.1236774
H	-1.1708656	3.7016008	0.5819837
H	4.9027055	-1.0784402	1.3358823
H	1.1488987	2.4928245	2.3821904
H	2.4258196	-2.7964453	2.2267516
H	0.5389989	4.0718172	0.3486655
H	4.2734952	-2.4277012	0.3865257
C	-0.4439910	-0.4572907	-1.2729366
C	-1.6254758	-0.2069362	-0.8763375
H	-0.2473634	-0.9283365	-2.2370200
C	-2.9230970	-0.0347675	-0.4227105
C	-3.5617361	-1.0916562	0.2841591
C	-3.6277603	1.1757843	-0.6723910
C	-4.8619647	-0.9292625	0.7312532
H	-3.0168860	-2.0117859	0.4659944
C	-4.9317277	1.3108361	-0.2316907
H	-3.1328135	1.9750797	-1.2134230
C	-5.5465297	0.2652161	0.4726788
H	-5.3520817	-1.7294912	1.2757102
H	-5.4779676	2.2277086	-0.4262446
H	-6.5677782	0.3833127	0.8215420

TSR0

43

Energy = -608.7614863992

B	-0.0061220	-0.0026369	-0.0459400
N	-0.0062674	-0.0017109	-1.3857048
N	-0.0042194	-0.0049661	1.2934737
C	2.3799253	-0.5178545	-1.8938200
C	-2.1203319	0.1157917	2.5786915
C	0.6413615	-2.3706308	-1.8533345
C	-1.5213407	-1.9810644	1.2828927
C	-0.9354491	0.9060230	-2.1674625
C	0.9946381	0.7889711	2.0949622
C	0.9281583	-0.9046695	-2.1670429
C	-0.9979313	-0.8036518	2.0965440
C	-2.3893502	0.5552743	-1.8596454
C	2.1212273	-0.1336315	2.5611409
C	-0.6132745	2.3717254	-1.8882217
C	1.5108663	1.9727713	1.2859564
H	2.5572509	0.5381704	-2.1158773
H	-2.7186811	0.4685589	1.7321511
H	-0.4093951	-2.6152245	-2.0308551
H	-0.7102327	-2.6519067	0.9868536
H	-0.7196678	0.6777820	-3.2138482
H	0.4364424	1.1568487	2.9613952
H	3.0452467	-1.1207762	-2.5186796
H	-1.7308261	0.9834702	3.1186331
H	1.2605352	-3.0091099	-2.4901813
H	-2.2350960	-2.5489236	1.8852544
H	-3.0535765	1.1622772	-2.4815947
H	1.7361649	-1.0055997	3.0973666
H	0.4392854	2.5911760	-2.0869898
H	2.2292975	2.5365229	1.8866424
H	2.6401277	-0.7079965	-0.8454449
H	-2.7740407	-0.4392231	3.2577287
H	0.8873140	-2.5983990	-0.8096253
H	-2.0473396	-1.6381594	0.3834583
H	0.6879764	-0.7023010	-3.2134551
H	-0.4333535	-1.1784581	2.9558793
H	-2.6241943	0.7693195	-0.8097705
H	2.7808817	0.4159478	3.2388756
H	-1.2289287	3.0103152	-2.5283831
H	2.0295177	1.6370847	0.3795933
H	-2.5932027	-0.5002530	-2.0601702
H	2.7122030	-0.4798592	1.7067395
H	-0.8375297	2.6247639	-0.8456441
H	0.6968505	2.6452293	1.0016789

TSRA$_0$

57

Energy = -917.3371699261

B	1.1013958	-0.0536258	-0.1425083
N	1.9691587	1.0200867	-0.2304885
N	0.9286983	-1.3022786	0.3922835
C	0.2653340	2.7368743	0.4988912
C	2.5920043	-2.4719645	1.9079229
C	2.6631113	2.9108527	1.2065133
C	1.4642670	-0.3534216	2.6760836
C	3.2624324	0.8398930	-0.9981235
C	0.3197852	-2.5141521	-0.2514354
C	1.7074846	2.4582252	0.0915001
C	1.3321625	-1.6064942	1.8214662
C	4.0821516	-0.3460790	-0.5090389
C	-1.1650440	-2.6716009	0.0766220
C	2.9825595	0.7690350	-2.5012323
C	0.6092863	-2.6012452	-1.7476626
H	-0.4163136	2.6752919	-0.3479803
H	2.6810257	-2.8588850	2.9277769
H	2.3699654	2.4690834	2.1629901
H	0.5634271	0.2661691	2.6186454
H	3.8265275	1.7532416	-0.7952247
H	0.8506067	-3.3429176	0.2263985
H	0.2068457	3.7450860	0.9182839
H	3.4860083	-1.8863833	1.6862309
H	3.7027578	2.6415200	1.0026933
H	1.6062857	-0.6511350	3.7188516
H	5.0189478	-0.3871592	-1.0727206
H	-1.3563887	-2.5441989	1.1463246
H	2.3761471	1.6177796	-2.8342764
H	0.0418656	-1.8614170	-2.3170390
H	-0.0619526	2.0349221	1.2752665
H	2.5573959	-3.3286964	1.2294347
H	2.6092199	3.9998509	1.2992704

H	2.3276547	0.2436856	2.3743249
H	1.9345967	3.0243782	-0.8206472
H	0.4839125	-2.1881776	2.2001833
H	3.5545489	-1.2917167	-0.6632123
H	-1.4895238	-3.6773570	-0.2076461
H	3.9259530	0.7928413	-3.0548785
H	1.6767974	-2.4670370	-1.9484568
H	4.3232671	-0.2431828	0.5519499
H	-1.7670089	-1.9491489	-0.4726299
H	2.4644954	-0.1620320	-2.7581950
H	0.3185556	-3.5933591	-2.1062500
C	-0.4267757	0.4199067	-1.6518876
C	-1.5681163	0.4732190	-1.1876578
H	0.2257940	0.6393367	-2.4735972
C	-2.8362415	0.4684121	-0.5721298
C	-3.1551957	1.3827122	0.4558783
C	-3.8156612	-0.4508399	-1.0143725
C	-4.4177751	1.3609461	1.0339688
H	-2.4128818	2.0979291	0.7896192
C	-5.0773590	-0.4536432	-0.4348193
H	-3.5742884	-1.1406755	-1.8162823
C	-5.3787478	0.4463571	0.5919212
H	-4.6580690	2.0613035	1.8273680
H	-5.8281386	-1.1564314	-0.7816641
H	-6.3655156	0.4384070	1.0447789

$TSRA_1$

57

Energy = -917.3456476322

B	0.2087758	-0.1807765	1.0975613
N	0.1049870	0.7951300	2.0447436
N	-0.0609755	-1.4489181	0.6828725
C	1.1170764	3.0558215	1.4454599
C	-2.2656082	-1.6780176	1.8650663
C	-1.2838776	2.4522670	0.8639566
C	-2.1625357	-1.3823286	-0.6464654
C	0.2376452	0.3148913	3.4778163
C	1.0268453	-2.4090594	0.3030787
C	-0.1299182	2.2601238	1.8460477
C	-1.4740313	-1.9608203	0.5922008
C	1.5493663	0.8087448	4.0891625
C	1.1742050	-3.4628220	1.4047990
C	-0.9704406	0.6997720	4.3339665
C	0.8061317	-3.0360181	-1.0721432
H	1.3879144	2.8841503	0.4021934
H	-2.4161203	-0.6025103	1.9994408
H	-1.0397687	1.9995322	-0.1031106
H	-2.2776728	-0.2976532	-0.5422959
H	0.2743144	-0.7764171	3.3998978
H	1.9413107	-1.8111246	0.2653689
H	1.9736086	2.8069813	2.0767401
H	-1.7592621	-2.0804386	2.7466784
H	-2.2006978	1.9894302	1.2400598
H	-1.5866070	-1.5800770	-1.5534312
H	2.4080127	0.5123655	3.4796569
H	1.3828620	-2.9918207	2.3699771
H	-1.9125579	0.4209308	3.8574294
H	0.6851657	-2.2696135	-1.8393830
H	0.9006910	4.1213375	1.5711766
H	-3.2515550	-2.1455233	1.7885182
H	-1.4709558	3.5179029	0.7029924
H	-3.1572840	-1.8238551	-0.7610295
H	-0.4481224	2.6194681	2.8265827
H	-1.3747736	-3.0431473	0.4786953
H	1.6657919	0.3744112	5.0868068
H	2.0030596	-4.1334933	1.1588780
H	-0.8977478	0.1671748	5.2869707
H	1.6780811	-3.6459150	-1.3256004
H	1.5499128	1.8978044	4.1960133
H	0.2676801	-4.0693692	1.5007157
H	-0.9900021	1.7700247	4.5583375
H	-0.0715104	-3.6895473	-1.0866030
C	1.9193155	0.5769892	-0.3475325
C	1.3459506	0.6872898	-1.4229877
H	2.6999466	0.6506718	0.3798413
C	0.5998854	0.7435533	-2.6246072
C	0.7977276	-0.2358297	-3.6214099
C	-0.3315312	1.7790759	-2.8467251
C	0.0587938	-0.1902605	-4.7974338
H	1.5403961	-1.0111074	-3.4668278
C	-1.0681199	1.8111297	-4.0247774
H	-0.4623582	2.5521808	-2.0978282
C	-0.8797953	0.8258077	-4.9978913
H	0.2158743	-0.9454299	-5.5610958
H	-1.7865913	2.6080215	-4.1885711
H	-1.4576006	0.8552994	-5.9165270

$TSRA_2$

57

Energy = -917.3468205699

B	1.0685384	0.1173752	-0.2004860
N	1.1694599	1.4509529	0.1444835
N	1.4288072	-1.1704494	0.0928076
C	3.5494049	1.8968499	0.8841173
C	2.5880577	-1.0048981	2.3468139
C	2.8718305	2.1087100	-1.5422732
C	0.1177341	-1.5250130	2.1702438
C	-0.0670541	2.2253915	0.4696627
C	1.6303556	-2.2126461	-0.9629439
C	2.4241368	2.2483962	-0.0844457
C	1.4948698	-1.6667393	1.5171841
C	0.0631001	2.8341851	1.8698477
C	3.0746922	-2.7210555	-0.9162051
C	-0.4080823	3.2756358	-0.5899995
C	0.6072903	-3.3441531	-0.8744347
H	3.9048175	0.8755100	0.7226720
H	2.3666254	0.0514239	2.5161686
H	3.1462549	1.0681726	-1.7583195
H	-0.1499358	-0.4664566	2.2696511
H	-0.8712176	1.4826565	0.4956410
H	1.4841953	-1.6971404	-1.9151379
H	3.2293294	2.0012847	1.9236063
H	3.5641934	-1.0910665	1.8631760
H	2.0789064	2.4134579	-2.2311767
H	-0.6537352	-2.0234736	1.5771296
H	0.2693762	2.0613624	2.6157422
H	3.7823864	-1.8924344	-1.0116366
H	-0.5063745	2.8210573	-1.5789891
H	-0.4085070	-2.9491277	-0.9434516
H	4.3882682	2.5786006	0.7122283
H	2.6409048	-1.5003179	3.3213390
H	3.7509276	2.7327768	-1.7281865
H	0.1285710	-1.9661803	3.1715540
H	2.1316533	3.2854828	0.0951731
H	1.7323756	-2.7288348	1.4261653
H	-0.8708165	3.3378218	2.1371309
H	3.2396448	-3.4178182	-1.7434702
H	-1.3586057	3.7518322	-0.3292720
H	0.7652418	-4.0364983	-1.7065019
H	0.8668657	3.5764626	1.9047688
H	3.2840041	-3.2539288	0.0169805
H	0.3485513	4.0644707	-0.6376701
H	0.7010427	-3.9130540	0.0554267
C	-0.1403065	0.0795624	-1.9441414

C	-1.2973087	-0.1316169	-1.5704688
H	0.5450464	0.2810889	-2.7461596
C	-2.5600031	-0.3309819	-0.9786864
C	-3.0539600	-1.6333156	-0.7431896
C	-3.3509226	0.7875552	-0.6263548
C	-4.2979079	-1.8058849	-0.1504839
H	-2.4588285	-2.4925449	-1.0315372
C	-4.5953304	0.6001048	-0.0408760
H	-2.9812620	1.7864037	-0.8315649
C	-5.0678202	-0.6936270	0.2031894
H	-4.6728583	-2.8076803	0.0325061
H	-5.2016318	1.4601244	0.2247370
H	-6.0406717	-0.8348803	0.6637249

TSRAa

57

Energy = -917.3471294719

B	0.9977618	-0.0545135	-0.2732752
N	1.4065347	1.2333163	-0.0160500
N	1.1024469	-1.3728086	0.1168359
C	0.4223971	3.1219518	1.2728118
C	1.8007569	-2.3712423	2.3322043
C	0.8736675	3.3768036	-1.2180511
C	-0.0730846	-0.6833693	2.2329143
C	2.8524108	1.5595984	0.2661478
C	1.3820707	-2.5278573	-0.7915407
C	0.4951330	2.4200276	-0.0882585
C	0.6551767	-1.8011352	1.4922451
C	3.4253617	0.7397264	1.4163787
C	0.1180097	-3.1495397	-1.3950960
C	3.6913242	1.4154346	-1.0061593
C	2.4095523	-2.1515843	-1.8553628
H	0.1309723	2.4226825	2.0606079
H	1.3809187	-2.8483298	3.2234806
H	1.8546774	3.8319073	-1.0504607
H	-0.8951848	-0.2742841	1.6349271
H	2.8458669	2.6110258	0.5612445
H	1.8400559	-3.2794882	-0.1408906
H	-0.3303174	3.9143207	1.2184392
H	2.4823270	-1.5818056	2.6562719
H	0.8838788	2.8626110	-2.1832889
H	-0.4947833	-1.0851669	3.1583605
H	4.4402167	1.0876999	1.6311847
H	-0.6176463	-3.3846894	-0.6198446
H	3.2704400	1.9961012	-1.8304087
H	2.0403488	-1.3579643	-2.5129218
H	1.3723660	3.5884193	1.5501014
H	2.3731060	-3.1281466	1.7890861
H	0.1364170	4.1841221	-1.2658419
H	0.6090347	0.1283040	2.4988884
H	-0.4922439	2.0096795	-0.2949865
H	-0.0663529	-2.6047983	1.3005092
H	3.4793137	-0.3193358	1.1513664
H	0.3856235	-4.0874692	-1.8912592
H	4.7093265	1.7698188	-0.8166861
H	3.3432488	-1.8195527	-1.3933130
H	2.8247460	0.8513230	2.3229705
H	-0.3424595	-2.4877229	-2.1316886
H	3.7467737	0.3664783	-1.3121082
H	2.6263776	-3.0218363	-2.4813528
C	-0.2375440	0.1245295	-2.0268672
C	-1.3599362	0.1043478	-1.5214800
H	0.4227163	0.1930189	-2.8687759
C	-2.5298727	0.0479345	-0.7374722
C	-3.1650458	1.2393820	-0.3217660
C	-3.0547956	-1.2013813	-0.3399642
C	-4.2891997	1.1748348	0.4909742
H	-2.7744107	2.1972739	-0.6493739
C	-4.1761463	-1.2500178	0.4776436
H	-2.5722399	-2.1121961	-0.6751181
C	-4.7913298	-0.0659698	0.8961693
H	-4.7776557	2.0899936	0.8096036
H	-4.5758188	-2.2100455	0.7880755
H	-5.6679879	-0.1101900	1.5349556

TSRa

43

Energy = -608.7578892282

B	0.0189056	0.0394114	0.0776029
N	0.1238143	0.0548702	1.4137765
N	-0.0399749	0.0460970	-1.2614315
C	2.4063807	-0.9024867	1.1635081
C	0.4619376	1.1256236	-3.5125937
C	2.0159429	1.1921262	2.5386335
C	-0.7601206	2.3903378	-1.7039515
C	-1.0531992	0.2656624	2.3279814
C	-0.4322061	-1.2089275	-2.0040519
C	1.4533933	-0.1572140	2.0906572
C	0.3022273	1.3360464	-2.0100187
C	-2.1628332	1.0206504	1.6066580
C	0.7980846	-2.0672117	-2.3020067
C	-1.5274774	-1.0831633	2.8710695
C	-1.4726204	-1.9783106	-1.1929859
H	2.0026144	-1.8794789	0.8816904
H	0.8263117	2.0670918	-3.9333253
H	2.2667536	1.8082027	1.6687223
H	-0.8116055	2.6009440	-0.6315035
H	-0.6715779	0.8793095	3.1497316
H	-0.8870064	-0.8673322	-2.9347595
H	3.3616035	-1.0587142	1.6711763
H	-0.4905107	0.8937468	-3.9975798
H	1.3060913	1.7406835	3.1639235
H	-0.5106097	3.3223791	-2.2195246
H	-3.0164654	1.1415175	2.2785068
H	1.2096326	-2.4750812	-1.3729504
H	-0.7124974	-1.6420241	3.3392845
H	-1.0562145	-2.3025181	-0.2306664
H	2.6069082	-0.3222881	0.2539077
H	1.1898864	0.3490431	-3.7551712
H	2.9257062	1.0294243	3.1238218
H	-1.7450044	2.0554390	-2.0441803
H	1.2360357	-0.7781437	2.9651052
H	1.2660012	1.6580239	-1.6046981
H	-2.5109468	0.4657581	0.7265596
H	1.5821487	-1.4984358	-2.8064671
H	-2.3001383	-0.9158338	3.6270706
H	-2.3633189	-1.3699928	-1.0114606
H	-1.8296743	2.0133896	1.2927691
H	0.5104416	-2.9033414	-2.9463339
H	-1.9547687	-1.6912654	2.0676067
H	-1.7717102	-2.8770157	-1.7391245

TSRA

57

Energy = -917.3464078053

B	1.0858202	0.0119662	-0.2445392
N	1.3007908	1.3505424	-0.1048797
N	1.3149318	-1.2686998	0.1524275
C	3.5769720	1.4155664	0.9453426
C	0.1077854	-3.1220855	-1.1109732
C	3.2918875	1.6794504	-1.5639145
C	2.3565333	-2.2301466	-1.8814652
C	0.1810686	2.3209220	0.1114601
C	1.4885390	-1.4451642	1.6508807

C	2.6883567	1.9332328	-0.1827661
C	1.4429329	-2.5036605	-0.6874454
C	0.3301423	2.9914314	1.4805212
C	0.2918083	-2.1856228	2.2482798
C	0.0698108	3.3269788	-1.0330889
C	2.8148371	-2.1199747	2.0060722
H	3.7763406	0.3470547	0.8217454
H	-0.3979863	-2.5138590	-1.8622613
H	3.4384767	0.6058836	-1.7272152
H	1.9236640	-1.4743368	-2.5454216
H	-0.7247917	1.7128159	0.1330489
H	1.5025162	-0.4243159	2.0457253
H	3.1151245	1.5791632	1.9228600
H	-0.5588998	-3.2557406	-0.2563103
H	2.6432598	2.0683651	-2.3537987
H	3.3391631	-1.8827436	-1.5501104
H	0.3837920	2.2445864	2.2780432
H	-0.6478169	-1.6853020	1.9965460
H	-0.0654007	2.8162939	-1.9898911
H	3.6593097	-1.6569164	1.4896852
H	4.5367270	1.9402729	0.9235464
H	0.3065106	-4.1081762	-1.5422045
H	4.2669601	2.1695750	-1.6407985
H	2.4899359	-3.1465464	-2.4633579
H	2.5462764	3.0082152	-0.0521446
H	1.9450972	-3.2211950	-0.0355573
H	-0.5393895	3.6302155	1.6620866
H	0.3920994	-2.2096109	3.3378603
H	-0.7959562	3.9736831	-0.8596501
H	2.9749750	-2.0178189	3.0835914
H	1.2231480	3.6221087	1.5289220
H	0.2501829	-3.2201087	1.8940237
H	0.9537934	3.9691000	-1.0958506
H	2.8063841	-3.1893164	1.7768702
C	-0.4519912	0.0225802	-2.0831120
C	-1.4908614	-0.0143534	-1.4411463
H	0.2386589	0.0586765	-2.8982749
C	-2.6259460	-0.0335682	-0.5917387
C	-3.0697788	-1.2391461	-0.0116415
C	-3.3155626	1.1664958	-0.3159630
C	-4.1674430	-1.2349037	0.8418808
H	-2.5520719	-2.1639615	-0.2380137
C	-4.4154776	1.1556608	0.5339075
H	-2.9870431	2.0902145	-0.7814305
C	-4.8387008	-0.0410154	1.1191468
H	-4.5040490	-2.1649723	1.2889377
H	-4.9451004	2.0803789	0.7400536
H	-5.6943741	-0.0440127	1.7869956

TSRb

43

Energy = -608.7547398574

B	-0.0316164	-0.0546256	-0.0548011
N	-0.1098161	1.2804626	-0.0547855
N	-0.0525433	-1.3938975	-0.0145779
C	2.1885696	2.2122818	0.2008683
C	-0.0067488	-1.8949715	-2.4520246
C	1.1986965	1.8159198	-2.1022058
C	-0.8484601	-3.6585815	-0.8566321
C	-1.3270837	1.8996093	0.6047778
C	0.5374071	-2.1077980	1.1785683
C	0.9207600	2.2034042	-0.6522670
C	-0.7444995	-2.1639669	-1.1415097
C	-0.9091076	2.7907808	1.7720712
C	1.7868949	-1.3719908	1.6557577
C	-2.1760373	2.6251612	-0.4377245
C	-0.5116008	-2.2239529	2.2856487
H	2.8865152	2.9559779	-0.1946412
H	-0.5070640	-2.4223722	-3.2695448
H	1.6705546	0.8277500	-2.1550483
H	-1.4558622	-4.0978895	-1.6531228
H	-1.8983126	1.0495471	0.9951282
H	0.8214984	-3.0977425	0.8204385
H	2.6795989	1.2339277	0.1699908
H	1.0279558	-2.2463416	-2.3895359
H	0.2775291	1.8027967	-2.6915548
H	0.1298701	-4.1475182	-0.8778207
H	-0.3231295	3.6496620	1.4306854
H	1.5403385	-0.3592584	1.9990703
H	-2.4595063	1.9515911	-1.2513198
H	-1.4296925	-2.6976867	1.9293539
H	1.9690502	2.4624922	1.2416667
H	-0.0029967	-0.8274310	-2.6939806
H	1.8871617	2.5385389	-2.5491490
H	-1.3407296	-3.8744871	0.0940358
H	0.4593483	3.1929236	-0.6270269
H	-1.7566051	-1.7525662	-1.1977846
H	-0.3240442	2.2318420	2.5077900
H	2.5365023	-1.3078147	0.8618249
H	-3.0874286	2.9942159	0.0415427
H	-0.1120994	-2.8217109	3.1103217
H	-1.8082879	3.1735857	2.2632762
H	2.2223242	-1.9076268	2.5035202
H	-1.6476291	3.4860886	-0.8586807
H	-0.7626372	-1.2292695	2.6719179

TSRc

43

Energy = -608.7078087015

B	-0.4628626	0.1217993	-0.2389788
N	0.0120603	1.4592054	-0.3697280
N	-0.0088981	-1.1764961	-0.1111202
C	1.7281858	1.7315146	1.4608691
C	-1.6863195	-2.2135712	1.4069587
C	2.2440224	2.2940809	-0.9658813
C	-1.9419888	-2.3882529	-1.1153093
C	-1.3261406	1.8748347	-0.1921974
C	1.4407470	-1.5133713	-0.1813963
C	1.1776773	2.2485576	0.1302014
C	-0.9662200	-2.3109717	0.0603526
C	-1.7642643	2.4953853	1.0935320
C	1.9277104	-2.1688734	1.1134439
C	-2.1465654	2.1531893	-1.4128608
C	1.7424861	-2.3665364	-1.4177551
H	2.1801153	0.7427306	1.3464300
H	-2.3130299	-1.3137356	1.4418455
H	2.6380456	1.2932233	-1.1701633
H	-2.5821784	-1.4980265	-1.1508412
H	-1.7267042	0.2790031	-0.1469160
H	1.9564774	-0.5567831	-0.3020138
H	0.9510202	1.6711052	2.2275789
H	-0.9704478	-2.1674811	2.2323277
H	1.8322554	2.7005905	-1.8931652
H	-1.4050794	-2.4666760	-2.0647905
H	-1.2312729	2.0954693	1.9554858
H	1.7112921	-1.5378789	1.9805130
H	-1.8211659	1.5537892	-2.2631981
H	1.4102471	-1.8613800	-2.3293921
H	2.5043979	2.4150691	1.8171316
H	-2.3357296	-3.0821964	1.5541524
H	3.0747919	2.9272982	-0.6407138
H	-2.5936379	-3.2607494	-1.0065628
H	0.7939675	3.2631993	0.2766407
H	-0.3545786	-3.2167850	0.0594800

H	-2.8438575	2.4020583	1.2252675
H	3.0090055	-2.3272730	1.0584616
H	-3.2160859	2.0348631	-1.2277744
H	2.8212220	-2.5373688	-1.4866787
H	-1.5428678	3.5698078	1.0140135
H	1.4557031	-3.1444138	1.2680644
H	-1.9613608	3.2123277	-1.6487776
H	1.2534524	-3.3442896	-1.3607331

TSRd

43

Energy = -608.6982743468

B	0.5005708	0.0198717	-0.0264420
N	0.3204498	-0.0036942	1.3527160
N	-0.0659912	-0.3229257	-1.2932562
C	2.8230436	0.2578152	1.6178393
C	2.2254018	-0.2983511	-2.3299394
C	1.2335953	1.7856321	2.8488642
C	0.5836728	1.6139046	-2.7396980
C	-0.9352943	-0.3399179	2.0882512
C	-1.2814311	-0.7619853	-2.0437683
C	1.4450579	0.3861948	2.2637766
C	0.9369417	0.3776181	-1.9863276
C	-2.0087156	0.7376439	1.9110835
C	-1.2906314	-2.2925547	-2.1340879
C	-1.4193475	-1.7484786	1.7447600
C	-2.5952832	-0.1882165	-1.5231635
H	2.9436931	-0.7093233	1.1182858
H	3.0593071	0.4057800	-2.3807016
H	1.2327048	2.5336752	2.0483406
H	-0.3428780	2.0667220	-2.3881264
H	-0.6421518	-0.3438231	3.1433314
H	-1.1259997	-0.3722456	-3.0557939
H	3.5826802	0.3319434	2.4022091
H	2.0821778	-0.7049838	-3.3438155
H	0.2883990	1.8571569	3.3939171
H	1.4082757	2.3308727	-2.6875809
H	-2.9044072	0.4682682	2.4799402
H	-1.4075758	-2.7452291	-1.1460085
H	-0.6284741	-2.4821165	1.9260263
H	-2.8795369	-0.6252358	-0.5640892
H	3.0219520	1.0608475	0.8991387
H	2.4466973	-1.1239147	-1.6543682
H	2.0429876	2.0232592	3.5464862
H	0.4825431	1.3507670	-3.8026044
H	1.3996343	-0.3466297	3.0790047
H	1.5187034	0.6683839	-0.3819591
H	-2.2912660	0.8504007	0.8629892
H	-0.3628171	-2.6635177	-2.5780094
H	-2.2831809	-2.0052996	2.3654381
H	-2.5438858	0.8993170	-1.4192099
H	-1.6498854	1.7053714	2.2705154
H	-2.1290527	-2.6112158	-2.7606803
H	-1.7264960	-1.8254558	0.6994713
H	-3.3846277	-0.4247810	-2.2427634

TSRrot

43

Energy = -608.7334831481

B	0.0076189	-0.1160678	0.0799913
N	0.1222687	1.2277101	0.0546279
N	-0.1064641	-1.4619378	0.1073872
C	1.7352502	1.8922716	-1.7417619
C	-1.5897521	-2.3086848	-1.7088176
C	-0.7730782	1.7600188	-2.2174444
C	0.8843694	-1.8827705	-2.1611790
C	-0.0111260	1.9853761	1.3664838
C	-0.3427961	-2.2349353	1.3833183
C	0.3193690	2.0573166	-1.1923842
C	-0.1698504	-2.3092173	-1.1461471
C	1.2513568	2.7993740	1.6415020
C	0.9034402	-3.0402083	1.7451419
C	-1.2913077	2.8189946	1.3660279
C	-0.7664599	-1.3104984	2.5178430
H	1.9111645	0.8706277	-2.0914635
H	-1.8609864	-1.3175928	-2.0872429
H	-0.6981798	0.7352626	-2.5975842
H	0.6645530	-0.8928299	-2.5757189
H	-0.0994935	1.2207892	2.1419709
H	-1.1720232	-2.9106144	1.1454948
H	2.4812033	2.1291681	-0.9793256
H	-2.3162411	-2.5999932	-0.9446751
H	-1.7662477	1.8975773	-1.7816540
H	1.8812653	-1.8674194	-1.7122649
H	2.1362165	2.1578716	1.6673065
H	1.2188785	-3.6945306	0.9280497
H	-2.1677006	2.1928705	1.1772538
H	-1.6351091	-0.7023663	2.2421891
H	1.8768747	2.5699115	-2.5892005
H	-1.6573742	-3.0226760	-2.5353343
H	-0.6682512	2.4361573	-3.0706847
H	0.8888028	-2.5881001	-2.9966993
H	0.1953765	3.0860296	-0.8476553
H	0.0770795	-3.3133650	-0.7915567
H	1.1478252	3.2893648	2.6142381
H	0.6856719	-3.6683357	2.6146155
H	-1.4069664	3.2938062	2.3450289
H	-1.0389089	-1.9082651	3.3913308
H	1.3995344	3.5798497	0.8892405
H	1.7309321	-2.3694744	1.9973658
H	-1.2552294	3.6117438	0.6127625
H	0.0641062	-0.6623976	2.8229721

3^{+}

56

Energy = -933.5154459320

B	-0.7165185	0.0251535	0.0039229
N	-1.0777204	1.5209437	0.2254301
N	-1.7041222	-0.9621394	0.1457435
C	-0.8055676	1.1701573	2.6759126
C	-1.0393635	-2.6552680	-1.5751460
C	0.7977487	2.6525630	1.3885522
C	-0.3583948	-2.9520488	0.8655983
C	-1.6082270	2.2326820	-0.7233626
C	-3.0958205	-0.6744017	0.5787146
C	-0.6454174	2.1558051	1.5226553
C	-1.4059780	-2.4021223	-0.1084147
C	-1.9176017	1.6211440	-2.0467460
C	-4.1142063	-1.0068376	-0.5201246
C	-1.9204283	3.6873528	-0.5534781
C	-3.4499704	-1.3932528	1.8879053
H	-0.1824097	0.2828339	2.5263013
H	-1.8147014	-2.2639019	-2.2409150
H	1.4784977	1.8078579	1.2586755
H	0.6093937	-2.4631066	0.7267806
H	-3.1389330	0.4020498	0.7675605
H	-1.8458518	0.8616854	2.7974168
H	-0.9445267	-3.7313179	-1.7532656
H	0.9154487	3.3307896	0.5386262
H	-0.6773319	-2.7986245	1.9007423
H	-1.6797229	0.5577117	-2.0952705
H	-5.1172989	-0.7144009	-0.1942437
H	-1.0380279	4.2521451	-0.2390192
H	-2.7150838	-1.1831062	2.6692605

H	-0.4851786	1.6606257	3.5989222
H	-0.0875119	-2.1856854	-1.8357470
H	1.0700887	3.1905378	2.3007682
H	-0.2281580	-4.0262645	0.6992019
H	-1.3135105	3.0036339	1.6847952
H	-2.3421223	-2.9325738	0.0845023
H	-1.3529276	2.1629092	-2.8154427
H	-3.8853737	-0.4801155	-1.4503859
H	-2.2935159	4.1023296	-1.4896869
H	-4.4323902	-1.0568800	2.2337785
H	-2.9779751	1.7735053	-2.2783248
H	-4.1334758	-2.0812401	-0.7298113
H	-2.6885470	3.8209289	0.2176775
H	-3.5025475	-2.4776109	1.7483453
N	0.6633482	-0.1616655	-0.1944690
C	1.5819688	-0.2305498	-1.0682736
C	3.0027168	-0.3673929	-0.7447233
C	3.9405588	-0.3819553	-1.7889919
C	3.4418680	-0.4877484	0.5851856
C	5.2994241	-0.5095769	-1.5101974
H	3.5968087	-0.2895671	-2.8165589
C	4.7970674	-0.6151876	0.8611278
H	2.7055451	-0.4884726	1.3836569
C	5.7273525	-0.6265901	-0.1861192
H	6.0229088	-0.5190553	-2.3195575
H	5.1372831	-0.7073697	1.8881929
H	6.7858489	-0.7308758	0.0332972
H	1.3530984	-0.1991982	-2.1454094

5^{+}
68
Energy = -1220.089132255

B	1.5569581	-0.0014886	-0.0474823
N	1.7567621	-1.5260763	-0.0218281
N	2.6432503	0.8787784	-0.1336711
C	3.3521386	-2.7101225	1.4976365
C	1.7313742	2.8951413	-1.3373354
C	1.5043669	-1.2577715	2.4472554
C	1.9054667	2.8622825	1.2156249
C	1.6048892	-2.2049477	-1.1196390
C	4.0398323	0.3943141	-0.2868740
C	1.9190392	-2.2024276	1.3220436
C	2.4879918	2.3630345	-0.1125393
C	1.3575649	-1.4914062	-2.4081613
C	4.6501633	0.8339185	-1.6235539
C	1.6401216	-3.6936035	-1.1876079
C	4.9177629	0.8062457	0.9004995
H	4.0528383	-1.8790057	1.6109693
H	2.1898955	2.5314331	-2.2612132
H	2.1356502	-0.3635070	2.4718873
H	0.8719527	2.5368731	1.3697124
H	3.9784364	-0.6965965	-0.2976303
H	3.6735511	-3.3286605	0.6556369
H	1.7693957	3.9889273	-1.3411369
H	0.4589829	-0.9579874	2.3510791
H	2.5034225	2.5001120	2.0567903
H	1.6181759	-0.4325371	-2.3626087
H	5.6472796	0.3961596	-1.7318975
H	1.5294523	-4.1918955	-0.2265577
H	4.4793399	0.4775201	1.8476403
H	3.3983850	-3.3178215	2.4055786
H	0.6768170	2.6027354	-1.3451367
H	1.6282642	-1.7841038	3.3973900
H	1.9134770	3.9565674	1.2308013
H	1.2275225	-3.0477265	1.3116792
H	3.5046553	2.7585601	-0.1778628
H	0.2875730	-1.5775229	-2.6390970
H	4.0341089	0.5028856	-2.4651292
H	0.8626203	-4.0355570	-1.8773410
H	5.9091007	0.3532104	0.8009489
H	1.9059699	-1.9784266	-3.2190368
H	4.7578518	1.9219093	-1.6802594
H	2.5992624	-3.9952030	-1.6282305
H	5.0524661	1.8917994	0.9440000
H	-0.1157311	1.3544395	0.0146493
N	0.1841605	0.3804748	0.0031922
N	-0.8176085	-0.5530949	0.0579776
C	-2.0429953	-0.1206527	0.1011760
C	-3.1298065	-1.1120958	0.1284969
C	-2.8624090	-2.4910796	0.0255552
C	-4.4639753	-0.6932341	0.2623956
C	-3.8986838	-3.4156772	0.0564324
H	-1.8330712	-2.8185562	-0.0776602
C	-5.5021143	-1.6244858	0.2924030
H	-4.6868799	0.3660607	0.3459927
C	-5.2253114	-2.9873632	0.1895648
H	-3.6783362	-4.4764311	-0.0252071
H	-6.5275874	-1.2824554	0.3973395
H	-6.0329480	-3.7130471	0.2120296
C	-2.3537583	1.3407262	0.1125236
C	-2.7342918	1.9949617	-1.0674554
C	-2.1975166	2.0862019	1.2906392
C	-2.9563196	3.3721888	-1.0676100
H	-2.8552798	1.4224335	-1.9828494
C	-2.4224690	3.4632632	1.2879055
H	-1.9054895	1.5828065	2.2085255
C	-2.8003018	4.1077913	0.1088508
H	-3.2516106	3.8699487	-1.9865537
H	-2.3051846	4.0303297	2.2065952
H	-2.9746419	5.1796166	0.1070243

$(C_6F_5)_4B^{-}$
45
Energy = -2937.868911310

B	-0.0000600	0.0000305	-0.0000041
C	1.0525524	0.1361949	1.2709968
C	-1.0527380	1.2709849	-0.1362816
C	1.0526934	-0.1361992	-1.2708786
C	-1.0528185	-1.2708663	0.1361579
C	1.3403280	1.2905743	2.0007745
C	1.8718266	-0.9521197	1.5887978
C	-1.3396441	2.0014328	-1.2904449
C	-1.8729318	1.5880497	0.9515654
C	1.3403279	-1.2905538	-2.0007509
C	1.8722464	0.9519787	-1.5884338
C	-1.3396021	-2.0015503	1.2901985
C	-1.8731795	-1.5876566	-0.9516442
C	2.3266951	1.3584945	2.9853578
F	0.6710995	2.4505126	1.7846965
C	2.8635706	-0.9337678	2.5614432
F	1.7166371	-2.1246118	0.9224573
C	-2.3256885	2.9863365	-1.3584264
F	-0.6699423	1.7855987	-2.4501565
C	-2.8644941	2.5608752	0.9330990
F	-1.7190505	0.9206098	2.1235994
C	2.3267234	-1.3585281	-2.9853012
F	0.6709538	-2.4504260	-1.7847694
C	2.8640529	0.9335604	-2.5610150
F	1.7173248	2.1243742	-0.9218623
C	-2.3255358	-2.9865762	1.3580469
F	-0.6699431	-1.7857857	2.4499529
C	-2.8647078	-2.5605178	-0.9332826
F	-1.7195478	-0.9198482	-2.1235013
C	3.0939750	0.2384076	3.2737007

F	2.5501678	2.5104558	3.6577245
F	3.6051110	-2.0337305	2.8229462
C	-3.0939366	3.2738941	-0.2388034
F	-2.5477192	3.6599660	-2.5099269
F	-3.6067064	2.8219063	2.0327201
C	3.0942245	-0.2385462	-3.2734616
F	2.5500085	-2.5104411	-3.6578137
F	3.6058951	2.0333793	-2.8222547
C	-3.0939545	-3.2738509	0.2384683
F	-2.5472364	-3.6606414	2.5093513
F	-3.6070795	-2.8212819	-2.0328598
F	4.0513972	0.2866192	4.2229878
F	-4.0514609	4.2230693	-0.2872408
F	4.0516216	-0.2867864	-4.2227735
F	-4.0514802	-4.2230296	0.2868127

$Si(CH_3)_4$
17
Energy = -449.3294971281

Si	-0.0000016	0.0000198	0.0000826
C	0.0000037	0.0000449	1.8864857
H	-0.8853980	-0.5116287	2.2833919
H	0.8857633	-0.5110153	2.2833852
H	-0.0003526	1.0225933	2.2835140
C	-0.0000001	-1.7785258	-0.6287732
H	-0.8857944	-2.3232363	-0.2795239
H	0.0003801	-1.8116479	-1.7252277
H	0.8854156	-2.3234521	-0.2788994
C	-1.5402209	0.8892543	-0.6288145
H	-1.5688143	1.9287157	-0.2795334
H	-1.5693125	0.9054852	-1.7252424
H	-2.4547117	0.3949745	-0.2786133
C	1.5402167	0.8892531	-0.6288192
H	1.5689643	0.9060756	-1.7252464
H	1.5691541	1.9285179	-0.2789791
H	2.4547083	0.3945718	-0.2791868

$((C_6F_5)_2BH)_2$
48
Energy = -2963.817946085
48
Energy = -2963.817946085

B	-0.8946584	0.0181428	0.0012668
B	0.8932965	-0.0183848	0.0013576
C	-1.6585131	-0.0277310	1.3793360
C	1.6563590	0.0270532	1.3794150
C	-1.6552874	0.0937782	-1.3773645
C	1.6532554	-0.0934388	-1.3772282
C	-2.5790044	0.9694503	1.7074973
C	2.5831974	-0.9653550	1.7044057
C	-2.6164176	-0.8647113	-1.7043674
C	2.6187914	0.8614432	-1.7019548
C	-1.4647962	-1.0276868	2.3344982
C	1.4582591	1.0233972	2.3375162
C	-1.4176168	1.0814401	-2.3354168
C	1.4127001	-1.0783058	-2.3374699
C	-3.2693419	0.9920417	2.9143658
C	3.2752677	-0.9860156	2.9098990
C	-3.3039433	-0.8625931	-2.9130211
C	3.3076377	0.8577361	-2.9094348
C	-2.1371210	-1.0443577	3.5521110
C	2.1320881	1.0411587	3.5538716
C	-2.0851937	1.1217081	-3.5550976
C	2.0815479	-1.1194414	-3.5560211
C	-3.0435658	-0.0251028	3.8415574
C	3.0454620	0.0275104	3.8393856
C	-3.0329804	0.1404489	-3.8433978
C	3.0343099	-0.1426547	-3.8413104
F	-2.7994748	1.9762325	0.8349140
F	2.8083954	-1.9694467	0.8295737
F	-2.8813924	-1.8583122	-0.8290875
F	2.8866877	1.8532997	-0.8252185
F	-0.6071872	-2.0424850	2.0835567
F	0.5943028	2.0343593	2.0902494
F	-0.5189706	2.0603306	-2.0855218
F	0.5093573	-2.0542595	-2.0903681
F	-3.6973335	-0.0237499	5.0080842
F	3.7034127	0.0293342	5.0035200
F	-3.6831157	0.1620587	-5.0117469
F	3.6882584	-0.1673065	-5.0074418
F	-4.2117534	-1.8077466	-3.1948092
F	-1.8323848	2.0894822	-4.4484044
F	-4.1373887	1.9735979	3.1972532
F	-1.9281067	-2.0254898	4.4422070
F	1.9183489	2.0195637	4.4464170
F	4.1510844	-1.9623401	3.1884888
F	4.2211920	1.7988131	-3.1878993
F	1.8254973	-2.0852578	-4.4510943
H	-0.0213917	-0.9787316	0.0007450
H	0.0182305	0.9785234	0.0020282

C_6H_5F
12
Energy = -331.6801843517

C	0.1582799	-0.8945580	0.0000342
C	1.5464601	-0.9288332	0.0004904
C	2.2355276	0.2855721	-0.0000241
C	1.5384413	1.4957032	-0.0010291
C	0.1418997	1.4945054	-0.0014945
C	-0.5654106	0.2906010	-0.0010055
F	-0.5238735	-2.0763804	0.0007101
H	2.0658112	-1.8814692	0.0011805
H	3.3215490	0.2815867	0.0003132
H	2.0813199	2.4357901	-0.0014970
H	-0.4044482	2.4331142	-0.0021899
H	-1.6501012	0.2642673	-0.0013995

Table S3. DFT (at the TPSS-D3/def2-TZVP level) computed chemical shifts (Calc., in ppm) and atomic assignment for the cations of **1**$^+$**, 2**$^+$**, 3**$^+$**, 5**$^+$ and the counter anion $B(C_6F_5)_4^-$ as well as a comparison with experiment (experimental chemical shifts (Expt.) and deviations with DFT-computations (Dev.) in ppm).

Species	atom symbol	Calc. ppm	atom no.	Expt. ppm	Assign.	Dev. ppm
1+	B	36.67	1	37.32	B^+	-0.65
1+	C	59.71	11	51.70	CH	8.01
1+	C	59.71	9	--	CH	--
1+	C	59.69	10	--	CH	--
1+	C	59.56	8	--	CH	--
1+	C	25.82	15	--	CH_3	--
1+	C	25.82	12	--	CH_3	--
1+	C	25.82	4	--	CH_3	--
1+	C	25.81	7	--	CH_3	--
1+	C	23.94	13	23.10	CH_3	0.84
1+	C	23.87	6	--	CH_3	--
1+	C	23.85	14	--	CH_3	--
1+	C	23.84	5	--	CH_3	--
1+	H	3.60	20	3.54	CH	0.06
1+	H	3.60	34	--	CH	--
1+	H	3.60	21	--	CH	--
1+	H	3.59	35	--	CH	--
1+	H	1.83	22	--	CH_3	--
1+	H	1.83	26	--	CH_3	--
1+	H	1.83	25	--	CH_3	--
1+	H	1.82	43	--	CH_3	--
1+	H	1.73	31	--	CH_3	--
1+	H	1.73	28	--	CH_3	--
1+	H	1.73	24	--	CH_3	--
1+	H	1.73	37	--	CH_3	--
1+	H	1.50	41	--	CH_3	--
1+	H	1.50	32	--	CH_3	--
1+	H	1.50	17	--	CH_3	--
1+	H	1.50	38	--	CH_3	--
1+	H	1.45	39	--	CH_3	--
1+	H	1.45	19	--	CH_3	--
1+	H	1.44	40	1.39	CH_3	0.05
1+	H	1.44	16	--	CH_3	--
1+	H	1.26	36	--	CH_3	--
1+	H	1.26	30	--	CH_3	--
1+	H	1.26	33	--	CH_3	--
1+	H	1.26	29	--	CH_3	--
1+	H	0.87	27	--	CH_3	--

1+	H	0.87	18	--	CH_3	--
1+	H	0.87	42	--	CH_3	--
1+	H	0.86	23	--	CH_3	--
1+	N	132.83	3	132.80	N15 Ref.	0.03
1+	N	132.75	2	132.80	N15 Ref.	-0.05
2+	B	32.15	1	32.30	--	-0.15
2+	C	193.54	8	190.30	C_3	3.24
2+	C	155.49	45	150.00	C_{14}	5.49
2+	C	135.29	54	135.60	C_{18}	-0.31
2+	C	134.41	47	132.30	C_{15}	2.11
2+	C	133.23	49	130.80	C_{16}, trans	2.43
2+	C	130.57	50	129.30	C_{17}	1.27
2+	C	130.52	52	128.50	C_{17}	2.02
2+	C	125.00	48	127.40	C_{16}, cis	-2.40
2+	C	115.73	44	129.00	C_{13}	-13.27
2+	C	65.02	10	56.80	C_5	8.22
2+	C	59.75	9	51.70	C_8	8.05
2+	C	54.99	11	46.30	C_{11}	8.69
2+	C	33.26	12	28.90	C_2	4.36
2+	C	26.63	5	25.00	H_{10}	1.63
2+	C	25.08	6	--	C_4	--
2+	C	24.91	7	24.60	C_{12}	0.31
2+	C	24.09	14	23.30	C_1	0.79
2+	C	22.43	13	--	C_7	--
2+	C	22.41	15	20.90	C_9	1.51
2+	C	21.20	4	--	C_6	--
2+	H	8.09	51	7.57	H_{16}, cis	0.52
2+	H	7.89	57	--	H_{18}	--
2+	H	7.80	55	--	H_{17}	--
2+	H	7.73	56	--	H_{17}	--
2+	H	7.24	53	7.32	H_{16}, trans	-0.08
2+	H	7.27	46	6.89	H_{13}	0.38
2+	H	6.62	20	6.53	H_{14}	0.09
2+	H	4.26	34	4.40	H_5	-0.14
2+	H	3.73	35	3.68	H_{11}	0.05
2+	H	3.35	21	3.46	H_8	-0.11
2+	H	2.91	26	--	H_2	--
2+	H	2.56	40	2.66	H_2	0.04
2+	H	2.54	36	--	H_2	--
2+	H	2.69	28	--	H_1	--
2+	H	2.53	38	2.52	H_1	-0.13
2+	H	2.53	42	--	H_1	--
2+	H	2.04	19	--	H_{12}	--

2+	H	1.51	33	1.60	H_{12}	--
2+	H	1.44	25	--	H_{12}	--
2+	H	1.90	17	--	H_{10}	--
2+	H	1.44	31	1.54	H_{10}	-0.16
2+	H	1.22	23	--	H_{10}	--
2+	H	1.59	22	--	H_6	--
2+	H	1.53	16	--	H_6	--
2+	H	1.36	30	--	H_6	--
2+	H	1.68	18	--	H_4	--
2+	H	1.42	32	1.48	H_4	--
2+	H	1.39	24	--	H_4	--
2+	H	1.55	43	--	H_9	--
2+	H	1.26	29	1.30	H_9	-0.04
2+	H	1.22	39	--	H_9	--
2+	H	1.51	41	--	H_7	--
2+	H	1.17	37	1.20	H_7	-0.03
2+	H	0.88	27	--	H_7	--
2+	N	234.53	2	--	N-C_3	--
2+	N	143.52	3	--	N-C_8	--
3+	B	24.44	1	25.80	B^+	-1.36
3+	C	192.35	8	190.00	C_3	2.35
3+	C	163.30	44	162.40	C_{13}	0.90
3+	C	137.62	52	135.80	C_{17}	1.82
3+	C	135.51	45	133.80	C_{14}	6.11
3+	C	135.29	46	129.40	C_{15}, trans	--
3+	C	130.86	48	129.30	C_{16}	1.56
3+	C	130.54	50	--	C_{16}	--
3+	C	126.62	47	--	C_{15}, cis	--
3+	C	65.01	10	56.70	C_5	8.31
3+	C	57.94	9	49.90	C_8	8.04
3+	C	53.48	11	45.10	C_{11}	8.38
3+	C	32.48	12	28.60	C_2	3.88
3+	C	27.59	5	24.30	C_{10}	3.29
3+	C	24.10	6	23.10	C_4	1.00
3+	C	23.72	14	22.90	C_1	0.82
3+	C	22.90	15	22.10	C_9	0.80
3+	C	22.51	13	21.40	C_7	1.11
3+	C	21.50	7	21.10	C_{12}	0.40
3+	C	21.31	4	20.40	C_6	0.91
3+	H	9.01	56	8.75	H_{13}	0.26
3+	H	8.14	51	7.70	H_{15}, cis	0.44
3+	H	8.07	55	--	H_{17}	--
3+	H	7.92	53	--	H_{16}	--

3+	H	7.85	54	--	H_{16}	--
3+	H	7.79	49	7.50	H_{15}, trans	0.29
3+	H	4.23	33	4.33	H_5	-0.10
3+	H	3.57	34	3.45	H_{11}	0.12
3+	H	3.18	20	3.25	H_8	-0.07
3+	H	3.22	25	--	H_2	--
3+	H	2.67	39	2.66	H_2	0.01
3+	H	2.48	35	--	H_2	--
3+	H	2.42	41	2.48	H_1	-0.06
3+	H	2.39	27	--	H_1	--
3+	H	2.36	37	--	H_1	--
3+	H	2.12	16	--	H_6	--
3+	H	1.62	21	1.60	H_6	0.02
3+	H	1.51	29	--	H_6	--
3+	H	1.52	42	--	H_9	--
3+	H	1.21	28	1.34	H_9	-0.13
3+	H	1.20	38	--	H_9	--
3+	H	1.33	22	--	H_{10}	--
3+	H	1.30	17	1.24	H_{10}	0.06
3+	H	1.28	30	--	H_{10}	--
3+	H	1.76	18	--	H_4	--
3+	H	1.30	31	1.24	H_4	0.06
3+	H	0.82	23	--	H_4	--
3+	H	1.54	40	--	H_7	--
3+	H	1.19	26	1.21	H_7	-0.02
3+	H	0.95	36	--	H_7	--
3+	H	1.61	19	--	H_{12}	--
3+	H	1.05	32	1.17	H_{12}	-0.12
3+	H	1.04	24	--	H_{12}	--
3+	N	305.05	43	--	N-C_{13}	--
3+	N	239.03	2	--	N-C_3	--
3+	N	106.17	3	--	N-C_8	--
5+	B	23.30	1	24.10	B^+	-0.80
5+	C	196.92	8	192.50	C_3	4.42
5+	C	159.71	46	153.90	C_{13}	5.81
5+	C	136.53	47	136.50	C_{14b}	0.03
5+	C	134.67	58	132.20	C_{14a}	2.47
5+	C	132.02	54	129.9	C_{17b}	2.12
5+	C	131.34	49	128.7	C_{15b}	2.64
5+	C	131.17	65	130.4	C_{17a}	0.77
5+	C	131.16	61	128.50	C_{16a}	2.66
5+	C	130.60	63	128.50	C_{16a}	2.10
5+	C	129.93	52	126.70	C_{16b}	3.23

5+	C	129.56	59	130.3	C_{15a}	-0.74
5+	C	128.84	60	130.3	C_{15a}	-1.36
5+	C	128.54	50	126.70	C_{16b}	1.84
5+	C	122.08	48	128.7	C_{15b}	-6.62
5+	C	64.71	10	56.80	C_5	7.91
5+	C	58.36	9	49.97	C_8	8.39
5+	C	51.86	11	43.41	C_{11}	8.45
5+	C	30.19	12	28.30	C_2	1.89
5+	C	24.65	14	23.40	C_1	1.25
5+	C	24.32	4	22.80	C_4	1.52
5+	C	24.13	7	22.50	C_{12}	1.63
5+	C	23.36	5	21.53	C_{10}	1.83
5+	C	22.68	13	21.30	C_9	1.38
5+	C	22.21	15	21.00	C_7	1.21
5+	C	21.24	6	20.70	C_6	0.54
5+	H	8.05	51	7.70	H_{15b}	0.35
5+	H	7.94	66	--	H_{16a}	--
5+	H	7.92	67	--	H_{16a}	--
5+	H	7.91	68	--	H_{17a}	--
5+	H	7.69	57	--	H_{17b}	--
5+	H	7.57	55	--	H_{16b}	--
5+	H	7.56	56	--	H_{16b}	--
5+	H	7.36	62	--	H_{15a}	--
5+	H	7.35	64	--	H_{15a}	--
5+	H	7.01	53	7.24	H_{15b}	-0.23
5+	H	6.83	43	6.78	H-N	0.05
5+	H	4.57	33	4.47	H_5	0.10
5+	H	3.39	34	3.37	H_{11}	0.02
5+	H	3.38	20	3.31	H_8	0.07
5+	H	2.95	27	--	H_1	--
5+	H	2.62	37	2.69	H_1	-0.07
5+	H	2.40	41	--	H_1	--
5+	H	2.78	25	--	H_2	--
5+	H	2.48	35	2.55	H_2	-0.07
5+	H	2.41	39	--	H_2	--
5+	H	1.89	23	--	H_6	--
5+	H	1.65	18	1.58	H_6	0.07
5+	H	1.40	31	--	H_6	--
5+	H	1.56	29	--	H_4	--
5+	H	1.53	16	1.53	H_4	0.00
5+	H	1.41	21	--	H_4	--
5+	H	1.49	42	--	H_7	--
5+	H	1.13	38	1.19	H_7	-0.06
5+	H	1.08	28	--	H_7	--

5+	H	1.40	40	--	H_9	--
5+	H	1.11	26	1.09	H_9	0.02
5+	H	0.81	36	--	H_9	--
5+	H	1.08	24	--	H_{10}	--
5+	H	1.06	19	0.97	H_{10}	0.09
5+	H	0.97	32	--	H_{10}	--
5+	H	0.84	17	--	H_{12}	--
5+	H	0.84	22	0.91	H_{12}	-0.07
5+	H	0.58	30	--	H_{12}	--
5+	N	286.58	45	--	N-C_{13}	--
5+	N	226.76	2	226.90	N-C_3	-0.14
5+	N	139.92	44	137.70	N-H	2.22
5+	N	101.25	3	106.60	N-C_8	-5.35
B(C6F5)4-	B	-14.40	1	-16.65	B^-	2.25
B(C6F5)4-	C	155.15	7	148.10	*o*	7.05
B(C6F5)4-	C	155.15	11	--	*o*	--
B(C6F5)4-	C	155.14	13	--	*o*	--
B(C6F5)4-	C	155.14	9	--	*o*	--
B(C6F5)4-	C	153.63	8	--	*o*	--
B(C6F5)4-	C	153.63	12	--	*o*	--
B(C6F5)4-	C	153.62	6	--	*o*	--
B(C6F5)4-	C	153.62	10	--	*o*	--
B(C6F5)4-	C	144.02	36	138.10	*p*	5.92
B(C6F5)4-	C	144.02	30	--	*p*	--
B(C6F5)4-	C	144.02	39	--	*p*	--
B(C6F5)4-	C	144.02	33	--	*p*	--
B(C6F5)4-	C	142.29	22	136.20	*m*	6.09
B(C6F5)4-	C	142.29	26	--	*m*	--
B(C6F5)4-	C	142.29	18	--	*m*	--
B(C6F5)4-	C	142.29	14	--	*m*	--
B(C6F5)4-	C	141.77	24	--	*m*	--
B(C6F5)4-	C	141.77	16	--	*m*	--
B(C6F5)4-	C	141.77	28	--	*m*	--
B(C6F5)4-	C	141.77	20	--	*m*	--
B(C6F5)4-	C	127.40	3	n.o.	*ipso*	--
B(C6F5)4-	C	127.40	5	--	*ipso*	--
B(C6F5)4-	C	127.40	2	--	*ipso*	--
B(C6F5)4-	C	127.40	4	--	*ipso*	--
B(C6F5)4-	F	-180.31	41	-166.90	*m*	-13.41
B(C6F5)4-	F	-180.31	35	--	*m*	--
B(C6F5)4-	F	-180.31	32	--	*m*	--
B(C6F5)4-	F	-180.30	38	--	*m*	--
B(C6F5)4-	F	-179.18	34	--	*m*	--

B(C6F5)4-	F	-179.18	40	--	*m*	--
B(C6F5)4-	F	-179.17	31	--	*m*	--
B(C6F5)4-	F	-179.17	37	--	*m*	--
B(C6F5)4-	F	-177.24	43	-163.10	*p*	-14.14
B(C6F5)4-	F	-177.24	45	--	*p*	--
B(C6F5)4-	F	-177.24	42	--	*p*	--
B(C6F5)4-	F	-177.23	44	--	*p*	--
B(C6F5)4-	F	-136.41	23	-132.60	*o*	-3.81
B(C6F5)4-	F	-136.40	15	--	*o*	--
B(C6F5)4-	F	-136.38	19	--	*o*	--
B(C6F5)4-	F	-136.37	27	--	*o*	--
B(C6F5)4-	F	-130.29	29	--	*o*	--
B(C6F5)4-	F	-130.29	21	--	*o*	--
B(C6F5)4-	F	-130.22	25	--	*o*	--
B(C6F5)4-	F	-130.22	17	--	*o*	--

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