Supporting information for:

Alkylideneborate Zwitterions and C-C Coupling by Atypical Diboration of Electron-Rich Alkynes

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Methods and Materials: Dipiperidinoacetylene,[1] $B_2Cl_2Mes_2$,[2] $B_2Cl_2Dur_2$,[2] F_2BBMes_2[2,3] were synthesized according to literature procedures. B_2Cat_2 was a generous gift from Allychem Co., Ltd. (Dalian, China). All non-deuterated solvents were distilled and degassed from appropriate drying agents and stored over activated molecular sieves under argon atmospheres. Deuterated solvents were dried under an argon atmosphere over activated molecular sieves and degassed by three *freeze-pump-thaw* cycles. Unless otherwise noted all manipulations were carried out either in an argon-filled glovebox or with Schlenk techniques as described by Shriver and Drezdzon.[2]

Physical methods: All solution NMR spectra were acquired on a Bruker Avance I 500 spectrometer (^{1}H: 500.13 MHz, ^{11}B: 160.5 MHz, ^{13}C: 125.8 MHz, ^{19}F: 470.6 MHz) or on a Bruker Avance 400 NMR spectrometer (^{1}H: 400.1 MHz, ^{11}B: 128.4 MHz, ^{13}C: 125.8 MHz). ^{1}H NMR and ^{13}C{^{1}H} NMR spectra were referenced to external TMS via the residual protons of the solvent (^{1}H) or the solvent itself (^{13}C). ^{11}B{^{1}H} NMR spectra were referenced to external $BF_3{\cdot}OEt_2$ and ^{19}F{^{1}H} NMR spectra to external $CFCl_3$. ^{1}H NMR and ^{13}C{^{1}H} NMR signals were assigned with assistance from DEPT135 and HSQC experiments. Elemental analysis was conducted on an Elementar vario MICRO cube elemental analyser. UV/Vis spectra were acquired on a JASCO-V660 UV/Vis spectrometer.

Synthetic Procedures

Synthesis of **2**:

To a benzene solution (2 mL) of B_2Cat_2 (15.5 mg, 0.07 mmol) was added a benzene solution (2 mL) of **1** (25.0 mg, 0.13 mmol). The solution was stirred for 2 h and over the course of the reaction a color change to bright yellow was observed. All volatile components were removed under dynamic vacuum and the resulting yellow oil was washed with pentane, yielding a complicated mixture of products as yellow amorphous solids. Crystals of **2** suitable for X-ray diffraction could be grown from a concentrated hexane solution at − 30 °C. By manual selection of crystals, enough material for NMR characterization of compound **2** could be obtained.

^{1}H NMR (400.1 MHz, 296 K, toluene-d_8): δ = 7.04-7.02 (m, 4 H, $BO_2C_6\mathit{H}_4$), 6.82-6.80 (m, 4 H, $BO_2C_6\mathit{H}_4$), 2.65-2.63 (m, 16 H, 2,6-$NC_5\mathit{H}_{10}$), 1.08-1.00 (m, 24 H, 3,4,5-$NC_5\mathit{H}_{10}$) ppm.

^{11}B NMR (128.4 MHz, 296 K, toluene-d_8): δ = 11.4 ppm.

^{13}C{^{1}H} NMR (100.6 MHz, 296 K, toluene-d_8): δ = 153.6 (s, C_q, C=C), 137.5 (s, C_q, C_6H_4), 119.5 (s, CH, C_6H_4), 109.9 (s, CH, C_6H_4), 46.1 (s, CH_2, 2,6-NC_5H_{10}), 26.3 (s, CH_2, 3,5-NC_5H_{10}), 24.5 (s, CH_2, 4-NC_5H_{10}) ppm.

Elemental analysis: By dissolving the mixture in THF and precipitation at − 30 °C, a solid sample with the elemental composition corresponding to a 1:1 ratio of B_2Cat_2 and **1** could be obtained. Calcd: C 67.02, H 6.56, N 6.51; found: C 66.83, H 6.79, N 6.83.

HRMS (LIFDI): *m/z* Calcd for $C_{36}H_{48}B_2N_4O_4$ $[M]^-$ 622.3862; found 622.3856.

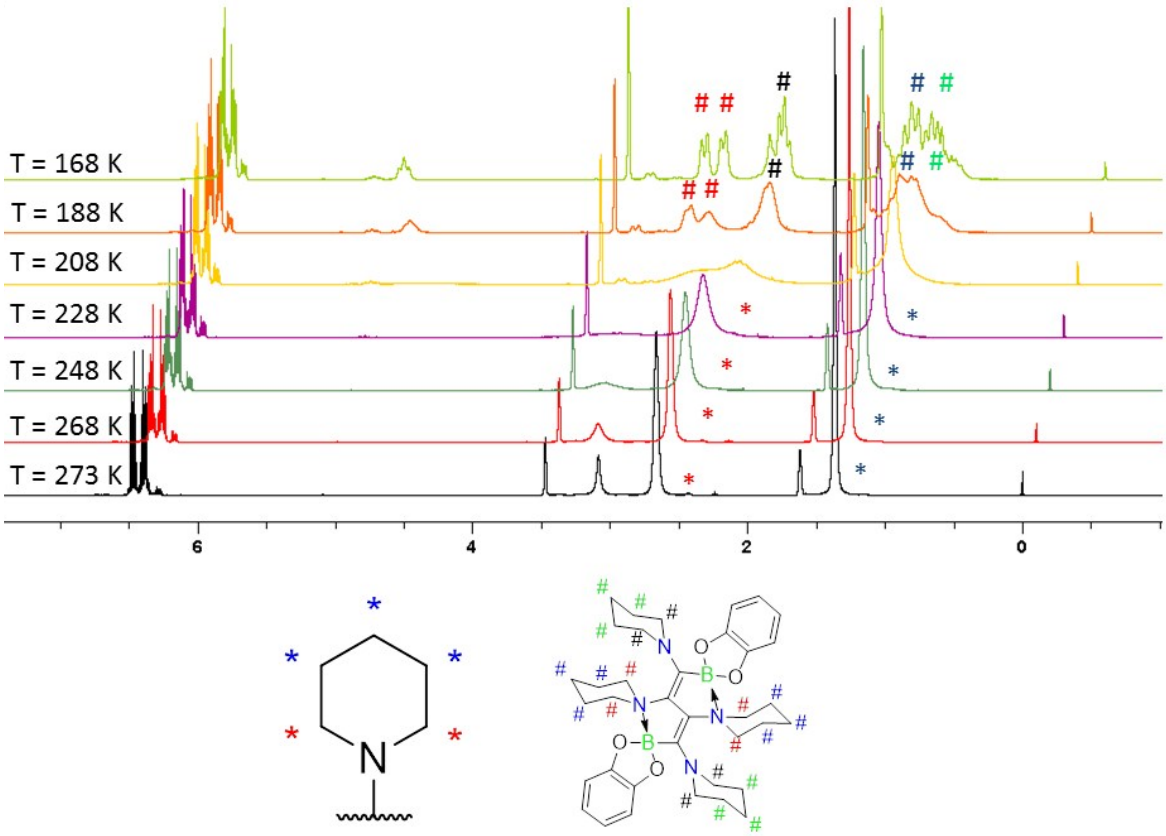


Figure S1. ^{1}H NMR spectra of **2** at different temperatures ranging from 168-273 K.

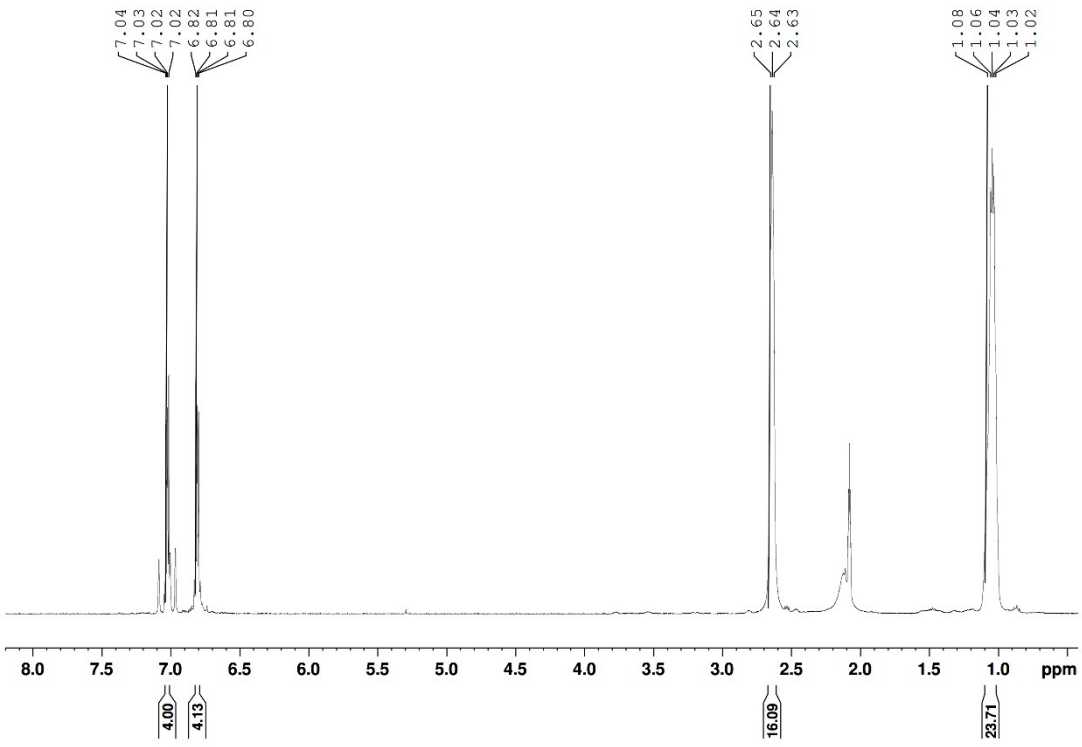


Figure S2. ^{1}H NMR spectrum of **2** in toluene-d_8. The multiplet at 2.08 ppm and the corresponding singlets at 6.97, 7.01 and 7.09 ppm, which overlap with the resonances of compound **2**, are due to residual solvent.

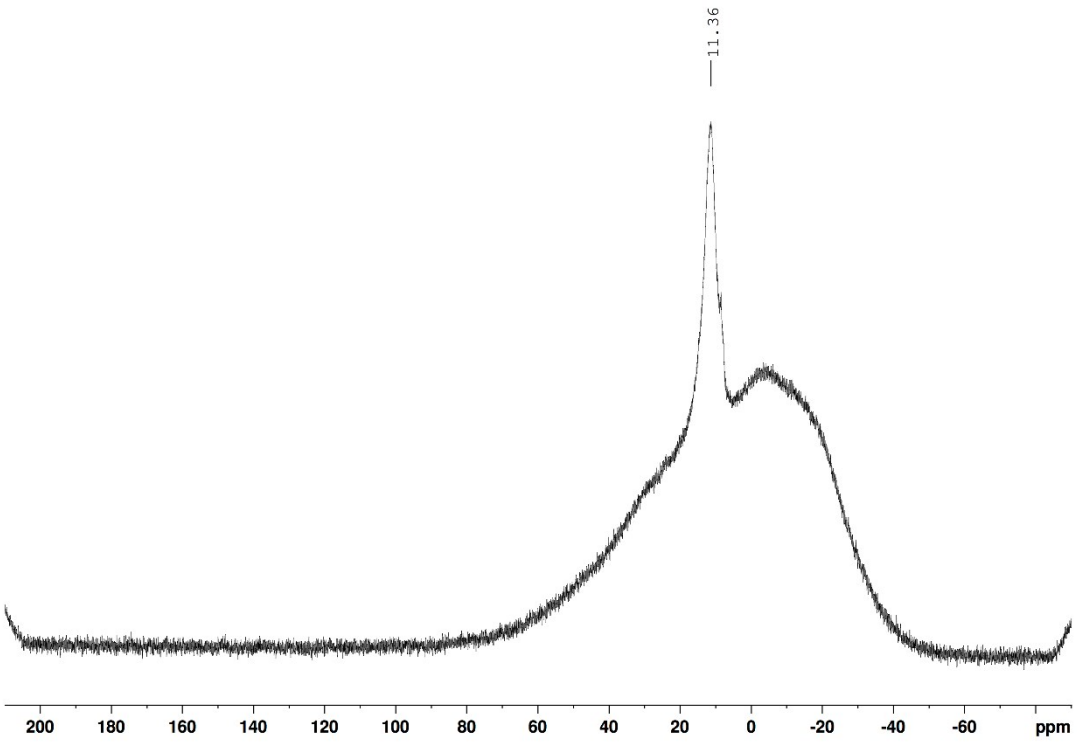


Figure S3. ^{11}B NMR spectrum of **2** in toluene-d_8.

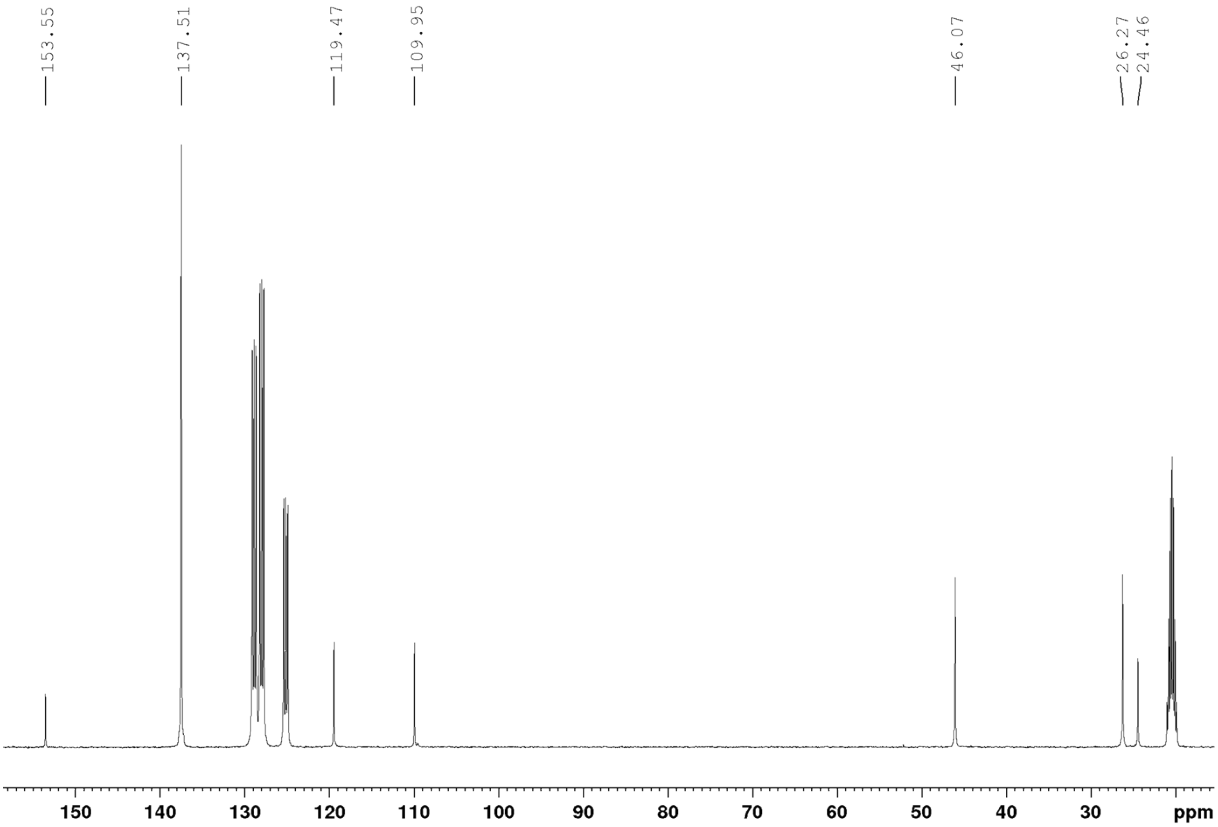


Figure S4. ^{13}C{^{1}H} NMR spectrum of **2** in toluene-d_8. The singlets at 20.43, 125.13, 127.96, 128.81 and 137.48 ppm, which overlap with the resonances of compound **2**, are due to residual solvent.

Synthesis of **3**:

To a pentane (2 mL) solution of **1** (58.1 mg, 0.30 mmol) was added a pentane (2 mL) solution of $B_2Cl_2Mes_2$ (100 mg, 0.30 mmol). The resulting orange suspension was stirred for 2 h at rt and filtered. Removal of volatiles yielded a yellow solid, which was recrystallized from pentane at − 30 °C to yield pure **3** as a yellow solid (107 mg, 0.19 mmol, 68%).

^{1}H NMR (500.1 MHz, 296 K, CD_2Cl_2): δ = 6.82 (s, 1 H, aryl-C*H*), 6.77 (s, 2 H, aryl-C*H*), 6.76 (s, 1 H, aryl-C*H*), 4.15 (dt, ^2J = 4.1 Hz, ^3J = 12.2 Hz, 1 H, NC_5H_{10}), 4.08 (dt, ^2J = 3.2 Hz, ^3J = 13.0 Hz, 1 H, NC_5H_{10}), 3.83-3.77 (m, 1 H, NC_5H_{10}), 3.37-3.31 (m, 1 H, NC_5H_{10}), 3.10-3.05 (m, 1 H, NC_5H_{10}), 2.99-2.93 (m, 1 H, NC_5H_{10}), 2.85-2.79 (m, 1 H, NC_5H_{10}), 2.75 (s, 3 H, aryl-CH_3), 2.46-2.39 (m, 1 H, NC_5H_{10}), 2.43 (s, 3 H, aryl-CH_3), 2.33 (s, 3 H, aryl-CH_3), 2.27 (s, 3 H, aryl-CH_3), 2.24 (s, 3 H, aryl-CH_3), 2.22 (s, 3 H, aryl-CH_3), 2.20-2.14 (m, 1 H, NC_5H_{10}), 1.75-1.34 (m, 7 H, NC_5H_{10}), 1.26-1.18 (m, 2 H, NC_5H_{10}), 1.14-0.94 (m, 2 H, NC_5H_{10}) ppm.

^{11}B NMR (160.5 MHz, 296 K, CD_2Cl_2): δ = 48.5 (s, *B*MesCl), 7.6 (s, N–*B*MesCl) ppm.

^{13}C{^{1}H} NMR (125.8 MHz, 296 K, CD_2Cl_2): δ = 145.7 (s, C_q), 143.5 (s, C_q), 138.0 (s, C_q), 137.9 (s, C_q), 137.8 (s, C_q), 137.3 (s, C_q), 131.3 (s, aryl-*C*H), 130.1 (s, aryl-*C*H), 127.8 (s, aryl-*C*H), 127.5 (s, aryl-*C*H), 55.5 (s, CH_2, NC_5H_{10}), 53.0 (s, CH_2, NC_5H_{10}), 50.5 (s, CH_2, NC_5H_{10}), 26.8 (s, aryl-*C*H_3), 26.3 (s, CH_2, NC_5H_{10}), 26.1 (s, CH_2, NC_5H_{10}), 24.6 (s, aryl-*C*H_3), 24.3 (s, CH_2, NC_5H_{10}), 23.9 (s, CH_2, NC_5H_{10}), 23.6 (s, CH_2, NC_5H_{10}), 22.2 (s, aryl-*C*H_3), 22.0 (s, CH_2, NC_5H_{10}), 21.2 (s, aryl-*C*H_3), 20.8 (s, aryl-*C*H_3).

UV-Vis: λ_{max} (CH_2Cl_2) = 330 nm (ε = 6393 L·(cm·mol)$^{-1}$).

Elemental analysis: calcd for $C_{30}H_{42}B_2Cl_2N_2$: C 68.87, H 8.09, N 5.35; found: C 69.73, H 8.39, N 5.34.

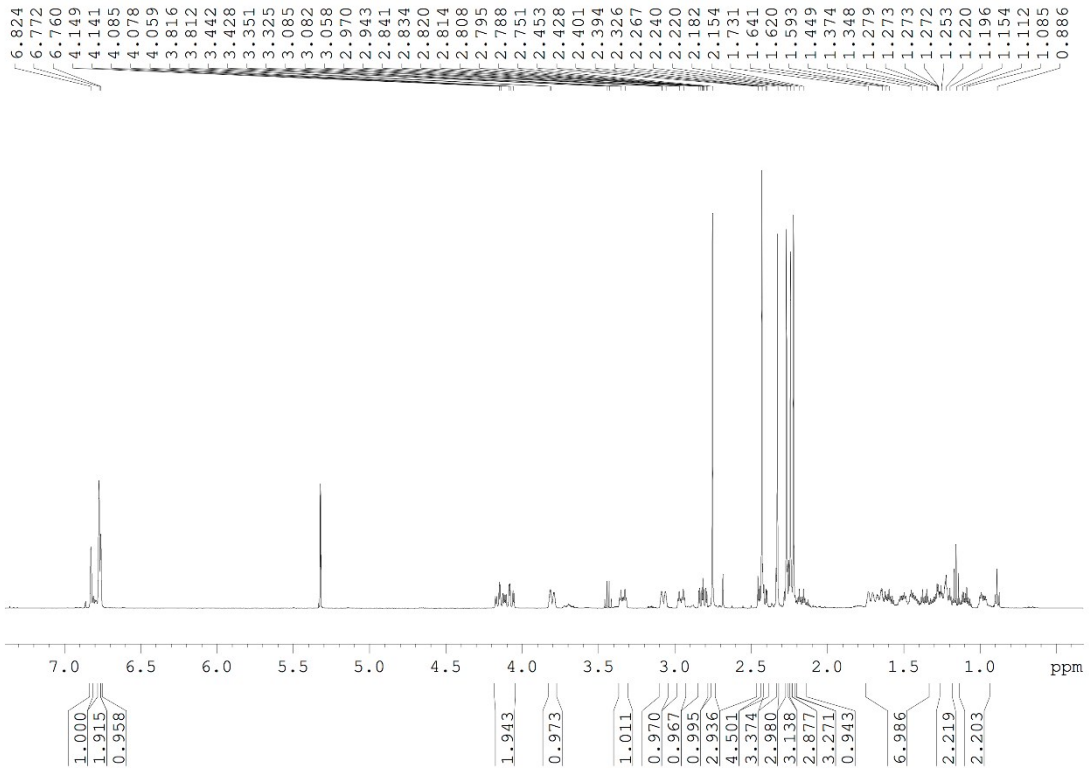


Figure S5. ^{1}H NMR spectrum of **3** in CD_2Cl_2. The triplet at 0.89 ppm and the corresponding multiplet at 1.27 ppm, which overlaps with the resonances of compound **3**, are due to residual pentane, while the triplet at 1.15 ppm and the corresponding quartet at 3.43 ppm are due to residual diethyl ether.

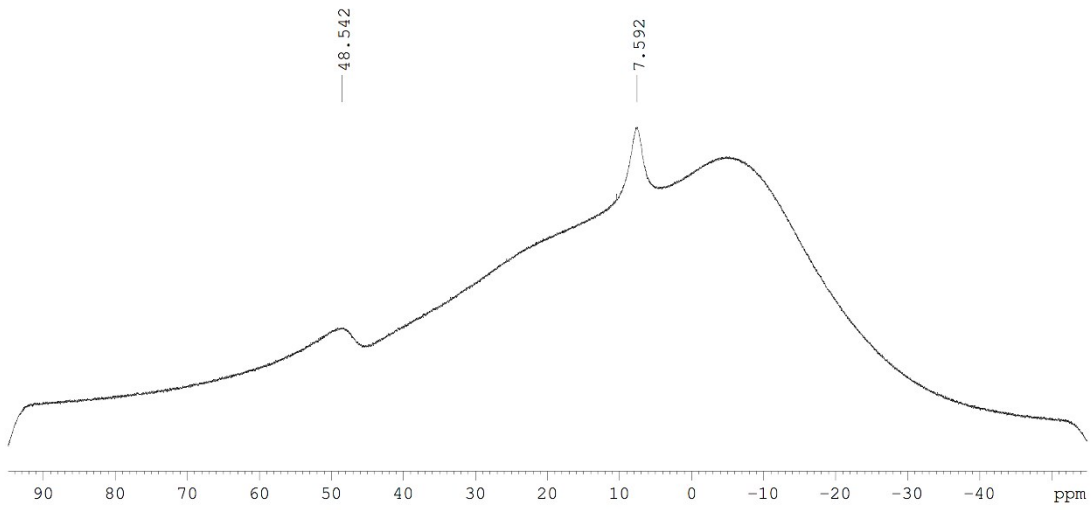


Figure S6. $^{11}B\{^{1}H\}$ NMR spectrum of **3** in CD_2Cl_2.

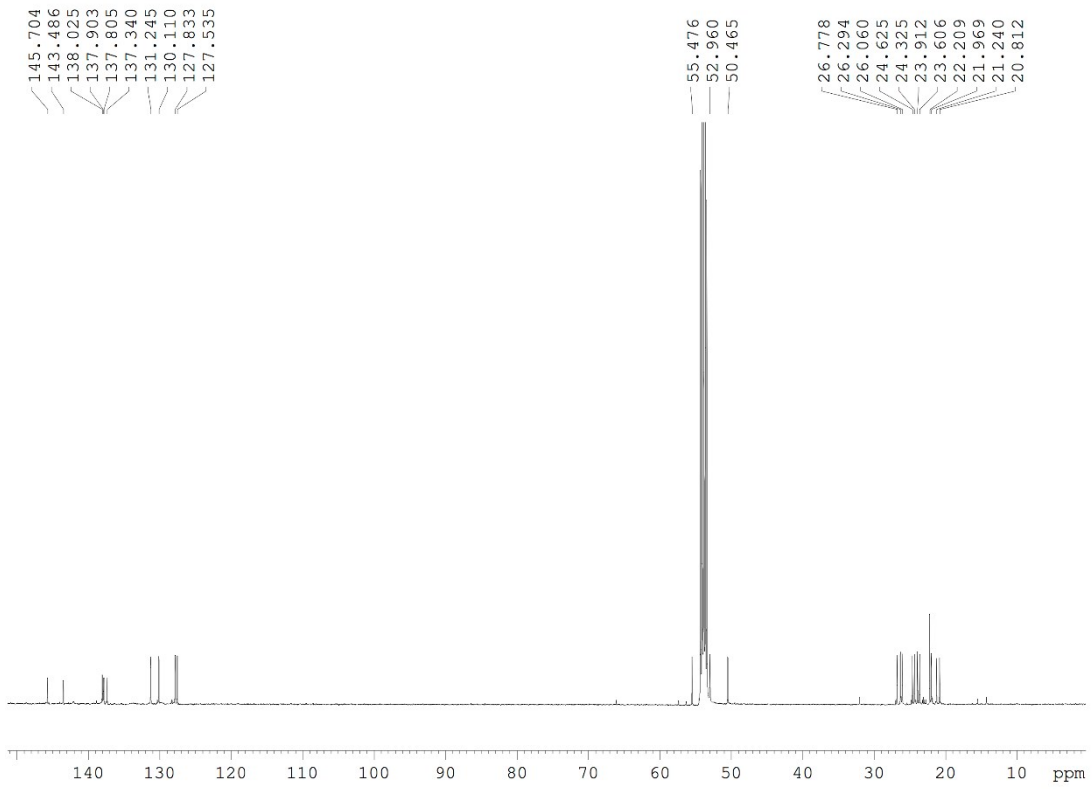


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in CD_2Cl_2.

Synthesis of **4**:

To a pentane (2 mL) solution of **1** (53.6 mg, 0.28 mmol) was added a pentane solution (2 mL) of $B_2Cl_2Dur_2$ (100 mg, 0.28 mmol). The resulting orange suspension was stirred for 2 h at rt and filtered. Removal of volatiles yielded a yellow solid which was recrystallized from pentane at − 30 °C to yield pure **4** as a yellow solid (94 mg, 0.17 mmol, 62%).

^{1}H NMR (500.1 MHz, 296 K, CD_2Cl_2): δ = 6.92 (s, 1 H, aryl-C*H*), 6.85 (s, 1 H, aryl-C*H*), 4.27-4.15 (m, 2 H, NC_5H_{10}), 3.93-3.87 (m, 1 H, NC_5H_{10}), 3.29-3.23 (m, 1 H, NC_5H_{10}), 3.17-3.11 (m, 1 H, NC_5H_{10}), 2.90-2.84 (m, 1 H, NC_5H_{10}), 2.74-2.68 (m, 1 H, NC_5H_{10}), 2.62 (s, 3 H, aryl-CH_3), 2.42-2.36 (m, 1 H, NC_5H_{10}), 2.35 (s, 3 H, aryl-CH_3), 2.26 (s, 3 H, aryl-CH_3), 2.21 (s, 3 H, aryl-CH_3), 2.19 (s, 3 H, aryl-CH_3), 2.18-2.16 (m, 9 H, aryl-CH_3), 1.77-1.70 (m, 2 H, NC_5H_{10}), 1.57-1.20 (m, 8 H, NC_5H_{10}), 1.09-1.00 (m, 1 H, NC_5H_{10}), 0.95-0.89 (m, 1 H, NC_5H_{10}) ppm.

^{11}B NMR (160.5 MHz, 296 K, CD_2Cl_2): δ = 48.7 (s, *B*DurCl), 7.8 (s, N–*B*DurCl) ppm.

^{13}C{^{1}H} NMR (125.8 MHz, 296 K, CD_2Cl_2): δ = 141.7 (s, C_q), 140.0 (s, C_q), 134.9 (s, C_q), 134.0 (s, C_q), 133.8 (s, C_q), 133.8 (s, C_q), 133.6 (s, C_q), 133.5 (s, C_q), 132.1 (s, aryl-*C*H), 131.5 (s, aryl-*C*H), 55.3 (s, CH_2, NC_5H_{10}), 54.5 (s, CH_2, NC_5H_{10}), 52.8 (s, CH_2, NC_5H_{10}), 50.4 (s, CH_2, NC_5H_{10}), 26.3 (s, CH_2, NC_5H_{10}), 25.9 (s, CH_2, NC_5H_{10}), 24.0 (s, CH_2, NC_5H_{10}), 23.9 (s, CH_2, NC_5H_{10}), 23.6 (s, CH_2, NC_5H_{10}), 22.0 (s, CH_2, NC_5H_{10}), 21.4 (s, aryl-*C*H_3), 21.2 (s, aryl-*C*H_3), 20.8 (s, aryl-*C*H_3), 19.6 (s, aryl-*C*H_3), 19.6 (s, aryl-*C*H_3), 19.5 (s, aryl-*C*H_3), 19.5 (s, aryl-*C*H_3) ppm.

Elemental analysis: calcd for $C_{32}H_{46}B_2Cl_2N_2$: C 69.72, H 8.41, N 5.08; found: C 68.85, H 8.48, N 4.72.

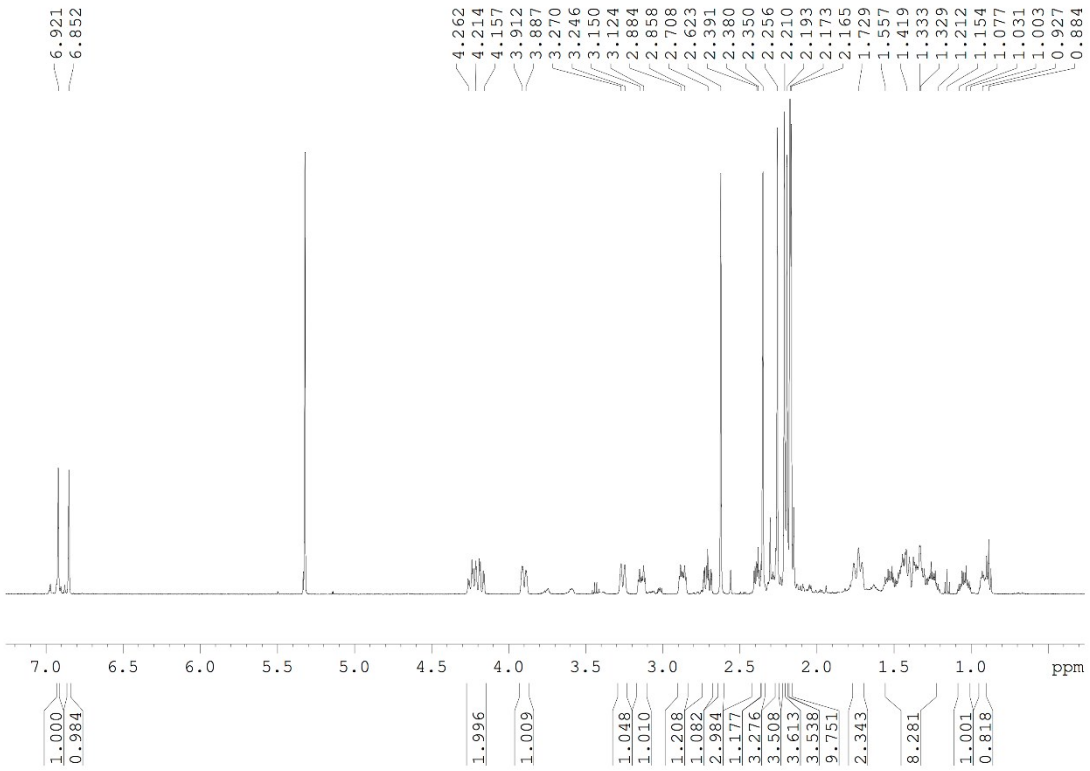


Figure S8. ^{1}H NMR spectrum of **4** in CD_2Cl_2. The triplet at 0.89 ppm and the corresponding multiplet at 1.30 ppm, which overlaps with the resonances of compund **4**, are due to residual pentane.

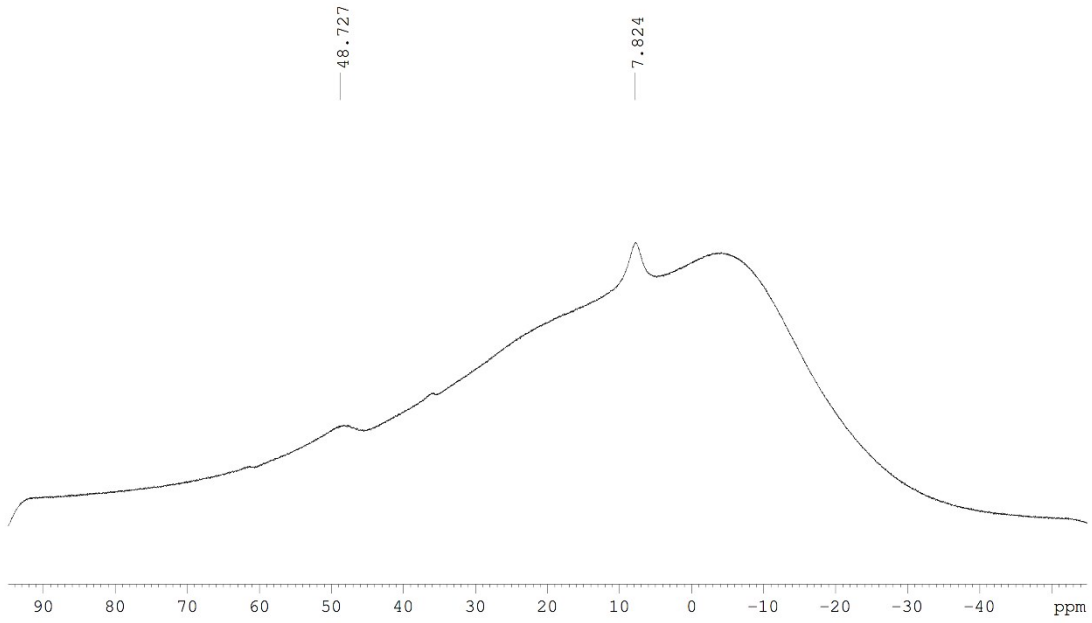


Figure S9. ^{11}B NMR spectrum of **4** in CD_2Cl_2.

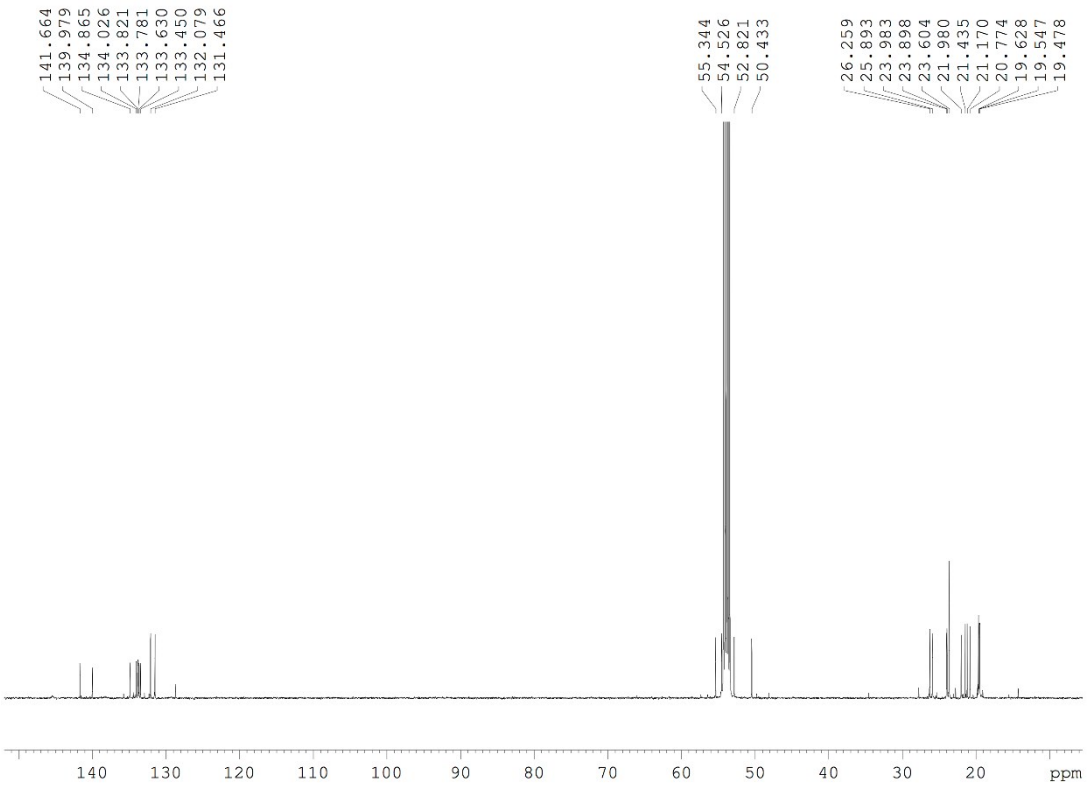


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2.

Synthesis of **5**:

To a pentane solution (5 mL) of **1** (90.4 mg, 0.47 mmol) was added a pentane solution (5 mL) of F_2BBMes_2 (70.0 mg, 0.24 mmol) and the resulting red suspension was stirred for 4 h at rt. Removal of volatiles yielded a red solid that was extracted with hexanes (3 x 2 mL) and recrystallized from CH_2Cl_2 (2 mL) at − 30 °C to yield pure **5** as a colorless solid (25.3 mg, 0.04 mmol, 16%).

^{1}H NMR (500.1 MHz, 296 K, C_6D_6): δ = 7.04 (s, 1 H, aryl-C*H*), 6.91 (s, 1 H, aryl-C*H*), 6.84 (s, 1 H, aryl-C*H*), 6.77 (s, 1 H, aryl-C*H*), 4.33-4.26 (m, 1 H, NC_5H_{10}), 3.95-3.85 (m, 2 H, NC_5H_{10}), 3.70-3.63 (m, 1 H, NC_5H_{10}), 3.50-3.43 (m, 1 H, NC_5H_{10}), 3.29-3.21 (m, 1 H, NC_5H_{10}), 3.06-2.97 (m, 1 H, NC_5H_{10}), 2.90-2.83 (m, 2 H, NC_5H_{10}), 2.83-2.68 (m, 3 H, NC_5H_{10}), 2.66 (s, 3 H, aryl-CH_3), 2.59 (s, 3 H, aryl-CH_3), 2.51-2.42 (m, 4 H, NC_5H_{10}), 2.40 (s, 3 H, aryl-CH_3), 2.21 (s, 3 H, aryl-CH_3), 2.19 (s, 3 H, aryl-CH_3), 2.16-2.08 (m, 1 H, NC_5H_{10}), 2.04 (s, 3 H, aryl-CH_3), 2.01-1.86 (m, 2 H, NC_5H_{10}), 1.54-1.24 (m, 14 H, NC_5H_{10}), 1.18-1.10 (m, 2 H, NC_5H_{10}), 1.10-0.96 (m, 4 H, NC_5H_{10}), 0.88-0.79 (m, 1 H, NC_5H_{10}) ppm.

^{11}B NMR (160.5 MHz, 296 K, C_6D_6): δ = 5.8 (br s), − 4.8 (s) ppm.

^{13}C{^{1}H} NMR (125.8 MHz, 296 K, C_6D_6): δ = 144.0 (s, C_q), 141.5 (s, C_q), 141.4 (s, C_q), 134.0 (s, C_q), 132.7 (s, C_q), 131.9 (s, aryl-*C*H), 131.3 (s, aryl-*C*H), 129.8 (aryl-*C*H), 110.2 (s, C_q), 58.0 (s, CH_2, NC_5H_{10}), 57.8 (s, CH_2, NC_5H_{10}), 57.1 (s, CH_2, NC_5H_{10}), 51.7 (s, CH_2, NC_5H_{10}), 51.4 (s, CH_2, NC_5H_{10}), 50.8 (s, CH_2, NC_5H_{10}), 27.7 (s, aryl-*C*H_3), 26.9 (s, CH_2, NC_5H_{10}), 26.6 (s, aryl-*C*H_3), 25.9 (s, CH_2, NC_5H_{10}), 25.6 (s, aryl-*C*H_3), 25.4 (s, CH_2, NC_5H_{10}), 25.2 (s, CH_2, NC_5H_{10}), 25.1 (s, CH_2, NC_5H_{10}), 24.0 (s, CH_2, NC_5H_{10}), 23.4 (s, CH_2, NC_5H_{10}), 23.3 (s, CH_2, NC_5H_{10}), 20.9 (s, aryl-*C*H_3) ppm.

^{19}F NMR (470.6 MHz, 296 K, C_6D_6): δ = –140.9 (br s, FWHH = 173.6 Hz), –147.0 (br s, FWHH = 161.3 Hz) ppm.

^{19}F{^{11}B} NMR (470.6 MHz, 296 K, C_6D_6): δ = –141.0 (d, $^2J_{F\text{-}F}$ = 48 Hz), –147.0 (d, $^2J_{F\text{-}F}$ = 48 Hz) ppm.

Elemental analysis: calcd for $C_{42}H_{62}B_2F_2N_4$: C 73.90, H 9.16, N 8.21; found: C 73.94, H 9.58, N 8.25.

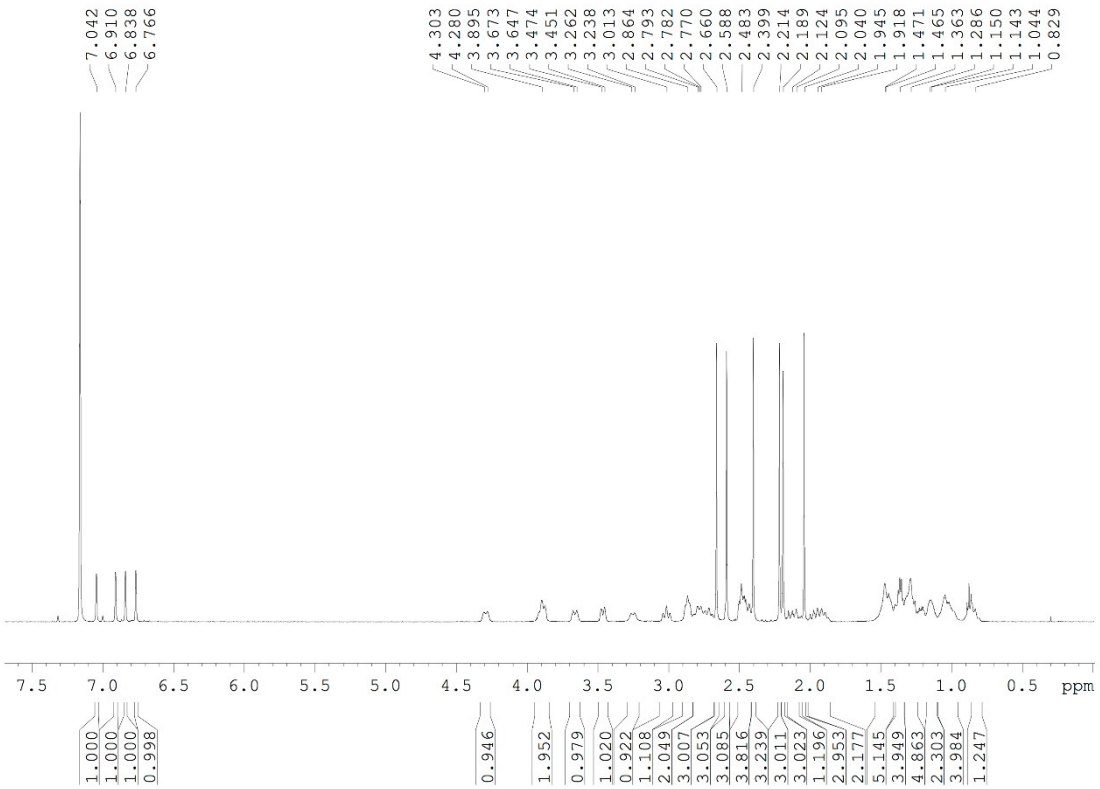


Figure S11. ^{1}H NMR spectrum of **5** in C_6D_6.

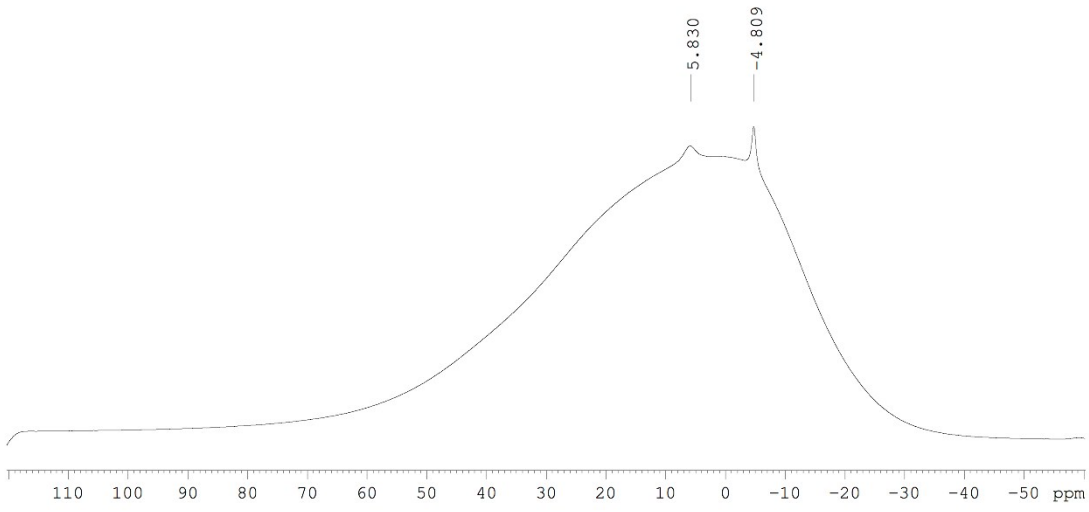


Figure S12. ^{11}B NMR spectrum of **5** in C_6D_6.

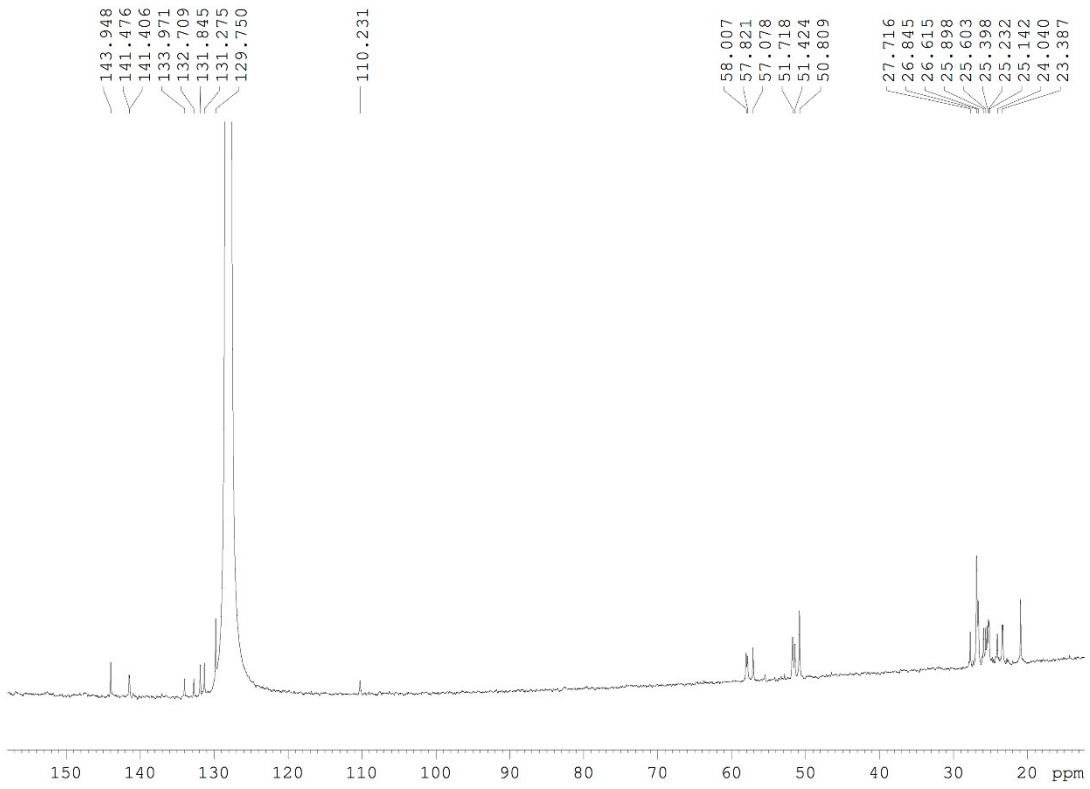


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in C_6D_6.

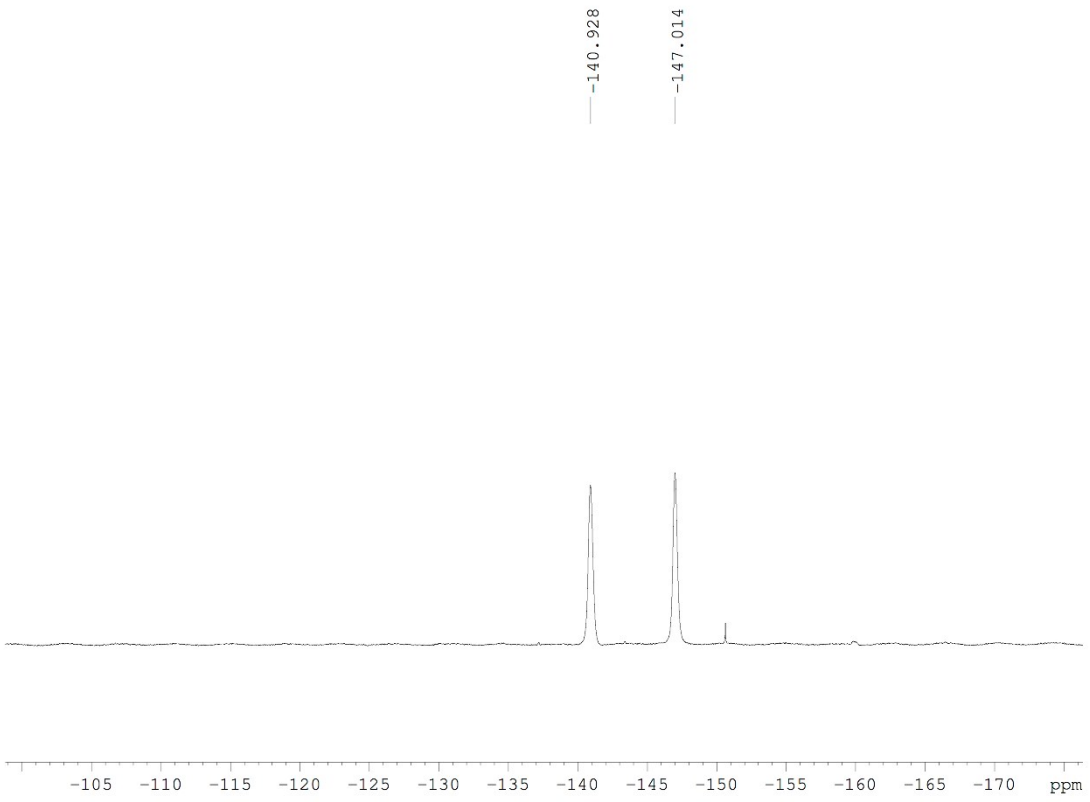


Figure S14. ^{19}F NMR spectrum of **5** in C_6D_6.

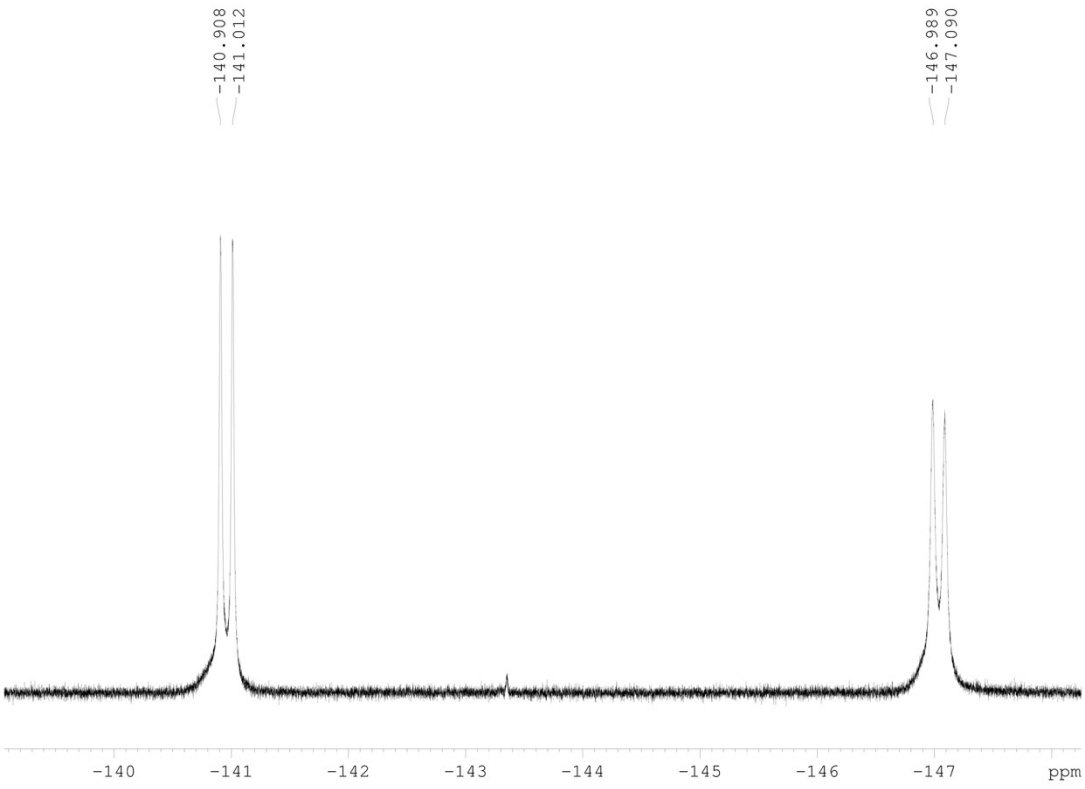


Figure S15. $^{19}F\{^{11}B\}$ NMR spectrum of **5** in C_6D_6.

UV-vis spectroscopy

The UV-vis spectrum was measured on a JASCO V-660 UV/Vis spectrometer in CH_2Cl_2 at 25 °C.

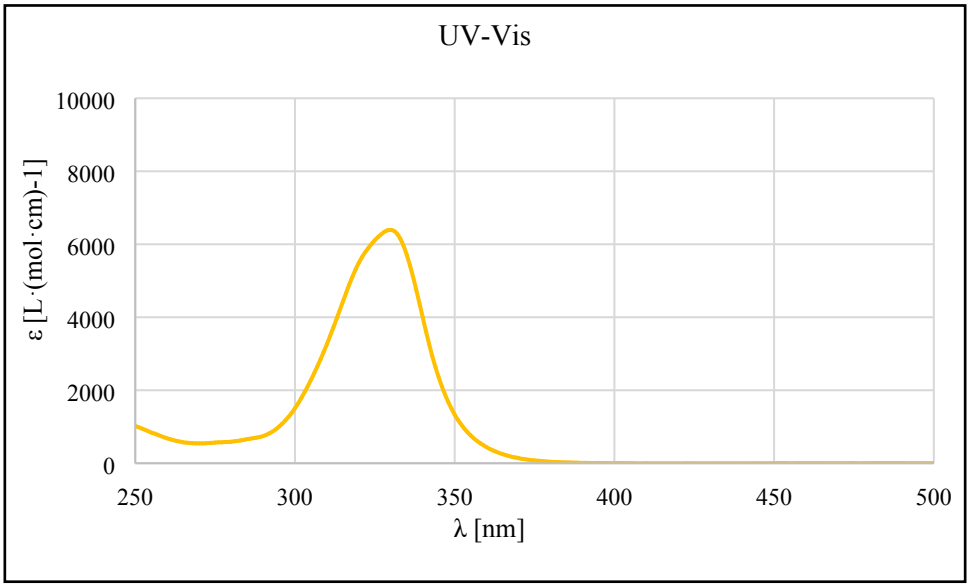


Figure S16. UV-Vis absorption spectrum of **3** in CH_2Cl_2 at 25 °C. Absorption maximum at 330 nm ($\varepsilon = 6393$ L·(cm·mol)$^{-1}$).

Crystallographic Details

Crystal data were collected on a BRUKER X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation or on a BRUKER D8 QUEST diffractometer. The structures were solved using intrinsic phasing methods, refined with the SHELXL program and expanded using Fourier techniques.[4,5] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealized geometric positions.

Crystal data for 2: Formula: $C_{54}H_{66}B_2N_4O_4$, $M_r = 856.72$, yellow plate, 0.275×0.27×0.10 mm^3, orthorhombic space group *Cmca*, $a = 10.924(4)$ Å, $b = 15.753(7)$ Å, $c = 27.040(9)$ Å, $V = 4653(3)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.223$ g·cm^{-3}, $\mu = 0.076$ mm^{-1}, $F(000) = 1840$, $T = 103(2)$ K, $R_1 = 0.0629$, $wR^2 = 0.1123$, 2596 independent reflections [$2\theta \leq 53.462°$] and 156 parameters. CCDC-1560439.

Crystal data for 3: Formula: $C_{30}H_{42}B_2Cl_2N_2$, $M_r = 523.17$, colorless block, 0.137×0.119×0.048 mm^3, tetragonal space group $P4_32_12$, $a = 12.362(3)$ Å, $b = 12.362(3)$ Å, $c = 38.073(7)$ Å, $\alpha = 90°$, $\beta = 90°$, $\gamma = 90°$, $V = 5818(3)$ Å^3, $Z = 8$, $\rho_{calcd} = 1.195$ g·cm^{-3}, $\mu = 0.245$ mm^{-1}, $F(000) = 2240$, $T = 100(2)$ K, $R_1 = 0.0348$, $wR^2 = 0.0714$, 5726 independent reflections [$2\theta \leq 52.032°$] and 331 parameters. CCDC-1560442.

Crystal data for 4: Formula: $C_{32}H_{46}B_2Cl_2N_2$, $M_r = 551.23$, colorless block, 0.40×0.25×0.20 mm^3, triclinic space group $P\bar{1}$, $a = 9.198(2)$ Å, $b = 10.869(2)$ Å, $c = 16.114(4)$ Å, $\alpha = 97.766(14)°$, $\beta = 102.763(8)°$, $\gamma = 100.085(8)°$, $V = 1521.2(6)$ Å^3, $Z = 2$, $\rho_{calcd} = 1.203$ g·cm^{-3}, $\mu = 0.237$ mm^{-1}, $F(000) = 592$, $T = 296(2)$ K, $R_1 = 0.0397$, $wR^2 = 0.0966$, 5998 independent reflections [$2\theta \leq 52.042°$] and 351 parameters. CCDC-1560441.

Crystal data for 5: Formula: $C_{42}H_{62}B_2F_2N_4$, $M_r = 682.57$, colorless block, 0.212×0.19×0.185 mm^3, monoclinic space group $P2_1/n$, $a = 9.595(4)$ Å, $b = 24.297(10)$ Å, $c = 16.928(11)$ Å, $\beta = 106.09(2)°$, $V = 3792(3)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.196$ g·cm^{-3}, $\mu = 0.076$ mm^{-1}, $F(000) = 1480$, $T = 100(2)$ K, $R_1 = 0.0548$, $wR^2 = 0.1028$, 7690 independent reflections [$2\theta \leq 52.744°$] and 457 parameters. CCDC-1560440.

Computational Methodology

Theoretical calculations were carried out in the Gaussian09 computational package.[6] Geometry optimizations were run in the gas phase with the default options set up in the program. The hybrid PBE0 exchange-correlation density-functional was chosen, which, by mixing a fraction of exact (Hartree-Fock) exchange (25%), significantly reduces the delocalization error of semi-local functionals.[7] Moreover, the 6-31G(d) basis set was selected for performing the geometry optimizations. Also, the D3 version of Grimme's dispersion correction[8] with the original damping function was added to the DFT model after each scf cycle. Then, as a second step, we calculated harmonic frequencies of each optimized species, presumed to be critical points on the potential energy surface for two reasons: first, depending on the number of negative eigenvalues, it is possible to classify each optimized structure as minimum (zero) or transition state (one and only one); second, in order to obtain the thermal and entropic corrections for expressing the total energy, according to classical thermodynamics, as Gibbs free energy. For the reaction field calculation, we have used Truhlar and coworkers' SMD solvation model[9] and the default options for benzene as the solvent (ε=2.2706), carrying out single-point calculations over the optimized geometries at the same level of theory (D3-PBE0/6-31G(d)). We then executed single-point calculations with the same density-functional but with a larger basis set, 6-311+G(d), with the aim of improving the numerical values reported herein for all of the structures calculated in the reaction routes. Therefore, our final reported free energies were calculated at the D3-PBE0/6-311+G(d) level. We have used the programs Chemcraft[10] and CYLView[11] for visualizing our results and plotting the optimized geometries shown in the energy profiles for each reaction mechanism. ^{11}B NMR signals were calculated at the GIAO-D3-PBE0/def2-svp level using $BF_3{\cdot}OEt_2$ as the standard for obtaining the chemical shifts and comparing with our experimental data.

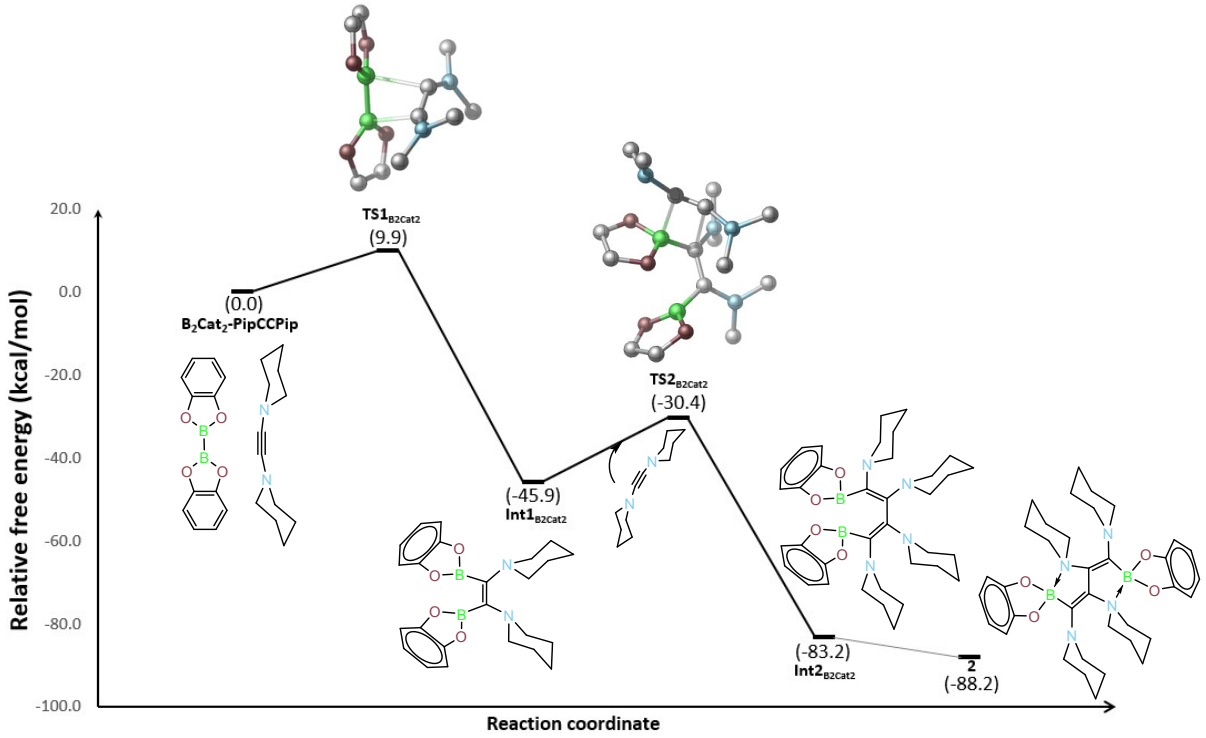


Figure S17. Energy profile of the reaction between B_2Cat_2 and PipCCPip to form **2**, calculated at the D3-PBE0/6-311+G(d) level. Transition states are shown as truncated models. Colour code: green = boron, grey = carbon, blue = nitrogen, dark red = oxygen.

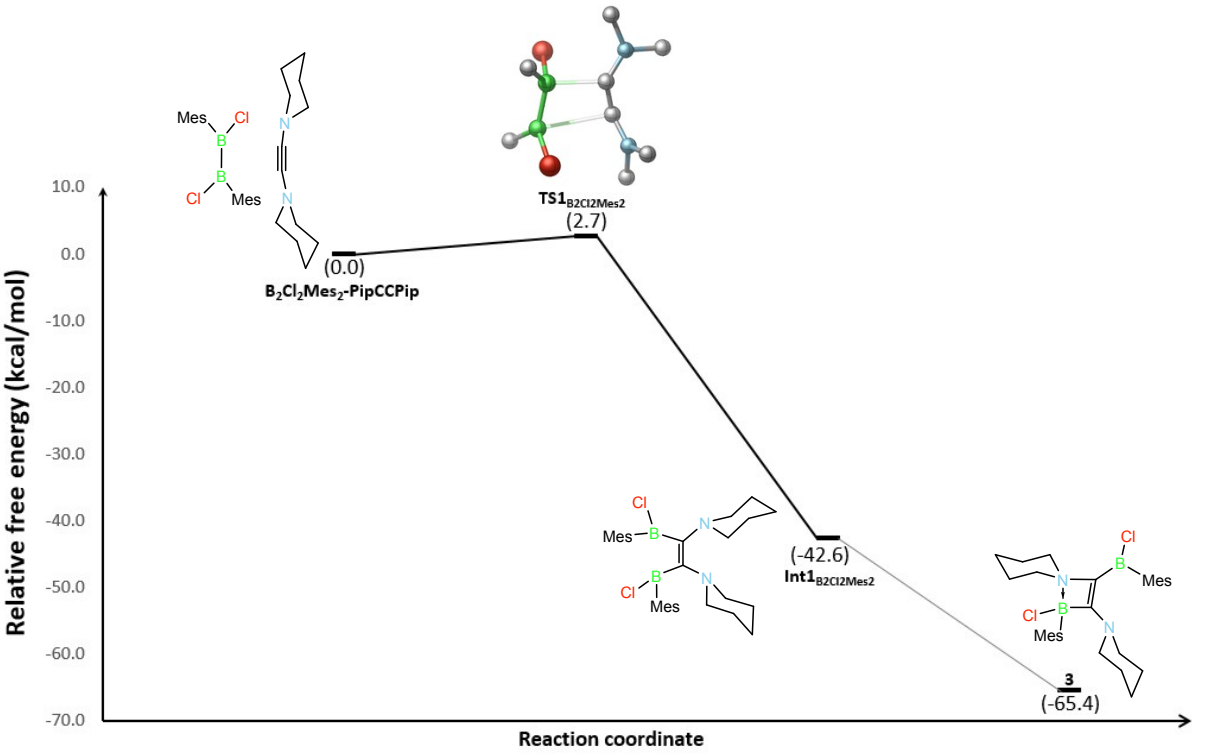


Figure S18. Energy profile of the reaction between $B_2Cl_2Mes_2$ and PipCCPip to form **3**, calculated at the D3-PBE0/6-311+G(d) level. Transition states are shown as truncated models. Colour code: green = boron, grey = carbon, blue = nitrogen, red = chlorine.

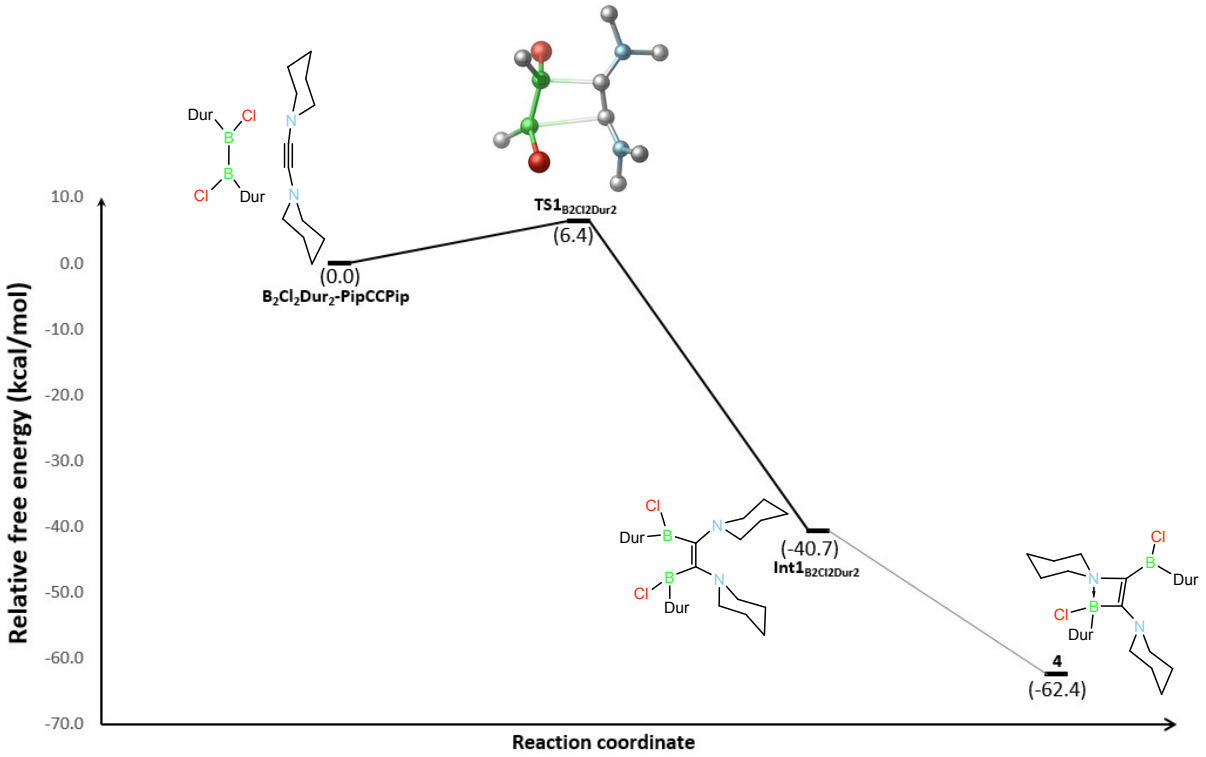


Figure S19. Energy profile of the reaction between $B_2Cl_2Dur_2$ and PipCCPip to form **4**, calculated at the D3-PBE0/6-311+G(d) level. Transition states are shown as truncated models. Colour code: green = boron, grey = carbon, blue = nitrogen, red = chlorine.

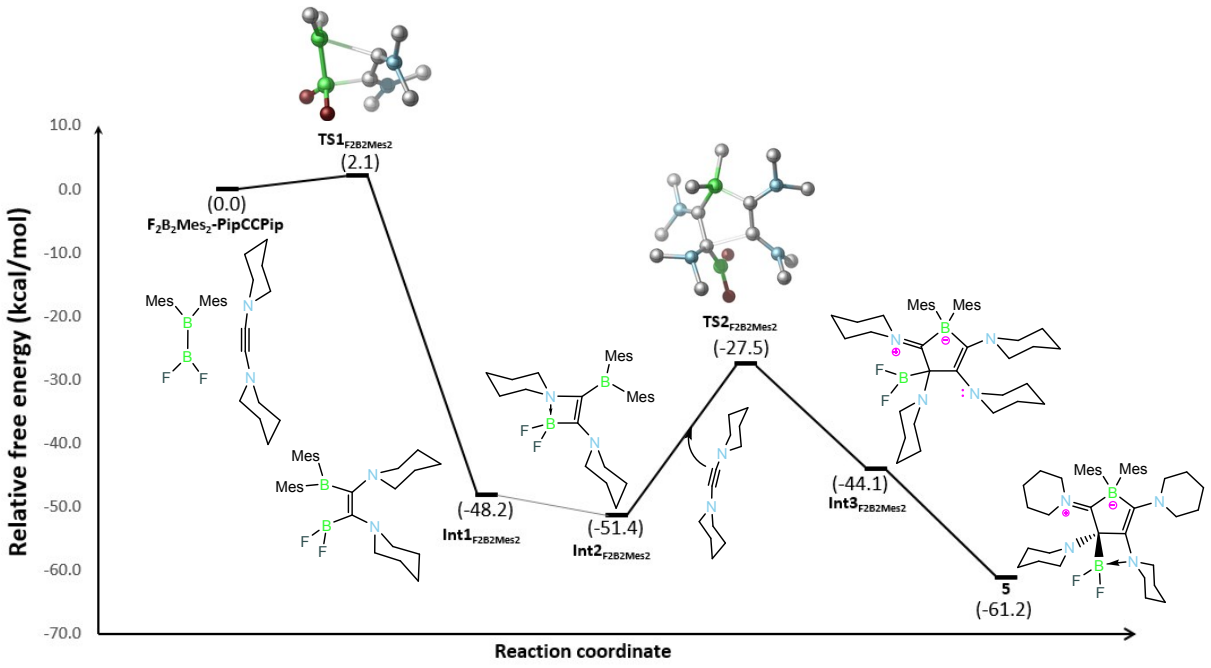
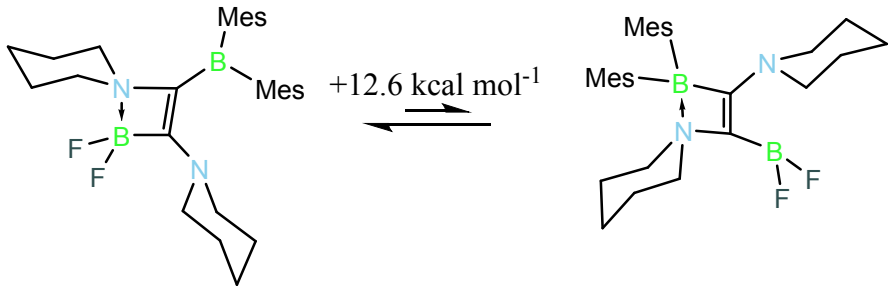
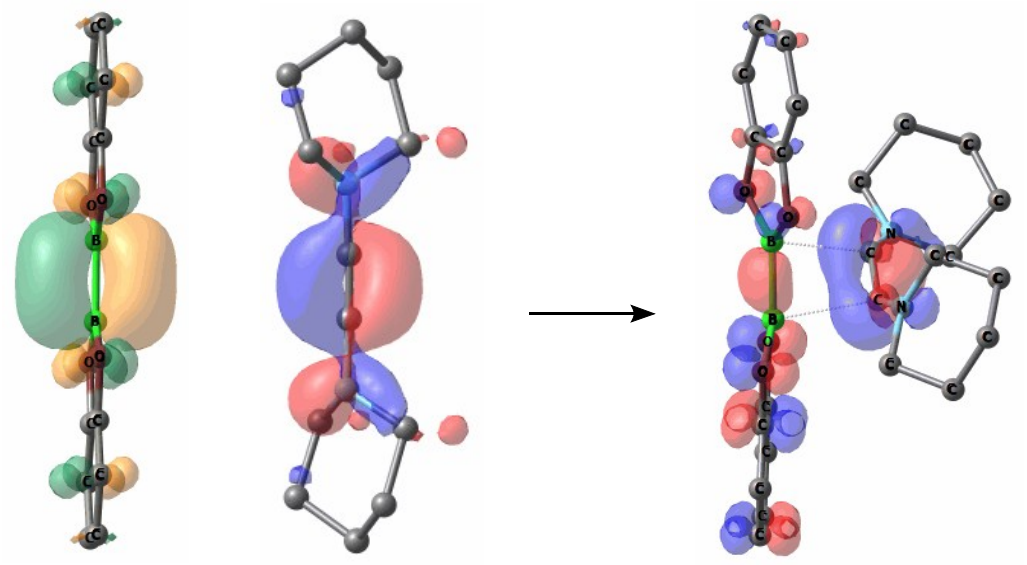


Figure S20. Energy profile of the reaction between $B_2F_2Mes_2$ and PipCCPip to form **5**, calculated at the D3-PBE0/6-311+G(d) level. Transition states are shown as truncated models. Colour code: green = boron, grey = carbon, blue = nitrogen, dark red = fluorine.



Int1$_{F2B2Mes2}$ **Int1$_{F2B2Mes2}$ isomer**

Figure S21. Energy difference between the two isomers of the initial product of the reaction between PipCCPip and $B_2F_2Mes_2$, calculated at the D3-PBE0/6-311+G(d) level.



LUMO
B_2Cat_2

HOMO
PipCCPip

HOMO
TS1$_{B2Cat2}$

Figure S22. LUMO of B_2Cat_2 and HOMO of PipCCPip (left), and the HOMO of the transition state **TS1$_{B2Cat2}$**. An isosurface of 0.05 a.u. was chosen for each MO graph.

Table S1. Cartesian coordinates (xyz) of the optimized geometries for all the species involved in the reaction mechanisms reported herein, calculated at the D3-PBE0/6-31G(d) level.

$B_2Cl_2Mes_2$-PipCCPip

E(scf) = –2246.27407798 a.u.

Cl	-0.496484	0.484428	1.955529
C	3.243809	0.651385	0.282903
B	-0.941285	-0.075543	0.319409
Cl	-1.970972	2.432667	-1.048086
C	2.508779	1.555675	-0.071369
B	-2.224389	0.848553	-0.290102
C	3.445709	-1.727161	0.347229
H	3.657875	-1.965992	-0.711131
H	2.360905	-1.695009	0.460475
N	3.969139	-0.404383	0.680332
C	4.060745	-2.789410	1.246560
H	3.685801	-3.775863	0.945826
H	3.728154	-2.614339	2.278275
C	5.584987	-2.737837	1.181866
H	6.029486	-3.473344	1.863068
H	5.913101	-3.005789	0.166177
C	6.078980	-1.331204	1.514387
H	7.169129	-1.265691	1.411231
H	5.832258	-1.093021	2.557447
C	5.422096	-0.296123	0.609019
H	5.696842	0.719581	0.907447
H	5.767816	-0.441670	-0.431681
C	1.875064	3.210921	-1.681869
H	0.926852	3.680937	-1.979467
H	2.121824	2.451732	-2.429388
N	1.642965	2.533692	-0.403307
C	2.975780	4.262300	-1.569368
H	3.105325	4.777508	-2.529579
H	3.920837	3.748774	-1.344156
C	2.650905	5.259990	-0.456306
H	1.765416	5.846032	-0.745922
H	3.472776	5.975030	-0.329390
C	2.361359	4.534453	0.858711
H	3.271852	4.033452	1.215735
H	2.055015	5.245409	1.636323
C	1.279142	3.477057	0.659450
H	1.097718	2.903334	1.570975
H	0.330986	3.948566	0.365982
C	-3.680911	0.341824	-0.038788
C	-4.201150	-0.707599	-0.823654
C	-5.483860	-1.188503	-0.565449

$TS1_{B2Cl2Mes2}$

E(scf) = –2246.26615737 a.u. υ_{min} = –169.9 cm^{-1}

Cl	0.369156	0.636497	2.170154
C	-1.782949	0.030330	0.343244
B	0.221309	0.698168	0.304522
Cl	0.695019	-0.905692	-2.232657
C	-1.591820	-1.243455	-0.010925
B	1.023077	-0.591893	-0.472797
C	-2.645430	2.001080	1.500095
H	-3.464897	2.548174	1.008017
H	-1.700060	2.414910	1.146191
N	-2.721373	0.607258	1.066951
C	-2.776941	2.123968	3.014515
H	-2.813460	3.187511	3.278407
H	-1.876004	1.702106	3.472740
C	-4.016067	1.393528	3.526923
H	-4.060626	1.437588	4.621057
H	-4.923480	1.890881	3.152134
C	-4.005973	-0.058043	3.052774
H	-4.912235	-0.585806	3.373804
H	-3.145071	-0.584287	3.484839
C	-3.899988	-0.121173	1.533714
H	-3.825286	-1.152759	1.179233
H	-4.792923	0.330477	1.075039
C	-2.706463	-1.590730	-2.160320
H	-2.037436	-1.570526	-3.031554
H	-3.050361	-0.572329	-1.972485
N	-1.909854	-2.016022	-1.000111
C	-3.869729	-2.547291	-2.396499
H	-4.411098	-2.232545	-3.296323
H	-4.571168	-2.471064	-1.554165
C	-3.377231	-3.986079	-2.528558
H	-2.759761	-4.077110	-3.433628
H	-4.223733	-4.671038	-2.651044
C	-2.545239	-4.373005	-1.308778
H	-3.180490	-4.382785	-0.412542
H	-2.129735	-5.380928	-1.421246
C	-1.401793	-3.388149	-1.095729
H	-0.845516	-3.593530	-0.180685
H	-0.697886	-3.425265	-1.938100
C	2.312625	-1.302867	0.075427
C	3.565899	-0.902747	-0.457769
C	4.740504	-1.437789	0.061176

H	-5.881590	-1.990046	-1.185861
C	-6.267205	-0.670207	0.463823
C	-5.743371	0.373021	1.227748
H	-6.344761	0.798061	2.029990
C	-4.472434	0.892071	0.991474
C	-3.410318	-1.272050	-1.973484
H	-3.926993	-2.118912	-2.435233
H	-2.421421	-1.621940	-1.655609
H	-3.255793	-0.517002	-2.755089
C	-7.628940	-1.232701	0.760127
H	-7.575882	-1.995847	1.547321
H	-8.069168	-1.705209	-0.123744
H	-8.316641	-0.455029	1.108764
C	-3.965213	2.032820	1.833622
H	-4.667150	2.271201	2.638266
H	-3.826423	2.936908	1.229584
H	-2.996805	1.800901	2.291709
C	-0.276248	-1.360437	-0.251275
C	0.302644	-1.308085	-1.540812
C	0.937620	-2.432915	-2.060690
H	1.402631	-2.369850	-3.043064
C	0.996143	-3.632783	-1.353538
C	0.377188	-3.691009	-0.105446
H	0.385496	-4.629590	0.446325
C	-0.248351	-2.581302	0.461993
C	0.243147	-0.051539	-2.364545
H	0.937578	-0.102843	-3.208810
H	0.489863	0.835949	-1.775586
H	-0.763394	0.098163	-2.776870
C	1.732872	-4.818356	-1.908066
H	1.349193	-5.758957	-1.500462
H	2.799867	-4.762003	-1.654740
H	1.661052	-4.862408	-2.999763
C	-0.898500	-2.739357	1.812704
H	-1.055601	-3.797858	2.041665
H	-1.870774	-2.238313	1.862467
H	-0.275669	-2.313442	2.606522

$Int1_{B2Cl2Mes2}$

E(scf) = –2246.36061817 a.u.

Cl	-0.649286	0.849334	-2.431464
C	1.035746	0.636278	-0.255041
B	-0.504337	0.863366	-0.638690
Cl	0.809680	-3.036369	1.615872
C	1.450485	-0.608766	0.237646
B	0.404119	-1.676862	0.484756
C	1.213620	3.035077	-0.804868
H	5.694642	-1.101020	-0.342802
C	4.733006	-2.386432	1.085532
C	3.502297	-2.771426	1.600599
H	3.467909	-3.499970	2.410084
C	2.300259	-2.237929	1.126408
C	3.680865	0.117311	-1.564907
H	4.677273	0.570887	-1.564448
H	2.949565	0.927455	-1.474281
H	3.523165	-0.343495	-2.546572
C	6.019539	-2.962305	1.607433
H	5.853364	-3.568541	2.503462
H	6.735476	-2.172383	1.862773
H	6.501282	-3.602074	0.857248
C	1.027307	-2.729691	1.761597
H	1.098206	-2.687782	2.854130
H	0.841716	-3.779194	1.491644
H	0.156098	-2.139661	1.466086
C	0.424814	2.146678	-0.360267
C	-0.411178	2.682571	-1.370947
C	-0.156869	3.945598	-1.908386
H	-0.824007	4.330374	-2.678812
C	0.929681	4.716718	-1.510334
C	1.786900	4.164609	-0.565418
H	2.672493	4.723069	-0.264209
C	1.563654	2.910774	0.008117
C	-1.585573	1.934053	-1.944297
H	-1.956882	2.437419	-2.843248
H	-2.422868	1.866666	-1.239273
H	-1.303022	0.916520	-2.222372
C	1.169964	6.086295	-2.080261
H	2.239338	6.317761	-2.129899
H	0.698943	6.861351	-1.461467
H	0.755475	6.179740	-3.089699
C	2.603550	2.435864	0.994500
H	3.554500	2.946543	0.808329
H	2.785885	1.359820	0.942236
H	2.302636	2.649547	2.025509

3

E(scf) = –2246.39794757 a.u.

Cl	-1.832435	0.346930	2.643346
C	-0.019227	-0.288624	0.672509
B	-1.556563	0.169041	0.786442
Cl	1.709106	3.115595	-1.263975
C	0.411340	0.915780	0.088540
B	1.677160	1.467931	-0.498796
C	1.982536	-1.527931	1.435091

H	1.555557	3.748352	-0.036815	H	2.094978	-1.495511	2.530777
H	0.124144	2.989390	-0.718487	H	2.523558	-0.685572	1.016716
N	1.799981	1.734576	-0.492572	N	0.562613	-1.380964	1.143710
C	1.631106	3.541481	-2.182544	C	2.522856	-2.849295	0.904929
H	1.200477	4.537822	-2.340537	H	3.585508	-2.925974	1.161496
H	1.206664	2.870754	-2.942393	H	2.460184	-2.843735	-0.191085
C	3.151718	3.576000	-2.309236	C	1.725195	-4.017232	1.478232
H	3.445964	3.852661	-3.328498	H	2.069362	-4.969375	1.057988
H	3.556118	4.350277	-1.640327	H	1.893636	-4.069683	2.563905
C	3.738545	2.223245	-1.917624	C	0.234815	-3.823256	1.208197
H	4.835138	2.256945	-1.918411	H	-0.357541	-4.603547	1.700472
H	3.436429	1.457895	-2.645010	H	0.042875	-3.912798	0.131082
C	3.259750	1.793604	-0.534620	C	-0.254236	-2.461648	1.696852
H	3.638646	0.812005	-0.259126	H	-1.294875	-2.292784	1.413886
H	3.594238	2.525852	0.218551	H	-0.195551	-2.412184	2.794180
C	3.180355	-0.565865	1.974356	C	-0.851430	2.818830	1.022773
H	2.799135	-1.362339	2.637029	H	-0.110276	3.487650	0.574206
H	2.691900	0.367708	2.278805	H	-0.469311	2.480938	1.986828
N	2.832840	-0.815226	0.582028	N	-0.929020	1.615533	0.141061
C	4.691768	-0.440299	2.147010	C	-2.178295	3.541552	1.171137
H	4.926529	-0.321645	3.212128	H	-2.009148	4.432216	1.788168
H	5.041974	0.467705	1.636660	H	-2.878010	2.906354	1.724324
C	5.409397	-1.654216	1.564260	C	-2.755510	3.920678	-0.187957
H	5.134304	-2.549505	2.140966	H	-2.106482	4.670452	-0.662659
H	6.496856	-1.540206	1.651733	H	-3.744364	4.379358	-0.073510
C	4.998549	-1.848622	0.108075	C	-2.837462	2.684999	-1.076353
H	5.340062	-0.992553	-0.491216	H	-3.577096	1.979702	-0.683283
H	5.469882	-2.746582	-0.310435	H	-3.163902	2.950813	-2.088888
C	3.482416	-1.979976	-0.000900	C	-1.488307	1.993504	-1.189404
H	3.177292	-2.033304	-1.051936	H	-1.573896	1.082016	-1.781395
H	3.172992	-2.923097	0.475581	H	-0.765227	2.653156	-1.676060
C	-1.016550	-1.865271	-0.168792	C	3.077051	0.755553	-0.561847
C	-2.197708	-1.820657	0.600852	C	4.072224	1.098121	0.377205
C	-3.409498	-2.218675	0.042928	C	5.307216	0.455000	0.341498
H	-4.314978	-2.154721	0.645129	H	6.061517	0.714431	1.083208
C	-3.489200	-2.698729	-1.257596	C	5.602397	-0.510831	-0.622599
C	-2.315160	-2.762825	-2.015707	C	4.620148	-0.823505	-1.559618
H	-2.357212	-3.139488	-3.031651	H	4.832599	-1.570589	-2.323333
C	-1.087508	-2.367737	-1.492377	C	3.367430	-0.207318	-1.543579
C	-2.190346	-1.354062	2.030202	C	3.790928	2.132488	1.434153
H	-2.936763	-0.566985	2.187276	H	4.595570	2.178349	2.174350
H	-1.215578	-0.948781	2.328366	H	2.853781	1.918681	1.964038
H	-2.425301	-2.180761	2.707021	H	3.682829	3.128701	0.989066
C	-4.799463	-3.155004	-1.843894	C	6.953389	-1.168648	-0.665431
H	-4.917410	-2.771686	-2.897287	H	6.910643	-2.141650	-1.165470
H	-5.664261	-2.793153	-1.221419	H	7.357701	-1.320730	0.341064
H	-4.840057	-4.276686	-1.881313	H	7.675068	-0.550053	-1.214189

C	0.155915	-2.535606	-2.318047
H	-0.090666	-2.832602	-3.344814
H	0.803980	-3.314071	-1.891368
H	0.742653	-1.616039	-2.360764
C	-1.662055	1.372882	0.276402
C	-1.379346	1.865315	1.586292
C	-2.403126	2.382106	2.380305
H	-2.157743	2.754540	3.372898
C	-3.726853	2.415701	1.957660
C	-4.011956	1.897723	0.697478
H	-5.045297	1.884701	0.355772
C	-3.025583	1.392186	-0.146304
C	-0.012367	1.854395	2.221455
H	-0.075651	2.216424	3.251447
H	0.704506	2.491463	1.695871
H	0.413978	0.847923	2.243203
C	-4.808237	2.994858	2.822222
H	-5.757797	2.467963	2.682638
H	-4.981950	4.049166	2.571218
H	-4.542516	2.950312	3.883038
C	-3.512878	0.861141	-1.468520
H	-4.595319	0.705192	-1.426526
H	-3.047991	-0.088826	-1.733224
H	-3.307509	1.565506	-2.281669
C	2.331923	-0.613113	-2.557874
H	2.795437	-1.060505	-3.443036
H	1.728932	0.239559	-2.888507
H	1.640256	-1.354306	-2.139058
C	-2.764507	-0.540737	-0.026576
C	-2.490280	-1.373573	-1.147752
C	-3.519059	-2.033019	-1.825167
H	-3.264840	-2.658968	-2.679160
C	-4.851166	-1.911566	-1.453262
C	-5.130296	-1.073125	-0.381639
H	-6.167685	-0.931398	-0.081932
C	-4.134860	-0.396691	0.328046
C	-1.107726	-1.609856	-1.705231
H	-1.171084	-2.119041	-2.671810
H	-0.498714	-2.236681	-1.047850
H	-0.543417	-0.687101	-1.855940
C	-5.940665	-2.656345	-2.170568
H	-6.874184	-2.083940	-2.185898
H	-6.154542	-3.612583	-1.675888
H	-5.660662	-2.879889	-3.205224
C	-4.644120	0.473978	1.450861
H	-5.710639	0.677146	1.309066
H	-4.128684	1.433108	1.512599
H	-4.519649	-0.008819	2.424832

$B_2Cl_2Dur_2$-PipCCPip

E(scf) = –2324.81066344 a.u.

Cl	-1.127097	-3.276339	1.630987
C	3.966516	-0.084426	-0.418465
B	-1.596565	-1.964380	0.541059
B	-0.482357	-0.870544	-0.111300
Cl	0.561036	-1.345359	-1.455971
C	3.520530	1.032276	-0.621400
C	3.887906	-2.200812	0.706971
H	2.806372	-2.089147	0.598665
H	4.152096	-1.919793	1.744143
N	4.523363	-1.293173	-0.243470
C	4.310232	-3.640038	0.442052
H	3.916079	-3.946848	-0.535635
H	3.858730	-4.294622	1.197417
C	5.830969	-3.770017	0.444903
H	6.212946	-3.545093	1.452049
H	6.132255	-4.798697	0.213894
C	6.442137	-2.792172	-0.555550
H	7.537845	-2.832950	-0.523110

$TS1_{B2Cl2Dur2}$

E(scf) = –2324.80828264 a.u. υ_{min} = –167.7 cm^{-1}

Cl	0.342938	0.657655	2.244553
C	-1.622639	-0.558760	0.556136
B	0.097765	0.661152	0.383821
B	1.174210	-0.377289	-0.429773
Cl	0.835382	-0.850742	-2.155121
C	-1.096231	-1.732631	0.193660
C	-2.888032	1.098089	1.821834
H	-2.236503	1.780533	1.275861
H	-2.602771	1.144725	2.882435
N	-2.639229	-0.257515	1.338381
C	-4.358375	1.460961	1.647287
H	-4.587155	1.524692	0.574748
H	-4.529110	2.457421	2.070453
C	-5.267097	0.426508	2.307055
H	-5.112594	0.449041	3.395604
H	-6.321453	0.669206	2.131774
C	-4.947880	-0.972796	1.784828
H	-5.544389	-1.732248	2.304388

H	6.132557	-3.066602	-1.572608	H	-5.197366	-1.035872	0.716533
C	5.981342	-1.368266	-0.270615	C	-3.467347	-1.287870	1.962683
H	6.400477	-1.028960	0.695120	H	-3.213469	-1.329379	3.033203
H	6.333642	-0.677734	-1.041599	H	-3.206876	-2.252521	1.519515
C	2.772960	3.193846	0.079362	C	-0.419626	-3.765689	-0.915153
H	3.648094	3.171039	0.735637	H	0.269294	-3.780468	-0.070209
H	1.891258	2.914368	0.679631	H	0.169317	-3.632952	-1.832624
N	2.992262	2.212557	-0.982169	N	-1.279654	-2.588901	-0.761372
C	2.561602	4.584957	-0.503373	C	-1.259441	-5.034655	-0.996269
H	2.351267	5.287504	0.312565	H	-0.595242	-5.892418	-1.151976
H	3.487644	4.915273	-0.992753	H	-1.767326	-5.188421	-0.034445
C	1.421188	4.574258	-1.518523	C	-2.290857	-4.933418	-2.117292
H	0.485168	4.314205	-1.002281	H	-1.771155	-4.882460	-3.084778
H	1.283473	5.569775	-1.957668	H	-2.922838	-5.828271	-2.142953
C	1.701685	3.538055	-2.602951	C	-3.146411	-3.681203	-1.938907
H	2.595256	3.830800	-3.170362	H	-3.751714	-3.772644	-1.026196
H	0.866801	3.479533	-3.312686	H	-3.842888	-3.558068	-2.776582
C	1.928228	2.164289	-1.987488	C	-2.275871	-2.434228	-1.830818
H	0.992558	1.805729	-1.527411	H	-1.730537	-2.257115	-2.768224
H	2.223728	1.432998	-2.744451	H	-2.867644	-1.544223	-1.609046
C	-3.086219	-1.674805	0.170372	C	-0.204503	2.113806	-0.240179
C	-3.604517	-2.171726	-1.036605	C	-1.286202	2.379158	-1.114246
C	-4.876687	-1.763968	-1.463086	C	-1.610244	3.700264	-1.464962
C	-5.584935	-0.854878	-0.679369	C	-0.811016	4.738936	-1.001028
H	-6.567534	-0.527326	-1.016141	H	-1.067610	5.763867	-1.266206
C	-5.084745	-0.349429	0.520183	C	0.328068	4.502436	-0.240496
C	-3.819882	-0.768923	0.957675	C	0.645439	3.185012	0.132103
C	-2.800631	-3.125516	-1.879365	C	-2.114034	1.273057	-1.715311
H	-2.627489	-2.728362	-2.887629	H	-2.458700	1.545654	-2.718004
H	-3.316230	-4.086721	-1.999517	H	-3.010832	1.043290	-1.122013
H	-1.817993	-3.340149	-1.444855	H	-1.531092	0.358700	-1.814679
C	-5.460535	-2.283329	-2.746316	C	-2.801428	4.015976	-2.330266
H	-6.455358	-1.865518	-2.927091	H	-2.977050	5.095629	-2.368605
H	-5.553763	-3.376699	-2.734457	H	-3.718159	3.542623	-1.957361
H	-4.830133	-2.031351	-3.608648	H	-2.663790	3.670619	-3.363619
C	-3.260664	-0.225467	2.245894	C	1.925659	2.978465	0.902941
H	-3.058347	0.850966	2.174479	H	2.730112	3.583394	0.468301
H	-2.320659	-0.708573	2.528537	H	2.264671	1.942577	0.903531
H	-3.960824	-0.374133	3.077044	H	1.822529	3.280632	1.952584
C	-5.883231	0.639957	1.321271	C	1.194933	5.659840	0.174556
H	-6.135168	0.248861	2.315277	H	1.379582	5.665228	1.255437
H	-6.819852	0.894761	0.816452	H	0.727564	6.613040	-0.091929
H	-5.322929	1.569734	1.483030	H	2.178583	5.627721	-0.312314
C	-0.543239	0.594517	0.427197	C	2.652162	-0.688502	0.018063
C	0.153781	0.906177	1.607005	C	2.977513	-1.626911	1.015241
C	-0.018296	2.164262	2.200960	C	4.323633	-1.863138	1.340871
C	-0.901795	3.066877	1.608873	C	5.315403	-1.144294	0.683343

H	-1.045426	4.040739	2.074875
C	-1.597323	2.776600	0.436117
C	-1.409862	1.525595	-0.172832
C	1.122568	-0.088550	2.183330
H	2.143738	0.131738	1.842577
H	0.896347	-1.112816	1.860525
H	1.121898	-0.089304	3.278118
C	0.739835	2.546720	3.441336
H	0.529184	3.581192	3.728678
H	1.822552	2.453066	3.292074
H	0.479050	1.905328	4.292762
C	-2.152330	1.202274	-1.441827
H	-3.235016	1.144735	-1.271567
H	-1.844075	0.245509	-1.871702
H	-1.980276	1.970699	-2.205763
C	-2.532571	3.788565	-0.163668
H	-3.542347	3.378449	-0.290919
H	-2.196015	4.110663	-1.157754
H	-2.607403	4.680118	0.466067
H	6.358285	-1.331141	0.936938
C	5.018743	-0.181018	-0.277638
C	3.677691	0.054343	-0.612305
C	1.921997	-2.404094	1.751193
H	0.910512	-2.112396	1.457580
H	1.998834	-2.242936	2.833399
H	2.034287	-3.485756	1.585369
C	4.696728	-2.873437	2.389677
H	5.783209	-2.941272	2.502194
H	4.323032	-3.875709	2.142997
H	4.275112	-2.614987	3.369505
C	3.368609	1.125235	-1.630453
H	4.001078	2.006097	-1.474754
H	2.332637	1.471397	-1.586715
H	3.549164	0.772088	-2.654054
C	6.132597	0.585968	-0.936297
H	6.108926	1.650286	-0.667260
H	6.071777	0.535554	-2.030187
H	7.108982	0.192882	-0.636358

$Int1_{B2Cl2Dur2}$

E(scf) = –2324.89912387 a.u.

Cl	0.615582	0.330153	2.663953
C	-1.140204	0.378068	0.573243
B	0.411189	0.619644	0.896520
B	-0.496575	-1.711920	-0.649598
Cl	-0.954228	-2.874331	-1.959331
C	-1.556261	-0.770425	-0.109758
C	-1.386056	2.608353	1.577219
H	-0.374128	2.742618	1.185091
H	-1.305280	2.556071	2.674698
N	-1.947160	1.358550	1.070586
C	-2.250911	3.802806	1.184052
H	-2.246061	3.904979	0.091070
H	-1.801915	4.713799	1.597702
C	-3.684671	3.625843	1.671213
H	-3.698320	3.637618	2.770884
H	-4.313311	4.459231	1.335923
C	-4.230949	2.291626	1.175112
H	-5.230582	2.099076	1.583503
H	-4.325977	2.312984	0.081161
C	-3.308794	1.142860	1.561853
H	-3.251589	1.064938	2.660582
H	-3.665213	0.200436	1.153329
C	-3.536935	-2.233703	-0.020153
H	-3.165427	-2.494460	0.978095
H	-3.233779	-3.045868	-0.701124

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E(scf) = –2324.93432008 a.u.

Cl	1.936261	0.834904	-2.509787
C	0.067044	-0.102386	-0.719063
B	1.578805	0.437702	-0.697372
B	-1.759326	1.434980	0.568223
Cl	-1.905710	2.982469	1.506889
C	-0.449835	1.010015	-0.025952
C	0.480402	-2.143597	-1.943633
H	1.507423	-1.896778	-1.674292
H	0.383147	-2.034332	-3.033857
N	-0.420377	-1.179593	-1.309980
C	0.137217	-3.571544	-1.526768
H	0.377504	-3.698550	-0.464046
H	0.782417	-4.262066	-2.082588
C	-1.336868	-3.892480	-1.763487
H	-1.535329	-3.908556	-2.845239
H	-1.577053	-4.892122	-1.382941
C	-2.222909	-2.833914	-1.112375
H	-3.281698	-3.000007	-1.341124
H	-2.122285	-2.869379	-0.019495
C	-1.824713	-1.444384	-1.592251
H	-1.957362	-1.378076	-2.683798
H	-2.436897	-0.675549	-1.133214
C	1.340901	1.989503	1.468028
H	1.436162	1.011572	1.941909
H	0.569635	2.554811	1.997897

N	-2.955769	-0.949279	-0.384741	N	0.859132	1.763933	0.074134
C	-5.059670	-2.147950	-0.011919	C	2.662855	2.739694	1.503559
H	-5.477227	-3.131769	0.235452	H	2.938707	2.887227	2.554547
H	-5.386417	-1.449769	0.771781	H	3.445336	2.117442	1.056761
C	-5.569483	-1.666965	-1.366685	C	2.561314	4.075557	0.775204
H	-5.304900	-2.408679	-2.134570	H	1.860597	4.730609	1.312462
H	-6.663167	-1.583603	-1.366301	H	3.532330	4.583860	0.767156
C	-4.926732	-0.327804	-1.716370	C	2.057768	3.857645	-0.647342
H	-5.264039	0.432133	-0.998054	H	2.811400	3.339938	-1.249025
H	-5.236615	0.007392	-2.714045	H	1.866199	4.815885	-1.145069
C	-3.404621	-0.424228	-1.666072	C	0.764825	3.062615	-0.657001
H	-3.048048	-1.046792	-2.505962	H	-0.027787	3.638130	-0.169208
H	-2.963713	0.572054	-1.793693	H	0.444951	2.829994	-1.673625
C	1.513168	1.373887	0.074568	C	2.771963	-0.369996	0.060965
C	1.134121	2.185796	-1.034129	C	2.463194	-1.410083	0.982149
C	2.061926	3.067647	-1.616793	C	3.455337	-2.307949	1.418180
C	3.364428	3.090435	-1.138472	C	4.758957	-2.149289	0.971087
H	4.078434	3.777936	-1.590003	H	5.520943	-2.858112	1.292635
C	3.797754	2.244117	-0.122161	C	5.123507	-1.086204	0.155645
C	2.878835	1.376246	0.484777	C	4.138787	-0.183679	-0.282659
C	-0.234381	2.165177	-1.663665	C	1.103257	-1.615962	1.603727
H	-0.146093	2.223934	-2.753229	H	1.194366	-1.646116	2.697185
H	-0.841916	3.024986	-1.353163	H	0.650119	-2.570944	1.309958
H	-0.792357	1.259558	-1.440813	H	0.387407	-0.834237	1.368613
C	1.680269	3.978343	-2.752093	C	3.132666	-3.436696	2.359184
H	2.490479	4.679132	-2.974678	H	4.010197	-4.069969	2.520650
H	0.782922	4.565900	-2.525246	H	2.326622	-4.075816	1.977072
H	1.468817	3.418971	-3.672784	H	2.803627	-3.072522	3.341402
C	3.425814	0.444444	1.531951	C	4.641232	0.983949	-1.092716
H	4.439621	0.132717	1.266215	H	5.555771	1.388512	-0.643251
H	2.834642	-0.461536	1.634940	H	3.922001	1.794897	-1.153178
H	3.477474	0.927972	2.515797	H	4.884461	0.697368	-2.123131
C	5.241523	2.289820	0.301371	C	6.566464	-0.929937	-0.242478
H	5.347445	2.406272	1.385881	H	6.685207	-0.828590	-1.327764
H	5.759405	3.126039	-0.178120	H	7.152890	-1.796222	0.078748
H	5.775999	1.371135	0.026236	H	7.023068	-0.039373	0.209336
C	1.007558	-1.890720	-0.209002	C	-3.116374	0.643438	0.497667
C	1.290140	-2.627856	0.963336	C	-3.373077	-0.412599	1.389126
C	2.604508	-3.054366	1.220229	C	-4.573857	-1.132437	1.287031
C	3.609830	-2.714553	0.320237	C	-5.499611	-0.761079	0.314822
H	4.630182	-3.034507	0.528528	H	-6.432366	-1.318405	0.238165
C	3.364391	-1.959546	-0.825752	C	-5.279741	0.303191	-0.558253
C	2.050330	-1.567659	-1.105887	C	-4.072450	1.011064	-0.468497
C	0.204115	-3.024905	1.924764	C	-2.376614	-0.789176	2.452360
H	0.036624	-4.110024	1.900910	H	-2.834554	-0.781538	3.449154
H	-0.743313	-2.532906	1.695015	H	-1.527641	-0.100436	2.476792
H	0.469712	-2.760864	2.954902	H	-1.975291	-1.799794	2.296046

C	2.930067	-3.853855	2.450489
H	3.986039	-4.140140	2.466558
H	2.332288	-4.771733	2.509478
H	2.724961	-3.284297	3.366167
C	1.774380	-0.801585	-2.368555
H	2.386130	0.107433	-2.420489
H	0.727400	-0.496816	-2.444025
H	2.006111	-1.406590	-3.254437
C	4.496821	-1.561243	-1.729135
H	4.603881	-0.468492	-1.765540
H	4.336854	-1.896581	-2.761198
H	5.446532	-1.980989	-1.383415

C	-4.860061	-2.287894	2.204396
H	-5.823537	-2.750312	1.969997
H	-4.887149	-1.974484	3.255815
H	-4.088339	-3.064909	2.128307
C	-3.801247	2.143610	-1.422962
H	-4.020995	1.860106	-2.459296
H	-2.755630	2.464621	-1.387018
H	-4.421559	3.019258	-1.191323
C	-6.318963	0.672876	-1.579412
H	-5.948459	0.538062	-2.604048
H	-6.616471	1.724812	-1.489208
H	-7.218362	0.059727	-1.468608

$Mes_2B_2F_2$-PipCCPip

E(scf) = –1525.72806228 a.u.

F	0.909060	1.410908	2.096961
C	0.332784	-2.018764	0.533345
B	1.354414	-0.885728	0.805581
F	1.974237	-0.162774	3.292820
C	0.463900	-2.941699	-0.545301
B	1.359442	0.155262	2.148547
N	-1.983674	3.532059	0.834689
C	-0.448612	-3.981045	-0.690675
H	-0.336004	-4.677102	-1.519191
N	-2.711763	-0.178703	-0.084570
C	1.556735	-2.846841	-1.581748
H	2.551950	-2.970498	-1.144731
H	1.558996	-1.875216	-2.078816
H	1.424951	-3.621752	-2.343161
C	-1.666985	-3.234823	1.227617
H	-2.508110	-3.343227	1.910072
C	-2.466110	-5.306058	0.042880
H	-2.069425	-6.212444	0.601820
H	-2.579104	-5.589383	-1.040405
H	-3.483601	-5.053071	0.469531
C	-1.518379	-4.150303	0.191410
C	-0.774668	-2.178138	1.411470
C	-1.049632	-1.236827	2.554759
H	-1.131916	-0.200821	2.205196
H	-0.266439	-1.292854	3.319846
H	-1.994892	-1.489002	3.040145
C	2.627542	-0.512832	-0.044761
C	3.870066	-1.087926	0.273447
C	3.952311	-2.135653	1.347564
H	3.305852	-2.994599	1.123343

$TS1_{Mes2B2F2}$

E(scf) = –1525.72710419 a.u. υ_{min} = –124.9 cm^{-1}

F	-0.480065	1.065557	2.851171
C	-1.770622	-1.472495	0.418347
B	-0.322378	-0.883496	0.769221
F	1.436158	-0.169300	2.684263
C	-1.976843	-2.503026	-0.551844
B	0.307056	0.285044	1.978151
N	1.908919	1.969100	0.476527
C	-3.265841	-2.828168	-0.984244
H	-3.381060	-3.601839	-1.742569
N	-1.434128	2.007460	-0.052421
C	-0.886570	-3.375645	-1.129614
H	-0.164878	-3.684767	-0.371990
H	-0.313647	-2.891232	-1.924928
H	-1.334881	-4.279394	-1.555973
C	-4.222088	-1.318070	0.570973
H	-5.096979	-0.885303	1.055271
C	-5.778170	-2.604926	-0.944395
H	-6.155721	-3.480018	-0.399694
H	-5.775052	-2.862939	-2.008838
H	-6.496330	-1.792502	-0.790849
C	-4.405647	-2.224522	-0.466622
C	-2.952928	-0.960506	1.029975
C	-2.926090	-0.045158	2.221777
H	-2.564361	0.956968	1.985360
H	-2.251883	-0.415509	2.994987
H	-3.930233	0.046405	2.649288
C	0.991475	-1.472844	0.055178
C	1.817343	-2.319375	0.827997
C	1.325957	-2.891782	2.132796
H	1.079553	-3.954680	2.006124

H	3.622014	-1.740668	2.319144	H	0.426737	-2.384340	2.491146
H	4.973506	-2.514030	1.471575	H	2.083545	-2.815091	2.918947
C	5.015066	-0.688974	-0.418272	C	3.063925	-2.732234	0.357121
H	5.972007	-1.151678	-0.169968	H	3.677575	-3.377636	0.985713
C	4.963859	0.289276	-1.414190	C	3.533616	-2.357711	-0.899426
C	6.215353	0.734136	-2.118858	C	4.901857	-2.758076	-1.376841
H	5.986904	1.230939	-3.067241	H	4.929800	-2.874991	-2.465801
H	6.878425	-0.111789	-2.331052	H	5.224174	-3.702819	-0.926256
H	6.784216	1.444296	-1.504922	H	5.652963	-2.001149	-1.112543
C	3.727703	0.859140	-1.709396	C	2.681632	-1.599238	-1.700370
H	3.665025	1.624455	-2.482349	H	2.992026	-1.357005	-2.717696
C	2.563899	0.476329	-1.040088	C	1.429872	-1.164758	-1.254090
C	1.239787	1.083514	-1.430604	C	0.556467	-0.457268	-2.264180
H	1.358423	2.097196	-1.828866	H	0.760531	-0.841257	-3.271227
H	0.534579	1.133053	-0.591990	H	0.723188	0.626833	-2.293832
H	0.754458	0.485922	-2.214763	H	-0.504434	-0.605523	-2.049339
C	-2.390870	1.096591	0.183252	C	-0.364482	1.287485	-0.009863
C	-4.045138	-0.634048	0.301576	C	-1.615927	3.280593	0.665283
H	-4.279511	-0.200551	1.277631	H	-0.750414	3.427705	1.313035
H	-4.000614	-1.726967	0.417830	H	-2.500651	3.173106	1.305975
C	-5.092175	-0.262187	-0.747722	C	-1.818874	4.411715	-0.335695
H	-5.165776	0.838087	-0.790067	H	-0.894452	4.545077	-0.914824
H	-6.076323	-0.642677	-0.457269	H	-1.996092	5.347204	0.207386
C	-4.685016	-0.801294	-2.118070	C	-2.981973	4.098028	-1.277257
H	-4.720123	-1.901360	-2.095319	H	-3.918624	4.091748	-0.701592
H	-5.397253	-0.481419	-2.885661	H	-3.082024	4.884026	-2.034230
C	-3.264742	-0.357734	-2.486073	C	-2.793602	2.735069	-1.942846
H	-3.238373	0.732907	-2.616261	H	-1.925023	2.761933	-2.615133
H	-2.948632	-0.809956	-3.434716	H	-3.665659	2.475636	-2.553592
C	-2.290198	-0.733027	-1.370727	C	-2.572305	1.642516	-0.902494
H	-2.239402	-1.824146	-1.263719	H	-3.454626	1.530312	-0.260547
H	-1.281489	-0.378086	-1.581122	H	-2.357870	0.669769	-1.345155
C	-2.116380	2.225884	0.562403	C	0.765498	1.409162	0.777870
C	-2.334136	4.472698	-0.229098	C	2.141118	2.741012	-0.745846
H	-2.637421	5.413820	0.244264	H	2.425034	3.761055	-0.448777
H	-3.199292	4.066932	-0.764009	H	1.199580	2.801437	-1.299680
C	-1.150946	4.718189	-1.162367	C	3.248036	2.109038	-1.585678
H	-0.899049	3.771853	-1.664019	H	2.898370	1.138990	-1.954535
H	-1.426175	5.439726	-1.942159	H	3.441703	2.747870	-2.455874
C	0.055844	5.214101	-0.363857	C	4.517278	1.899723	-0.762171
H	-0.173431	6.208591	0.053489	H	4.947549	2.875957	-0.492245
H	0.925829	5.340500	-1.014849	H	5.268724	1.377597	-1.365475
C	0.386044	4.256294	0.786327	C	4.206761	1.109650	0.506589
H	1.190184	4.661540	1.413173	H	5.098492	1.019833	1.137980
H	0.745787	3.302144	0.385418	H	3.878774	0.094078	0.253773
C	-0.848744	3.985072	1.638540	C	3.103419	1.787638	1.308352
H	-0.642635	3.229745	2.398195	H	2.814813	1.201757	2.178335

H	-1.157968	4.908912	2.149760	H	3.426232	2.787755	1.632673

$Int1_{Mes2B2F2}$

E(scf) = –1525.82199883 a.u.

F	-1.508147	-2.005115	-1.561444	F	0.592809	-3.300345	1.946870
C	1.762229	0.924834	-0.445413	C	-1.745909	1.137735	-0.297741
B	0.548050	0.092084	0.137020	B	-0.246561	0.700245	0.015991
F	-1.847982	-2.658471	0.575514	F	0.511468	-3.914147	-0.263485
C	3.082834	0.739467	0.024349	C	-2.532622	1.794058	0.681243
B	-1.473852	-1.663627	-0.255285	B	0.489940	-2.871459	0.642202
N	-3.086720	0.248020	-0.149769	N	2.579436	-1.334760	-0.005742
C	4.140051	1.436880	-0.560605	C	-3.849146	2.150825	0.402802
H	5.147414	1.287792	-0.173686	H	-4.437007	2.642152	1.177386
N	-1.050147	1.974403	1.095833	N	-0.848498	-1.895531	0.428730
C	3.402604	-0.204001	1.155647	C	-1.982643	2.093638	2.050647
H	3.356072	-1.250220	0.831416	H	-1.025250	2.620878	1.992206
H	2.702470	-0.100139	1.990552	H	-1.809752	1.174490	2.624645
H	4.409317	-0.018049	1.543453	H	-2.677691	2.710628	2.628496
C	2.647629	2.484424	-2.096883	C	-3.654608	1.287822	-1.808966
H	2.470913	3.157571	-2.934734	H	-4.079259	1.097788	-2.794360
C	5.099357	3.063552	-2.233095	C	-5.861504	2.297159	-1.108054
H	5.262653	4.017728	-1.715304	H	-6.555721	1.729287	-0.476361
H	4.918304	3.293447	-3.288277	H	-6.138217	2.117490	-2.151585
H	6.031818	2.493435	-2.164225	H	-6.028680	3.359233	-0.893528
C	3.947783	2.310459	-1.628488	C	-4.435756	1.904201	-0.839882
C	1.562316	1.823763	-1.521102	C	-2.332235	0.904197	-1.560103
C	0.189708	2.090790	-2.080416	C	-1.569966	0.291760	-2.710155
H	-0.334101	1.163996	-2.338382	H	-0.617993	-0.140397	-2.390859
H	0.246943	2.710055	-2.981004	H	-1.355779	1.047060	-3.476273
H	-0.443593	2.611482	-1.351808	H	-2.153444	-0.499424	-3.195311
C	0.727494	-1.502723	0.174935	C	0.842720	1.827051	0.299151
C	1.262057	-2.197311	-0.949636	C	1.104585	2.858678	-0.636004
C	1.343035	-1.546614	-2.300744	C	0.419627	2.901197	-1.975889
H	1.428742	-2.298770	-3.091028	H	0.762894	3.757536	-2.564553
H	2.213130	-0.883407	-2.361824	H	-0.667375	2.972944	-1.872103
H	0.455600	-0.942874	-2.505281	H	0.628841	1.996884	-2.559064
C	1.716406	-3.505511	-0.823184	C	2.052251	3.843235	-0.360037
H	2.096510	-4.021232	-1.703377	H	2.240144	4.616880	-1.103445
C	1.704028	-4.170256	0.402330	C	2.756994	3.871823	0.840950
C	2.173409	-5.591461	0.513539	C	3.785901	4.932803	1.112820
H	2.960126	-5.813135	-0.214771	H	3.498360	5.892533	0.670348
H	1.345516	-6.286065	0.321585	H	4.759033	4.657726	0.685494
H	2.557600	-5.810647	1.514886	H	3.932585	5.083798	2.187154
C	1.216378	-3.487506	1.514947	C	2.487861	2.870211	1.768245
H	1.209032	-3.988963	2.481014	H	3.015153	2.877677	2.721350
C	0.733191	-2.185959	1.426623	C	1.565523	1.851121	1.518546
C	0.202399	-1.558052	2.685225	C	1.392846	0.811648	2.598440

$Int2_{Mes2B2F2}$

E(scf) = –1525.85652206 a.u.

H	0.491763	-2.144077	3.563094
H	-0.890860	-1.509898	2.655567
H	0.560754	-0.534229	2.820749
C	-0.783036	0.680947	0.607007
C	-2.099378	2.078983	2.112842
H	-2.930632	1.422319	1.846695
H	-2.476897	3.112528	2.093864
C	-1.590809	1.750161	3.516962
H	-1.307093	0.691142	3.549450
H	-2.404401	1.885191	4.241493
C	-0.391963	2.622670	3.884672
H	-0.727209	3.665569	3.991812
H	0.020548	2.324380	4.856264
C	0.676442	2.558171	2.794936
H	1.131024	1.559023	2.768775
H	1.488700	3.267219	2.997981
C	0.060989	2.857378	1.428885
H	-0.337630	3.883015	1.433554
H	0.816462	2.811398	0.645573
C	-1.791762	-0.148271	0.121862
C	-4.136234	-0.721663	-0.440458
H	-5.045227	-0.379198	0.078767
H	-3.870509	-1.685478	-0.000806
C	-4.428694	-0.846753	-1.935869
H	-3.555672	-1.289874	-2.426597
H	-5.271857	-1.533002	-2.084115
C	-4.729833	0.522265	-2.541502
H	-5.683575	0.898207	-2.140656
H	-4.854343	0.443270	-3.628061
C	-3.619813	1.511880	-2.194226
H	-3.859979	2.516599	-2.564739
H	-2.681871	1.204086	-2.674526
C	-3.401267	1.569471	-0.683434
H	-2.595655	2.257927	-0.422556
H	-4.323376	1.924819	-0.196790

H	1.773571	1.186331	3.554123
H	1.942472	-0.105512	2.359733
H	0.348831	0.526433	2.742498
C	0.127416	-0.766471	0.131625
C	-1.715988	-2.300464	-0.704791
H	-1.064002	-2.463907	-1.565214
H	-2.386162	-1.463729	-0.925224
C	-2.524655	-3.548074	-0.379443
H	-1.839098	-4.390004	-0.233799
H	-3.153930	-3.785890	-1.245640
C	-3.373522	-3.333119	0.869053
H	-4.125630	-2.555183	0.671689
H	-3.918555	-4.248008	1.128772
C	-2.479387	-2.894941	2.023834
H	-1.791309	-3.702604	2.297296
H	-3.073506	-2.656815	2.914294
C	-1.662832	-1.667080	1.648147
H	-2.318937	-0.810422	1.451933
H	-0.968111	-1.402486	2.447978
C	1.286227	-1.537964	0.226886
C	3.123547	-0.231104	-0.788053
H	4.026211	0.140984	-0.284379
H	2.405836	0.585163	-0.804884
C	3.454819	-0.717872	-2.198736
H	2.514003	-0.989476	-2.697237
H	3.897793	0.106832	-2.770156
C	4.390098	-1.925719	-2.168906
H	5.370719	-1.611502	-1.781352
H	4.559746	-2.303877	-3.183880
C	3.827580	-3.027547	-1.272095
H	4.541844	-3.853859	-1.173020
H	2.904968	-3.441531	-1.699437
C	3.493984	-2.468931	0.107620
H	3.035193	-3.221796	0.751371
H	4.408034	-2.115023	0.605642

$TS2_{Mes2B2F2}$

E(scf) = –2103.92131217 a.u. υ_{min} = –181.7 cm^{-1}

F	3.386611	0.587577	2.294463
C	-1.067105	1.404472	-1.116613
N	0.297204	-1.948289	-1.496682
B	-0.874115	0.021366	-0.181042
F	1.628535	-0.578230	3.095997
C	-2.086242	2.343719	-0.811412
N	2.797490	-1.351328	0.093713
B	2.069369	0.352264	2.226310
N	1.439519	2.171516	0.428755

$Int3_{Mes2B2F2}$

E(scf) = –2103.95222458 a.u.

F	-3.083005	0.848928	-2.866846
C	0.620943	1.354706	1.452619
N	0.294869	-2.315780	0.986860
B	0.916332	0.184606	0.268563
F	-1.283886	-0.409687	-3.368391
C	1.230416	2.635123	1.381214
N	-2.289800	-1.926343	-0.371096
B	-1.951008	0.292278	-2.445414
N	-2.074629	1.419042	-0.103760

C	-2.365320	3.433356	-1.641345	C	1.082278	3.595089	2.386458
H	-3.174219	4.109024	-1.365086	H	1.593086	4.551289	2.275871
N	-0.905674	0.820599	2.421872	N	0.615645	1.471460	-2.105410
C	-2.966254	2.233016	0.404804	C	2.112666	3.058543	0.239896
H	-2.451910	2.588973	1.306555	H	1.517560	3.408861	-0.612634
H	-3.288771	1.206792	0.585519	H	2.755181	2.246207	-0.100715
H	-3.863656	2.849688	0.291285	H	2.757817	3.892535	0.534681
C	-0.621446	2.790040	-3.096380	C	-0.302220	2.123591	3.600269
H	-0.020641	2.962819	-3.988604	H	-0.918540	1.904173	4.471291
C	-1.968047	4.838627	-3.703103	C	0.157248	4.399710	4.595519
H	-1.340818	5.703322	-3.448560	H	1.024548	5.066505	4.647630
H	-3.012197	5.154323	-3.606390	H	0.020622	3.941686	5.580987
H	-1.780984	4.602330	-4.756203	H	-0.723978	5.026120	4.403516
C	-1.663142	3.666396	-2.814477	C	0.326356	3.359950	3.524837
C	-0.288283	1.710437	-2.270961	C	-0.198287	1.149095	2.600802
C	0.971444	0.989021	-2.670193	C	-1.055587	-0.061601	2.840703
H	1.713847	1.106769	-1.877679	H	-1.843436	-0.100181	2.085168
H	1.377426	1.417179	-3.592948	H	-1.528653	-0.003623	3.826772
H	0.853109	-0.082210	-2.823486	H	-0.519192	-1.008238	2.785439
C	-2.178938	-1.024925	-0.092937	C	2.486332	-0.321638	0.060319
C	-3.362968	-0.956107	-0.880015	C	3.564266	-0.052214	0.948721
C	-3.629863	0.037326	-1.990959	C	3.443085	0.691759	2.260263
H	-4.323589	-0.407052	-2.712838	H	4.276718	0.415123	2.914482
H	-2.735208	0.344073	-2.531571	H	2.514124	0.480037	2.792119
H	-4.095552	0.959059	-1.626078	H	3.476583	1.778937	2.136567
C	-4.399077	-1.885699	-0.710658	C	4.852685	-0.535208	0.686286
H	-5.289890	-1.782781	-1.329757	H	5.647623	-0.297303	1.392434
C	-4.332864	-2.936124	0.190838	C	5.155153	-1.316631	-0.419500
C	-5.475870	-3.892145	0.382329	C	6.555603	-1.783486	-0.699552
H	-6.098762	-3.601653	1.238639	H	7.139314	-1.876101	0.222457
H	-5.119713	-4.910467	0.573794	H	7.087712	-1.077565	-1.350926
H	-6.126451	-3.920312	-0.498095	H	6.561310	-2.756058	-1.203658
C	-3.148400	-3.062880	0.907194	C	4.095589	-1.646782	-1.256162
H	-3.033958	-3.902578	1.592342	H	4.280497	-2.296348	-2.111613
C	-2.092511	-2.159450	0.772090	C	2.795563	-1.188189	-1.031354
C	-0.870083	-2.517219	1.588762	C	1.770373	-1.724897	-2.005376
H	-1.151007	-3.176098	2.417934	H	2.258591	-2.036853	-2.935445
H	-0.330919	-1.668548	2.005892	H	0.974596	-1.028888	-2.261374
H	-0.144348	-3.065753	0.979763	H	1.268115	-2.606281	-1.597048
C	0.428516	-0.923012	-0.572097	C	-0.058987	-1.140717	0.335651
C	-0.765354	-1.957529	-2.489002	C	1.423340	-2.341313	1.906562
H	-1.196290	-0.959869	-2.553680	H	1.575682	-1.337100	2.301229
H	-1.569547	-2.645677	-2.182654	H	2.348432	-2.628541	1.380692
C	-0.238398	-2.379306	-3.861239	C	1.181485	-3.318749	3.052525
H	-1.080281	-2.415804	-4.563844	H	2.058146	-3.313207	3.712073
H	0.459916	-1.618632	-4.234796	H	0.323164	-2.978623	3.648640
C	0.471152	-3.727622	-3.794837	C	0.910405	-4.720166	2.517191

H	0.898710	-3.992123	-4.769560	H	0.697511	-5.420454	3.334090
H	-0.259729	-4.510560	-3.543475	H	1.810245	-5.090325	2.003662
C	1.548329	-3.690055	-2.715582	C	-0.249114	-4.666417	1.529151
H	2.017290	-4.674984	-2.592272	H	-0.417635	-5.646551	1.064497
H	2.336885	-2.981182	-3.001768	H	-1.167061	-4.401318	2.068875
C	0.944020	-3.241805	-1.389203	C	0.011416	-3.633982	0.436072
H	0.186403	-3.987336	-1.081819	H	0.884203	-3.973396	-0.151590
H	1.702560	-3.200879	-0.615028	H	-0.838803	-3.554224	-0.243012
C	1.581771	-0.718211	0.119442	C	-1.238495	-0.960186	-0.338966
C	3.910566	-0.784424	-0.655073	C	-2.912154	-2.269604	0.902137
H	4.507496	-0.121620	-0.005022	H	-3.637915	-1.501283	1.230063
H	3.494296	-0.180260	-1.465361	H	-2.124714	-2.301461	1.659842
C	4.821519	-1.871219	-1.216327	C	-3.639273	-3.608667	0.850306
H	4.269583	-2.451285	-1.966891	H	-2.911289	-4.418946	0.717250
H	5.668809	-1.397763	-1.727629	H	-4.136903	-3.776010	1.813544
C	5.303595	-2.799786	-0.106725	C	-4.635209	-3.645972	-0.300275
H	5.925459	-2.230282	0.599808	H	-5.410522	-2.880701	-0.145582
H	5.934184	-3.598770	-0.514180	H	-5.145979	-4.615088	-0.348406
C	4.104083	-3.383737	0.632842	C	-3.890337	-3.360299	-1.596135
H	3.541899	-4.036303	-0.048204	H	-3.154753	-4.155675	-1.777274
H	4.428504	-4.004662	1.477028	H	-4.573192	-3.343381	-2.454393
C	3.198534	-2.272947	1.159765	C	-3.161683	-2.020158	-1.521884
H	2.288197	-2.681461	1.607539	H	-2.551456	-1.931768	-2.423629
H	3.738675	-1.733261	1.951954	H	-3.926380	-1.217974	-1.541925
C	-0.303317	0.627686	1.261237	C	0.155204	0.806748	-1.059452
C	-2.246903	0.328597	2.770715	C	2.045150	1.580315	-2.451491
H	-2.633970	-0.254837	1.942145	H	2.620898	0.988832	-1.747446
H	-2.891189	1.204831	2.914818	H	2.336011	2.631810	-2.350045
C	-2.223278	-0.483370	4.061062	C	2.302084	1.144096	-3.889033
H	-1.581031	-1.360659	3.931143	H	1.995933	0.101151	-4.023758
H	-3.239583	-0.851793	4.241773	H	3.384035	1.186360	-4.058148
C	-1.722879	0.366092	5.221681	C	1.550268	2.045696	-4.857870
H	-2.431454	1.186746	5.405647	H	1.930415	3.073731	-4.770539
H	-1.667886	-0.221501	6.145067	H	1.708319	1.733340	-5.896084
C	-0.353512	0.934579	4.869506	C	0.066713	2.008934	-4.515228
H	0.386593	0.130731	4.834598	H	-0.343965	1.028424	-4.768009
H	-0.018016	1.654927	5.625303	H	-0.493516	2.754061	-5.092428
C	-0.373390	1.649087	3.522460	C	-0.178813	2.297627	-3.036804
H	-1.037679	2.524259	3.577692	H	0.106760	3.335886	-2.813764
H	0.615494	2.011544	3.250765	H	-1.237643	2.234746	-2.791678
C	1.156052	0.984856	1.187571	C	-1.358843	0.452206	-0.977980
C	0.737153	3.355302	0.917337	C	-1.860700	2.832166	-0.364787
H	1.161303	3.695322	1.886576	H	-2.395492	3.175104	-1.276897
H	-0.312586	3.102642	1.085255	H	-0.791501	3.011912	-0.509524
C	0.816662	4.495585	-0.087297	C	-2.327202	3.672573	0.818949
H	0.304034	4.180032	-1.001917	H	-1.704484	3.415562	1.682407
H	0.278304	5.363637	0.313174	H	-2.161128	4.733638	0.593391

C	2.268634	4.842343	-0.392336
H	2.745736	5.255711	0.509380
H	2.330902	5.614765	-1.168352
C	3.010099	3.581477	-0.820217
H	4.079581	3.782927	-0.960660
H	2.611007	3.231176	-1.780240
C	2.845761	2.476953	0.217616
H	3.347275	1.570822	-0.119436
H	3.339325	2.786416	1.159021
C	-3.794353	3.404400	1.132704
H	-4.420338	3.765403	0.302359
H	-4.106497	3.953817	2.029123
C	-4.013330	1.905779	1.307677
H	-5.077521	1.677181	1.447697
H	-3.476301	1.557722	2.198560
C	-3.490655	1.150403	0.090404
H	-3.625212	0.079598	0.235670
H	-4.093247	1.437666	-0.792621

5

E(scf) = –2103.98175409 a.u.

F	-3.624468	-1.358593	1.421544
C	2.448596	0.332264	-0.056715
N	0.710213	-1.349324	-2.148255
B	0.818887	0.592117	-0.252985
F	-1.672750	-2.314694	2.152872
C	3.462988	1.265447	-0.405016
N	0.274441	0.234536	2.432792
B	-2.268613	-1.479314	1.221888
N	-2.207294	1.108866	0.480428
C	4.803547	1.028815	-0.072379
H	5.544082	1.780859	-0.342341
N	-1.943370	-2.163892	-0.323564
C	3.222396	2.512595	-1.224038
H	2.800597	3.339495	-0.645765
H	2.525921	2.335961	-2.047104
H	4.169994	2.858460	-1.650817
C	4.258730	-1.097763	0.807170
H	4.562388	-2.048612	1.244528
C	6.662749	-0.336476	0.956865
H	7.340160	0.245296	0.322995
H	6.950737	-1.390942	0.883571
H	6.839917	-0.023895	1.994418
C	5.227469	-0.128842	0.564333
C	2.911950	-0.899607	0.498396
C	2.017346	-2.092189	0.743566
H	1.104420	-1.859793	1.295353
H	2.554703	-2.864387	1.304922
H	1.701707	-2.536068	-0.205925
C	0.316255	2.097968	-0.794045
C	0.409041	3.241363	0.043735
C	1.020717	3.198140	1.416577
H	1.275073	4.206384	1.759278
H	1.936776	2.605409	1.434571
H	0.326437	2.777827	2.152988
C	-0.043241	4.500245	-0.353783

$Int2_{Mes2B2F2}$ isomer

E(scf) = –1525.81638831 a.u.

F	-3.151850	2.929187	-0.191337
C	0.139035	-1.682326	0.573516
B	-2.195712	2.655288	0.713068
F	-2.185191	3.515953	1.742447
C	-0.805667	-2.135263	1.537679
B	0.241602	-0.130070	0.019799
N	-2.150948	-0.126295	-1.145789
C	-0.695437	-3.403201	2.120788
H	-1.415639	-3.683192	2.889502
N	0.067512	1.268707	1.200846
C	-2.087449	-1.424837	1.931792
H	-2.930037	-1.957327	1.469069
H	-2.161611	-0.386170	1.620859
H	-2.253192	-1.470695	3.015274
C	1.042826	-3.969890	0.632068
H	1.719540	-4.709777	0.205557
C	0.404527	-5.660060	2.398496
H	-0.525836	-5.967238	2.887726
H	1.183822	-5.626842	3.171004
H	0.689580	-6.441786	1.686012
C	0.259165	-4.326544	1.723728
C	0.986950	-2.705646	0.043520
C	1.810444	-2.591469	-1.224412
H	1.398046	-1.884031	-1.945042
H	1.848707	-3.574942	-1.706359
H	2.842936	-2.275971	-1.044662
C	1.593767	0.268144	-0.785021
C	1.607227	0.901620	-2.053221
C	0.347728	1.252467	-2.803130
H	0.586300	1.794600	-3.723609
H	-0.324578	1.880869	-2.210371
H	-0.217615	0.362199	-3.089463
C	2.811146	1.244732	-2.670331
H	2.781558	1.722696	-3.648760
C	4.046973	1.007615	-2.074165

H	0.060864	5.335952	0.338050
C	-0.607898	4.724745	-1.602416
C	-1.135221	6.072489	-2.004239
H	-0.538503	6.883340	-1.571913
H	-2.168497	6.211457	-1.659105
H	-1.136703	6.195300	-3.092562
C	-0.677495	3.627192	-2.447090
H	-1.094931	3.762831	-3.444246
C	-0.247226	2.346643	-2.074962
C	-0.419618	1.311846	-3.158486
H	-0.867303	1.768426	-4.046845
H	-1.066956	0.487380	-2.849723
H	0.535107	0.882919	-3.467994
C	0.116746	-0.676796	-1.113336
C	1.983697	-0.971259	-2.749322
H	2.476979	-0.223700	-2.136892
H	1.792013	-0.524472	-3.740232
C	2.872677	-2.193791	-2.950778
H	3.821936	-1.876331	-3.398809
H	3.111542	-2.631317	-1.973778
C	2.169993	-3.212866	-3.845317
H	2.756765	-4.135057	-3.931201
H	2.084922	-2.796044	-4.859784
C	0.769505	-3.517124	-3.315555
H	0.212793	-4.144802	-4.022957
H	0.853345	-4.079688	-2.375808
C	-0.006126	-2.226648	-3.057382
H	-0.145539	-1.692369	-4.014480
H	-1.001355	-2.427752	-2.672917
C	-0.064585	0.270733	1.164615
C	1.611937	0.564489	2.961162
H	1.495275	1.480765	3.554219
H	2.278259	0.770012	2.131279
C	2.178910	-0.538555	3.847320
H	2.363685	-1.432112	3.243279
H	3.154963	-0.197648	4.211729
C	1.237639	-0.868892	4.997968
H	1.173155	-0.008534	5.680132
H	1.620417	-1.712224	5.584057
C	-0.143002	-1.181772	4.437204
H	-0.121849	-2.101407	3.845139
H	-0.875158	-1.333802	5.238927
C	-0.646386	-0.048616	3.553388
H	-1.635138	-0.262866	3.164990
H	-0.703325	0.878894	4.141071
C	-1.082285	-0.958783	-0.503036
C	-1.230095	-3.465418	-0.233843
C	5.330752	1.353224	-2.774404
H	5.231207	2.269763	-3.366048
H	5.631555	0.554088	-3.464278
H	6.150577	1.495438	-2.062752
C	4.037978	0.429325	-0.811774
H	4.984655	0.252242	-0.301010
C	2.852175	0.065594	-0.168040
C	3.032944	-0.532967	1.209141
H	3.663261	-1.429464	1.162625
H	2.097574	-0.833769	1.676680
H	3.541578	0.177111	1.874506
C	-1.247228	1.495677	0.527054
C	1.048218	2.373964	0.995253
H	1.011160	2.649964	-0.059395
H	2.041455	1.954820	1.182030
C	0.850261	3.587208	1.895402
H	-0.070731	4.116335	1.641592
H	1.677170	4.279322	1.692878
C	0.832037	3.185656	3.366640
H	1.829846	2.822497	3.655210
H	0.612027	4.051048	4.002235
C	-0.186696	2.073387	3.589446
H	-1.200482	2.456041	3.444523
H	-0.128585	1.691659	4.616454
C	0.071074	0.908585	2.643568
H	1.066059	0.497630	2.846214
H	-0.644578	0.110158	2.806554
C	-1.213687	0.436752	-0.378026
C	-1.856144	-1.337836	-1.903717
H	-2.261052	-2.204808	-1.357707
H	-0.774846	-1.469809	-1.950674
C	-2.464896	-1.276597	-3.302008
H	-1.964518	-0.489179	-3.880191
H	-2.270542	-2.226462	-3.814251
C	-3.962165	-0.983227	-3.246726
H	-4.483595	-1.836339	-2.788012
H	-4.368343	-0.869982	-4.258504
C	-4.223130	0.267746	-2.412026
H	-5.299079	0.442192	-2.293451
H	-3.801219	1.152076	-2.907046
C	-3.582521	0.127349	-1.037147
H	-3.754599	1.012787	-0.436905
H	-4.031211	-0.732060	-0.511404

H	-0.393049	-3.327768	0.448455
H	-0.827982	-3.720409	-1.216955
C	-2.143141	-4.587743	0.237373
H	-2.468965	-4.380474	1.261875
H	-1.555227	-5.513403	0.264836
C	-3.349444	-4.731475	-0.682664
H	-3.014387	-5.039063	-1.684762
H	-4.024408	-5.514454	-0.318576
C	-4.075363	-3.395179	-0.769992
H	-4.499509	-3.134561	0.204688
H	-4.905170	-3.441683	-1.485518
C	-3.137988	-2.277245	-1.205877
H	-2.799101	-2.450454	-2.235512
H	-3.652431	-1.318881	-1.185307
C	-1.455850	-0.148407	0.713316
C	-3.219700	1.069811	-0.553647
H	-4.081761	0.440515	-0.250854
H	-2.771648	0.620234	-1.445481
C	-3.733467	2.464234	-0.889773
H	-2.905484	3.053118	-1.299039
H	-4.504621	2.383165	-1.666963
C	-4.282733	3.147207	0.356738
H	-5.168633	2.602074	0.716596
H	-4.605413	4.171575	0.132599
C	-3.208660	3.141175	1.436492
H	-3.586582	3.567350	2.374713
H	-2.359290	3.752620	1.105561
C	-2.704909	1.724781	1.697197
H	-1.884052	1.791227	2.416637
H	-3.507038	1.119967	2.166287

B_2Cat_2-PipCCPip

E(scf) = –1390.07917841 a.u.

O	-1.481564	-1.443961	1.632267
B	-0.544638	-0.409911	1.615631
N	0.165633	-1.659578	-1.776331
N	0.183438	2.052792	-0.901289
C	0.102612	-0.482247	-1.126802
C	0.093742	0.761871	-1.110994
C	1.591080	3.992907	-1.427856
H	1.651506	3.741796	-2.495366
H	2.526467	4.498390	-1.158035
C	1.462678	2.705044	-0.622814
H	1.522933	2.919774	0.454656
H	2.257332	1.995254	-0.860834

$TS1_{B2Cat2}$

E(scf) = –1390.06199544 a.u. υ_{min} = –106.2 cm^{-1}

O	1.423490	-1.268420	-1.862406
B	0.443989	-0.295665	-1.524409
N	0.841715	-1.399192	1.516578
N	-0.640411	1.750843	0.709601
C	0.417473	-0.438209	0.747290
C	-0.552031	0.445606	0.666941
C	-2.222658	3.520932	1.333690
H	-2.527000	3.014242	2.257702
H	-3.095668	4.077327	0.967746
C	-1.848091	2.465209	0.295600
H	-1.660987	2.932829	-0.684090
H	-2.645738	1.735817	0.170893

C	0.391712	4.907150	-1.183264	C	-1.056276	4.464002	1.612192
H	0.391427	5.229395	-0.131382	H	-0.823916	5.038802	0.707140
H	0.468937	5.815133	-1.792697	H	-1.329723	5.190639	2.385043
C	-2.205841	-2.938335	-2.848079	C	2.843283	-2.263744	3.396499
H	-3.291223	-2.954830	-3.004589	H	3.762820	-2.062930	3.972819
H	-1.804340	-3.842455	-3.330742	H	2.529180	-3.286765	3.663084
C	-1.878662	-2.976906	-1.354989	C	3.121752	-2.203973	1.894915
H	-2.250448	-3.902911	-0.898125	H	3.844307	-2.977568	1.604336
H	-2.377782	-2.142912	-0.844515	H	3.561192	-1.233430	1.621613
C	-0.373310	-2.852784	-1.125997	C	1.834106	-2.390223	1.096240
H	-0.128278	-2.813618	-0.064450	H	1.976585	-2.281223	0.018350
H	0.143675	-3.722754	-1.556678	H	1.405916	-3.386785	1.281595
C	-2.701228	-0.831808	1.689950	C	2.583431	-0.570162	-2.019896
C	-3.958481	-1.403395	1.671406	C	3.857875	-1.057150	-2.230340
H	-4.085472	-2.479117	1.607445	H	4.049240	-2.122416	-2.296600
C	-5.046738	-0.526387	1.735082	C	4.889937	-0.108433	-2.350540
H	-6.054347	-0.931597	1.721700	H	5.904047	-0.456504	-2.516138
O	2.028173	0.450926	1.487443	O	-2.272034	0.224254	-1.628250
B	1.112156	-0.601223	1.447660	B	-1.179262	-0.585292	-1.211131
C	3.243363	-0.114638	1.223913	C	-3.385995	-0.463871	-1.251962
C	4.474166	0.499489	1.098299	C	-4.707344	-0.061371	-1.327040
H	4.581749	1.573226	1.214383	H	-4.973352	0.910203	-1.734337
C	5.563923	-0.332037	0.818024	C	-5.675714	-0.971747	-0.874832
H	6.551174	0.107474	0.708588	H	-6.726539	-0.692317	-0.923991
O	1.771499	-1.815606	1.256483	O	-1.670050	-1.841642	-0.780723
C	3.087323	-1.492382	1.082005	C	-3.021620	-1.712064	-0.742940
C	4.156130	-2.322838	0.808488	C	-3.970828	-2.610127	-0.300295
H	4.022114	-3.393819	0.698057	H	-3.681149	-3.581019	0.091465
C	5.407816	-1.711732	0.676589	C	-5.314151	-2.218442	-0.370469
H	6.275912	-2.326903	0.457980	H	-6.082711	-2.898059	-0.028403
O	-1.181223	0.825272	1.756290	O	0.993072	0.998041	-1.720124
C	-0.912744	4.170464	-1.481999	C	0.174605	3.666707	2.038357
H	-0.962164	3.925126	-2.551309	H	-0.023979	3.169361	3.001871
H	-1.778664	4.803059	-1.251136	H	1.036154	4.322812	2.183429
C	-0.998371	2.881010	-0.673539	C	0.513263	2.612395	0.996160
H	-1.063565	3.111188	0.401075	H	0.806537	3.089959	0.048445
H	-1.877010	2.288302	-0.938090	H	1.337329	1.968093	1.312836
C	-1.588637	-1.705479	-3.510382	C	1.741799	-1.282666	3.796815
H	-1.762426	-1.715570	-4.593923	H	1.485739	-1.394714	4.859046
H	-2.057560	-0.794454	-3.113214	H	2.092213	-0.247893	3.650280
C	-0.091729	-1.644348	-3.216998	C	0.485962	-1.497813	2.937549
H	0.371165	-0.746291	-3.635048	H	-0.284048	-0.751304	3.146673
H	0.411328	-2.518641	-3.656028	H	0.061085	-2.495925	3.123269
C	-2.518278	0.547728	1.766973	C	2.321498	0.797491	-1.932191
C	-3.585352	1.422527	1.833669	C	3.325360	1.738413	-2.059903
H	-3.431616	2.494974	1.897687	H	3.115752	2.799743	-1.994496
C	-4.864259	0.854977	1.815489	C	4.629354	1.256008	-2.266867

H	-5.732480	1.505807	1.864563

$Int1_{B2Cat2}$

E(scf) = –1390.16308420 a.u.

O	-1.182277	0.973710	-0.608759
B	0.080730	1.450933	-0.225374
N	2.600627	0.970011	0.084121
N	1.814760	-1.863843	0.387144
C	1.258653	0.504865	-0.004547
C	0.933219	-0.827023	0.184595
C	1.192935	-4.082970	-0.523011
H	0.411077	-3.669738	-1.171721
H	0.871254	-5.087794	-0.221481
C	1.316742	-3.192801	0.713665
H	2.023726	-3.645180	1.425406
H	0.361784	-3.104189	1.243703
C	2.522151	-4.139961	-1.273899
H	3.261380	-4.679433	-0.662597
H	2.411065	-4.706769	-2.205969
C	5.034188	2.409434	0.699132
H	6.124200	2.515946	0.641009
H	4.659005	3.274214	1.266149
C	4.654066	1.126453	1.431501
H	5.025236	1.140237	2.463697
H	5.121276	0.267541	0.930793
C	3.142370	0.932044	1.440936
H	2.886657	-0.036507	1.883233
H	2.669439	1.712353	2.067342
C	-2.018340	2.053222	-0.572546
C	-3.376887	2.100924	-0.807832
H	-3.938042	1.201274	-1.040134
C	-3.979026	3.361162	-0.718691
H	-5.047144	3.450623	-0.894122
O	-1.383191	-0.963329	1.401589
B	-0.594192	-1.194966	0.280568
C	-2.627712	-1.413099	1.056064
C	-3.802500	-1.347814	1.778954
H	-3.831736	-0.895203	2.764454
C	-4.942687	-1.881994	1.169646
H	-5.890218	-1.848444	1.699441
O	-1.294275	-1.900706	-0.691657
C	-2.573701	-1.983330	-0.214871
C	-3.692289	-2.515389	-0.825675
H	-3.637763	-2.953257	-1.816882
C	-4.888951	-2.452699	-0.103301
H	-5.795162	-2.856331	-0.545550
O	0.031070	2.835917	-0.047087
H	5.448177	1.963770	-2.372960

$TS2_{B2Cat2}$

E(scf) = –1968.25872365 a.u. υ_{min} = –144.5 cm^{-1}

O	-2.486577	1.176347	0.836275
B	-1.879739	0.847982	-0.383276
N	-2.572145	-1.487117	-0.863452
N	0.189459	-2.106391	-1.729125
C	-1.486533	-0.609425	-0.798514
C	-0.172203	-0.907519	-1.081834
C	0.486769	-1.800579	-4.174092
H	0.567566	-0.710517	-4.064905
H	0.013568	-2.001795	-5.144234
C	-0.392473	-2.340532	-3.046054
H	-0.523739	-3.426896	-3.180888
H	-1.385211	-1.885134	-3.079139
C	1.875316	-2.432147	-4.102044
H	1.786809	-3.515979	-4.275732
H	2.526090	-2.037647	-4.892135
C	-4.937992	-3.083951	-0.479927
H	-5.760148	-3.455856	0.143363
H	-5.054182	-3.550465	-1.469925
C	-3.588757	-3.486197	0.109366
H	-3.496190	-4.578806	0.159601
H	-3.514145	-3.104325	1.135626
C	-2.436739	-2.922180	-0.719709
H	-1.471046	-3.129835	-0.256623
H	-2.432119	-3.424550	-1.703455
C	-2.775507	2.508319	0.747772
C	-3.291849	3.347330	1.715614
H	-3.536178	2.978535	2.706745
C	-3.476748	4.687134	1.353765
H	-3.878422	5.382666	2.085110
O	1.777894	0.788180	-1.586555
B	0.813816	0.233812	-0.704726
N	3.389408	0.284054	0.957132
N	0.468941	-1.507741	2.409258
C	2.257529	-0.458195	0.951331
C	1.520612	-1.094101	1.763678
C	-1.935468	-1.167358	2.844243
H	-2.220210	-1.270088	1.791368
H	-2.643994	-0.462258	3.293091
C	-0.540482	-0.564872	2.914679
H	-0.288000	-0.318066	3.958902
H	-0.473246	0.341741	2.312573
C	-1.986480	-2.523803	3.540383
H	-1.781416	-2.399982	4.614491

C	3.042714	-2.731226	-1.554226
H	2.370740	-2.214516	-2.252699
H	4.033610	-2.768681	-2.024245
C	3.120250	-1.915316	-0.265226
H	3.828904	-2.389539	0.431052
H	3.450123	-0.892797	-0.457268
C	4.411717	2.419382	-0.694218
H	4.622294	3.365238	-1.208439
H	4.845896	1.612108	-1.299549
C	2.903975	2.216798	-0.603476
H	2.463224	2.167899	-1.605410
H	2.453175	3.085459	-0.091374
C	-1.275487	3.187489	-0.251144
C	-1.860025	4.435480	-0.165080
H	-1.275649	5.314794	0.085073
C	-3.237233	4.501336	-0.407560
H	-3.738216	5.463150	-0.346579
H	-2.988692	-2.961062	3.460018
C	5.974726	-0.912775	1.499987
H	6.585399	-1.796192	1.722431
H	6.663302	-0.055081	1.461689
C	4.947404	-0.676364	2.608072
H	5.442713	-0.494419	3.570089
H	4.316742	-1.568126	2.729765
C	4.050260	0.503801	2.243041
H	3.277580	0.683991	2.995664
H	4.651629	1.420157	2.156172
C	1.898041	2.098696	-1.238216
C	2.744081	3.053450	-1.766993
H	3.439493	2.806400	-2.562839
C	2.649747	4.347155	-1.237527
H	3.295261	5.127478	-1.630899
O	0.301574	1.284092	0.124344
C	-0.948125	-3.462605	2.931562
H	-1.199949	-3.659246	1.882523
H	-0.935510	-4.428478	3.450826
C	0.442507	-2.847842	3.001219
H	0.758375	-2.770801	4.054542
H	1.181924	-3.453218	2.471719
C	5.286511	-1.061837	0.142649
H	6.027409	-1.141789	-0.662838
H	4.692580	-1.986771	0.127812
C	4.349412	0.114074	-0.130406
H	3.798820	-0.025576	-1.059357
H	4.923392	1.047590	-0.217408
C	0.998450	2.406595	-0.217899
C	0.890225	3.676898	0.307564
H	0.166721	3.902724	1.084621
C	1.741651	4.653258	-0.225374
H	1.686859	5.668490	0.156921
O	-1.952264	1.933070	-1.267159
C	2.486593	-2.182712	-2.725483
H	2.679647	-1.110839	-2.613031
H	3.447169	-2.705345	-2.621197
C	1.535110	-2.641382	-1.616371
H	1.456404	-3.741201	-1.658348
H	1.928883	-2.381741	-0.631197
C	-5.014890	-1.567148	-0.629844
H	-5.952361	-1.268801	-1.115208
H	-4.987387	-1.092164	0.360026
C	-3.830199	-1.055220	-1.440900
H	-3.842125	0.038235	-1.494286
H	-3.916631	-1.417123	-2.483894
C	-2.451382	2.966426	-0.529366

C	-2.630982	4.285273	-0.897025
H	-2.361681	4.631479	-1.889237
C	-3.153374	5.144792	0.075886
H	-3.305376	6.191818	-0.170222

$Int2_{B2Cat2}$

E(scf) = –1968.34772158 a.u.

O	-1.313749	-0.432555	2.144033
B	-0.165483	-0.903060	1.481396
N	2.316925	-0.261794	1.402063
N	1.400789	2.331988	0.291801
C	0.996490	0.007857	1.018092
C	0.641210	1.175612	0.345512
C	1.820118	4.438014	-0.913240
H	0.823352	4.848322	-0.709647
H	2.146205	4.836618	-1.881918
C	1.714309	2.921410	-1.000514
H	2.671005	2.513216	-1.377812
H	0.940009	2.621271	-1.710117
C	2.781710	4.853084	0.197159
H	3.800557	4.531096	-0.066298
H	2.810825	5.944837	0.296281
C	4.993299	-1.229223	1.971975
H	5.990261	-1.097155	2.409244
H	4.970535	-2.233164	1.523161
C	4.732140	-0.189705	0.887357
H	5.445199	-0.297126	0.060751
H	4.866462	0.816319	1.306352
C	3.317786	-0.330823	0.340577
H	3.100123	0.446152	-0.395585
H	3.238258	-1.299564	-0.185404
C	-2.013629	-1.546573	2.498422
C	-3.242404	-1.632870	3.123564
H	-3.787728	-0.740425	3.413515
C	-3.741459	-2.919837	3.357211
H	-4.704051	-3.033671	3.847485
O	1.314006	-0.432899	-2.144293
B	0.165933	-0.903311	-1.481253
N	-2.316690	-0.262853	-1.402497
N	-1.401783	2.331325	-0.292193
C	-0.996394	0.007402	-1.018458
C	-0.641665	1.175307	-0.345910
C	-1.821697	4.437243	0.912781
H	-0.825016	4.847743	0.709165
H	-2.147878	4.835824	1.881437
C	-1.715528	2.920671	1.000099
H	-2.672153	2.512236	1.377315

2

E(scf) = –1968.36151665 a.u.

O	0.095222	2.956536	1.382528
B	-0.014513	2.347952	0.060229
N	-2.596493	1.622874	-0.182554
N	-1.349436	-1.269974	-0.164630
C	-1.212150	1.294811	-0.110270
C	-0.719254	0.048208	-0.134973
C	-2.880665	-2.692183	-1.595472
H	-2.268397	-3.596147	-1.543404
H	-3.356648	-2.680009	-2.583699
C	-2.000320	-1.456038	-1.505071
H	-2.611668	-0.565610	-1.679106
H	-1.194082	-1.483065	-2.243183
C	-3.925037	-2.704012	-0.486014
H	-4.613083	-1.854942	-0.611908
H	-4.526370	-3.618396	-0.537904
C	-5.000855	3.203282	-0.509401
H	-6.095968	3.255207	-0.531642
H	-4.629040	4.220960	-0.697281
C	-4.480635	2.274436	-1.603710
H	-4.752535	2.651732	-2.597153
H	-4.935172	1.280159	-1.492541
C	-2.967638	2.132439	-1.510035
H	-2.597309	1.432534	-2.266890
H	-2.479138	3.102545	-1.707684
C	0.258283	4.285957	1.174869
C	0.451058	5.281841	2.113010
H	0.482618	5.047102	3.172486
C	0.604142	6.594039	1.640481
H	0.755700	7.399336	2.353831
O	-0.095222	-2.956536	1.382528
B	0.014513	-2.347952	0.060229
N	2.596493	-1.622874	-0.182554
N	1.349436	1.269974	-0.164630
C	1.212150	-1.294811	-0.110270
C	0.719254	-0.048208	-0.134973
C	2.880665	2.692183	-1.595472
H	2.268397	3.596147	-1.543404
H	3.356648	2.680009	-2.583699
C	2.000320	1.456038	-1.505071
H	2.611668	0.565610	-1.679106

H	-0.941216	2.620708	1.709761	H	1.194082	1.483065	-2.243183
C	-2.783383	4.852041	-0.197639	C	3.925037	2.704012	-0.486014
H	-3.802157	4.529843	0.065847	H	4.613083	1.854942	-0.611908
H	-2.812742	5.943783	-0.296817	H	4.526370	3.618396	-0.537904
C	-4.992505	-1.231785	-1.972385	C	5.000855	-3.203282	-0.509401
H	-5.989548	-1.100266	-2.409637	H	6.095968	-3.255207	-0.531642
H	-4.969172	-2.235723	-1.523595	H	4.629040	-4.220960	-0.697281
C	-4.731924	-0.192149	-0.887741	C	4.480635	-2.274436	-1.603710
H	-5.444913	-0.300007	-0.061130	H	4.752535	-2.651732	-2.597153
H	-4.866824	0.813813	-1.306700	H	4.935172	-1.280159	-1.492541
C	-3.317480	-0.332453	-0.340984	C	2.967638	-2.132439	-1.510035
H	-3.100255	0.444668	0.395156	H	2.597309	-1.432534	-2.266890
H	-3.237360	-1.301139	0.185019	H	2.479138	-3.102545	-1.707684
C	2.014110	-1.546949	-2.498148	C	-0.258283	-4.285957	1.174869
C	3.242818	-1.633299	-3.123415	C	-0.451058	-5.281841	2.113010
H	3.787874	-0.740882	-3.413956	H	-0.482618	-5.047102	3.172486
C	3.742172	-2.920274	-3.356386	C	-0.604142	-6.594039	1.640481
H	4.704724	-3.034145	-3.846731	H	-0.755700	-7.399336	2.353831
O	0.140192	-2.302985	-1.507394	O	-0.014513	-3.435750	-0.908197
C	-2.379369	4.198988	-1.516656	C	3.223135	2.599344	0.862452
H	-1.397177	4.576977	-1.831369	H	2.613099	3.492771	1.034980
H	-3.095542	4.449269	-2.309347	H	3.950641	2.549873	1.681478
C	-2.303022	2.682314	-1.369372	C	2.369715	1.345410	0.935718
H	-3.317618	2.285997	-1.195468	H	2.996447	0.452616	0.833726
H	-1.935998	2.217804	-2.287542	H	1.814111	1.295440	1.873758
C	-3.912531	-1.137709	-3.046181	C	4.506616	-2.738346	0.858144
H	-4.047172	-1.917319	-3.806010	H	4.798598	-3.450087	1.639683
H	-3.982260	-0.166749	-3.554858	H	4.962977	-1.770754	1.107517
C	-2.524877	-1.272600	-2.429668	C	2.992169	-2.580640	0.855749
H	-1.760496	-1.142024	-3.203445	H	2.635044	-2.205150	1.819708
H	-2.400661	-2.290367	-2.018460	H	2.516487	-3.565924	0.697109
C	1.303120	-2.682894	-2.109431	C	-0.215650	-4.573683	-0.195209
C	1.788225	-3.956587	-2.331218	C	-0.371642	-5.861632	-0.668362
H	1.228128	-4.831853	-2.018988	H	-0.337444	-6.070108	-1.733447
C	3.030931	-4.055814	-2.968294	C	-0.565865	-6.878275	0.279159
H	3.449174	-5.039571	-3.161189	H	-0.687784	-7.903053	-0.060320
O	-0.139391	-2.302697	1.508338	O	0.014513	3.435750	-0.908197
C	2.377817	4.200008	1.516199	C	-3.223135	-2.599344	0.862452
H	1.395520	4.577766	1.830858	H	-2.613099	-3.492771	1.034980
H	3.093897	4.450517	2.308902	H	-3.950641	-2.549873	1.681478
C	2.301884	2.683308	1.369001	C	-2.369715	-1.345410	0.935718
H	3.316599	2.287267	1.195198	H	-2.996447	-0.452616	0.833726
H	1.934920	2.218758	2.287176	H	-1.814111	-1.295440	1.873758
C	3.913258	-1.135763	3.045753	C	-4.506616	2.738346	0.858144
H	4.048315	-1.915306	3.805577	H	-4.798598	3.450087	1.639683
H	3.982448	-0.164771	3.554443	H	-4.962977	1.770754	1.107517
C	2.525676	-1.271409	2.429251	C	-2.992169	2.580640	0.855749

H	1.761249	-1.141240	3.203047	H	-2.635044	2.205150	1.819708
H	2.401991	-2.289245	2.018055	H	-2.516487	3.565924	0.697109
C	-1.302299	-2.682558	2.110453	C	0.215650	4.573683	-0.195209
C	-1.787106	-3.956248	2.332915	C	0.371642	5.861632	-0.668362
H	-1.226742	-4.831550	2.021264	H	0.337444	6.070108	-1.733447
C	-3.029874	-4.055420	2.969874	C	0.565865	6.878275	0.279159
H	-3.447895	-5.039170	3.163284	H	0.687784	7.903053	-0.060320

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