Electronic Supplementary Material (ESI) for ChemComm.

Utilization of BODIPY-Based Redox Events to Manipulate the Lewis Acidity of Fluorescent Boranes

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Supporting Information

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1) Experimental Methods

Synthetic Techniques

All preparations and manipulations were performed on a double manifold N_2/vacuum line with Schlenk-type glassware or in a N_2-filled VAC glovebox, unless indicated otherwise. Solvents were dried using an Innovative Technologies solvent system, and degassed before use. *N,N′*-bis-BODIPY-ethylenediamine, (±)-*N,N′*-bis-BODIPY-cyclohexane-1,2-diamine, and *N,N′*-bis-BODIPY-(*R,R*)-cyclohexane-1,2-diamine were prepared according to previously reported literature procedures.[1] All remaining reagents were purchased from Sigma Aldrich, Acros Organics, or Alfa Aesar and were used without further purification.

Spectroscopic Techniques

NMR spectra were obtained on a Varian 400 MR or a Vairan DD2 600 MHz spectrometer, and spectra were referenced to residual solvent (^{1}H, ^{13}C) or externally (^{11}B; $BF_3{\bullet}OEt_2$, ^{19}F; CCl_3F).[2] Chemical shifts are reported in parts per million (ppm). NMR solvents were purchased from Cambridge Isotope Laboratories, Inc., and used as received. All remaining reagents were purchased from Sigma Aldrich, Acros Organics, or Alfa Aesar and were used without further purification. All UV-Vis spectra were obtained on a Cary 60 UV-Vis spectrometer. Photoluminescent spectra were obtained with a Horiba FluoroMax-4 fluorometer equipped with a Xenon lamp. X-band (9.37 GHz) EPR spectra were collected on a Bruker EMX Plus spectrometer with a 12” magnet equipped with a standard rectangular (TE102) EPR cavity (Bruker ER 4102ST). Samples were prepared in dry degassed THF and run at room temperature and 77 K. A field modulation of 50 kHz and a microwave power of 10.0 mW was used during data collection. The EPR spectrum was simulated and fitted to experimental data using the simulation program EasySpin.[3] Fitting was implemented using the Nelder/Mead downhill simplex. Cyclic voltammetry (CV) experiments were carried out at room temperature in nitrogen-purged acetonitrile solutions

using a CH Instruments Model CHI600E electrochemical workstation. All CV experiments were performed using a glassy carbon working electrode (3.0 mm diameter). The electrode surface was polished routinely with 0.05 mm alumina–water slurry on a felt surface immediately before use and in between runs. The counter electrode was a graphite rod and the pseudo reference electrode was an Ag/AgCl electrode. The concentration of the sample and supporting electrolyte, tetrabutylammonium hexafluorophosphate, were 1.0 mM and 0.1 M, respectively. The supporting electrolyte was recrystallized from acetonitrile and stored in a desiccator prior to use. To employ moisture free conditions, the CV cell was dried in an oven (140 °C for 24 hours) prior to use. Voltammograms were referenced to 1.0 mM ferrocene/ferrocenium. All color names listed are taken in relation to a crayon of most similar color from a 120 Crayola crayon set.

1. Under a nitrogen atmosphere, a slurry of 0.34 g (0.77 mmol) of *N,N′*-bis-BODIPY-ethylenediamine in 2 mL of THF was added a slurry of 0.31 g (1.55 mmol) of $KN(SiMe_3)_2$ (KHMDS) in 8 mL of THF. Upon addition of the KHMDS solution, a dark red colored solution results. The solution was left to stir for 16 hours, the solution was then filtered and volatiles removed under reduced pressure, yielding 0.45 g of a brown solid. The brown solid was used without further purification and slurried (0.36 g, 0.70 mmol) in 10 mL of dry, degassed methylene chloride. To the slurry was added a solution of 110.0 mg (0.69 mmol) of $PhBCl_2$ in 6 mL of methylene chloride dropwise over the course of several minutes. Addition of $PhBCl_2$ resulted in a dark red solution. The reaction mixture was left to stir for 16 hours, where the solvent was removed under reduced pressure. The crude oily red solid was dissolved in a minimal amount of methylene chloride (~ 6 mL), filtered (discarding the filter cake), and precipitated using diethyl ether (~ 50 mL). Filtration of the slurry followed by washing with 20 mL of diethyl ether yielded 0.24 g (66% yield) of a brown-red solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (s, 4H), 7.19 (d, 2H), 7.03 (t, 1H), 7.02 (d, 4H), 6.37 (d, 4H), 4.42 (s, 4H). ^{11}B NMR (128 MHz, $CDCl_3$): δ 35.48 (br, 1B), 0.45 (t, 2B, J = 27 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 135.46 (s, 4C), 135.23 (s, 1C), 134.86 (s, 4C), 134.24 (s, 2C), 133.35

(s, 4C), 132.64 (s, 4C), 132.02 (s, 1C), 131.24 (s, 2C), 131.04 (s, 2C), 66.02 (s, 2C). ^{19}F NMR (376 MHz, $CDCl_3$): δ -147.7 (broad), -147.13 (broad). λ_{abs} (CH_2Cl_2) = 334, 411, 488 nm. $\lambda_{emission}$ (CH_2Cl_2) = 485 nm. ε (CH_2Cl_2) = 26442 L cm^{-1} mol^{-1}. τ (CH_2Cl_2) = 1.21 ± 0.025, 11.06 ± 0.028 ns.

2. Under a nitrogen atmosphere, a slurry of 0.30 g (0.61 mmol) of (±)-*N,N′*-bis-BODIPY-cyclohexane-1,2-diamine in 2 mL of THF was added to a slurry of 0.49 g (1.23 mmol) of $KN(SiMe_3)_2$ (KHMDS) in 8 mL of THF. Upon addition of the KHMDS solution, a dark brown colored solution results. The solution was left to stir for 16 hours and then filtered and volatiles removed under reduced pressure, yielding 0.35 g of a clear colorless solid. The colorless solid was used without further purification and slurried (0.35 g, 0.61 mmol) in 10 mL of dry, degassed methylene chloride. To the slurry was added a solution of 97.5 mg (0.61 mmol) of $PhBCl_2$ in 6 mL of methylene chloride dropwise over the course of several minutes. Addition of $PhBCl_2$ resulted in a bright orange solution. The reaction mixture was left to stir for 16 hours, where the solvent was removed under reduced pressure. The crude orange solid was dissolved in a minimal amount of methylene chloride (~ 5 mL), filtered (discarding the filter cake), and precipitated with pentanes (~ 15 mL). Filtration of the slurry followed by washing with 10 mL of pentane yielded 0.206 g (58% yield) of a bright orange solid. ^{1}H NMR (600 MHz, CD_2Cl_2): δ 7.79 (s, BODIPY (3,5-position), 2H), 7.57 (s, BODIPY (3,5-position), 2H), 7.41 (s, BODIPY (2,6-position), 2H), 7.16 (d, phenyl (2,6-position), 2H), 7.12 (t, phenyl (3,5-position), 2H), 7.03 (t, phenyl (4-position), 1H), 6.76 (s, BODIPY (1,7-position), 2H), 6.71 (s, BODIPY (1,7-position), 2H), 6.15 (s, BODIPY (2,6-position), 2H), 4.31 (s, NC*H*$CH_2CH_2CH_2CH_2C$*H*N, 2H), 2.43 (s, NCHC*H*$_2CH_2CH_2CH_2CHN$, 2H), 1.93 (s, $NCHCH_2CH_2CH_2C$*H*$_2CHN$, 2H), 1.48 (s, $NCHCH_2C$*H*$_2C$*H*$_2CH_2CHN$, 4H). ^{11}B NMR (192 MHz, CD_2Cl_2): δ 34.99 (br, 1B), -0.22 (t, 2B, J_{BF} = 28.5 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 149.03 (s, 2C), 145.58 (s, 2C), 143.74 (s, 2C), 136.91 (s, 1C), 135.54 (s, 2C), 133.35 (s, 2C), 131.80 (s, 2C), 130.74 (s, 2C), 130.70 (s, 2C), 129.60 (s, 2C), 128.09 (s, 2C), 119.54 (s, 2C), 119.08 (s, 2C), 73.45 (s, 2C), 29.30 (s, 2C), 25.58 (s, 2C). ^{19}F NMR (564 MHz, CD_2Cl_2): δ -145.96 (q, J_{BF} = 28.5

Hz), -146.15 (q, J_{BF} = 28.5 Hz), -146.72 (q, J_{BF} = 28.5 Hz), -146.91 (q, J_{BF} = 28.5 Hz). λ_{abs} (CH_2Cl_2) = 331, 417, 506 nm. $\lambda_{emission}$ (CH_2Cl_2) = 487, 531 nm. ε (CH_2Cl_2) = 24773500 L cm^{-1} mol^{-1}.

(*R,R*)-2. Under a nitrogen atmosphere, a slurry of 0.13 g (0.27 mmol) of *N,N'*-bis-BODIPY-(*R,R*)-cyclohexane-1,2-diamine in 2 mL of THF was added to a solution of 01.1 µL (0.56 mmol) of $KN(SiMe_3)_2$ (KHMDS) in 8 mL of THF. Upon addition to the KHMDS solution, a red colored solution results. The solution was left to stir for 16 hours and then filtered and volatiles removed under reduced pressure, yielding 0.95 g of a clear colorless solid. The colorless solid was used without further purification and slurried (0.95 g, 0.16 mmol) in 10 mL of dry, degassed methylene chloride. To the slurry was added a solution of 26.3 mg (0.16 mmol) of $PhBCl_2$ in 6 mL of methylene chloride dropwise over the course of several minutes. Addition of $PhBCl_2$ resulted in a bright red-orange solution. The reaction mixture was left to stir for 16 hours, where the solvent was removed under reduced pressure. The crude orange oil was extracted in a minimal amount of pentanes (~ 5 mL) and filtered. Concentration of the solution yielded 52 mg (54% yield) of a deep orange solid. ^{1}H NMR (600 MHz, CD_2Cl_2): δ 7.79 (s, BODIPY (3,5-position), 2H), 7.57 (s, BODIPY (3,5-position), 2H), 7.40 (s, BODIPY (2,6-position), 2H), 7.15 (d, phenyl (2,6-position), 2H), 7.12 (t, phenyl (3,5-position), 2H), 7.02 (t, phenyl (4-position), 1H), 6.75 (s, BODIPY (1,7-position), 2H), 6.70 (s, BODIPY (1,7-position), 2H), 6.14 (s, BODIPY (2,6-position), 2H), 4.32 (s, NC*H*$CH_2CH_2CH_2CH_2C$*H*N, 2H), 2.42 (s, NCHC*H*$_2CH_2CH_2CH_2$CHN, 2H), 1.93 (s, $NCHCH_2CH_2CH_2C$*H*$_2$CHN, 2H), 1.47 (s, $NCHCH_2C$*H*$_2C$*H*$_2CH_2$CHN, 4H). ^{11}B NMR (192 MHz, CD_2Cl_2): δ 35.94 (br, 1B), 0.83 (t, 2B, J_{BF} = 28.5 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 149.03 (s, 2C), 145.58 (s, 2C), 143.74 (s, 2C), 136.91 (s, 1C), 135.54 (s, 2C), 133.35 (s, 2C), 131.80 (s, 2C), 130.74 (s, 2C), 130.70 (s, 2C), 129.60 (s, 2C), 128.09 (s, 2C), 119.54 (s, 2C), 119.08 (s, 2C), 73.45 (s, 2C), 29.30 (s, 2C), 25.58 (s, 2C). ^{19}F NMR (564 MHz, CD_2Cl_2): δ -145.96 (q, J_{BF} = 28.5 Hz), -146.15 (q, J_{BF} = 28.5 Hz), -146.72 (q, J_{BF} = 28.5 Hz), -146.91 (q, J_{BF} = 28.5 Hz).

2Cl$_4$. Under a nitrogen atmosphere, 10 mg of the bright orange **2** was dissolved in 0.5 mL of deuterated chloroform ($CDCl_3$) with minimal water content. The resulting orange solution gradually became more red, and after 10 minutes the ^{19}F signals of **2** were not visible. **2Cl$_4$** was crystallized out of 1mL of CH_2Cl_2 layered with 5mL of pentanes and cooled to -13 °C. The resulting red rod crystals were analysed using single crystal X-Ray diffraction (Figure 1). ^1H NMR (600 MHz, $CDCl_3$): δ 8.08 (s, BODIPY (3,5-position), 2H), 7.84 (s, BODIPY (3,5-position), 2H), 7.39 (s, BODIPY (1,7-position), 2H), 7.19 (m, phenyl (2,6-position), 2H), 7.12 (m, phenyl (4-position), 1H), 7.05 (m, phenyl (3,5-position), 2H), 6.71 (d, BODIPY (2,6-position), 4H), 6.17 (s, BODIPY (1,7-position), 2H), 4.31 (s, NC*H*$CH_2CH_2CH_2CH_2$C*H*N, 2H), 2.51 (s, NCHCH_2C*H*$_2$C*H*$_2$$CH_2$CHN, 2H), 2.00 (s, NCH$CH_2$C*H*$_2$C*H*$_2$$CH_2$CHN, 2H), 1.53 (s, NCHC*H*$_2$$CH_2CH_2$C*H*$_2$CHN, 4H). ^{11}B NMR (192 MHz, $CDCl_3$): δ 36.39 (br, 1B), 1.82 (s, 2B). ^{13}C NMR (150 MHz, $CDCl_3$): δ 147.9 (s, 2C), 144.47 (s, 2C), 142.6 (s, 2C), 135.80 (s, 1C), 134.43 (s, 2C), 132.23 (s, 2C), 130.69 (s, 2C), 129.63 (s, 2C), 129.5 (s, 2C), 128.48 (s, 2C), 126.98 (s, 2C), 118.42 (s, 2C), 117.96 (s, 2C), 72.3 (s, 2C), 28.2 (s, 2C), 254.46 (s, 2C).

[2(F)]$^-$. Under a nitrogen atmosphere, 10 mg of the bright orange **2** was dissolved in 0.5 mL of CD_3CN and 4.5 mg (0.017 mmol) Bu_4NF in 0.1 mL CD_3CN was added. The resulting orange solution immediately began to lose color and was colorless within three minutes. The solution was analysed by NMR spectroscopy after 10 minutes. ^1H NMR (600 MHz, CD_3CN): δ 7.37 (m), 7.20 (m), 7.12 (m), 6.44 (br), 6.09 (br), 4.51 (br), 3.11 (d, Bu_4N^+, 8H), 2.25 (d), 1.62 (m, Bu_4N^+, 8H), 1.36 (m, Bu_4N^+, 8H), 0.97 (t, Bu_4N^+, 12H). ^{11}B NMR (192 MHz, CD_3CN): δ 4.10 (t, J = 60 Hz), 3.19 (q, J = 52 Hz), 0.32 (t, J_{BF} = 32 Hz). ^{19}F NMR (376 MHz, CD3CN): δ -137.9 (q, J = 11 Hz), -139.2 (br), -142.2 (q, J = 52 Hz), -151.8 (s, F^-).

[Cp$_2$Co][2]. Under a nitrogen atmosphere, a solution of 8.0 mg (0.04 mmol) of Cp_2Co in 2 mL of methylene chloride was added to a solution of 23.0 mg (0.04 mmol) of **2** in 3 mL of methylene

chloride. The reaction mixture was stirred for 18 hours before solvent was removed under reduced pressure, yielding a brown solid. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.29 (Cp_2Co^+), 7.17 (Cp_2Co^+), 2.46, 2.12, 1.98, 1.71, 1.57. ^{11}B NMR (128 MHz, CD_2Cl_2): δ -0.29 (br). ^{13}C NMR (150 MHz, CD_2Cl_2): δ 85.45, 79.56, 74.60, 60.24, 39.93. ^{19}F NMR (376 MHz, CD_2Cl_2): δ -141.0 (br), -144.48 (br), -148.4 (br).

[Cp_2Co][Cp^*_2Co][2]. Under a nitrogen atmosphere, a solution of 8.0 mg (0.02 mmol) of Cp^*_2Co in 2 mL of methylene chloride was added to a solution of 12 mg (0.02 mmol) of **[Cp_2Co][2]** in 3 mL of methylene chloride. The reaction mixture was stirred for 18 hours before solvent was removed under reduced pressure, yielding a black oily solid. ^{1}H NMR (400 MHz, CD_2Cl_2): Paramagnetic. ^{11}B NMR (128 MHz, CD_2Cl_2): δ -0.20 (br). ^{13}C NMR (150 MHz, CD_2Cl_2): δ 94.16, 85.49, 79.44, 74.49, 60.12, 39.79, 8.40. ^{19}F NMR (376 MHz, CD_2Cl_2): δ -142.7 (br), -145.04 (br), -147.95 (br).

Computational Methods. All structures were fully optimized without symmetry constraints using the M06-2X[4] functional as implemented in Gaussian 09,[5] using the 6-31G(d,p) basis set[6-7] for all non-metal atoms and the Stuttgart basis set with effective core potential (ECP)[8] for the iron atoms in ferrocene and ferrocenium. The exchange-correlation functional M06-2X was chosen for the good overall performance observed in the description of main group compounds and BODIPY complexes.[1, 4, 9-12] In all calculations, the ultrafine integration grid was employed to ensure the stability of the optimization procedure for the molecules of interest. Each stationary point was confirmed by a frequency calculation at the same level of theory to be a real local minimum on the potential energy surface. The 6-311++G(d,p) basis set for all non-hydrogen atoms was used to compute more accurate electronic energies for the optimized geometries.[13-14]

General Structural Refinement Information

X-ray diffraction data for **$2Cl_4$** were collected at 100 K on a Bruker D8 Venture using CuKα (λ = 1.54178) radiation. Data have been corrected for absorption using SADABS[15] area detector absorption correction program. Using Olex2,[16] the structure was solved with the ShelXT[17] structure solution program using Direct Methods and refined with the ShelXL[18] refinement package using least squares minimization. Hydrogen atoms were placed in calculated positions using a ridged group model and refined with isotropic thermal parameters. The majority of non-hydrogen atoms were refined with anisotropic thermal displacement parameters. All calculations and refinements were carried out using APEX3,[19] SHELXTL,[20] Olex2,[16] and PLATON.[21]

X-ray diffraction data for **1** were collected at 298 K on a Bruker Apex II using MoKα (λ = 0.71073) radiation. Data have been corrected for absorption using SADABS[15] area detector absorption correction program. Using Olex2,[16] the structure was solved using Direct Methods and refined with the ShelXL[18] refinement package using least squares minimization. Hydrogen atoms were placed in calculated positions using a ridged group model and refined with isotropic thermal parameters. The majority of non-hydrogen atoms were refined with anisotropic thermal displacement parameters, see below discussion for further details. All calculations and refinements were carried out using APEX2,[22] SHELXTL,[20] Olex2,[16] and PLATON.[21] The crystals for **1** weakly diffracted and refinements were unable to provide a solution with R_1 and wR_2 values below 11.69% and 37.39%, thus a picture showing the connectivity is provided as opposed to a complete crystallographic information file.

2) Multinuclear NMR Spectra of 1

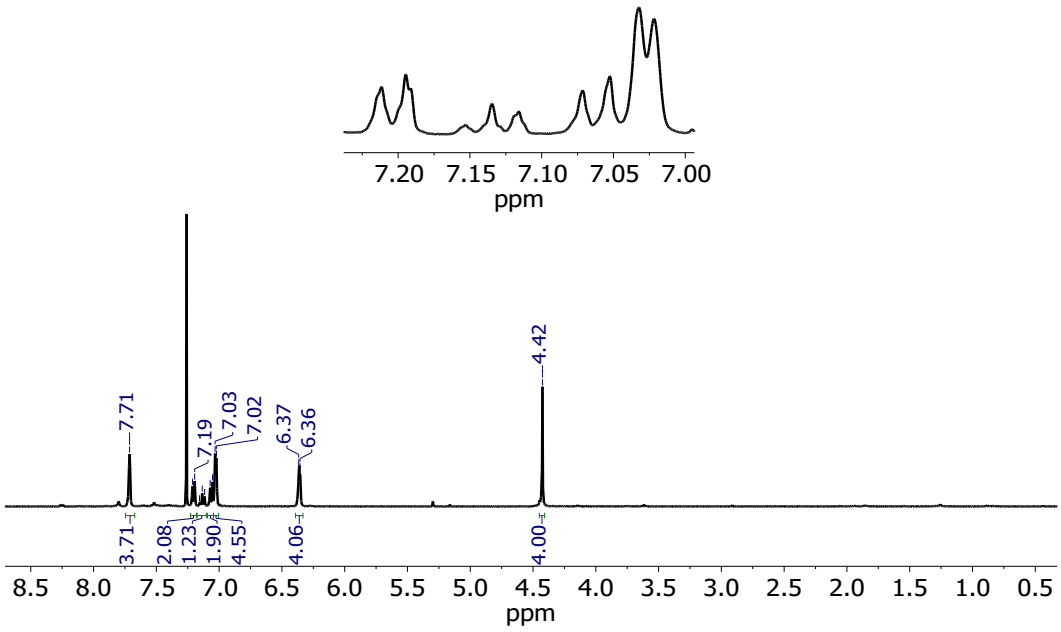


Figure S1. ^{1}H NMR spectra of **1** in $CDCl_3$.

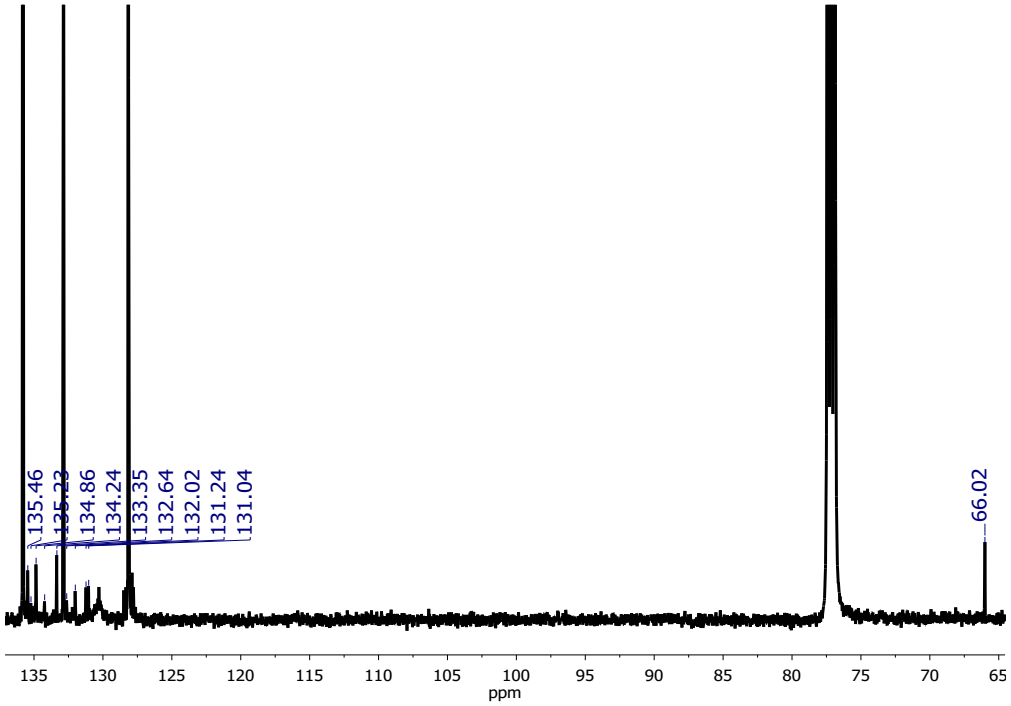


Figure S2. ^{13}C NMR spectra of **1** in $CDCl_3$.

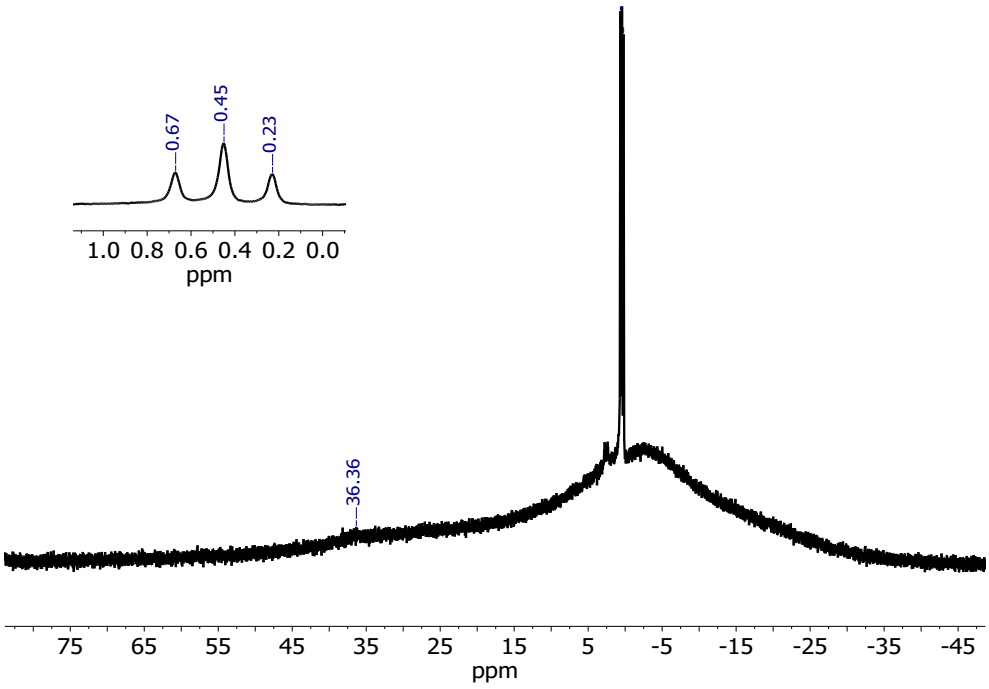


Figure S3. ^{11}B NMR spectrum of **1** in $CDCl_3$.

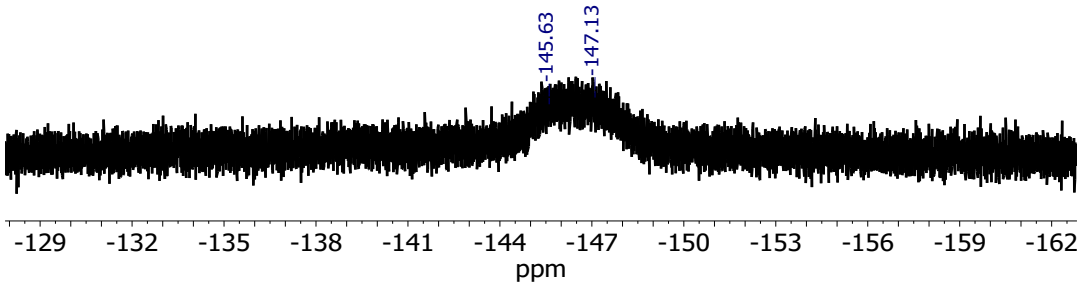


Figure S4. ^{19}F NMR spectrum of **1** in $CDCl_3$.

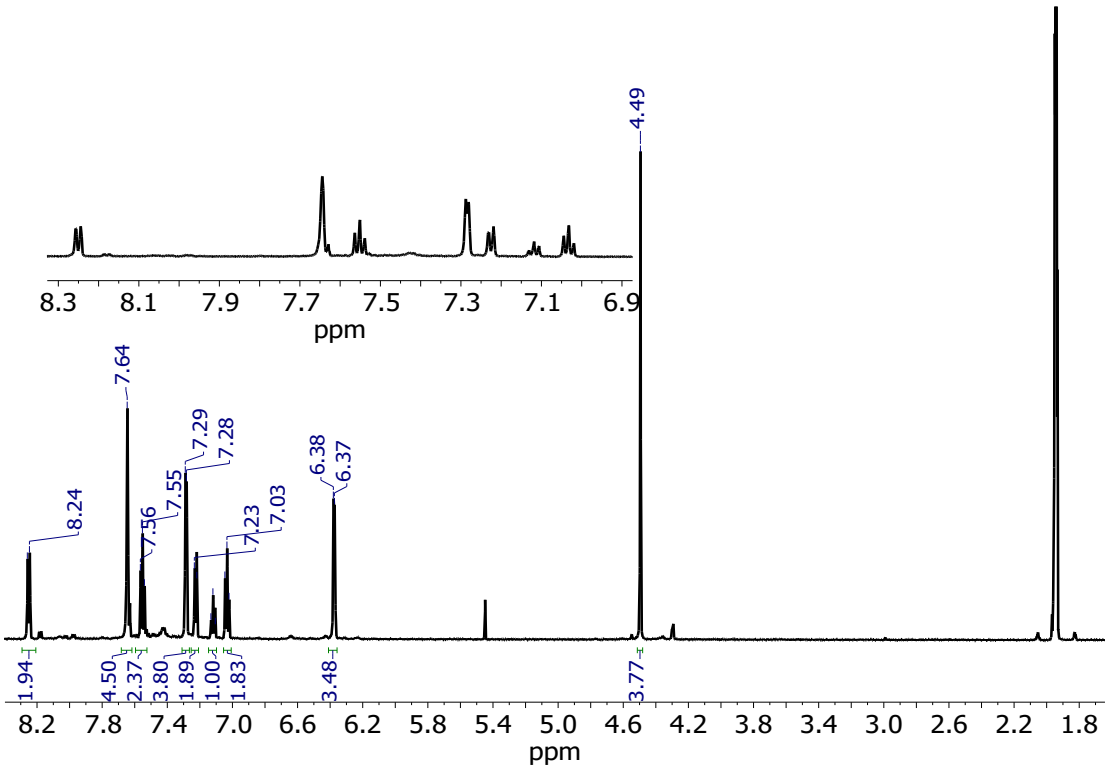


Figure S5. ^{1}H NMR spectra of **1** in CD_3CN.

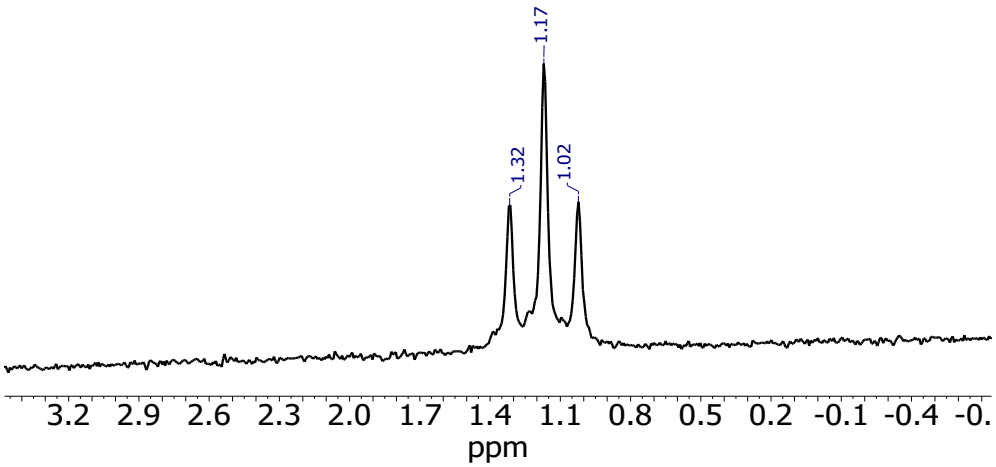


Figure S6. ^{11}B NMR spectrum of **1** in CD_3CN.

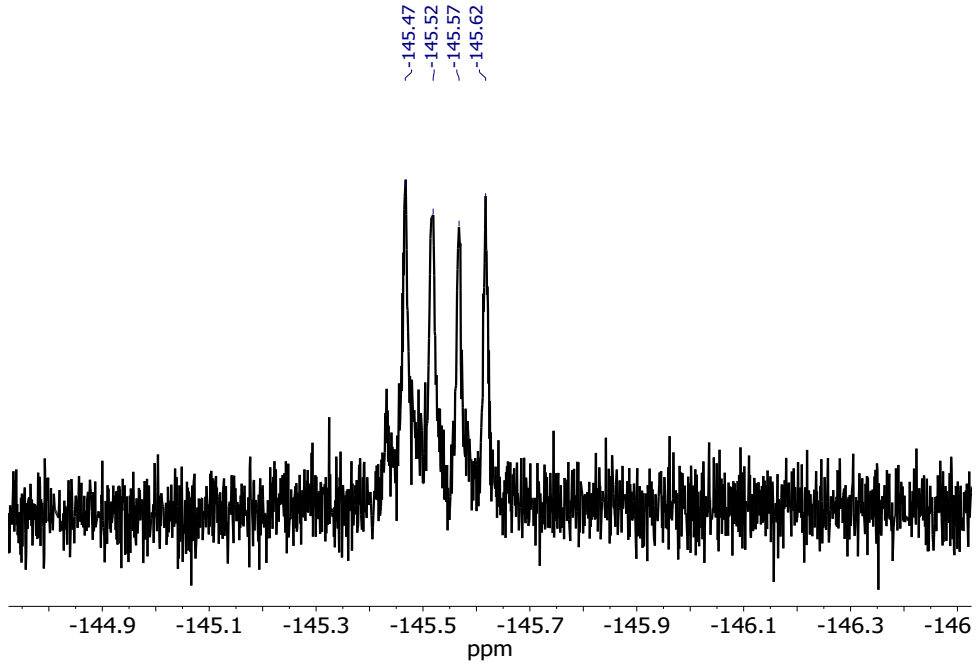


Figure S7. ^{19}F NMR spectrum of **1** in CD_3CN.

3) Multinuclear NMR Spectra of 2

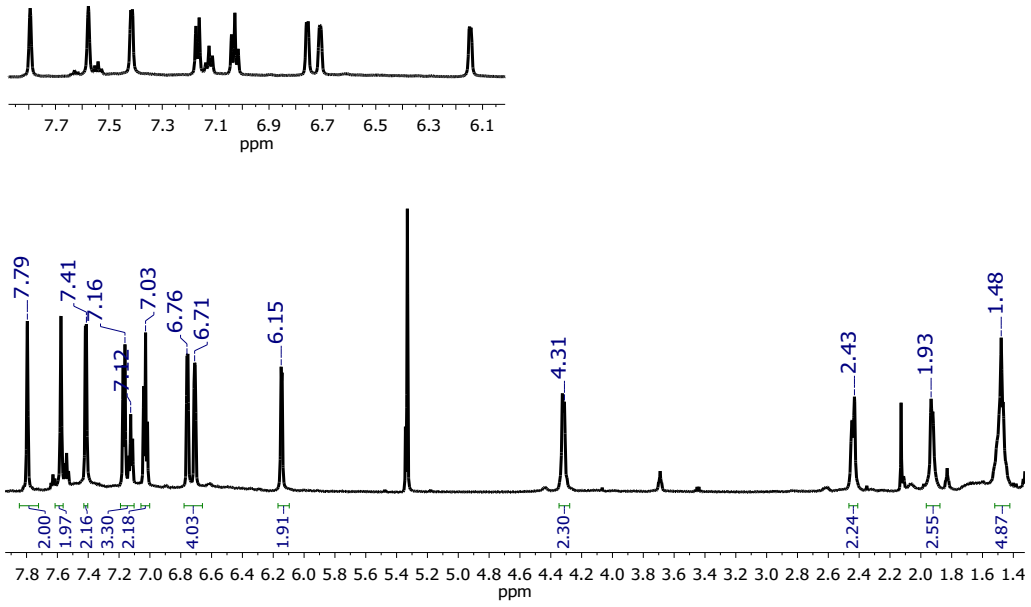


Figure S8. ^{1}H NMR spectra of **2** in CD_2Cl_2.

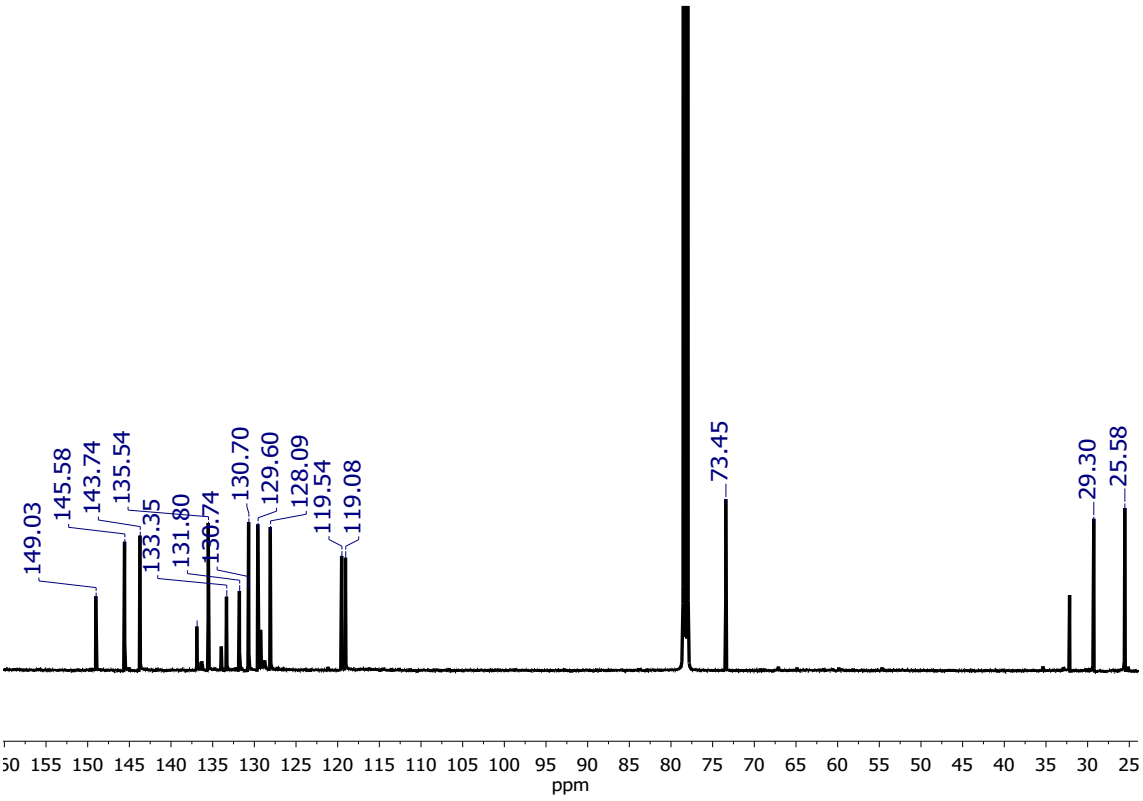


Figure S9. ^{13}C NMR spectra of **2** in $CDCl_3$.

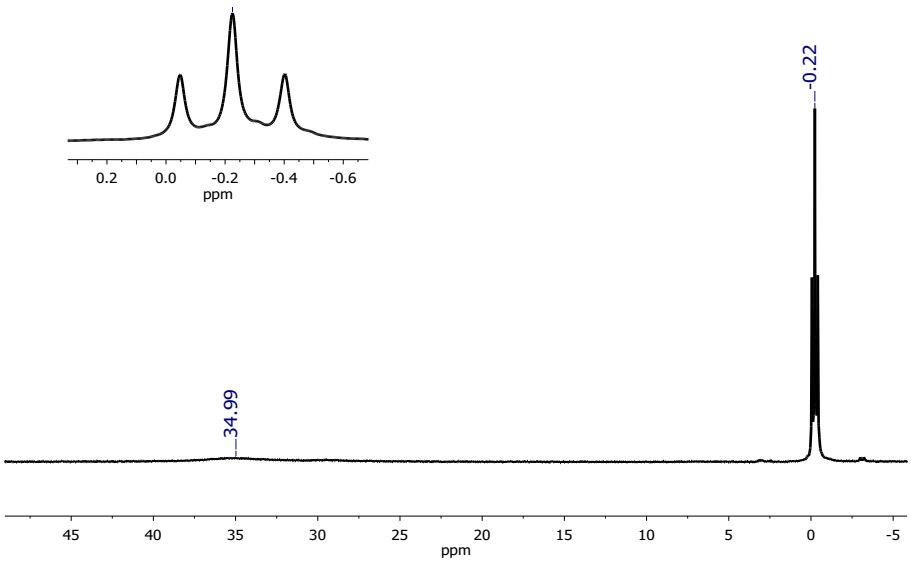


Figure S10. ^{11}B NMR spectra of **2** in CD_2Cl_2 with insert zoomed in on the peak at 0.22 ppm.

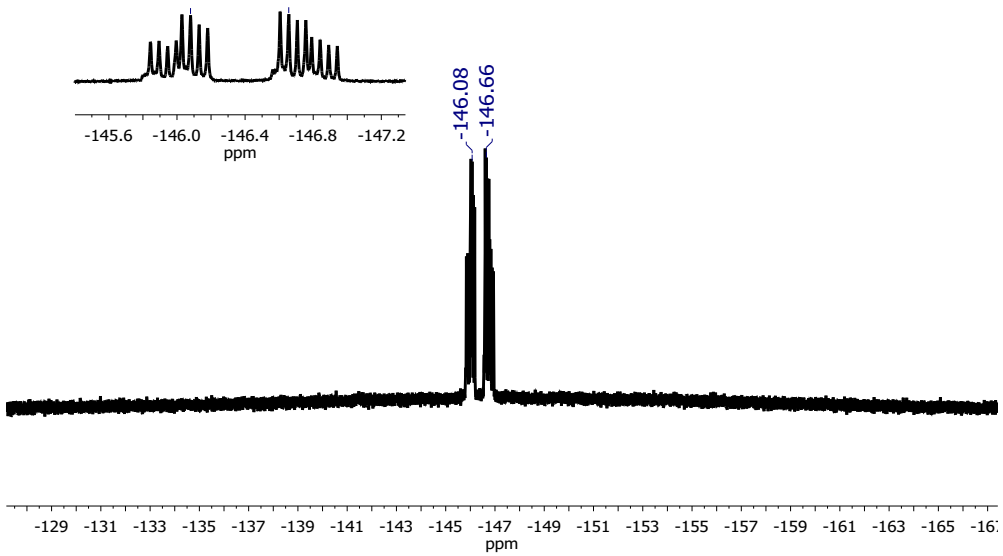


Figure S11. ^{19}F NMR spectra of **2** in CD_2Cl_2 with insert zoomed in on the quartet of AB quartets at -146.7 ppm.

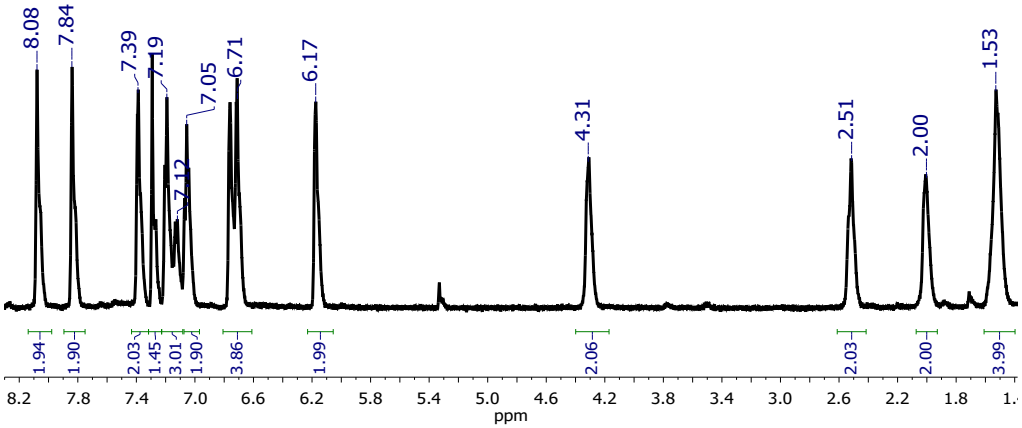


Figure S12. ^{1}H NMR spectrum of **$2Cl_4$** in $CDCl_3$.

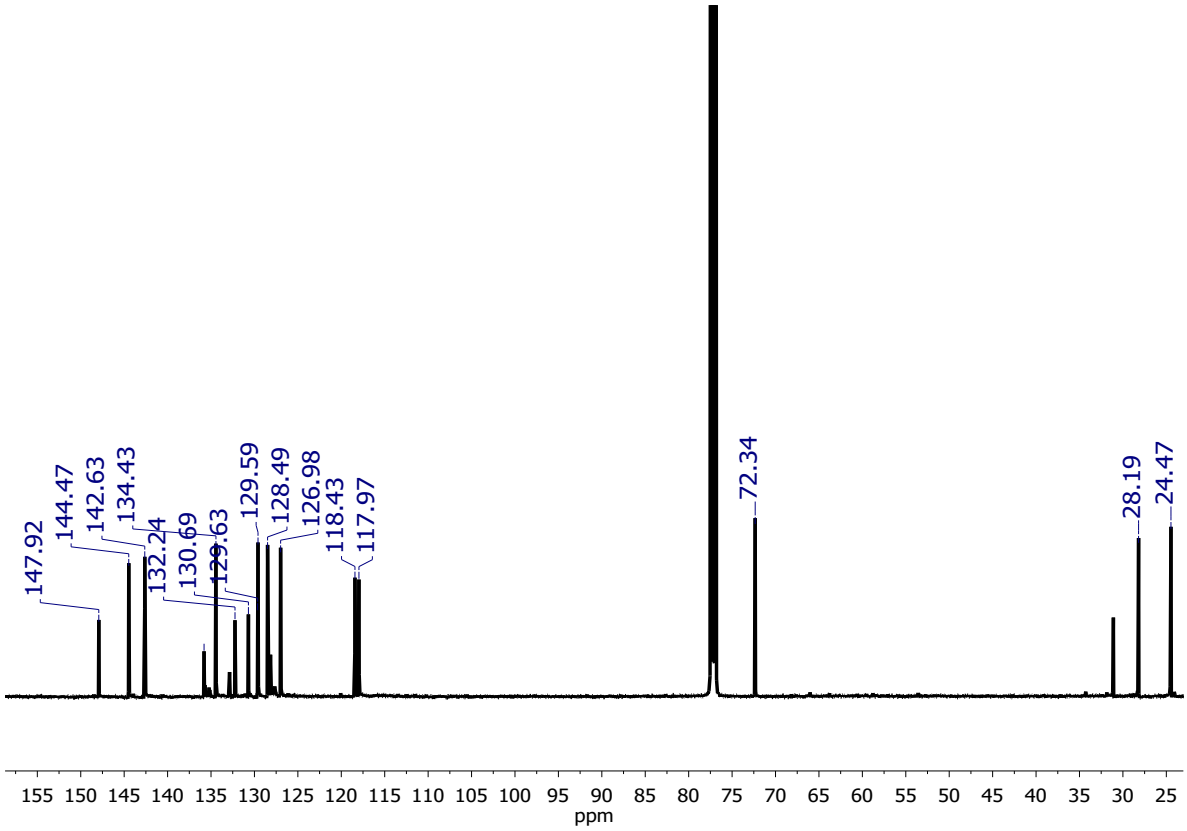


Figure S13. ^{13}C NMR spectrum of **2Cl₄** in $CDCl_3$.

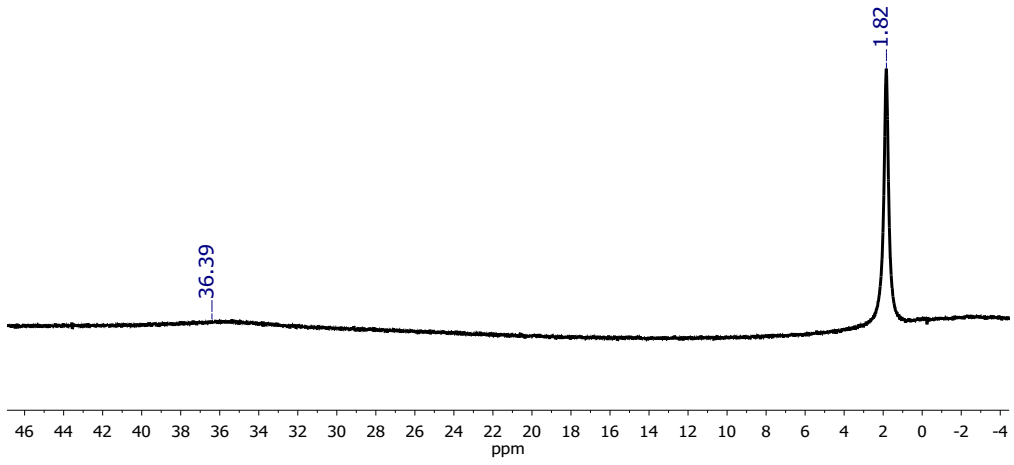


Figure S14. ^{11}B NMR spectrum of **2Cl₄** in $CDCl_3$.

4) Multinuclear NMR Spectra of Reduced Boranes

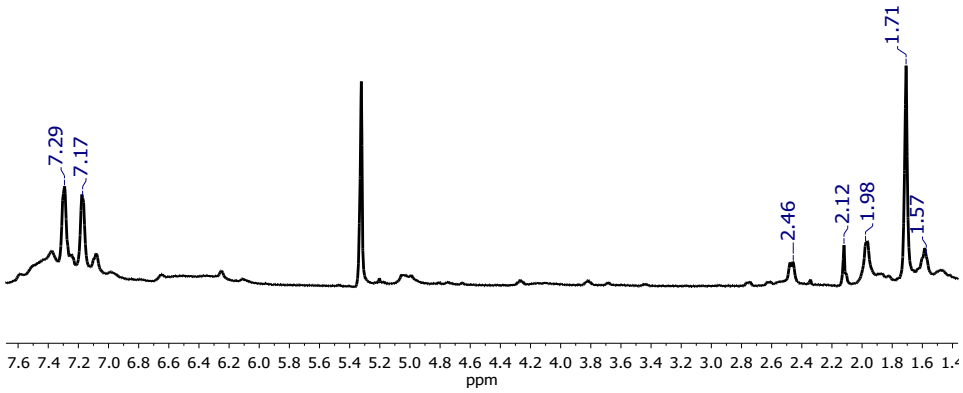


Figure S15. ^{1}H NMR spectrum of **[Cp$_2$Co][2]** in CD_2Cl_2.

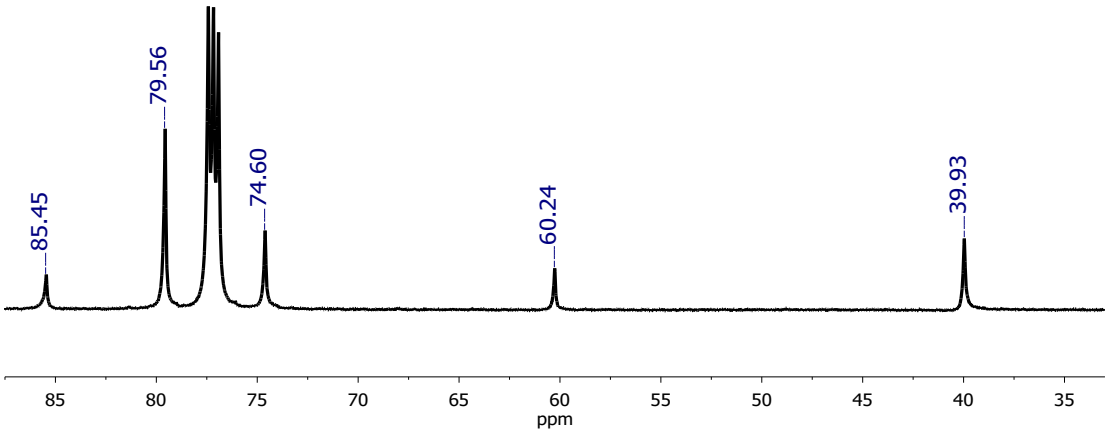


Figure S16. ^{13}C NMR spectrum of **[Cp$_2$Co][2]** in $CDCl_3$.

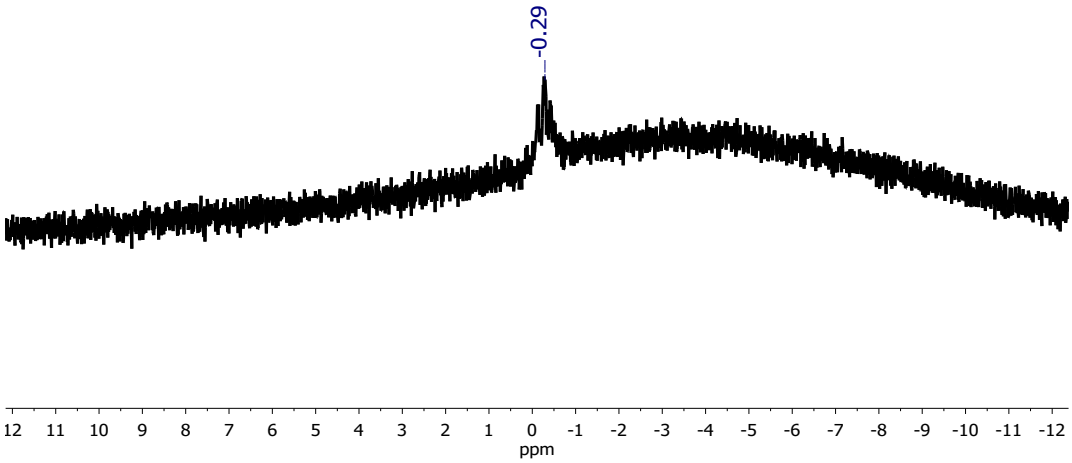


Figure S17. ^{11}B NMR spectrum of **[Cp$_2$Co][2]** in CD_2Cl_2.

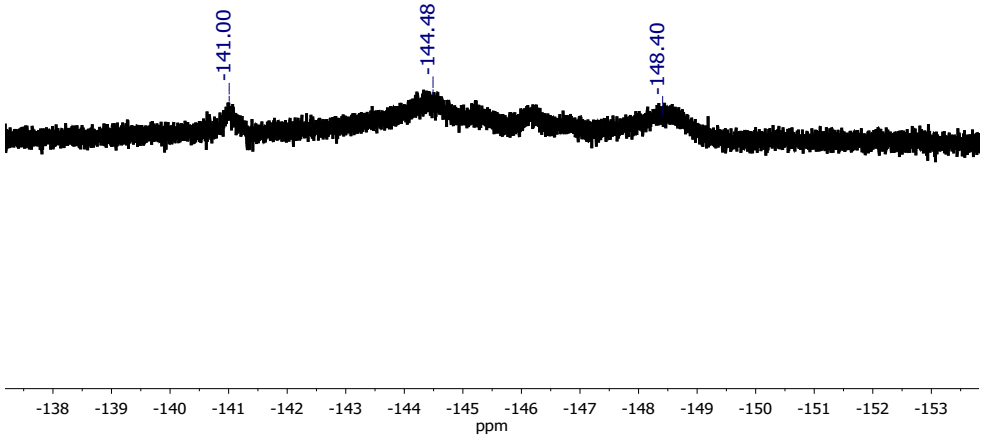


Figure S18. ^{19}F NMR spectrum of **[Cp$_2$Co][2]** in CD_2Cl_2.

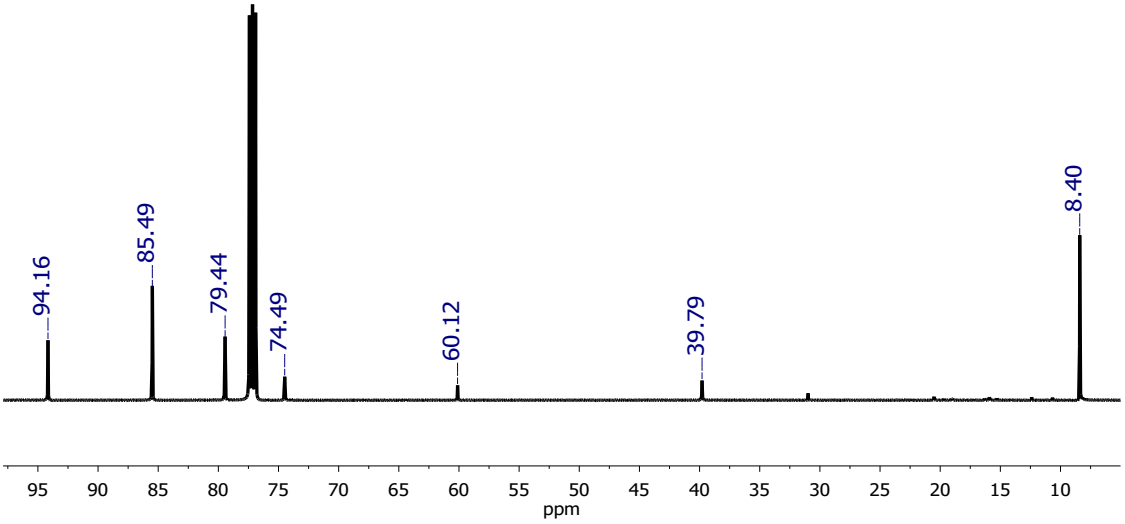


Figure S19. ^{13}C NMR spectrum of **[Cp$_2$Co][Cp$^*_2$Co][2]** in $CDCl_3$.

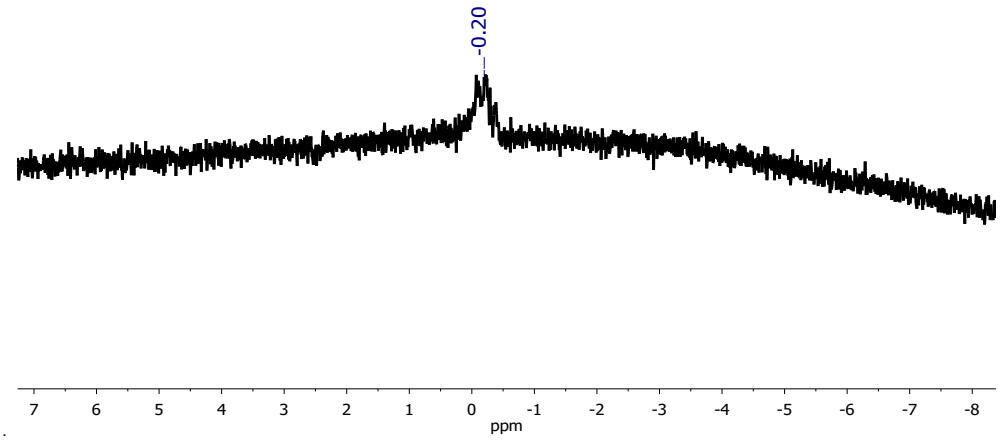


Figure S20. ^{11}B NMR spectrum of **[Cp$_2$Co][Cp$^*_2$Co][2]** in CD_2Cl_2.

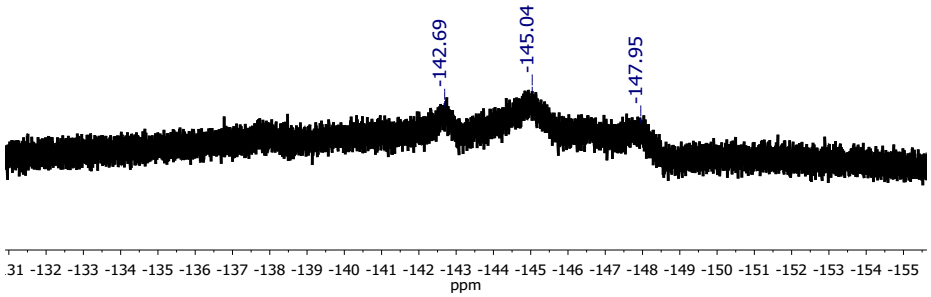


Figure S21. ^{19}F NMR spectrum of **[Cp$_2$Co][Cp$^*_2$Co][2]** in CD_2Cl_2.

5) Multinuclear NMR Spectra of Lewis Bases and 2

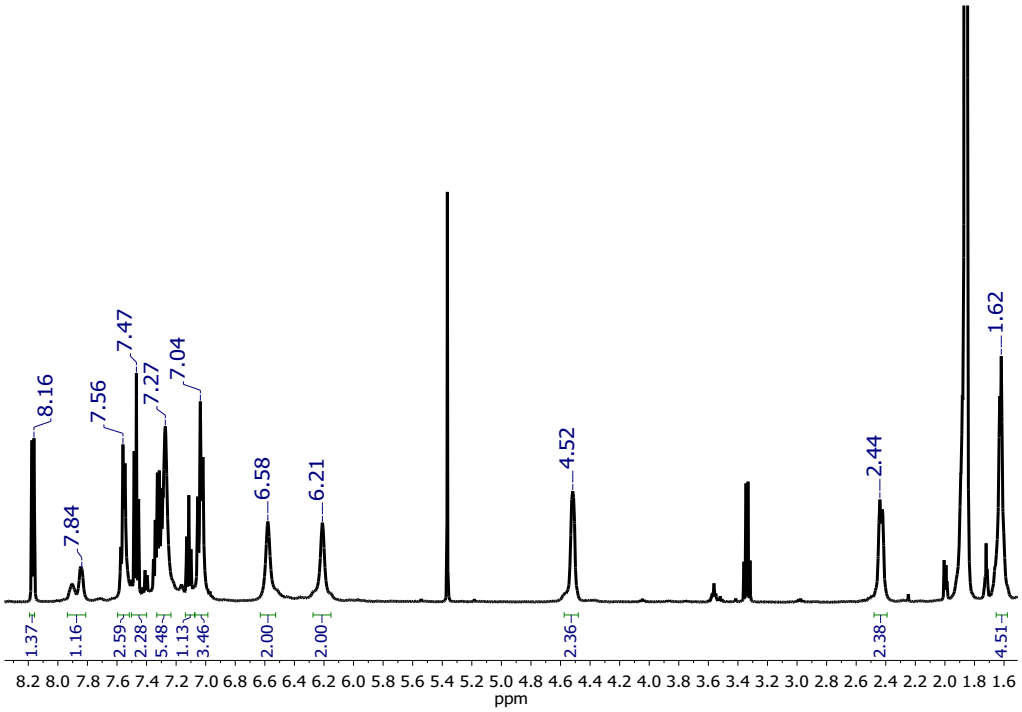


Figure S22. ^1H NMR spectrum of **2** in CD_3CN.

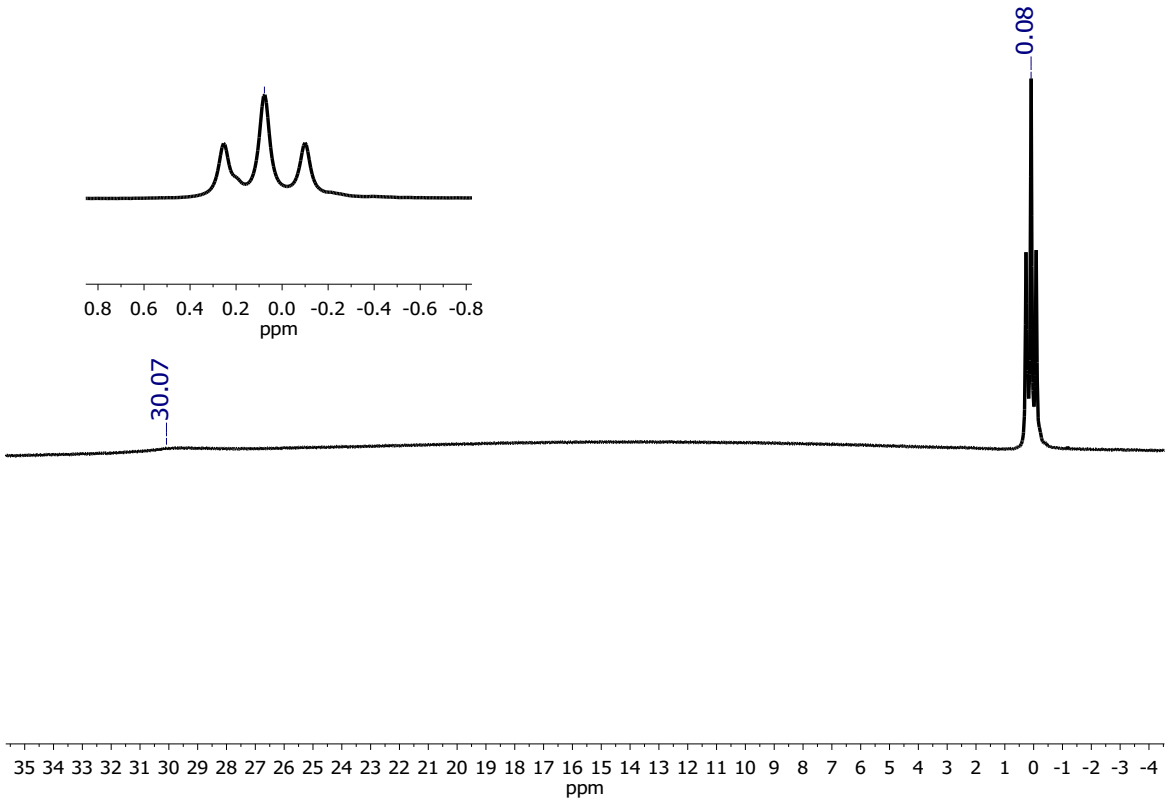


Figure S23. ^{11}B NMR spectra of **2** in CD_3CN.

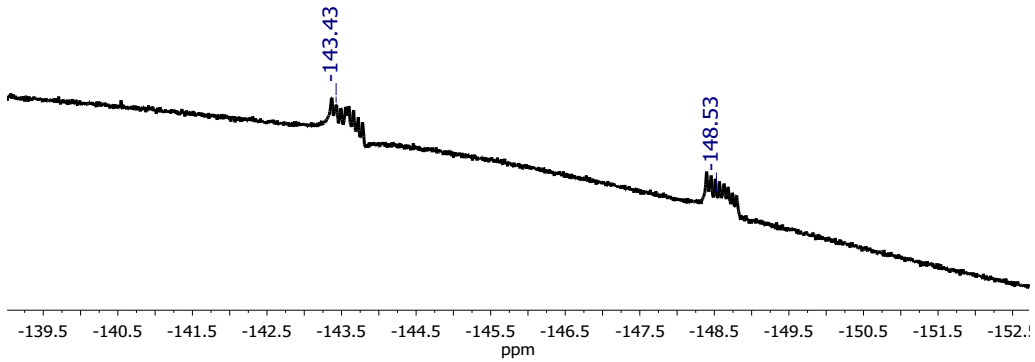


Figure S24. ^{19}F NMR spectrum of **2** in CD_3CN.

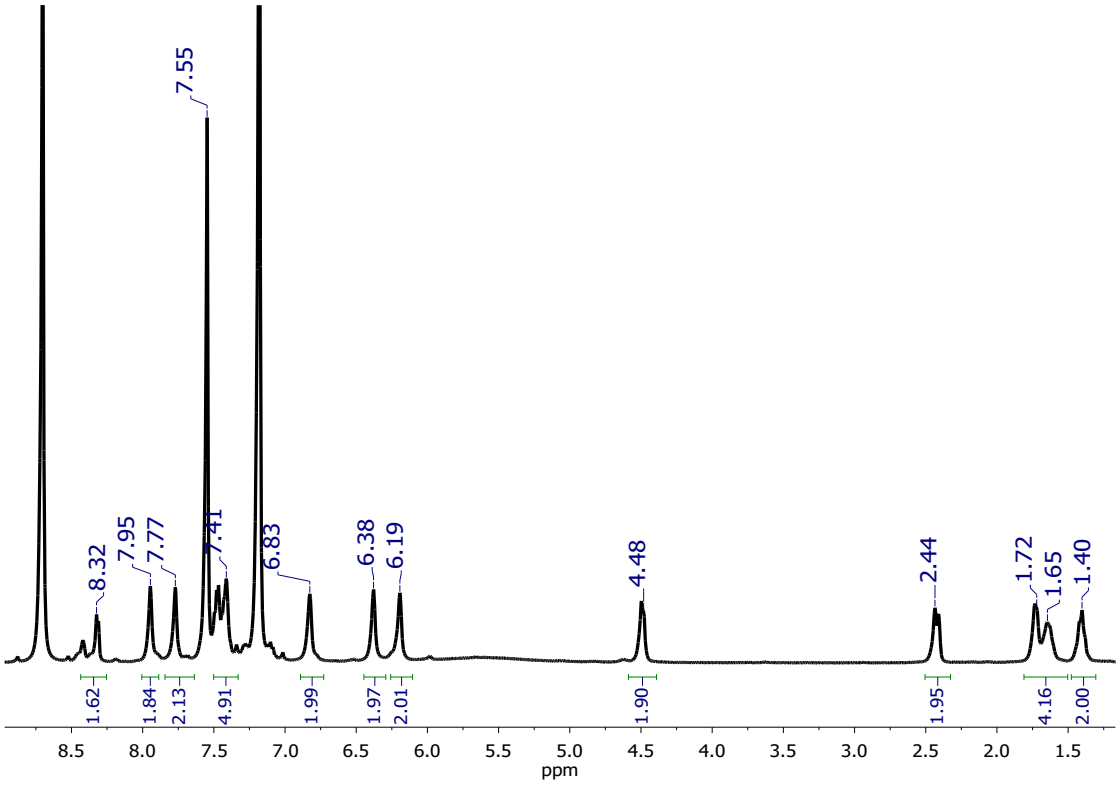


Figure S25. ^{1}H NMR spectrum of **2** in d-pyridine.

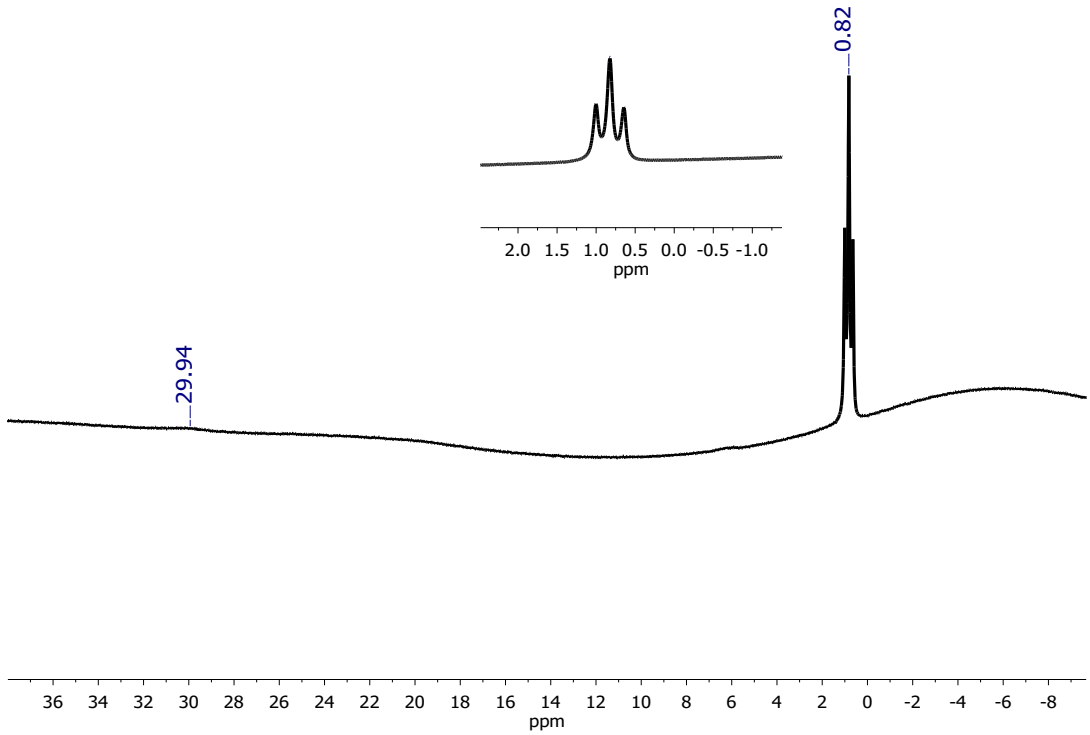


Figure S26. ^{11}B NMR spectrum of **2** in d-pyridine.

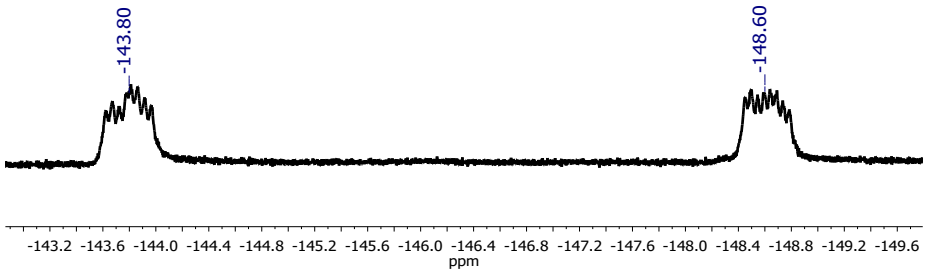


Figure S27. ^{19}F NMR spectrum of **2** in d-pyridine.

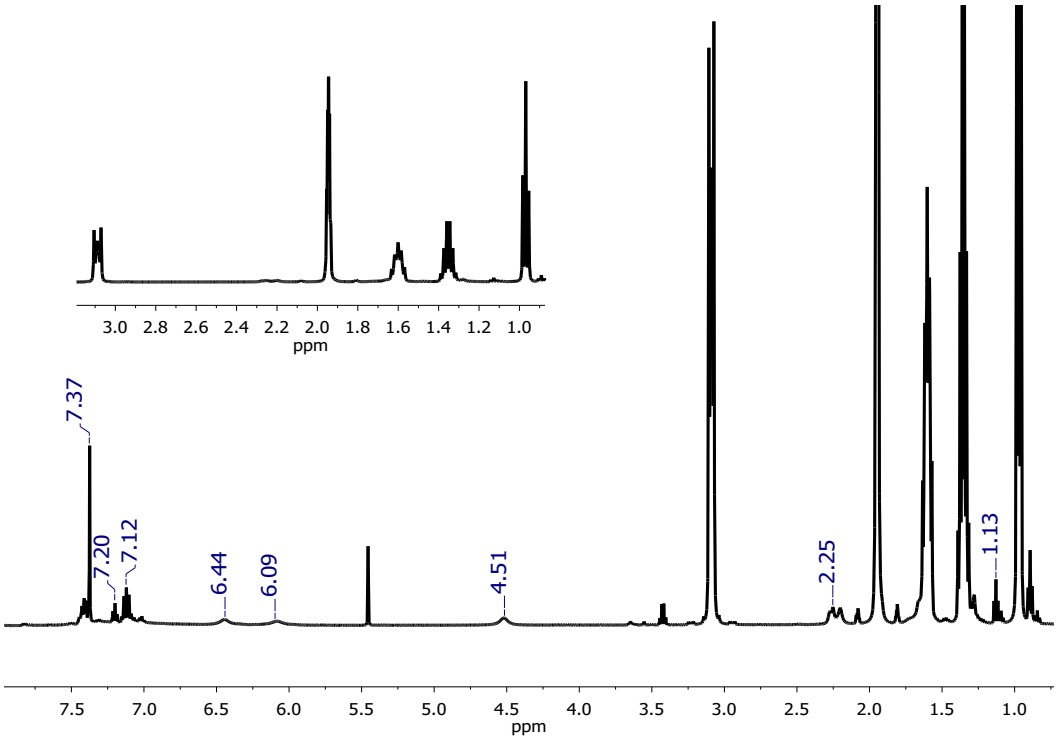


Figure S28. ^{1}H NMR spectrum of **[2(F)]**$^{-}$ in CD_3CN.

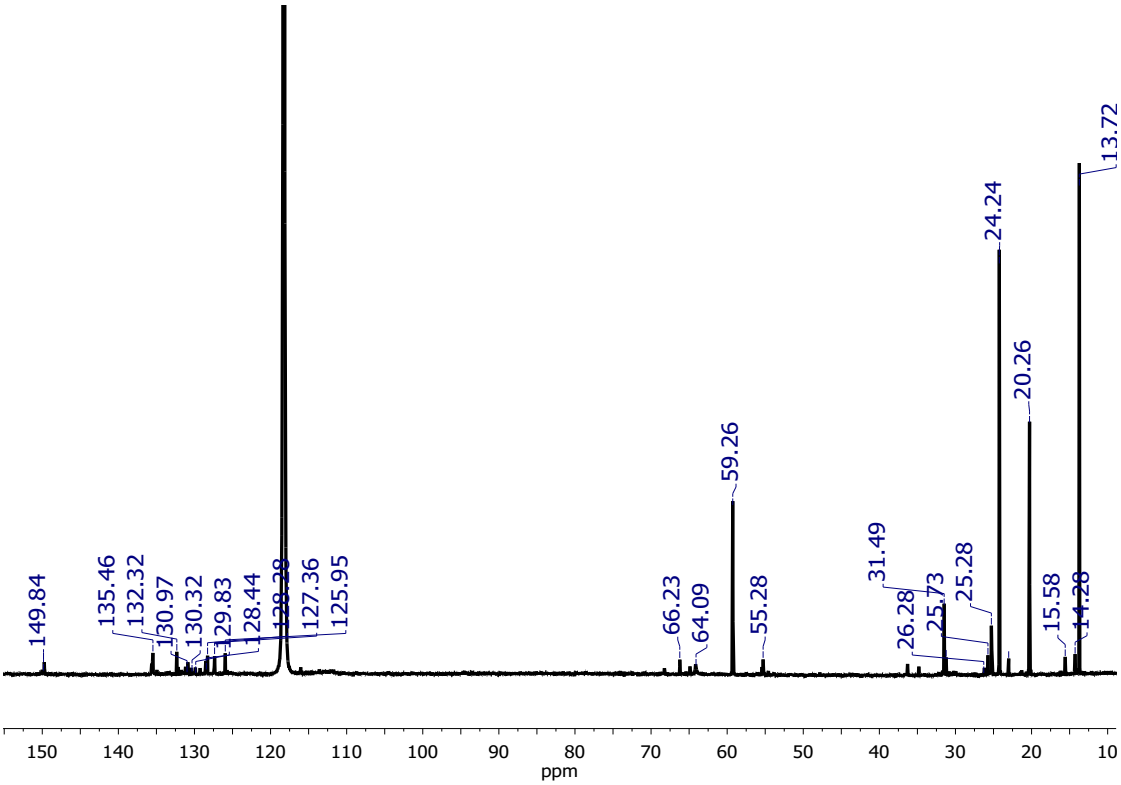


Figure S29. ^{13}C NMR spectrum of **[2(F)]**$^{-}$ in CD_3CN.

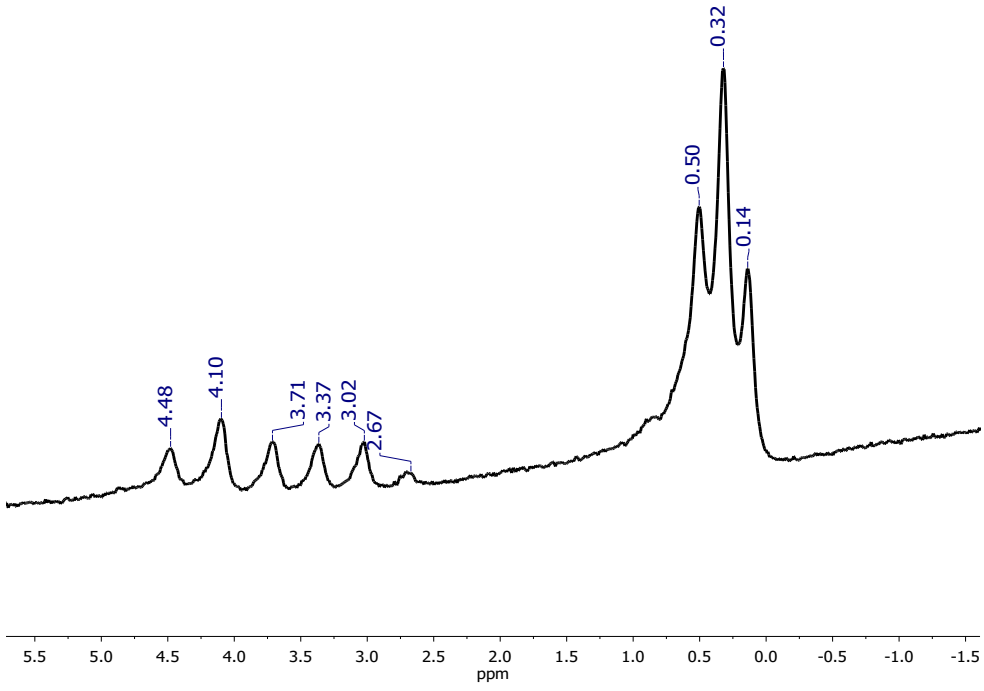


Figure S30. ^{11}B NMR spectrum of **[2(F)]**$^{-}$ in CD_3CN.

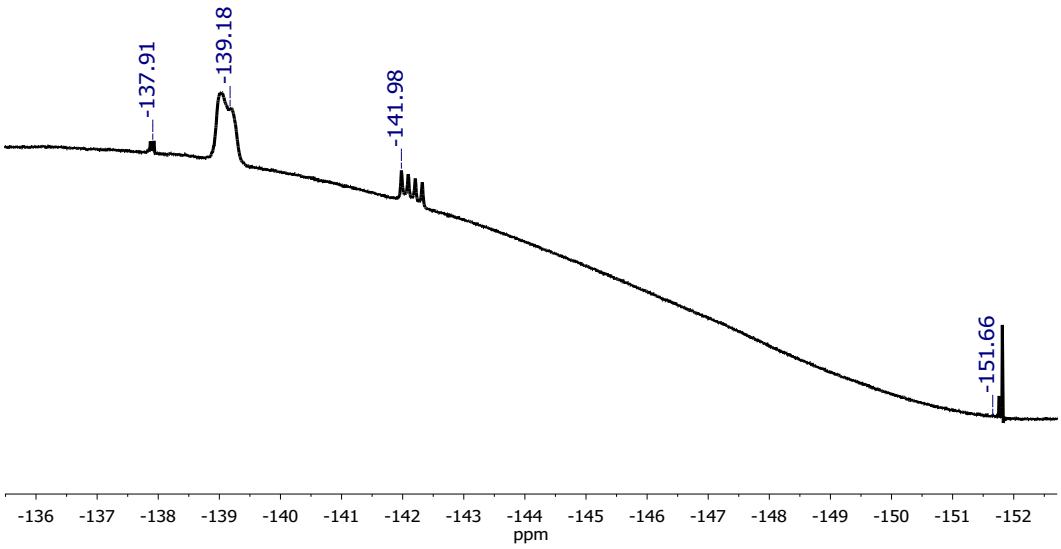


Figure S31. ^{19}F NMR spectrum of **[2(F)]**$^{-}$ in CD_3CN.

6) Cyclic Voltammograms of 2

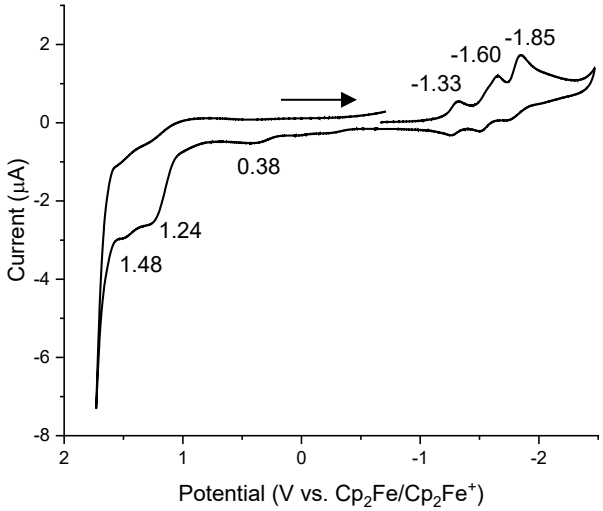


Figure S32. Cyclic voltammogram of **2** in CH_2Cl_2. Scan rate = 100 mV/s, electrolyte = $Bu_4NB(C_6F_5)_4$.

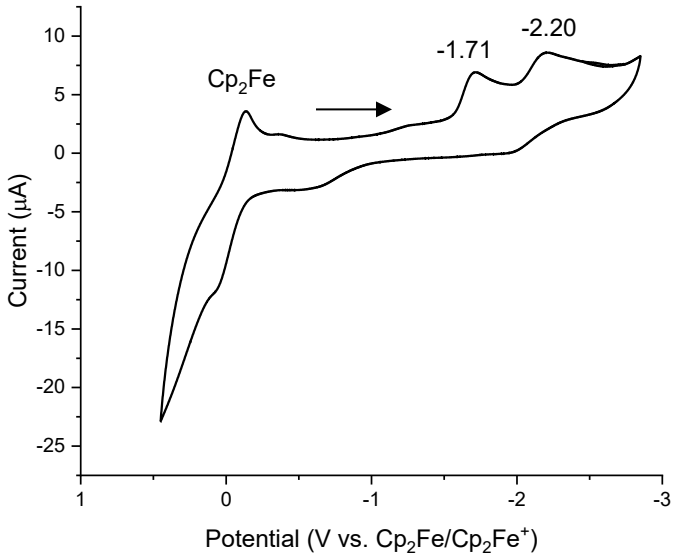


Figure S33. Cyclic voltammogram of **2** in pyridine. Scan rate = 750 mV/s, electrolyte = $Bu_4NB(C_6F_5)_4$.

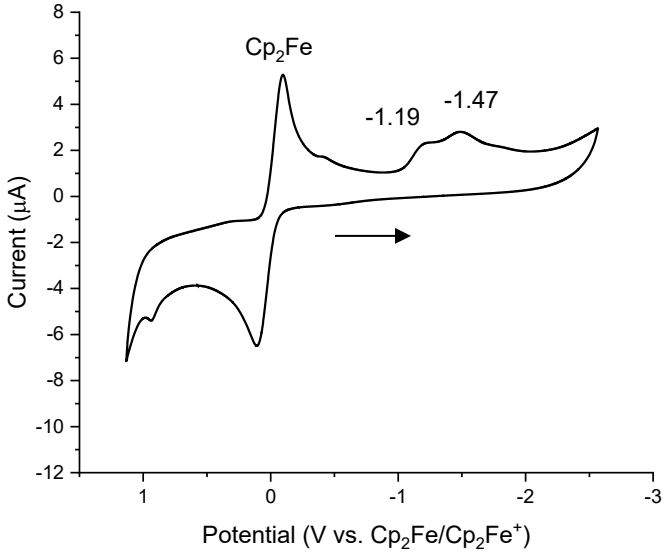


Figure S34. Cyclic voltammogram of **2** in MeCN. Scan rate = 100 mV/s, electrolyte = $Bu_4NB(C_6F_5)_4$.

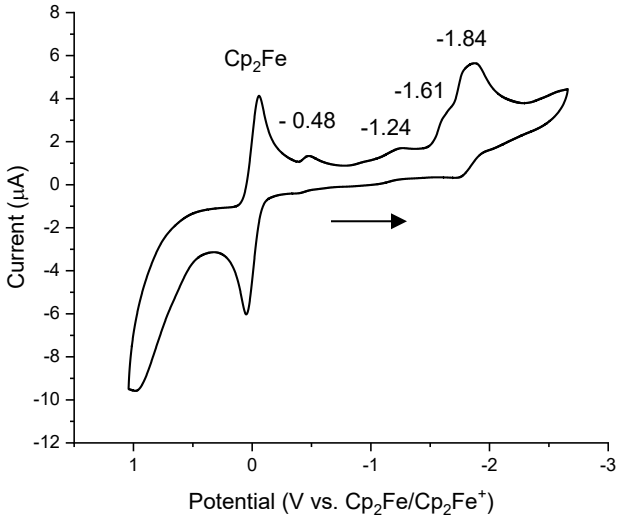


Figure S35. Cyclic voltammogram of **2** in MeCN with 1eq of Bu_4NF. Scan rate = 100 mV/s, electrolyte = $Bu_4NB(C_6F_5)_4$.

7) UV-Vis and Fluorescence Spectra of 1 and 2

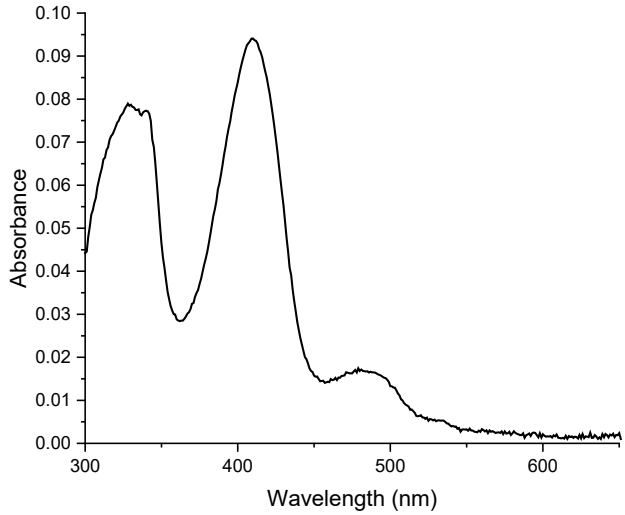


Figure S36. UV-Vis spectra of **1** (1.99 μM) in CH_2Cl_2.

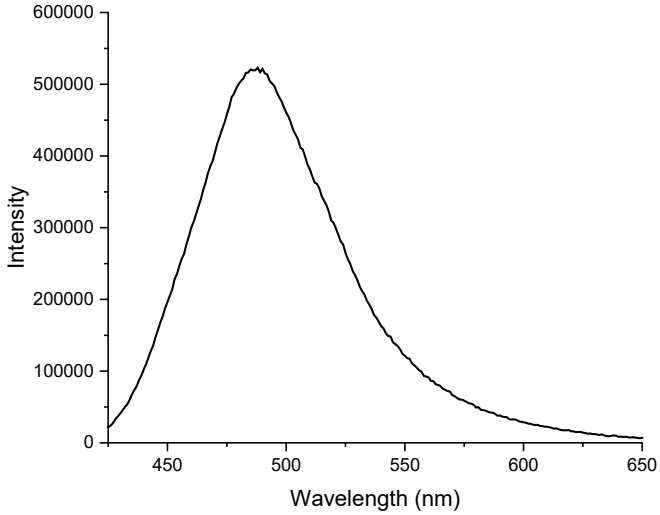


Figure S37. Emission spectra of **1** (1.99 μM) in CH_2Cl_2 excited at 410 nm.

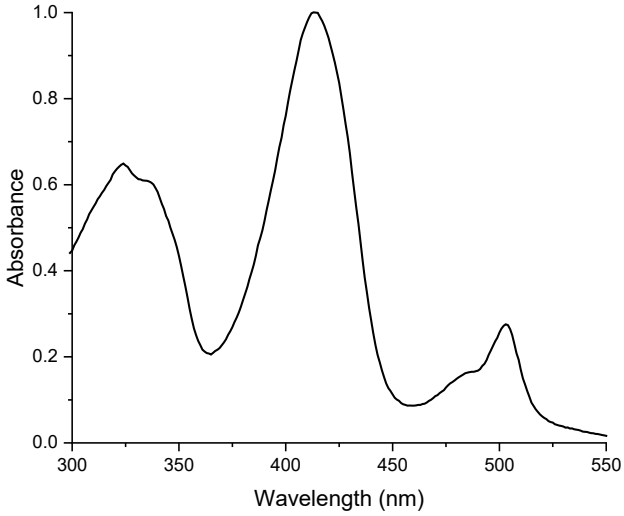


Figure S38. UV-Vis spectra of **2** (0.05 μM) in CH_2Cl_2.

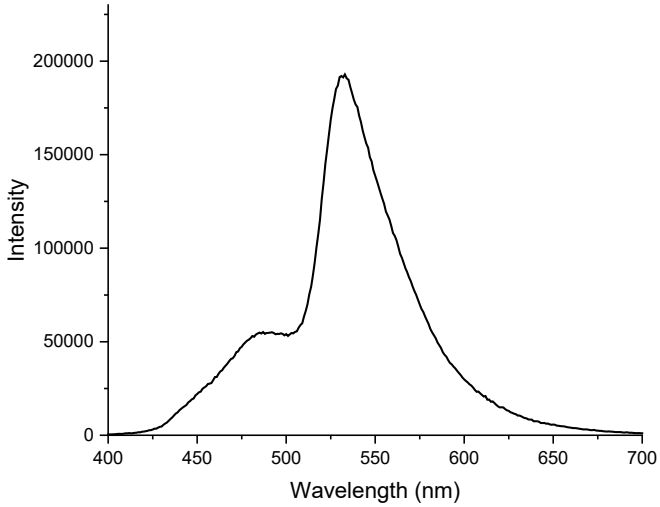


Figure S39. Emission spectra of **2** (0.05 μM) in CH_2Cl_2 excited at 413 nm.

8) Pictures of Selected Compounds

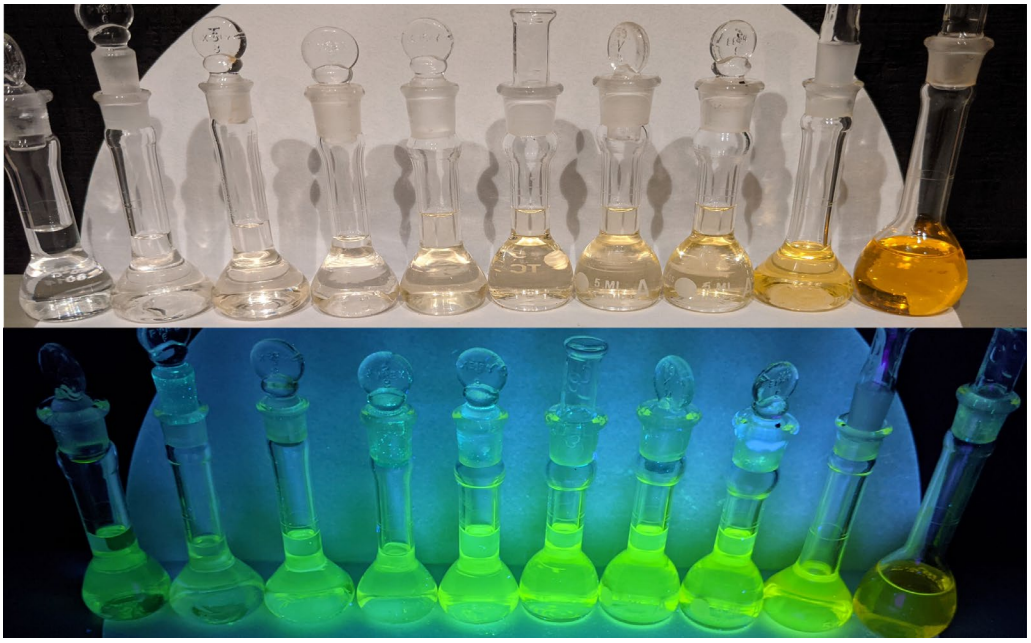


Figure S40. Picture of **2** (from 0.01 μM to 1 μM) in CH_2Cl_2 under lab light (top) and UV light (bottom).

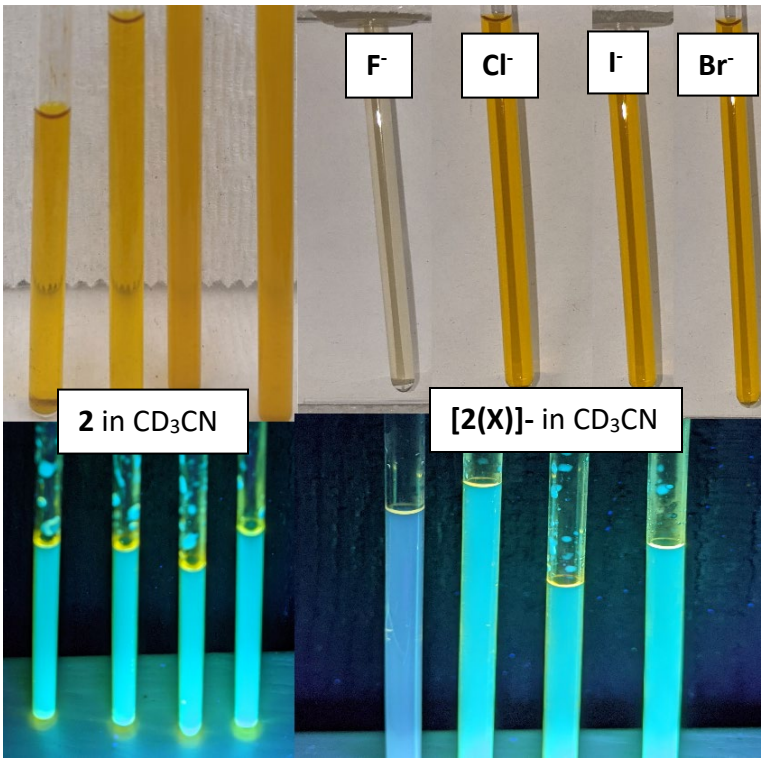


Figure S41. Pictures of **2** in CD_3CN under lab light (top) and UV light (bottom), before addition of halides (left) and after halide addition (right).

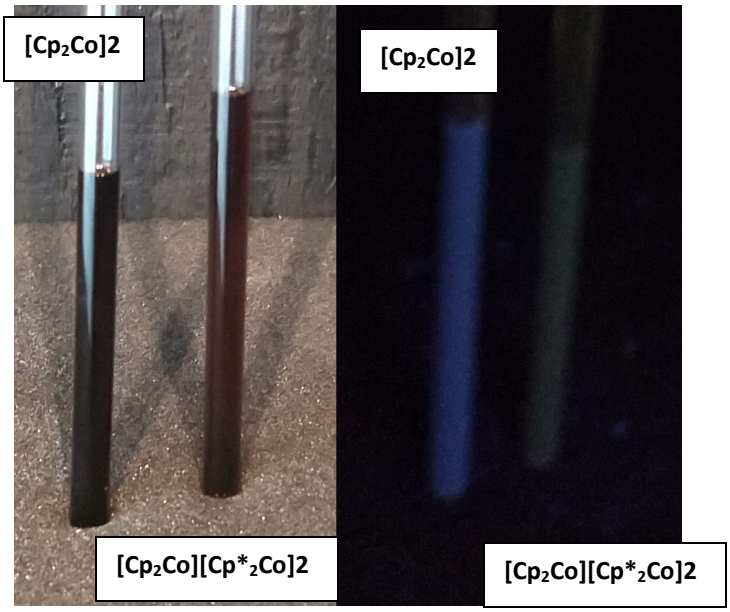


Figure S42. Pictures of **2** in CD_2Cl_2 under lab light (left) and UV light (right), after addition of Cp_2Co and Cp^*_2Co.

9) Picture of Molecular Structure of 1

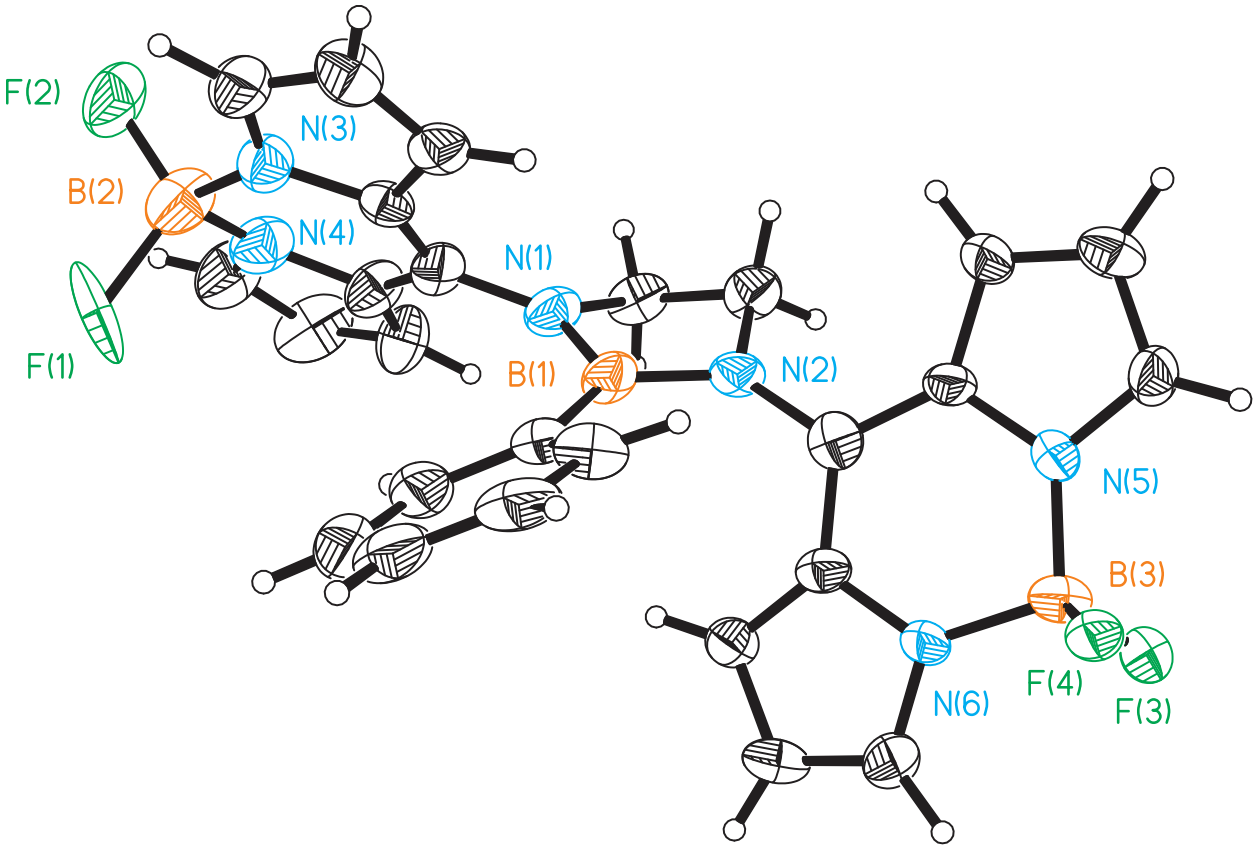


Figure S43. Picture of the molecular structure obtained from the weakly diffracting crystals of **1**. Thermal ellipsoids are drawn at 50% probability.

10) Frontier Molecular Orbitals of 1 and 2

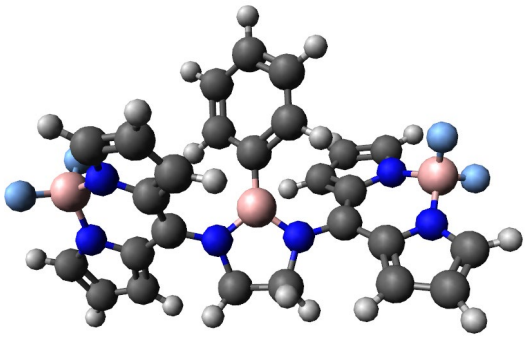
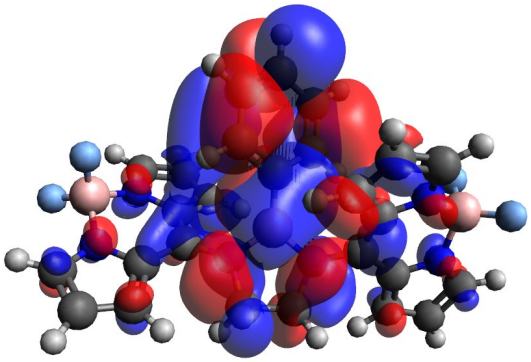
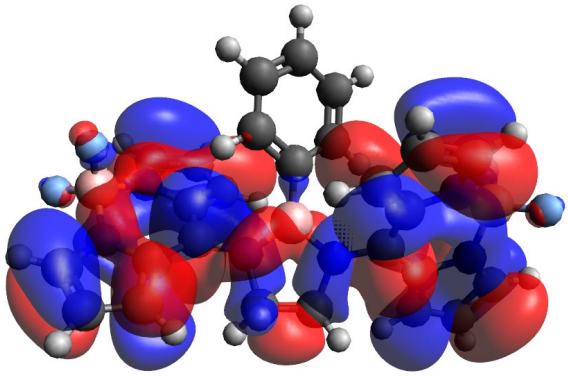
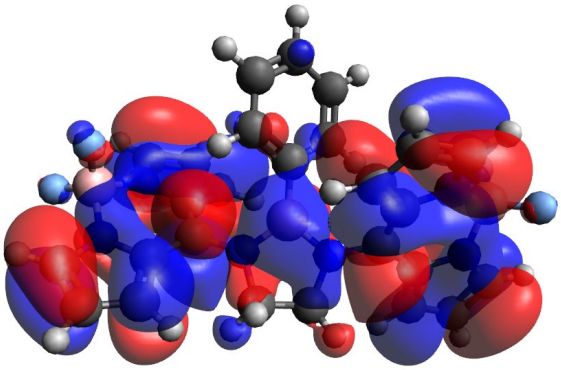
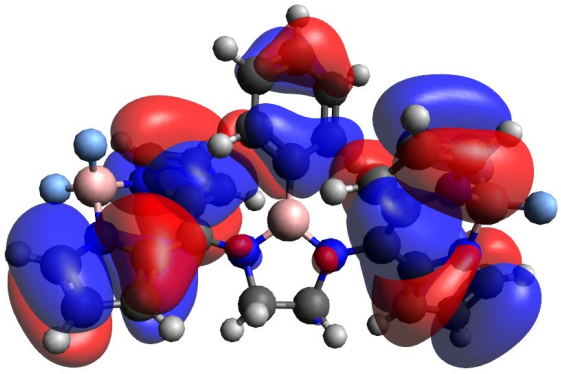
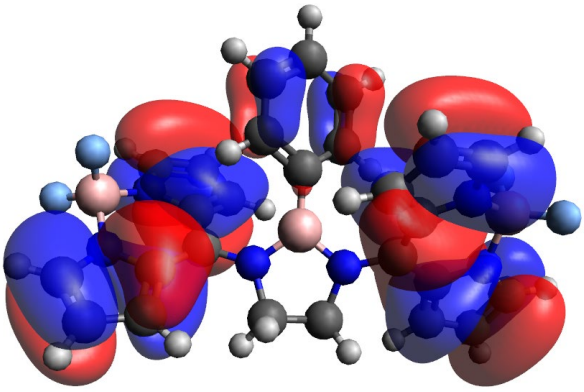
Orientation without Molecular Orbitals	LUMO+2
	
LUMO+1	**LUMO**
	
HOMO	**HOMO-1**
	

Figure S44. Frontier molecular orbitals of **1**. Isovalue = 0.01 e^{-}/a.u. C = black, N = blue, B = pink, F = green, and H = white.

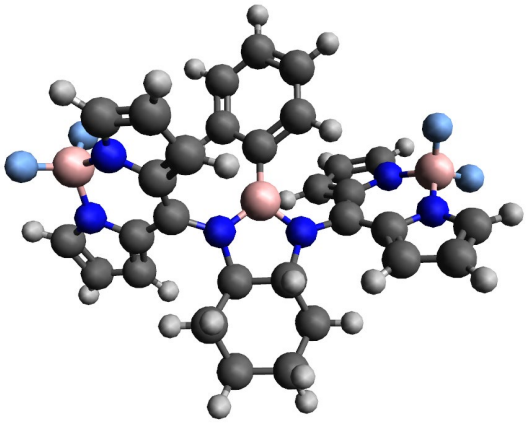
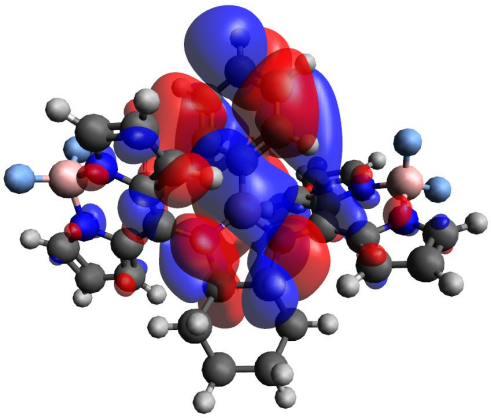
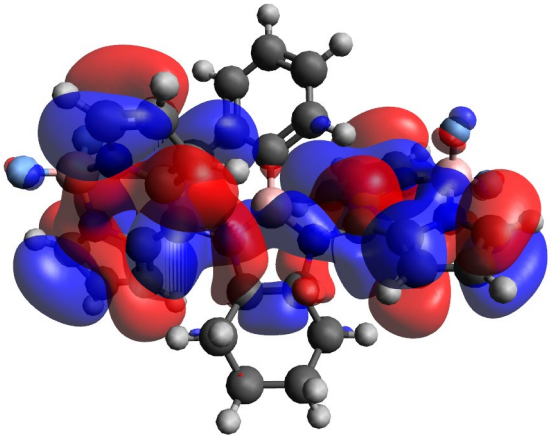
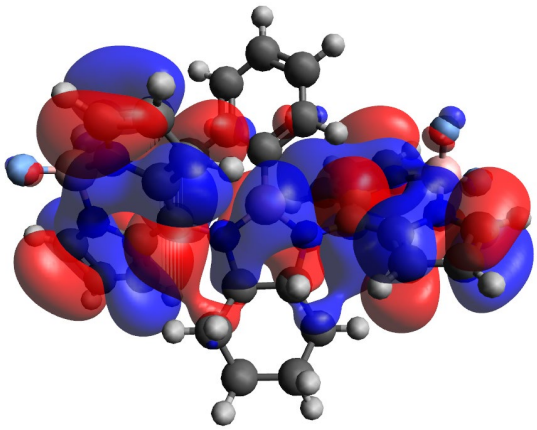
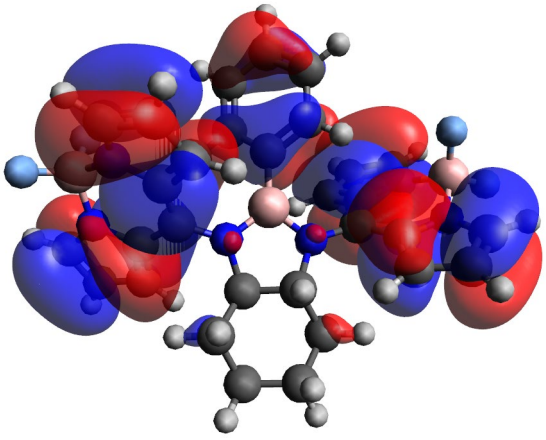
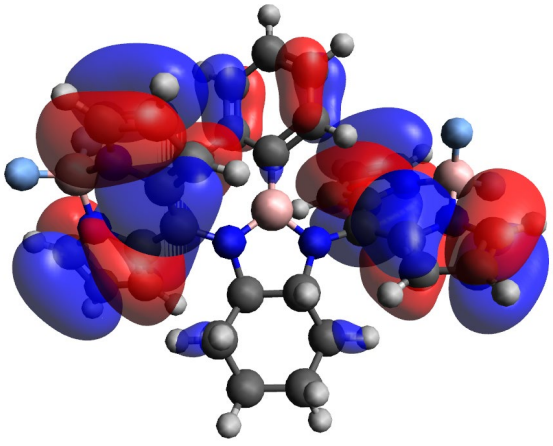
Orientation without Molecular Orbitals	LUMO+2
	
LUMO+1	**LUMO**
	
HOMO	**HOMO-1**
	

Figure S45. Frontier molecular orbitals of **2**. Isovalue = 0.01 e^{-}/a.u. C = black, N = blue, B = pink, F = green, and H = white.

11) Unpaired Spin Density plot for $[2]^{\bullet-}$ and $[2]^{\bullet\bullet 2-}$

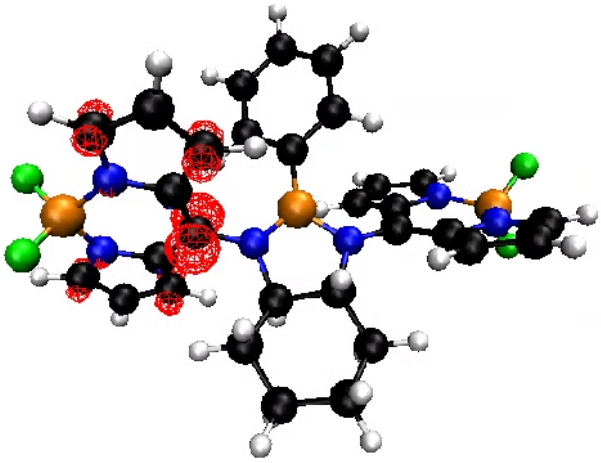


Figure S46. Unpaired spin density plot of $\mathbf{[2]^{\bullet-}}$. Isovalue = 0.01 e^-/a.u. C = black, N = blue, B = orange, F = green, and H = white.

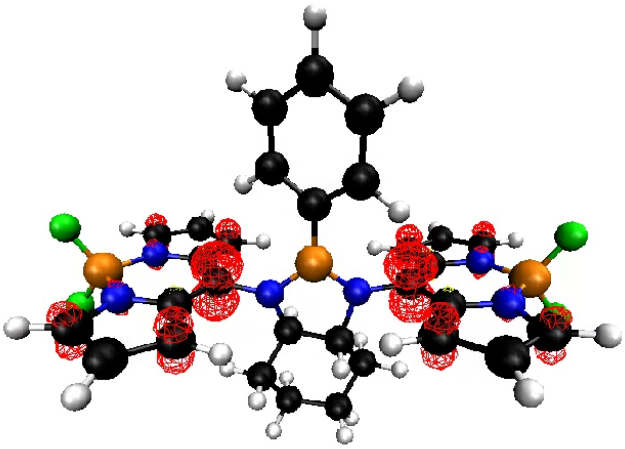


Figure S47. (Left) EPR spectrum of $\mathbf{[1]^{\bullet\bullet 2-}}$ in THF at 5 K. (Right) Unpaired spin density plot of $\mathbf{[2]^{\bullet\bullet 2-}}$. The positive and negative regions of spin density are shown as red and yellow mesh, respectively. Isovalue = 0.01 e^-/a.u. C = black, N = blue, B = orange, F = green, and H = white.

12) Table of Binding Affinity for Lewis Bases to 1 and 2

Table S1. Computed energies for the binding of Lewis bases to **1** and **2**. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

Complex	Lewis Base	Binding Affinity (kcal/mol)
1	H^-	−47.94
1Cl$_4$	H^-	−42.44
[1]$^{\bullet-}$	H^-	−24.00
[1]$^{\bullet\bullet 2-}$	H^-	+20.25
[1]$^{2-}$	H^-	+4.57
2	H^-	−54.52
2Cl$_4$	H^-	−38.25
[2]$^{\bullet-}$	H^-	−24.00
[2]$^{\bullet\bullet 2-}$	H^-	+20.25
[2]$^{2-}$	H^-	+4.57
1	F^-	−33.12
[1]$^{\bullet-}$	F^-	−12.27
[1]$^{\bullet\bullet 2-}$	F^-	+5.97
1	Cl^-	+3.63
1	Br^-	+10.73
2	F^-	−30.69
[2]$^{\bullet-}$	F^-	−17.31
[2]$^{\bullet\bullet 2-}$	F^-	+1.18
2	Cl^-	+5.09
2	Br^-	+13.84
1	Pyridine	+3.22
1	PMe_3	+20.40
1	MeCN	+15.95
2	PMe_3	+4.67
2	Pyridine	+4.64
[2]$^{\bullet-}$	Pyridine	+12.56
[2]$^{\bullet\bullet 2-}$	Pyridine	+21.34
BEt$_3$	F^-	−18.99
BEt$_3$	Cl^-	+3.08
BEt$_3$	Br^-	+7.48

13) Table of Computed Reduction Potentials

Table S2. Computed reduction potentials for BODIPY-containing boranes. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

Complex	Reduction Potential (V vs. Cp_2Fe/Cp_2Fe^+)
1	−1.41
[1]$^{\bullet-}$	−1.78
[1(F)]$^-$	−2.35
[1(F)]$^{\bullet 2-}$	−2.45
2	−1.41
[2]$^{\bullet-}$	−1.78
2(Py)	−1.80
[2(Py)]$^{\bullet-}$	−2.27
[2(F)]$^-$	−1.99
[2(F)]$^{\bullet 2-}$	−2.58

14) Table of Lewis Base Cone Angles and Free Binding Energies to 2

Table S3. List of cone angles and computed free energies for binding of ligands to **2**. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

Ligand	Cone Angle	ΔG (kcal/mol)
H^-	75	−54.5
F^-	92	−30.7
Cl^-	102	+9.0
Br^-	105	+17.2
PMe_3	118	+4.7

15) Gas Phase Energies of All Computed Structures

Table S4. Computed energies for all optimized structures. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
H^-	-0.4491144	-0.01	0.00236
F^-	-99.7233502	-0.014159	0.00236
Cl^-	-460.2172788	-0.015023	0.00236
Br^-	-2571.832849	-0.016176	0.00236
Pyridine	-248.177987	0.062386	0.094971
PMe_3	-460.9904557	0.084679	0.121523
MeCN	-132.6958226	0.021992	0.050523
Ferrocene	-1650.427881	0.135834	0.181188
Ferrocenium	-1650.165026	0.13675	0.181379
1	-1805.627547	0.393038	0.488363
[1]$^{\bullet-}$	-1805.698432	0.388474	0.485575
[1]$^{\bullet\bullet2-}$	-1805.672778	0.379794	0.481596
[1]$^{2-}$	-1805.645646	0.389389	0.483591
2	-1961.6211	0.48374	0.585792
[2]$^{\bullet-}$	-1961.688341	0.47758	0.582698
[2]$^{\bullet\bullet2-}$	-1961.665821	0.471184	0.579182
[2]$^{2-}$	-1961.636188	0.479089	0.580519
[1(H)]$^-$	-1806.317519	0.404924	0.49854
[1(H)]$^{\bullet2-}$	-1806.252412	0.396339	0.493265
[1(H)]$^{3-}$	-1806.053908	0.390902	0.488731
[1(H)]$^{\bullet\bullet3-}$	-1806.088909	0.390606	0.488721
1Cl$_4$	-3246.997371	0.384794	0.483805
[1Cl$_4$(H)]$^-$	-3247.680993	0.394108	0.493324
2Cl$_4$	-3402.991346	0.476072	0.581387
[2Cl$_4$(H)]$^-$	-3403.665942	0.484218	0.590122
[1(F)]$^-$	-1905.584637	0.396724	0.491798
[1(Cl)]$^-$	-2265.927518	0.394328	0.490664
[1(Br)]$^-$	-4377.545564	0.392677	0.49048
1(PMe$_3$)	-2266.625403	0.511742	0.614776
1(Py)	-2053.839024	0.484843	0.586602
1(NCMe)	-1938.336353	0.441386	0.540538

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
[2(H)]$^{-}$	-1962.288082	0.493748	0.594459
[2(H)]$^{\bullet 2-}$	-1962.240818	0.486093	0.590058
[2(H)]$^{3-}$	-1962.052457	0.481287	0.58554
[2(H)]$^{\bullet\bullet 3-}$	-1962.085018	0.479713	0.585377
[2(F)]$^{-}$	-2061.57206	0.486936	0.588903
[2(F)]$^{\bullet 2-}$	-2061.526648	0.478613	0.584972
[2(F)]$^{3-}$	-2061.344157	0.475607	0.580547
[2(F)]$^{\bullet\bullet 3-}$	-2061.376256	0.472327	0.580024
[2(Cl)]$^{-}$	-2421.915566	0.483357	0.587704
[2(Br)]$^{-}$	-4533.537238	0.483683	0.58798
2(PMe$_3$)	-2422.631173	0.590166	0.709557
2(Py)	-2209.828959	0.576704	0.683943
[2(Py)]$^{\bullet -}$	-2209.888761	0.572355	0.680406
[2(Py)]$^{2-}$	-2209.795407	0.564962	0.676395
[2(Py)]$^{\bullet\bullet 2-}$	-2209.846469	0.565929	0.676476

16) 3D Coordinates of All Computed Structures

The 3D coordinates are organized so that they can be readily visualized in a Mercury. For each complex, the first number is the number of atoms,followed by the complex name, and the 3D coordinates.

6
MeCN
N -1.43606 -0.00001 0.00000
C -0.28121 0.00002 -0.00001
C 1.18058 -0.00000 0.00000
H 1.55205 -0.79605 0.64709
H 1.55212 -0.16239 -1.01291
H 1.55211 0.95839 0.36585

11
Pyridine
C -1.170423 0.852042 -0.075369
C -1.176132 -0.539238 -0.009621
C 0.044281 -1.204546 0.023934
C 1.212551 -0.451429 -0.009642
C 1.104707 0.935676 -0.075389
N -0.058404 1.588788 -0.108268
H -2.108173 1.402496 -0.103007
H -2.115229 -1.080853 0.014355
H 0.084113 -2.288097 0.075216
H 2.188880 -0.922633 0.014317
H 1.999509 1.553496 -0.10304360

13
PMe_3
P -0.00013 -0.00006 -0.61446
C -1.61551 -0.16445 0.28407
C 0.95030 -1.31665 0.28394
C 0.66538 1.48120 0.28391
H -2.27928 0.65553 -0.00143
H -1.48352 -0.15075 1.37104
H -2.10039 -1.10152 -0.00105
H 0.57220 -2.30167 -0.00108
H 0.87270 -1.20881 1.37090
H 2.00422 -1.26786 -0.00130
H 0.61098 1.35995 1.37085
H 0.09650 2.36974 -0.00127
H 1.70753 1.64576 -0.00128

21
Ferrocene
C 0.000000 1.208045 1.756055
C -1.148919 0.373307 1.756055
C -0.710071 -0.977329 1.756055
C 0.710071 -0.977329 1.756055
C 1.148919 0.373307 1.756055
H 0.000000 2.288521 1.726326
H -2.176513 0.707192 1.726326
H -1.345159 -1.851452 1.726326
H 1.345159 -1.851452 1.726326
H 2.176513 0.707192 1.726326
Fe 0.000000 0.000000 0.000000
C -1.148919 0.373307 -1.756055
C 0.000000 1.208045 -1.756055
C -0.710071 -0.977329 -1.756055
H -2.176513 0.707192 -1.726326
C 1.148919 0.373307 -1.756055
H 0.000000 2.288521 -1.726326
C 0.710071 -0.977329 -1.756055
H -1.345159 -1.851452 -1.726326
H 2.176513 0.707192 -1.726326
H 1.345159 -1.851452 -1.726326

21
Ferrocenium
C 0.000000 1.211827 1.755329
C -1.152516 0.374475 1.755329
C -0.712294 -0.980389 1.755329
C 0.712294 -0.980389 1.755329
C 1.152516 0.374475 1.755329
H 0.000000 2.293010 1.729813
H -2.180782 0.708579 1.729813
H -1.347797 -1.855084 1.729813
H 1.347797 -1.855084 1.729813
H 2.180782 0.708579 1.729813
Fe 0.000000 0.000000 0.000000
C -1.152516 0.374475 -1.755329
C 0.000000 1.211827 -1.755329
C -0.712294 -0.980389 -1.755329
H -2.180782 0.708579 -1.729813
C 1.152516 0.374475 -1.755329
H 0.000000 2.293010 -1.729813
C 0.712294 -0.980389 -1.755329
H -1.347797 -1.855084 -1.729813
H 2.180782 0.708579 -1.729813
H 1.347797 -1.855084 -1.729813

60
PhB(Bo_2en) (**1**)
F 5.12518 1.35257 -0.89387

F	6.45664	0.27686	0.62815
F	-5.12545	1.35279	0.89356
F	-6.45667	0.27681	-0.62846
N	1.15482	-1.18552	-0.00684
N	-1.15488	-1.18543	0.00705
N	4.12735	0.60267	1.16155
N	4.79496	-1.00290	-0.57556
N	-4.79501	-1.00267	0.57556
N	-4.12733	0.60270	-1.16166
C	-2.13299	0.57014	-2.22721
C	-2.84486	0.09280	-1.10329
C	2.48649	-0.85230	0.11826
C	-3.00256	1.37691	-2.94386
C	3.49112	-1.46067	-0.67688
C	2.13308	0.57016	2.22725
C	-3.49122	-1.46053	0.67693
C	-0.97815	1.96836	0.70266
C	0.00009	1.24958	-0.00005
C	0.70151	-2.55549	-0.29920
C	-5.56335	-1.72495	1.39301
C	0.97843	1.96833	-0.70268
C	-0.70166	-2.55536	0.29980
C	-0.97618	3.35864	0.70898
C	0.97665	3.35859	-0.70879
C	2.84488	0.09274	1.10332
C	5.56318	-1.72518	-1.39310
C	-3.48324	-2.52575	1.60823
C	4.78943	-2.69608	-2.04676
C	0.00028	4.05459	0.00015
C	-2.48651	-0.85219	-0.11815
C	-4.22532	1.37027	-2.24761
C	3.00270	1.37696	2.94380
C	4.22542	1.37028	2.24746
C	-4.78970	-2.69590	2.04669
C	3.48301	-2.52583	-1.60825
B	0.00002	-0.30424	0.00001
B	5.20878	0.36700	0.06585
B	-5.20887	0.36709	-0.06606
H	-1.11300	0.32204	-2.48265
H	-2.80149	1.89766	-3.86755
H	1.11310	0.32210	2.48275
H	-1.75959	1.44106	1.24577
H	0.64620	-2.72967	-1.37982
H	1.36582	-3.29300	0.15550
H	-6.61795	-1.50359	1.48196
H	1.75980	1.44098	-1.24584
H	-0.64639	-2.72922	1.38047
H	-1.36602	-3.29295	-0.15470
H	-1.74070	3.89670	1.25946
H	1.74123	3.89663	-1.25920
H	6.61779	-1.50390	-1.48212
H	-2.63502	-3.11885	1.90973
H	5.15043	-3.43308	-2.74792
H	0.00038	5.14006	0.00023
H	-5.15788	1.86482	-2.48165
H	2.80173	1.89775	3.86748
H	5.15799	1.86487	2.48140
H	-5.15078	-3.43289	2.74783
H	2.63471	-3.11883	-1.90972

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[1]$^{\bullet-}$

F	5.593511	0.520472	-1.249933
F	6.457012	0.510756	0.861511
F	-5.952548	0.965513	-0.663786
F	-6.502215	-0.471589	1.007282
N	1.185646	-0.991749	0.314983
N	-1.128273	-0.873333	0.297662
N	4.145494	1.129726	0.587118
N	4.855669	-1.196777	0.264260
N	-4.381644	0.680853	1.157654
N	-4.734148	-1.122157	-0.511177
C	-3.116254	-2.411132	-1.417248
C	-3.373142	-1.334536	-0.555329
C	2.487938	-0.659087	0.386739
C	-4.365836	-2.852651	-1.895810
C	3.541623	-1.628199	0.262805
C	2.062198	1.746368	1.189606
C	-3.027363	0.431597	1.125249
C	-0.913200	2.022688	-1.147665
C	0.075957	1.029195	-1.125262
C	0.678623	-2.331505	0.657236
C	-4.616860	1.612135	2.119346
C	1.112272	1.107969	-2.069355
C	-0.765142	-2.064367	1.076646
C	-0.861115	3.059875	-2.076358
C	1.162741	2.137129	-3.001558
C	2.837002	0.699261	0.660598
C	5.657274	-2.261219	0.123237
C	-2.402325	1.233896	2.092703
C	4.892352	-3.423948	0.034146
C	0.174078	3.119295	-3.003724
C	-2.502281	-0.533725	0.225993
C	-5.329298	-2.036737	-1.320167
C	2.924397	2.817577	1.414670
C	4.200071	2.392943	1.031851
C	-3.421375	1.980776	2.718064
C	3.555926	-3.029562	0.111644
B	0.007930	-0.183368	-0.144575
B	5.337980	0.278555	0.086797
B	-5.456388	0.031132	0.240186
H	-2.134983	-2.793120	-1.666228

H	-4.551133	-3.667608	-2.581558
H	1.002224	1.714486	1.397053
H	-1.724904	1.991144	-0.427663
H	0.704404	-2.981769	-0.226535
H	1.281450	-2.777784	1.450450
H	-5.626200	1.946470	2.312210
H	1.896436	0.354250	-2.077289
H	-0.846337	-1.851416	2.150548
H	-1.432728	-2.893082	0.828757
H	-1.636536	3.819575	-2.074177
H	1.974832	2.175775	-3.720958
H	6.728812	-2.125778	0.079103
H	-1.343723	1.237514	2.317924
H	5.266628	-4.431652	-0.067897
H	0.212411	3.928193	-3.727730
H	-6.404108	-2.040406	-1.432838
H	2.668528	3.784149	1.821581
H	5.147046	2.912741	1.067257
H	-3.305655	2.699035	3.517600
H	2.705324	-3.688831	0.070839

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$[1]^{2-}$ (singlet)

F	6.590119	0.167984	-0.231938
F	6.004515	-1.501322	1.187856
F	-6.590284	0.167952	0.230059
F	-6.003895	-1.502805	-1.187710
N	1.148074	-0.682656	-0.236007
N	-1.148183	-0.682253	0.237128
N	4.491900	0.375260	0.963882
N	4.740274	-1.245468	-0.866350
N	-4.740536	-1.244627	0.866752
N	-4.491584	0.374195	-0.965067
C	-2.570867	1.178546	-1.824547
C	-3.111389	0.349006	-0.831346
C	2.508055	-0.516214	-0.145177
C	-3.652267	1.694554	-2.569924
C	3.373829	-1.249177	-1.042480
C	2.571277	1.179155	1.824007
C	-3.374179	-1.247812	1.043440
C	-1.051671	2.476842	0.578582
C	0.000082	1.740166	-0.000150
C	0.619687	-2.040463	-0.442439
C	-5.316875	-1.927188	1.892547
C	1.051813	2.476660	-0.579160
C	-0.620045	-2.039990	0.444732
C	-1.049547	3.867321	0.586573
C	1.049618	3.867136	-0.587699
C	3.111641	0.349272	0.831003
C	5.316370	-1.929074	-1.891583
C	-3.097341	-1.952820	2.221788
C	4.333224	-2.389374	-2.747468
C	0.000019	4.572240	-0.000706
C	-2.508098	-0.515686	0.145738
C	-4.807938	1.180201	-2.012978
C	3.652832	1.696047	2.568530
C	4.808438	1.181932	2.011227
C	-4.333951	-2.386284	2.749344
C	3.096719	-1.955570	-2.219938
B	0.000037	0.186758	0.000223
B	5.509134	-0.558034	0.278967
B	-5.509001	-0.558495	-0.279618
H	-1.524624	1.394217	-1.968978
H	-3.593259	2.386491	-3.399261
H	1.524998	1.394428	1.968835
H	-1.886319	1.944961	1.026481
H	0.322730	-2.199614	-1.485716
H	1.359975	-2.791303	-0.156449
H	-6.392478	-2.021474	1.937785
H	1.886489	1.944643	-1.026840
H	-0.323121	-2.198285	1.488147
H	-1.360455	-2.790949	0.159384
H	-1.877057	4.403058	1.044538
H	1.877106	4.402737	-1.045861
H	6.391982	-2.023105	-1.937152
H	-2.121993	-2.088183	2.664643
H	4.489040	-2.956876	-3.655427
H	-0.000004	5.659479	-0.000932
H	-5.844491	1.319185	-2.287467
H	3.593958	2.388415	3.397516
H	5.845080	1.321598	2.285037
H	-4.490003	-2.952792	3.657884
H	2.121264	-2.091759	-2.662285

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$[1]^{\bullet 2-}$ (triplet)

F	-6.29069	-0.11615	0.87249
F	-6.38034	0.70828	-1.23695
F	6.28598	0.10918	0.87908
F	6.38569	-0.68517	-1.24134
N	-1.14898	-0.16019	-0.88627
N	1.14892	0.17125	-0.88372
N	-4.44522	1.26390	0.11350
N	-4.75677	-1.02992	-0.76632
N	4.75597	1.04220	-0.75274
N	4.44678	-1.26451	0.09366
C	2.47490	-2.35014	0.28176
C	3.08200	-1.14259	-0.08939
C	-2.52627	-0.06144	-0.58400
C	3.50940	-3.21471	0.69699
C	-3.38970	-1.14217	-0.92142

C	-2.47226	2.34476	0.31705
C	3.38871	1.15544	-0.90561
C	1.02583	0.60709	2.24779
C	-0.00020	-0.01290	1.52069
C	-0.76113	0.10144	-2.28008
C	5.32348	2.22251	-1.12675
C	-1.02672	-0.64387	2.23764
C	0.76109	-0.06952	-2.28134
C	1.02560	0.60146	3.63988
C	-1.02753	-0.65915	3.62966
C	-3.08066	1.14354	-0.07216
C	-5.32541	-2.20473	-1.15554
C	3.10065	2.43923	-1.38735
C	-4.33926	-3.08649	-1.56696
C	-0.00125	-0.03407	4.33394
C	2.52632	0.06939	-0.58304
C	4.69906	-2.51602	0.56705
C	-3.50575	3.20379	0.74606
C	-4.69610	2.50827	0.60606
C	4.33640	3.10887	-1.52591
C	-3.10291	-2.41970	-1.42030
B	0.00001	-0.00087	-0.04739
B	-5.52118	0.21273	-0.24843
B	5.52149	-0.20569	-0.24930
H	1.41124	-2.54518	0.26308
H	3.40416	-4.22920	1.05794
H	-1.40842	2.53903	0.30107
H	1.83547	1.09590	1.71141
H	-1.26769	-0.58575	-2.96653
H	-1.04910	1.12873	-2.55052
H	6.39649	2.34551	-1.07730
H	-1.83600	-1.12450	1.69339
H	1.26773	0.62776	-2.95746
H	1.04905	-1.09268	-2.56698
H	1.83169	1.08767	4.18244
H	-1.83405	-1.15343	4.16424
H	-6.39849	-2.32756	-1.10700
H	2.10612	2.81676	-1.58141
H	-4.49822	-4.09561	-1.92412
H	-0.00170	-0.04213	5.42135
H	5.71562	-2.81984	0.77521
H	-3.39935	4.21251	1.12252
H	-5.71229	2.80974	0.81940
H	4.49436	4.12265	-1.87009
H	-2.10876	-2.79545	-1.61972

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1Cl$_4$

Cl	4.91537	1.77994	-1.21116
Cl	6.84321	0.45809	0.77451
Cl	-4.91609	1.78037	1.20880
Cl	-6.84338	0.45782	-0.77682
N	1.15406	-1.16880	0.03200
N	-1.15431	-1.16843	-0.03052
N	4.09460	0.67372	1.19723
N	4.79316	-0.91199	-0.53455
N	-4.79383	-0.91177	0.53360
N	-4.09459	0.67307	-1.19870
C	-2.09287	0.62722	-2.24867
C	-2.82056	0.13166	-1.14615
C	2.47982	-0.82309	0.16741
C	-2.93678	1.48045	-2.94294
C	3.49957	-1.41276	-0.62116
C	2.09350	0.62783	2.24837
C	-3.50006	-1.41181	0.62148
C	-0.99442	1.98442	0.68162
C	0.00018	1.26677	0.00037
C	0.71045	-2.53782	-0.27732
C	-5.57684	-1.61313	1.36348
C	0.99498	1.98417	-0.68087
C	-0.71112	-2.53763	0.27849
C	-0.99447	3.37461	0.68456
C	0.99556	3.37434	-0.68357
C	2.82087	0.13153	1.14602
C	5.57614	-1.61411	-1.36379
C	-3.51902	-2.47742	1.54653
C	4.82648	-2.61027	-1.99754
C	0.00070	4.06987	0.00060
C	-2.48001	-0.82245	-0.16689
C	-4.16189	1.48715	-2.25739
C	2.93730	1.48234	2.94125
C	4.16201	1.48901	2.25501
C	-4.82701	-2.60809	1.99892
C	3.51866	-2.47965	-1.54470
B	-0.00005	-0.28428	0.00052
B	5.13283	0.45402	0.09237
B	-5.13325	0.45404	-0.09397
H	-1.07786	0.36122	-2.50536
H	-2.71643	2.02666	-3.84710
H	1.07875	0.36155	2.50581
H	-1.78897	1.46062	1.20938
H	0.68803	-2.70962	-1.35952
H	1.35882	-3.27714	0.19720
H	-6.62106	-1.35415	1.47020
H	1.78924	1.46020	-1.20890
H	-0.68857	-2.70963	1.36064
H	-1.35980	-3.27667	-0.19605
H	-1.77625	3.91001	1.21313
H	1.77751	3.90953	-1.21210
H	6.62017	-1.35474	-1.47136
H	-2.68845	-3.10286	1.83097
H	5.20384	-3.33901	-2.69841

H	0.00096	5.15539	0.00078
H	-5.07709	2.01993	-2.47517
H	2.71718	2.02937	3.84497
H	5.07701	2.02256	2.47171
H	-5.20432	-3.33612	2.70056
H	2.68835	-3.10604	-1.82781

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[1(H)]$^{-}$

F	4.132532	-2.940940	-1.155183
F	6.027903	-1.667293	-1.168533
F	-6.027797	-1.667608	-1.168520
F	-4.132301	-2.941068	-1.154974
N	1.195388	0.151913	0.750459
N	-1.195333	0.151832	0.750466
N	3.922074	-0.561765	-1.547667
N	4.495205	-1.392896	0.665381
N	-4.495191	-1.392867	0.665410
N	-3.922063	-0.561882	-1.547641
C	-2.376995	1.004182	-2.007401
C	-2.815635	0.088055	-1.040595
C	2.402347	-0.170380	0.327859
C	-3.235178	0.884074	-3.108074
C	3.406819	-0.753938	1.214119
C	2.376856	1.004209	-2.007245
C	-3.406785	-0.753935	1.214034
C	1.194595	3.131672	0.398476
C	-0.000060	2.410571	0.248786
C	0.768796	-0.079019	2.124384
C	-5.341039	-1.744416	1.649657
C	-1.194732	3.131607	0.398526
C	-0.768779	-0.078993	2.124399
C	1.201087	4.499497	0.663604
C	-1.201286	4.499457	0.663655
C	2.815755	0.088186	-1.040482
C	5.341098	-1.744459	1.649533
C	-3.607881	-0.698993	2.603473
C	4.833964	-1.324236	2.872252
C	-0.000123	5.191104	0.794925
C	-2.402267	-0.170451	0.327757
C	-4.165037	-0.098192	-2.786162
C	3.234910	0.884129	-3.108047
C	4.164808	-0.098119	-2.786292
C	-4.833789	-1.324163	2.872296
C	3.608031	-0.699097	2.603568
B	-0.000028	0.804859	-0.034669
B	4.682671	-1.710978	-0.844628
B	-4.682577	-1.711143	-0.844509
H	-1.562309	1.702170	-1.902440
H	-3.192409	1.450808	-4.026382
H	1.562262	1.702278	-1.902107
H	2.146207	2.611457	0.305841
H	1.164362	-1.031630	2.483970
H	1.149575	0.719350	2.771936
H	-6.254395	-2.269201	1.409669
H	-2.146332	2.611371	0.305938
H	-1.149521	0.719438	2.771900
H	-1.164422	-1.031548	2.484072
H	2.146292	5.024517	0.771026
H	-2.146526	5.024399	0.771135
H	6.254466	-2.269209	1.409510
H	-2.980564	-0.216385	3.334566
H	5.300199	-1.447093	3.838734
H	-0.000118	6.257367	1.002386
H	-4.991444	-0.497807	-3.356310
H	3.192010	1.450868	-4.026347
H	4.991133	-0.497741	-3.356552
H	-5.299891	-1.447007	3.838844
H	2.980594	-0.216685	3.334692
H	0.000037	0.458311	-1.177060

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[1H]$^{\bullet 2-}$

F	-4.871666	-2.720095	0.501728
F	-6.435920	-1.069084	0.487882
F	6.102845	-1.457276	1.144478
F	5.623056	-2.549266	-0.782464
N	-1.223784	0.328470	-0.635426
N	1.143860	0.165962	-0.563133
N	-4.223675	-0.511151	1.262366
N	-4.633815	-0.926129	-1.101624
N	4.843103	-0.263553	-0.542057
N	3.793694	-2.087357	0.742074
C	1.580448	-2.396639	1.042148
C	2.544041	-1.553787	0.477683
C	-2.469445	0.006384	-0.397379
C	2.275792	-3.458236	1.665057
C	-3.419749	-0.376030	-1.457275
C	-2.532223	0.690667	2.117730
C	3.601573	0.315550	-0.727853
C	-0.964809	3.142242	0.428064
C	0.097949	2.244128	0.599917
C	-0.684389	0.371024	-2.001740
C	5.794778	0.582670	-1.029633
C	1.342148	2.802490	0.940970
C	0.817468	0.672197	-1.868183
C	-0.809052	4.518952	0.599580
C	1.512204	4.173416	1.114215
C	-3.000200	0.054421	0.965260
C	-5.364483	-1.149926	-2.211365
C	3.795754	1.559132	-1.350729
C	-4.650428	-0.743946	-3.325661

C	0.432983	5.041521	0.946700
C	2.410658	-0.340316	-0.271711
C	3.624984	-3.236842	1.457094
C	-3.496252	0.492534	3.120944
C	-4.516759	-0.255070	2.554204
C	5.189085	1.715730	-1.539017
C	-3.417991	-0.257777	-2.856457
B	0.025036	0.618865	0.368404
B	-5.084274	-1.359901	0.315580
B	5.131858	-1.615598	0.144613
H	0.513658	-2.233176	1.001458
H	1.842811	-4.287574	2.209766
H	-1.615707	1.249291	2.205299
H	-1.946866	2.755304	0.157536
H	-0.857755	-0.597953	-2.483264
H	-1.200678	1.148742	-2.575810
H	6.839644	0.312838	-0.963523
H	2.200254	2.140318	1.041014
H	0.966402	1.761958	-1.971006
H	1.398156	0.178858	-2.654582
H	-1.658848	5.183319	0.456261
H	2.493243	4.567219	1.369289
H	-6.349295	-1.586007	-2.122713
H	3.018963	2.273018	-1.584333
H	-4.978167	-0.787074	-4.354680
H	0.562456	6.113502	1.077702
H	4.487363	-3.818280	1.753154
H	-3.454671	0.857414	4.137278
H	-5.441481	-0.622581	2.976309
H	5.694203	2.563474	-1.984633
H	-2.643538	0.150708	-3.479651
H	-0.058286	-0.009275	1.390745

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[1H]$^{3-}$ (singlet)

F	5.635368	-2.279555	-0.890061
F	6.567089	-0.344353	-0.180729
F	-6.278847	-1.074001	-1.244873
F	-5.794652	-2.530621	0.415841
N	1.156928	0.070385	0.614240
N	-1.209530	0.131246	0.512554
N	4.375075	-0.226638	-1.199315
N	4.642749	-1.174914	1.024741
N	-4.920272	-0.264736	0.596793
N	-3.974362	-1.829747	-1.041980
C	-1.780996	-2.135756	-1.487910
C	-2.694413	-1.376273	-0.738315
C	2.461898	-0.206381	0.381329
C	-2.538822	-3.054849	-2.258531
C	3.335788	-0.852338	1.368197
C	2.580277	0.851832	-2.003004
C	-3.653672	0.255530	0.824456
C	1.090066	3.055557	-0.138028
C	-0.010749	2.231420	-0.429225
C	0.601684	-0.104267	1.945741
C	-5.841900	0.499441	1.270060
C	-1.225721	2.893879	-0.689679
C	-0.841513	0.410807	1.870029
C	0.998204	4.449045	-0.133618
C	-1.330903	4.282851	-0.694522
C	3.068272	0.134203	-0.901258
C	5.266306	-1.762864	2.081991
C	-3.803979	1.375971	1.665018
C	4.387953	-1.843604	3.139969
C	-0.212910	5.074001	-0.420674
C	-2.495968	-0.325146	0.208413
C	-3.869190	-2.844239	-1.960998
C	3.610351	0.907939	-2.966551
C	4.695113	0.238932	-2.438117
C	-5.189790	1.513329	1.938980
C	3.172272	-1.272524	2.706488
B	-0.030587	0.573171	-0.353942
B	5.339074	-1.021885	-0.331297
B	-5.267800	-1.441358	-0.323583
H	-0.708732	-2.019719	-1.454049
H	-2.152108	-3.787107	-2.959202
H	1.597759	1.280034	-2.091953
H	2.045914	2.586487	0.089041
H	0.576962	-1.166531	2.230450
H	1.209165	0.434046	2.692002
H	-6.894594	0.260922	1.197762
H	-2.115440	2.287685	-0.856551
H	-0.855987	1.488598	2.122149
H	-1.495184	-0.110119	2.579255
H	1.877500	5.049720	0.098464
H	-2.292379	4.752003	-0.898207
H	6.296626	-2.076340	1.986018
H	-3.004246	2.028770	1.984700
H	4.592331	-2.255299	4.120878
H	-0.290053	6.160685	-0.418613
H	-4.761565	-3.342992	-2.316131
H	3.561227	1.391277	-3.934278
H	5.683911	0.059005	-2.837868
H	-5.658733	2.277664	2.550179
H	2.295238	-1.174846	3.318851
H	-0.031710	0.065041	-1.451081

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[1]$^{\bullet\bullet 3-}$ (triplet)

F	-6.68809	-0.71845	0.83962

F	-6.08928	0.73808	-0.79099
F	6.52921	-0.07308	0.90437
F	6.12542	-2.09311	-0.03321
N	-1.22797	-0.52183	-0.37074
N	1.17730	-0.46583	-0.41362
N	-4.54569	0.38619	1.05913
N	-4.85958	-1.35306	-0.60677
N	4.87180	-0.17911	-0.85872
N	4.38289	-1.11898	1.35218
C	2.34338	-1.55097	2.20199
C	3.02219	-1.02324	1.09929
C	-2.58320	-0.56771	-0.09034
C	3.32349	-1.96380	3.13762
C	-3.48582	-1.50080	-0.74668
C	-2.60167	1.10509	1.91989
C	3.51619	0.00633	-1.08537
C	-0.92025	2.50063	-0.64803
C	0.04401	1.79231	0.08460
C	-0.70344	-1.22027	-1.53207
C	5.57463	0.41302	-1.87004
C	1.16669	2.52261	0.51026
C	0.67650	-0.61403	-1.76174
C	-0.78027	3.85871	-0.93659
C	1.32098	3.87842	0.22873
C	-3.16660	0.29414	0.92553
C	-5.50087	-2.37624	-1.24653
C	3.38739	0.73808	-2.27712
C	-4.56388	-3.20783	-1.81856
C	0.34285	4.55746	-0.49811
C	2.53373	-0.47637	-0.14597
C	4.55756	-1.68711	2.58377
C	-3.66605	1.68224	2.65402
C	-4.84102	1.21997	2.10105
C	4.69319	0.98571	-2.76462
C	-3.29013	-2.67035	-1.51195
B	-0.02239	0.17323	0.37727
B	-5.58244	-0.21610	0.11829
B	5.51353	-0.87807	0.34728
H	1.26997	-1.60183	2.29406
H	3.14591	-2.40276	4.11278
H	-1.54857	1.24374	2.09544
H	-1.80724	1.96572	-0.98297
H	-0.57387	-2.29854	-1.33892
H	-1.36302	-1.11041	-2.40314
H	6.65596	0.38912	-1.85844
H	1.94635	1.99841	1.06207
H	0.55310	0.35194	-2.28557
H	1.32605	-1.25349	-2.37151
H	-1.55412	4.37557	-1.50294
H	2.21125	4.40632	0.56744
H	-6.58080	-2.42530	-1.22520
H	2.45911	1.09024	-2.69919
H	-4.76466	-4.11120	-2.38372
H	0.45738	5.61740	-0.72217
H	5.55760	-1.85755	2.95996
H	-3.57524	2.35289	3.50062
H	-5.87454	1.40989	2.35745
H	4.95860	1.53496	-3.66071
H	-2.34548	-3.10948	-1.78420
H	0.01857	-0.04972	1.56822

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[1Cl$_4$(H)]$^-$

Cl	4.70989	-1.09321	-2.86256
Cl	6.97517	-0.83218	-0.82666
Cl	-6.88631	-0.40147	-1.40900
Cl	-5.01427	-2.79230	-1.77045
N	1.20196	-0.71072	0.62573
N	-1.21713	-0.53142	0.41371
N	4.48864	0.39539	-0.49675
N	4.52024	-2.02609	-0.23194
N	-4.83863	-1.02350	0.38667
N	-4.12731	-0.13256	-1.76175
C	-2.13415	0.77375	-2.27773
C	-2.83526	0.07210	-1.29030
C	2.50044	-0.78793	0.35573
C	-3.01336	0.98122	-3.34802
C	3.25289	-2.03027	0.33694
C	3.01907	1.71719	0.57372
C	-3.57174	-0.81934	0.89237
C	-0.57929	2.28864	1.16009
C	0.00937	1.72856	0.01976
C	0.52478	-1.84456	1.23282
C	-5.68774	-1.25075	1.41106
C	0.54092	2.61680	-0.92477
C	-0.84325	-1.30574	1.59180
C	-0.60243	3.66595	1.37332
C	0.51800	3.99440	-0.73108
C	3.24202	0.42169	0.10106
C	5.02048	-3.27666	-0.19271
C	-3.65994	-0.89499	2.28715
C	4.11508	-4.12297	0.42625
C	-0.04740	4.52372	0.42724
C	-2.47399	-0.43443	0.01335
C	-4.22034	0.39632	-2.99887
C	4.13006	2.48809	0.20668
C	5.00782	1.64001	-0.45519
C	-4.99790	-1.16777	2.60964
C	2.99525	-3.34841	0.75223
B	0.08556	0.13542	-0.20556
B	5.11834	-0.87134	-1.04578
B	-5.15730	-1.03892	-1.10355

H	-1.12270	1.12936	-2.20852
H	-2.80032	1.50715	-4.26648
H	2.16762	2.03562	1.15338
H	-1.03518	1.63457	1.90255
H	0.42855	-2.67434	0.51881
H	1.06211	-2.19223	2.11928
H	-6.73059	-1.44719	1.21130
H	1.00964	2.21008	-1.81902
H	-0.76273	-0.66080	2.47747
H	-1.56266	-2.10039	1.79207
H	-1.05883	4.07028	2.27250
H	0.94604	4.65538	-1.47915
H	5.99087	-3.47911	-0.62206
H	-2.86350	-0.72031	2.99301
H	4.25284	-5.17564	0.62264
H	-0.06460	5.59793	0.58685
H	-5.14678	0.31367	-3.54849
H	4.28828	3.53623	0.41186
H	5.98099	1.83156	-0.88295
H	-5.41777	-1.28168	3.59785
H	2.12504	-3.71882	1.26381
H	0.24546	-0.17306	-1.36135

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[1(F)]$^-$

F	5.36119	0.94100	-1.55211
F	6.55055	0.61980	0.36666
F	-4.78256	1.19617	1.19461
F	-6.37968	0.40757	-0.23990
N	1.26811	-0.99711	0.14875
N	-1.09652	-1.17154	-0.34419
N	4.20774	1.12973	0.57149
N	4.92538	-1.04772	-0.25988
N	-4.65271	-1.10526	0.49571
N	-4.13359	0.68330	-1.07427
C	-2.30607	0.72106	-2.38991
C	-2.87693	0.14666	-1.24698
C	2.56329	-0.66420	0.19914
C	-3.24391	1.62600	-2.89779
C	3.64267	-1.55986	-0.17617
C	2.24664	1.44620	1.62748
C	-3.39106	-1.65244	0.37152
C	-1.06893	1.63634	0.91195
C	-0.20181	1.33061	-0.14413
C	0.88386	-2.39066	0.00385
C	-5.42621	-1.93839	1.20992
C	0.42464	2.39629	-0.79770
C	-0.60732	-2.38968	0.28133
C	-1.28546	2.94965	1.31784
C	0.22718	3.71361	-0.39242
C	2.93288	0.62370	0.72303
C	5.76631	-2.02643	-0.62502
C	-3.40812	-2.89017	1.04337
C	5.06501	-3.21786	-0.77716
C	-0.62684	3.99353	0.67073
C	-2.39748	-0.90940	-0.39298
C	-4.35165	1.57712	-2.05290
C	3.11879	2.47351	1.99385
C	4.31689	2.23939	1.31966
C	-4.69743	-3.06825	1.56043
C	3.72449	-2.92916	-0.50574
B	0.11076	-0.16172	-0.62530
B	5.32357	0.46157	-0.25540
B	-5.04611	0.35733	0.12382
F	0.50664	-0.21747	-1.97077
H	-1.33271	0.48078	-2.78857
H	-3.14130	2.24099	-3.77965
H	1.23962	1.28754	1.97843
H	-1.60065	0.83800	1.42788
H	1.08052	-2.74891	-1.01631
H	1.41905	-3.02390	0.71573
H	-6.44816	-1.66427	1.42962
H	1.09163	2.18098	-1.62854
H	-0.80716	-2.37499	1.36144
H	-1.08706	-3.27134	-0.15256
H	-1.97898	3.15655	2.12743
H	0.73872	4.52231	-0.90681
H	6.81543	-1.80700	-0.76443
H	-2.61062	-3.60729	1.12717
H	5.47866	-4.17928	-1.04381
H	-0.79000	5.02035	0.98597
H	-5.28669	2.11776	-2.09091
H	2.91422	3.28665	2.67429
H	5.25003	2.78438	1.34101
H	-5.05855	-3.92116	2.11607
H	2.92777	-3.65098	-0.52785

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[1(Cl)]$^-$

F	5.51114	0.16809	-1.87368
F	6.63923	-0.34209	0.03865
F	-6.69470	-0.14205	-0.61651
F	-5.51919	-1.80798	-1.64197
N	1.15747	-0.95382	0.20003
N	-1.24201	-0.75746	0.13400
N	4.45531	0.64085	0.25688
N	4.69949	-1.66213	-0.53138
N	-4.85268	-1.12316	0.57713
N	-4.43749	0.32804	-1.31991
C	-2.50319	1.29228	-1.94582
C	-3.06995	0.34380	-1.07440
C	2.49304	-0.82935	0.08792

C	-3.54025	1.83958	-2.70106
C	3.34634	-1.90134	-0.35909
C	2.66141	1.36479	1.40836
C	-3.51392	-1.09127	0.88911
C	-0.63555	2.07599	0.86574
C	0.08486	1.51769	-0.19777
C	0.53655	-2.26164	0.36020
C	-5.54780	-1.53816	1.64957
C	0.88323	2.37709	-0.96260
C	-0.79900	-1.88279	0.96689
C	-0.54306	3.43139	1.17438
C	0.98245	3.73195	-0.66209
C	3.12104	0.38916	0.50941
C	5.28276	-2.78202	-0.97983
C	-3.38839	-1.49709	2.22847
C	4.33407	-3.79530	-1.10311
C	0.27298	4.26314	0.41266
C	-2.54230	-0.51069	-0.03749
C	-4.71211	1.20677	-2.29255
C	3.72886	2.22454	1.66611
C	4.81663	1.73833	0.93830
C	-4.67544	-1.77717	2.70473
C	3.11010	-3.24299	-0.72348
B	0.03543	-0.05724	-0.46891
B	5.39658	-0.26638	-0.56684
B	-5.44789	-0.71782	-0.79190
Cl	0.18650	-0.48147	-2.33442
H	-1.46750	1.57084	-2.00889
H	-3.45333	2.61046	-3.45213
H	1.66790	1.41235	1.82508
H	-1.27775	1.43906	1.47141
H	0.38280	-2.75889	-0.60619
H	1.12620	-2.90119	1.02136
H	-6.62293	-1.62641	1.59115
H	1.44517	1.96802	-1.79803
H	-0.63165	-1.56206	2.00171
H	-1.53004	-2.69238	0.95277
H	-1.11297	3.83856	2.00472
H	1.62047	4.37331	-1.26297
H	6.34096	-2.78500	-1.20091
H	-2.48301	-1.54138	2.81116
H	4.51570	-4.80960	-1.42630
H	0.34944	5.32034	0.65017
H	-5.72951	1.31881	-2.64054
H	3.72587	3.08987	2.31208
H	5.83557	2.09484	0.88332
H	-4.94233	-2.10478	3.69869
H	2.17038	-3.76686	-0.71143

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[1(Br)]$^-$

F	5.60408	0.10979	-1.73288
F	6.61086	-0.39110	0.24640
F	-6.68994	-0.10752	-0.57517
F	-5.56741	-1.88314	-1.46535
N	1.13962	-0.94807	0.32080
N	-1.24744	-0.74600	0.23016
N	4.44098	0.64299	0.32634
N	4.67854	-1.68247	-0.41452
N	-4.86527	-1.03548	0.68542
N	-4.42718	0.24195	-1.32965
C	-2.47330	1.09472	-2.05380
C	-3.05809	0.25228	-1.08790
C	2.47690	-0.82347	0.18503
C	-3.50033	1.58269	-2.86011
C	3.31991	-1.89989	-0.25303
C	2.62468	1.42973	1.40197
C	-3.52549	-0.99799	0.99274
C	-0.61681	2.17114	0.65962
C	0.10630	1.48265	-0.32246
C	0.51783	-2.24645	0.55073
C	-5.56374	-1.35491	1.78799
C	0.93946	2.23120	-1.16309
C	-0.81692	-1.82511	1.13337
C	-0.49196	3.54945	0.81995
C	1.07404	3.60679	-1.00706
C	3.10126	0.40596	0.56668
C	5.24137	-2.80824	-0.87294
C	-3.40278	-1.29938	2.35948
C	4.27302	-3.80181	-1.01608
C	0.36197	4.27031	-0.01008
C	-2.54653	-0.50843	0.02411
C	-4.68481	1.02189	-2.38659
C	3.68717	2.30154	1.63326
C	4.78950	1.77460	0.95568
C	-4.69236	-1.52357	2.85755
C	3.05846	-3.23088	-0.63752
B	0.03137	-0.10796	-0.40388
B	5.40551	-0.30170	-0.42864
B	-5.45993	-0.72903	-0.70864
Br	0.22866	-0.77962	-2.39116
H	-1.43173	1.33685	-2.15395
H	-3.39945	2.27044	-3.68634
H	1.62129	1.50130	1.79098
H	-1.28495	1.61948	1.31861
H	0.35410	-2.78493	-0.39097
H	1.10901	-2.85488	1.23952
H	-6.64026	-1.43079	1.73824
H	1.48964	1.71480	-1.94511
H	-0.65095	-1.44482	2.14755
H	-1.55523	-2.62755	1.16234
H	-1.06483	4.06039	1.58860

H	1.73912	4.16210	-1.66181
H	6.30056	-2.83096	-1.08861
H	-2.49678	-1.30957	2.94270
H	4.43759	-4.81390	-1.35481
H	0.46525	5.34460	0.11312
H	-5.70049	1.11989	-2.74396
H	3.67333	3.20150	2.22985
H	5.81012	2.12713	0.90454
H	-4.96153	-1.76871	3.87438
H	2.10500	-3.72988	-0.64163

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1(PMe_3)

F	4.24174	0.70792	-2.78213
F	6.21973	0.69213	-1.61544
F	-6.21995	0.69183	-1.61508
F	-4.24245	0.70780	-2.78254
N	1.20982	-0.91817	-0.06113
N	-1.20967	-0.91800	-0.06129
N	4.16925	1.14396	-0.42749
N	4.64487	-1.09158	-1.23345
N	-4.64472	-1.09163	-1.23346
N	-4.16911	1.14404	-0.42792
C	-2.54679	1.72041	1.00803
C	-3.01245	0.69676	0.16610
C	2.50266	-0.62075	-0.18852
C	-3.44161	2.79182	0.89254
C	3.46666	-1.57477	-0.69844
C	2.54691	1.72002	1.00858
C	-3.46658	-1.57471	-0.69823
C	1.18911	-0.39988	2.83860
C	-0.00006	-0.18754	2.11519
C	0.76314	-2.28877	-0.29496
C	-5.43996	-2.12049	-1.55238
C	-1.18935	-0.39983	2.83842
C	-0.76316	-2.28876	-0.29451
C	1.19596	-0.71074	4.19558
C	-1.19644	-0.71073	4.19539
C	3.01257	0.69650	0.16651
C	5.44013	-2.12036	-1.55253
C	-3.56950	-2.98429	-0.67947
C	4.81718	-3.31825	-1.20670
C	-0.00029	-0.85255	4.88922
C	-2.50250	-0.62056	-0.18866
C	-4.42431	2.39592	-0.01102
C	3.44155	2.79158	0.89307
C	4.42435	2.39578	-0.01046
C	-4.81707	-3.31829	-1.20619
C	3.56956	-2.98436	-0.68005
B	0.00008	-0.08044	0.47522
B	4.87995	0.39874	-1.59034
B	-4.88011	0.39864	-1.59048
P	0.00012	1.66178	-0.79188
C	-0.00014	3.31841	0.00908
C	-1.39394	1.73460	-1.99529
C	1.39451	1.73463	-1.99487
H	-1.69681	1.67990	1.66957
H	-3.40314	3.72680	1.43185
H	1.69680	1.67952	1.66994
H	2.15091	-0.33979	2.34393
H	1.17261	-2.65088	-1.24220
H	1.13672	-2.93122	0.50822
H	-6.39918	-1.93690	-2.01487
H	-2.15105	-0.33973	2.34356
H	-1.13640	-2.93064	0.50930
H	-1.17308	-2.65144	-1.24132
H	2.14433	-0.85474	4.70346
H	-2.14489	-0.85478	4.70309
H	6.39939	-1.93669	-2.01490
H	-2.86407	-3.69055	-0.27565
H	5.22641	-4.31066	-1.31934
H	-0.00038	-1.09458	5.94718
H	-5.29613	2.91887	-0.37719
H	3.40296	3.72655	1.43236
H	5.29619	2.91879	-0.37648
H	-5.22630	-4.31073	-1.31858
H	2.86400	-3.69075	-0.27671
H	0.89640	3.86172	-0.29371
H	0.00081	3.22200	1.09551
H	-0.89777	3.86070	-0.29226
H	-1.05319	2.32247	-2.84953
H	-2.27267	2.21611	-1.57054
H	-1.67618	0.74211	-2.35128
H	1.67684	0.74210	-2.35068
H	2.27316	2.21622	-1.57007
H	1.05399	2.32237	-2.84930

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1(Py)

F	2.41004	-2.98874	-1.20562
F	4.69813	-3.14577	-1.01025
F	-4.43757	-3.24258	-1.28716
F	-2.23067	-3.03428	-0.64098
N	1.04101	0.23835	1.24051
N	-1.32326	0.53161	0.95725
N	3.66746	-0.96300	-0.94433
N	3.41567	-2.48497	0.92598
N	-3.92559	-1.91711	0.66775
N	-3.32416	-1.10854	-1.53206
C	-2.57088	0.96076	-1.96250
C	-2.69901	-0.02020	-0.97225
C	2.14155	-0.43098	0.88568

C	-3.11635	0.42846	-3.13834
C	2.63242	-1.57828	1.61368
C	3.15800	1.22213	-0.85211
C	-3.33879	-0.82158	1.25827
C	1.25462	3.21756	1.13172
C	0.15122	2.63202	0.49508
C	0.36487	-0.08653	2.49523
C	-4.82576	-2.43790	1.52030
C	-0.90877	3.48421	0.14705
C	-1.03335	0.51698	2.39362
C	1.32942	4.59132	1.35385
C	-0.84345	4.85851	0.35829
C	2.90247	-0.03303	-0.28270
C	3.81988	-3.44050	1.77328
C	-3.92729	-0.64170	2.51834
C	3.34400	-3.16487	3.05523
C	0.28436	5.41822	0.95420
C	-2.39741	-0.05734	0.45121
C	-3.55431	-0.85866	-2.83107
C	4.08964	1.02176	-1.87922
C	4.36727	-0.34349	-1.90920
C	-4.87322	-1.66438	2.67590
C	2.58283	-1.99885	2.95912
B	0.03862	1.03601	0.31663
B	3.56448	-2.47702	-0.62536
B	-3.48390	-2.43262	-0.73170
N	0.18850	0.45977	-1.14585
C	0.14156	-1.44717	-2.57482
C	0.44373	-0.63379	-3.66159
C	0.02578	-0.86645	-1.32761
C	0.62065	0.73203	-3.46531
C	0.48343	1.24863	-2.19103
H	-2.15881	1.95040	-1.84030
H	-3.20603	0.92490	-4.09319
H	2.74617	2.16672	-0.53139
H	2.07012	2.58289	1.47070
H	0.29465	-1.17573	2.59558
H	0.91546	0.30934	3.35413
H	-5.37303	-3.32929	1.25027
H	-1.82392	3.06488	-0.26185
H	-1.06290	1.54629	2.76452
H	-1.74419	-0.09106	2.94284
H	2.19989	5.01259	1.84680
H	-1.67915	5.48991	0.07339
H	4.41516	-4.26634	1.41072
H	-3.75419	0.17911	3.19952
H	3.53619	-3.74108	3.94752
H	0.33798	6.48876	1.12425
H	-4.01983	-1.60928	-3.45329
H	4.53053	1.77794	-2.51158
H	5.02452	-0.91228	-2.55102
H	-5.52533	-1.81787	3.52236
H	2.11559	-1.48600	3.78441
H	0.00445	-2.51664	-2.66333
H	0.54622	-1.06210	-4.65283
H	-0.20710	-1.46311	-0.45237
H	0.86751	1.39631	-4.28372
H	0.60213	2.30270	-1.96928

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1(NCMe)

F	3.61806	-3.40229	-0.76869
F	5.69065	-2.53409	-1.22787
F	-5.63536	-2.33008	-0.96583
F	-3.41799	-2.87712	-1.22231
N	1.28558	0.07403	0.76452
N	-1.11682	0.13455	0.96987
N	3.76011	-1.14536	-1.60463
N	4.47697	-1.65377	0.65613
N	-4.13191	-1.89325	0.86848
N	-4.00342	-0.56112	-1.14823
C	-2.81481	1.32434	-1.40580
C	-2.96978	0.17549	-0.61265
C	2.45917	-0.33980	0.28741
C	-3.77612	1.25831	-2.42296
C	3.49779	-0.83162	1.16722
C	2.40241	0.54401	-2.18841
C	-3.12317	-1.15651	1.46099
C	1.35189	2.99363	-0.10235
C	0.14363	2.32125	0.14132
C	0.95753	0.02858	2.18686
C	-4.77125	-2.59929	1.81171
C	-0.92273	3.08602	0.63778
C	-0.54278	-0.25906	2.25723
C	1.46710	4.36997	0.07019
C	-0.81600	4.46298	0.81730
C	2.78065	-0.30039	-1.12943
C	5.40664	-1.86203	1.59886
C	-3.17364	-1.42187	2.84579
C	5.07458	-1.15036	2.75121
C	0.37844	5.11176	0.52081
C	-2.34257	-0.26595	0.62882
C	-4.48407	0.07262	-2.23050
C	3.15775	0.17296	-3.30520
C	3.97662	-0.87997	-2.90108
C	-4.21942	-2.32065	3.06033
C	3.86686	-0.50118	2.48682
B	0.04899	0.71438	0.08238
B	4.42066	-2.28092	-0.76684
B	-4.34399	-1.99079	-0.66098
N	-0.16771	0.00754	-1.30086
C	-1.38522	-1.35454	-3.14188

C	-0.68115	-0.59876	-2.12834
H	-2.10328	2.12085	-1.25457
H	-3.95810	1.99765	-3.18870
H	1.70165	1.36366	-2.14700
H	2.23207	2.43677	-0.41049
H	1.51940	-0.76146	2.68286
H	1.20182	0.98994	2.65385
H	-5.57821	-3.26250	1.53488
H	-1.85851	2.59663	0.89698
H	-1.00765	0.30351	3.07176
H	-0.72825	-1.32559	2.42087
H	2.41374	4.86000	-0.13392
H	-1.66304	5.02474	1.19811
H	6.25083	-2.50372	1.39140
H	-2.57399	-0.97236	3.61968
H	5.65119	-1.10134	3.66244
H	0.46732	6.18458	0.65909
H	-5.30023	-0.35989	-2.79154
H	3.13898	0.63298	-4.28182
H	4.70797	-1.45221	-3.45336
H	-4.54567	-2.71934	4.00875
H	3.36404	0.18902	3.14676
H	-0.67207	-1.80725	-3.83243
H	-2.05384	-0.66105	-3.66086
H	-1.98838	-2.11525	-2.62992

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PhB(Bo$_2$dach) (2)

F	6.40054	-0.81554	0.63757
F	4.98389	-2.01078	-0.70623
N	1.15742	0.86104	0.07606
N	4.74671	0.37494	-0.66927
N	4.07813	-0.99084	1.27206
C	3.44238	1.80784	-1.83437
C	4.71983	1.82997	-2.37861
C	5.48852	0.92016	-1.63585
C	4.15788	-1.69372	2.40204
C	2.95211	-1.58925	3.12229
C	2.11160	-0.78106	2.37432
C	2.82472	-0.41222	1.21089
C	2.47831	0.46165	0.16416
C	3.46562	0.89619	-0.75429
C	0.00028	-1.56968	0.00044
C	-1.00856	-2.29044	0.65742
C	-1.00837	-3.68088	0.66200
C	0.00053	-4.37716	0.00070
C	0.71964	2.22749	-0.25927
C	1.46812	3.41411	0.32769
C	0.75143	4.68634	-0.15703
B	0.00012	-0.01408	0.00042
B	5.13255	-0.92142	0.12582
F	-6.40048	-0.81439	-0.63997
F	-4.98578	-2.01131	0.70437
N	-1.15740	0.86074	-0.07516
N	-4.74693	0.37432	0.66885
N	-4.07772	-0.99086	-1.27272
C	-3.44271	1.80641	1.83508
C	-4.72031	1.82843	2.37899
C	-5.48893	0.91915	1.63552
C	-4.15710	-1.69337	-2.40295
C	-2.95103	-1.58884	-3.12269
C	-2.11073	-0.78095	-2.37416
C	-2.82426	-0.41240	-1.21088
C	-2.47821	0.46117	-0.16380
C	-3.46581	0.89537	0.75449
C	1.00926	-2.29037	-0.65641
C	1.00930	-3.68081	-0.66074
C	-0.71996	2.22732	0.26016
C	-1.46869	3.41377	-0.32681
C	-0.75226	4.68617	0.15785
B	-5.13297	-0.92138	-0.12723
H	2.59756	2.39556	-2.16106
H	5.06629	2.42822	-3.20761
H	6.52036	0.62215	-1.76125
H	5.06524	-2.22805	2.64808
H	2.74514	-2.04357	4.07920
H	1.11055	-0.46077	2.62523
H	-1.81286	-1.76620	1.16906
H	-1.79980	-4.21737	1.17474
H	0.00063	-5.46269	0.00080
H	0.66919	2.33525	-1.35442
H	2.51577	3.42618	0.01851
H	1.44928	3.34657	1.42235
H	1.22300	5.56796	0.28576
H	0.88980	4.77011	-1.24322
H	-2.59786	2.39377	2.16233
H	-5.06690	2.42625	3.20824
H	-6.52085	0.62124	1.76046
H	-5.06444	-2.22749	-2.64954
H	-2.74372	-2.04292	-4.07965
H	-1.10954	-0.46074	-2.62458
H	1.81348	-1.76611	-1.16812
H	1.80085	-4.21725	-1.17338
H	-0.66954	2.33511	1.35531
H	-2.51633	3.42565	-0.01759
H	-1.44988	3.34621	-1.42147
H	-1.22403	5.56768	-0.28496
H	-0.89064	4.76995	1.24404

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[2]$^{\bullet-}$

F	-6.17800	0.48698	-1.26333

F	-6.33437	-1.19364	0.26419
N	-1.20223	0.63116	-0.01464
N	-4.81253	0.61162	0.72965
N	-4.30956	-1.01576	-1.05459
C	-3.28241	1.69929	1.97795
C	-4.53201	1.85039	2.57821
C	-5.44461	1.15760	1.77810
C	-4.45111	-1.91266	-2.03972
C	-3.21782	-2.14752	-2.65852
C	-2.28903	-1.33232	-2.01818
C	-2.97912	-0.63819	-1.00749
C	-2.52428	0.32894	-0.07120
C	-3.47062	0.92713	0.81725
C	-0.04323	-1.82357	0.19318
C	0.96070	-2.62540	-0.36843
C	0.97358	-4.00141	-0.16327
C	-0.01098	-4.59830	0.62014
C	-0.66200	1.98669	0.24525
C	-1.41164	3.21913	-0.23881
C	-0.55382	4.44091	0.13953
B	-0.02245	-0.28105	-0.03539
B	-5.49071	-0.28795	-0.34737
F	6.22224	0.90269	0.63709
F	6.29343	-1.27004	-0.02284
N	1.11754	0.53024	-0.17918
N	4.69163	0.18757	-1.09733
N	4.37300	-0.53145	1.25373
C	3.03927	0.74683	-2.52927
C	4.26349	0.74430	-3.23007
C	5.24844	0.39453	-2.31938
C	4.61742	-0.99514	2.50686
C	3.43193	-1.05141	3.22585
C	2.41086	-0.59499	2.37125
C	3.02031	-0.27715	1.14753
C	2.49029	0.21034	-0.07371
C	3.33412	0.39681	-1.20281
C	-1.02492	-2.44294	0.97861
C	-1.00967	-3.81653	1.19598
C	0.69346	1.90893	-0.46180
C	1.59092	3.04598	-0.01041
C	0.88773	4.35951	-0.38653
B	5.45970	-0.17965	0.20218
H	-2.33877	2.08030	2.34026
H	-4.75845	2.38283	3.48987
H	-6.50775	1.00970	1.90501
H	-5.42727	-2.32037	-2.26380
H	-3.03381	-2.82982	-3.47467
H	-1.23417	-1.24957	-2.23580
H	1.74273	-2.16128	-0.96464
H	1.75958	-4.60545	-0.60550
H	0.00228	-5.67167	0.78603
H	-0.45364	2.08527	1.32283
H	-2.40447	3.30727	0.20636
H	-1.54168	3.15759	-1.32649
H	-1.03427	5.35373	-0.22696
H	-0.53137	4.51811	1.23520
H	2.05086	0.93430	-2.92663
H	4.41433	0.95887	-4.27889
H	6.31360	0.27277	-2.45490
H	5.62593	-1.24819	2.80166
H	3.32238	-1.39452	4.24514
H	1.35289	-0.52657	2.58418
H	-1.81417	-1.84366	1.42788
H	-1.77708	-4.27693	1.81071
H	0.51757	2.02130	-1.54460
H	2.56679	2.97236	-0.49767
H	1.75515	2.97497	1.07220
H	1.46378	5.21432	-0.01866
H	0.87020	4.44120	-1.48138

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[2]$^{2-}$ (singlet)

F	-6.02192	1.09533	-1.10764
F	-6.56671	-0.74925	0.09854
N	-1.16113	0.41507	0.17797
N	-4.77301	0.64111	0.92188
N	-4.44965	-0.74851	-1.08002
C	-3.14315	1.29247	2.32666
C	-4.39260	1.56420	2.92797
C	-5.36555	1.14358	2.03858
C	-4.72478	-1.51153	-2.17185
C	-3.54285	-1.91412	-2.76696
C	-2.48930	-1.37063	-2.00134
C	-3.07363	-0.63923	-0.95834
C	-2.51656	0.17704	0.08176
C	-3.40592	0.72101	1.07388
C	0.00010	-1.99950	0.00012
C	1.06711	-2.73295	-0.54937
C	1.06518	-4.12392	-0.55889
C	0.00018	-4.82747	0.00015
C	-0.65435	1.78295	0.40381
C	-1.50191	2.97803	-0.01442
C	-0.70198	4.24907	0.31031
B	0.00003	-0.43934	0.00013
B	-5.50718	0.06724	-0.30847
F	6.02310	1.09457	1.10690
F	6.56625	-0.74990	-0.10014
N	1.16104	0.41527	-0.17759
N	4.77281	0.64162	-0.92208
N	4.44983	-0.74842	1.07962
C	3.14271	1.29357	-2.32631
C	4.39207	1.56549	-2.92775

C	5.36516	1.14447	-2.03871
C	4.72512	-1.51146	2.17139
C	3.54328	-1.91396	2.76675
C	2.48963	-1.37036	2.00134
C	3.07381	-0.63898	0.95824
C	2.51653	0.17738	-0.08166
C	3.40569	0.72164	-1.07379
C	-1.06686	-2.73300	0.54963
C	-1.06485	-4.12397	0.55918
C	0.65406	1.78311	-0.40315
C	1.50147	2.97822	0.01531
C	0.70140	4.24922	-0.30920
B	5.50735	0.06700	0.30770
H	-2.16191	1.44269	2.75489
H	-4.56419	1.99657	3.90484
H	-6.44325	1.15053	2.11884
H	-5.75264	-1.70643	-2.44474
H	-3.44897	-2.55190	-3.63568
H	-1.43054	-1.51264	-2.15521
H	1.91341	-2.20072	-0.97472
H	1.90435	-4.65981	-0.99455
H	0.00021	-5.91481	0.00016
H	-0.38345	1.89807	1.46554
H	-2.45714	2.99125	0.51273
H	-1.71451	2.91324	-1.08909
H	-1.25814	5.13484	-0.01807
H	-0.60887	4.32587	1.40276
H	2.16142	1.44402	-2.75431
H	4.56349	1.99826	-3.90447
H	6.44285	1.15139	-2.11918
H	5.75302	-1.70646	2.44408
H	3.44952	-2.55172	3.63548
H	1.43087	-1.51222	2.15545
H	-1.91318	-2.20080	0.97499
H	-1.90399	-4.65990	0.99486
H	0.38313	1.89842	-1.46486
H	2.45671	2.99164	-0.51183
H	1.71406	2.91325	1.08997
H	1.25745	5.13499	0.01934
H	0.60828	4.32620	-1.40163

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[2]$^{\bullet 2-}$ (triplet)

F	-6.46174	0.95815	0.08057
F	-6.30150	-1.30225	0.03342
N	-1.15937	0.41040	-0.10214
N	-4.59965	-0.07139	1.24294
N	-4.67525	-0.02058	-1.23193
C	-2.72978	0.04172	2.50323
C	-3.84656	-0.07968	3.35931
C	-4.96974	-0.14561	2.55138
C	-5.12965	0.00336	-2.51512
C	-4.06186	0.15273	-3.38647
C	-2.89406	0.22584	-2.59877
C	-3.30026	0.11487	-1.26168
C	-2.54609	0.12912	-0.05829
C	-3.22469	0.04542	1.19142
C	-0.00008	-2.00883	-0.00060
C	1.05597	-2.73345	-0.57439
C	1.05599	-4.12625	-0.57839
C	-0.00029	-4.82649	-0.00120
C	-0.72429	1.77305	0.22689
C	-1.46606	2.95678	-0.36689
C	-0.75800	4.22802	0.13712
B	-0.00000	-0.43760	-0.00027
B	-5.56363	-0.11464	0.03150
F	6.46176	0.95815	-0.07965
F	6.30156	-1.30228	-0.03408
N	1.15940	0.41028	0.10213
N	4.59982	-0.07062	-1.24293
N	4.67517	-0.02153	1.23198
C	2.73008	0.04341	-2.50333
C	3.84695	-0.07744	-3.35939
C	4.97004	-0.14395	-2.55138
C	5.12944	0.00152	2.51523
C	4.06155	0.15030	3.38658
C	2.89384	0.22397	2.59880
C	3.30017	0.11393	1.26168
C	2.54612	0.12901	0.05823
C	3.22485	0.04617	-1.19147
C	-1.05625	-2.73354	0.57287
C	-1.05647	-4.12634	0.57628
C	0.72439	1.77316	-0.22609
C	1.46621	2.95649	0.36838
C	0.75821	4.22807	-0.13487
B	5.56367	-0.11469	-0.03143
H	-1.68352	0.10158	2.77315
H	-3.83780	-0.11759	4.44052
H	-6.01438	-0.24336	2.81225
H	-6.18864	-0.08435	-2.71498
H	-4.12501	0.19910	-4.46569
H	-1.86829	0.33199	-2.92281
H	1.88405	-2.19923	-1.03156
H	1.88532	-4.66326	-1.03063
H	-0.00036	-5.91406	-0.00143
H	-0.73825	1.89398	1.32781
H	-2.51827	2.94983	-0.06366
H	-1.44108	2.89558	-1.46225
H	-1.21276	5.11982	-0.31013
H	-0.92027	4.30375	1.22098
H	1.68385	0.10348	-2.77332
H	3.83830	-0.11462	-4.44061

H	6.01470	-0.24155	-2.81222
H	6.18840	-0.08636	2.71514
H	4.12460	0.19592	4.46583
H	1.86803	0.32991	2.92282
H	-1.88425	-2.19939	1.03025
H	-1.88587	-4.66342	1.02830
H	0.73836	1.89473	-1.32694
H	2.51842	2.94968	0.06515
H	1.44123	2.89465	1.46371
H	1.21301	5.11958	0.31290
H	0.92048	4.30443	-1.21869

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$2Cl_4$

Cl	6.82118	-0.64412	0.77886
Cl	4.87748	-2.20278	-1.00543
N	1.15723	1.04711	0.08382
N	4.74899	0.54953	-0.66269
N	4.07869	-0.82072	1.26412
C	3.44852	1.99248	-1.81675
C	4.72562	2.00958	-2.36570
C	5.49209	1.09546	-1.63437
C	4.14430	-1.56543	2.37244
C	2.93544	-1.47538	3.08254
C	2.10354	-0.63980	2.35409
C	2.82239	-0.23777	1.20828
C	2.47589	0.64514	0.17161
C	3.46670	1.07971	-0.74187
C	0.00008	-1.38264	0.00018
C	-1.00734	-2.10208	0.66089
C	-1.00902	-3.49237	0.66267
C	0.00023	-4.18795	0.00028
C	0.72143	2.41369	-0.25523
C	1.46588	3.60050	0.33671
C	0.75251	4.87278	-0.15288
B	0.00001	0.16989	0.00013
B	5.09991	-0.72761	0.12458
Cl	-6.82111	-0.64442	-0.77919
Cl	-4.87758	-2.20274	1.00560
N	-1.15726	1.04701	-0.08374
N	-4.74909	0.54951	0.66240
N	-4.07855	-0.82105	-1.26410
C	-3.44879	1.99273	1.81632
C	-4.72595	2.00990	2.36512
C	-5.49231	1.09563	1.63388
C	-4.14403	-1.56595	-2.37231
C	-2.93508	-1.47600	-3.08228
C	-2.10327	-0.64029	-2.35386
C	-2.82226	-0.23809	-1.20821
C	-2.47590	0.64498	-0.17162
C	-3.46682	1.07971	0.74165
C	1.00758	-2.10202	-0.66046
C	1.00941	-3.49231	-0.66215
C	-0.72158	2.41363	0.25529
C	-1.46618	3.60036	-0.33664
C	-0.75293	4.87271	0.15294
B	-5.09991	-0.72776	-0.12469
H	2.60720	2.58873	-2.13642
H	5.07287	2.60825	-3.19381
H	6.52036	0.78837	-1.76655
H	5.04634	-2.11460	2.60506
H	2.71938	-1.95931	4.02257
H	1.10166	-0.32449	2.60730
H	-1.80994	-1.57999	1.17794
H	-1.80326	-4.02650	1.17370
H	0.00029	-5.27351	0.00032
H	0.67736	2.52046	-1.35063
H	2.51582	3.61334	0.03532
H	1.43967	3.53312	1.43116
H	1.22153	5.75407	0.29299
H	0.89760	4.95677	-1.23814
H	-2.60752	2.58906	2.13596
H	-5.07331	2.60873	3.19307
H	-6.52060	0.78854	1.76600
H	-5.04603	-2.11516	-2.60494
H	-2.71890	-1.96009	-4.02220
H	-1.10137	-0.32501	-2.60701
H	1.81014	-1.57988	-1.17754
H	1.80371	-4.02640	-1.17314
H	-0.67752	2.52041	1.35069
H	-2.51611	3.61308	-0.03521
H	-1.43999	3.53297	-1.43109
H	-1.22203	5.75395	-0.29294
H	-0.89802	4.95670	1.23820

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$[2(H)]^-$

F	-5.62406	0.87781	-1.85393
F	-6.46792	-0.92843	-0.74483
N	-1.18888	0.56222	-0.02256
N	-4.83387	0.42702	0.38544
N	-4.16522	-1.00575	-1.46809
C	-3.45614	1.10760	2.01615
C	-4.77417	1.18941	2.48520
C	-5.59163	0.75978	1.44550
C	-4.26343	-1.90007	-2.46397
C	-2.99172	-2.29346	-2.87219
C	-2.07910	-1.58190	-2.08893
C	-2.82277	-0.77868	-1.20825
C	-2.44971	0.17484	-0.19090
C	-3.51120	0.63443	0.69708
C	0.01597	-1.76409	0.30223

C	0.74313	-2.82743	-0.24618	H	0.61043	2.34916	-0.83298
C	0.74888	-4.09094	0.33822	H	2.32832	3.23048	0.89621
C	0.00807	-4.32430	1.49399	H	1.17266	2.78371	2.14701
C	-0.80798	1.80600	0.65707	H	0.90750	5.20074	1.52340
C	-1.59717	3.07493	0.32506	H	0.67027	4.74556	-0.15948
C	-0.99909	4.24747	1.11448				
B	0.11251	-0.29413	-0.33605	71			
B	-5.34773	-0.14428	-0.95913	**[2(H)]$^{\bullet 2-}$**			
F	6.61056	-0.36371	-0.14506	F	-6.28113	-1.16047	0.06860
F	5.31144	-1.25919	-1.78637	F	-6.38555	0.88742	-0.90030
N	1.22455	0.69277	0.32169	N	-1.12977	-0.46932	0.18308
N	4.70562	0.90507	-0.91797	N	-4.50295	-0.53057	-1.45850
N	4.40022	-1.10500	0.45245	N	-4.66857	0.51204	0.77014
C	3.21748	2.53184	-1.35805	C	-2.60054	-1.13730	-2.50533
C	4.41225	2.83482	-2.01453	C	-3.68584	-1.32745	-3.39048
C	5.29763	1.80039	-1.72212	C	-4.83092	-0.94510	-2.71370
C	4.71963	-2.08860	1.30734	C	-5.15920	1.14166	1.87453
C	3.65737	-2.32013	2.18456	C	-4.12310	1.40625	2.75630
C	2.65038	-1.42014	1.83688	C	-2.94065	0.90963	2.16720
C	3.11972	-0.67717	0.74196	C	-3.30308	0.35928	0.93051
C	2.53910	0.47484	0.12186	C	-2.50236	-0.24587	-0.08158
C	3.40753	1.31891	-0.66683	C	-3.13122	-0.63804	-1.30604
C	-0.73880	-2.03088	1.45222	C	-0.02405	1.87457	0.24598
C	-0.74348	-3.29010	2.04766	C	0.77814	2.23399	1.33664
C	0.64433	2.01858	0.21936	C	0.65459	3.47217	1.96427
C	1.26419	3.10263	1.10090	C	-0.29234	4.39043	1.51717
C	0.50537	4.41475	0.87567	C	-0.64743	-1.82090	0.09518
B	5.32063	-0.50035	-0.62919	C	-1.42182	-2.86910	0.88108
H	-2.56595	1.34363	2.57898	C	-0.71389	-4.22159	0.74376
H	-5.09662	1.50916	3.46525	B	-0.02825	0.41029	-0.44532
H	-6.66559	0.65553	1.39271	B	-5.51057	-0.07519	-0.37938
H	-5.23866	-2.19330	-2.82681	F	5.67875	-1.02431	-1.75568
H	-2.75948	-3.02263	-3.63430	F	6.65511	0.65777	-0.56931
H	-1.00674	-1.65925	-2.12683	N	1.27120	-0.46747	-0.02074
H	1.33923	-2.64943	-1.13956	N	4.89493	-0.59084	0.49581
H	1.33540	-4.89156	-0.10353	N	4.37438	0.96577	-1.30126
H	0.00908	-5.30753	1.95614	C	3.43972	-1.17269	2.09457
H	-0.78404	1.64842	1.74571	C	4.74346	-1.37520	2.58233
H	-2.65620	2.97570	0.55774	C	5.60916	-1.00363	1.56382
H	-1.51461	3.25597	-0.75413	C	4.57612	1.93281	-2.21805
H	-1.52853	5.17163	0.86103	C	3.35985	2.49478	-2.57867
H	-1.17349	4.07010	2.18488	C	2.36675	1.81985	-1.85079
H	0.37065	-0.30323	-1.52335	C	3.01396	0.86784	-1.05610
H	2.32965	3.14248	-1.36655	C	2.53834	-0.13658	-0.11333
H	4.61727	3.70400	-2.62187	C	3.55716	-0.69229	0.78829
H	6.31474	1.63798	-2.05039	C	-0.96593	2.81949	-0.18584
H	5.69377	-2.55444	1.25395	C	-1.10798	4.05613	0.43882
H	3.63340	-3.04932	2.98071	C	0.78114	-1.70226	0.63222
H	1.68718	-1.29060	2.30616	C	1.51671	-3.01724	0.36813
H	-1.33540	-1.23502	1.89712	C	0.77124	-4.13297	1.11931
H	-1.33634	-3.46666	2.94102	B	5.46451	-0.01624	-0.82150

H	-1.54856	-1.27518	-2.70920
H	-3.63933	-1.68773	-4.41031
H	-5.86396	-0.93178	-3.03288
H	-6.21752	1.35082	1.95146
H	-4.21421	1.91401	3.70819
H	-1.92550	0.96644	2.53382
H	1.51964	1.52900	1.71199
H	1.29745	3.72031	2.80611
H	-0.39737	5.35497	2.00839
H	-0.56947	-2.18428	-0.95250
H	-2.44843	-2.92015	0.50478
H	-1.47594	-2.55269	1.93163
H	-1.20981	-4.98461	1.35590
H	-0.79371	-4.55369	-0.30017
H	2.51761	-1.33977	2.63061
H	5.02165	-1.73632	3.56235
H	6.68879	-0.98782	1.52602
H	5.58089	2.15104	-2.55242
H	3.20923	3.31042	-3.27148
H	1.30885	2.01605	-1.86449
H	-1.61763	2.56035	-1.01857
H	-1.86262	4.75670	0.08974
H	0.68799	-1.52208	1.71303
H	2.55992	-2.99788	0.68148
H	1.50023	-3.21043	-0.71186
H	1.26691	-5.09431	0.93808
H	0.85657	-3.93628	2.19800
H	-0.07536	0.46559	-1.66745

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$[2(H)]^{3-}$ (singlet)

F	-6.13393	0.25966	-1.34037
F	-6.58405	-0.99016	0.49839
N	-1.24077	0.25807	-0.39074
N	-4.77591	0.60341	0.64546
N	-4.51302	-1.42690	-0.67963
C	-3.11760	1.75763	1.61868
C	-4.34548	2.16259	2.19000
C	-5.33805	1.42978	1.56771
C	-4.82122	-2.60522	-1.28682
C	-3.66080	-3.20139	-1.74370
C	-2.59084	-2.34461	-1.40341
C	-3.13893	-1.24167	-0.74090
C	-2.53730	-0.04231	-0.18168
C	-3.40554	0.78336	0.65123
C	0.03267	-1.93383	0.54170
C	0.81886	-3.07044	0.30608
C	0.90292	-4.11267	1.22837
C	0.18085	-4.05014	2.41893
C	-0.74675	1.63639	-0.37612
C	-1.51957	2.67777	-1.18232
C	-0.78859	4.02215	-1.03002
B	0.02290	-0.72484	-0.53963
B	-5.54864	-0.38916	-0.23778
F	6.42378	0.67159	-0.44514
F	6.32466	-1.30366	0.65147
N	1.13921	0.31283	-0.26915
N	4.62658	-0.85945	-1.03408
N	4.58760	0.33336	1.11691
C	2.87606	-1.21120	-2.41537
C	4.04367	-1.76154	-3.00580
C	5.09162	-1.52565	-2.14020
C	4.97669	0.85849	2.32447
C	3.86870	1.35093	2.98514
C	2.74466	1.11977	2.15114
C	3.21598	0.48618	0.98878
C	2.51201	0.03051	-0.17025
C	3.25836	-0.65659	-1.17910
C	-0.66176	-1.88433	1.75752
C	-0.60234	-2.92756	2.68099
C	0.67293	1.51243	-0.91634
C	1.43327	2.80860	-0.68245
C	0.69757	3.93992	-1.41758
B	5.52186	-0.29193	0.07543
H	-2.13487	2.09892	1.90318
H	-4.48470	2.89348	2.97689
H	-6.40885	1.41677	1.71655
H	-5.85342	-2.92348	-1.34519
H	-3.58698	-4.15955	-2.24294
H	-1.53894	-2.50374	-1.57711
H	1.38808	-3.11686	-0.62227
H	1.53768	-4.97324	1.02227
H	0.23481	-4.86462	3.14029
H	-0.63596	2.00449	0.65512
H	-2.55538	2.76464	-0.84355
H	-1.53644	2.36771	-2.23527
H	-1.29094	4.80094	-1.62086
H	-0.86383	4.33166	0.02283
H	0.05096	-1.18126	-1.68647
H	1.86853	-1.20711	-2.80275
H	4.10969	-2.27777	-3.95794
H	6.14303	-1.76913	-2.21978
H	6.01865	0.83066	2.61535
H	3.86886	1.81093	3.96794
H	1.70046	1.31410	2.35322
H	-1.26703	-1.00692	1.98149
H	-1.16631	-2.86403	3.61039
H	0.59689	1.37942	-2.02326
H	2.46335	2.70163	-1.03931
H	1.49277	3.00903	0.39446
H	1.18412	4.90794	-1.23336
H	0.76345	3.75524	-2.49975

71
[2H]$^{\bullet 3-}$ (triplet)

F	-6.17795	1.24854	-0.99623
F	-6.58830	-0.90205	-0.41308
N	-1.20455	0.50414	-0.06291
N	-4.83556	0.26568	0.77851
N	-4.49539	-0.42185	-1.54177
C	-3.23441	0.54424	2.32935
C	-4.49654	0.54404	2.97455
C	-5.45055	0.36757	1.99422
C	-4.75466	-0.89721	-2.79651
C	-3.56503	-1.04559	-3.48136
C	-2.52592	-0.63874	-2.60931
C	-3.12447	-0.25597	-1.40422
C	-2.55967	0.23491	-0.16771
C	-3.46487	0.36906	0.95326
C	-0.03816	-1.90955	-0.09610
C	0.80263	-2.86272	-0.68831
C	0.84004	-4.18903	-0.26330
C	0.00957	-4.61091	0.77355
C	-0.72101	1.58613	0.77602
C	-1.46265	2.92163	0.71793
C	-0.73550	3.91975	1.63164
B	0.03764	-0.35098	-0.55021
B	-5.56353	0.05552	-0.55627
F	6.36438	0.91134	0.54609
F	6.49546	-0.77063	-0.96468
N	1.19587	0.41399	0.21093
N	4.66296	0.79937	-1.18938
N	4.67661	-0.83620	0.64331
C	2.83700	1.69170	-2.16083
C	3.97888	2.07035	-2.90577
C	5.07563	1.50491	-2.28166
C	5.10044	-1.75703	1.55803
C	4.01587	-2.21263	2.28796
C	2.87354	-1.53487	1.80525
C	3.30474	-0.68620	0.77902
C	2.56199	0.21469	-0.05292
C	3.28234	0.89798	-1.09330
C	-0.86313	-2.36164	0.94533
C	-0.84630	-3.68892	1.37420
C	0.71810	1.77554	0.30445
C	1.47516	2.70586	1.24487
C	0.75539	4.06125	1.28695
B	5.59109	0.02672	-0.23587
H	-2.26707	0.62263	2.80169
H	-4.68190	0.64551	4.03767
H	-6.52733	0.29024	2.05849
H	-5.77625	-1.08730	-3.09785
H	-3.45303	-1.42330	-4.49130
H	-1.46278	-0.64167	-2.79093
H	1.45907	-2.53750	-1.49425
H	1.52263	-4.89477	-0.73465
H	0.02965	-5.64669	1.11029
H	-0.64996	1.29181	1.84141
H	-2.50317	2.80552	1.03206
H	-1.46347	3.27968	-0.32046
H	-1.22457	4.90335	1.59638
H	-0.82674	3.56229	2.66802
H	0.23924	-0.28417	-1.76549
H	1.80110	1.88995	-2.39172
H	3.99864	2.67412	-3.80556
H	6.12701	1.54032	-2.53426
H	6.15046	-2.01132	1.62067
H	4.04524	-2.96345	3.06886
H	1.84123	-1.65249	2.10263
H	-1.53509	-1.65206	1.42556
H	-1.50556	-4.00625	2.18099
H	0.66058	2.28352	-0.68122
H	2.50990	2.82440	0.90487
H	1.50622	2.24864	2.24342
H	1.24442	4.74105	1.99911
H	0.84297	4.52937	0.29591

71
[2Cl$_4$(H)]$^-$

Cl	5.78768	0.81316	2.11767
Cl	6.81237	-1.64582	0.61425
N	1.20591	0.33609	0.14373
N	4.83020	0.05045	-0.39155
N	4.16445	-1.37609	1.46657
C	3.43259	0.89054	-1.92773
C	4.73948	0.95647	-2.43109
C	5.57128	0.43519	-1.45130
C	4.25105	-2.26494	2.47633
C	2.97875	-2.58981	2.92444
C	2.07448	-1.84115	2.16310
C	2.82123	-1.08481	1.25082
C	2.45377	-0.10368	0.26105
C	3.50386	0.33401	-0.64627
C	-0.12920	-1.94591	-0.11047
C	-0.95302	-2.92754	0.45525
C	-1.06413	-4.19901	-0.10052
C	-0.33359	-4.52397	-1.24080
C	0.85652	1.62775	-0.46311
C	1.70358	2.84384	-0.08237
C	1.13398	4.07918	-0.79306
B	-0.11951	-0.46312	0.49567
B	5.32349	-0.56068	0.91286
Cl	-7.04399	-0.33954	0.09978
Cl	-5.29041	-1.74930	2.16717

N	-1.19900	0.56808	-0.15084
N	-4.68016	0.76458	1.10202
N	-4.41540	-1.13959	-0.41630
C	-3.14645	2.31317	1.65476
C	-4.32969	2.59224	2.34555
C	-5.24298	1.61028	1.98580
C	-4.72642	-2.10732	-1.29875
C	-3.65302	-2.32099	-2.16136
C	-2.64372	-1.43779	-1.77534
C	-3.12021	-0.72132	-0.67034
C	-2.51904	0.37040	0.02567
C	-3.36972	1.16851	0.87247
C	0.60990	-2.30375	-1.24549
C	0.51103	-3.57333	-1.80992
C	-0.57898	1.86919	0.01776
C	-1.17471	3.02389	-0.78598
C	-0.35692	4.29020	-0.50719
B	-5.28646	-0.58207	0.69445
H	2.53617	1.19240	-2.44672
H	5.04640	1.32755	-3.39753
H	6.64241	0.29871	-1.43715
H	5.22159	-2.59763	2.81570
H	2.73796	-3.29810	3.70290
H	1.00130	-1.86534	2.23767
H	-1.54288	-2.67729	1.33574
H	-1.72491	-4.93295	0.35157
H	-0.41574	-5.51421	-1.67985
H	0.80124	1.52865	-1.55689
H	2.75298	2.71658	-0.34477
H	1.65371	2.96818	1.00664
H	1.70447	4.96728	-0.50346
H	1.27623	3.95458	-1.87558
H	-0.35184	-0.43318	1.68926
H	-2.24116	2.89603	1.70104
H	-4.50836	3.41293	3.02387
H	-6.25920	1.44477	2.31443
H	-5.70290	-2.56969	-1.26854
H	-3.62282	-3.03040	-2.97454
H	-1.67077	-1.30479	-2.22246
H	1.27339	-1.57207	-1.70567
H	1.09477	-3.82296	-2.69169
H	-0.51413	2.13603	1.08677
H	-2.22759	3.18286	-0.54622
H	-1.12275	2.76222	-1.85049
H	-0.74219	5.12620	-1.09991
H	-0.48424	4.56792	0.54851

71
[2(F)]$^-$

F	-6.10021	-0.29292	-0.22515
F	-5.91572	0.93416	1.68764
N	-1.21065	-0.51517	-0.80542
N	-4.31046	1.31150	-0.09152
N	-4.24029	-0.73967	1.26352
C	-2.75996	1.96793	-1.60450
C	-3.80489	2.89104	-1.60636
C	-4.74355	2.43872	-0.67309
C	-4.41564	-1.43583	2.40019
C	-3.25539	-2.14660	2.70493
C	-2.33078	-1.84645	1.69865
C	-2.96901	-0.98567	0.79505
C	-2.39361	-0.19213	-0.25871
C	-3.07909	0.99533	-0.64262
C	0.13859	1.64997	-0.13384
C	0.11359	1.43559	1.24868
C	0.22441	2.48981	2.15093
C	0.36162	3.79286	1.67984
C	-0.83956	-1.83341	-1.31646
C	-1.67857	-3.09081	-1.13314
C	-1.02417	-4.19945	-1.97415
B	0.01046	0.41612	-1.14641
B	-5.22647	0.30438	0.66913
F	6.22374	0.60215	0.88219
F	4.45525	1.29442	2.13908
N	1.17465	-0.69850	-0.89943
N	4.30181	-0.84405	1.03401
N	4.20406	1.22076	-0.27032
C	2.95123	-2.63344	0.95491
C	4.00910	-2.91347	1.82618
C	4.81241	-1.77992	1.84952
C	4.65975	2.26896	-0.97606
C	3.82776	2.49645	-2.07124
C	2.81764	1.53116	-2.01596
C	3.06127	0.75061	-0.87809
C	2.40231	-0.45270	-0.44171
C	3.14048	-1.32774	0.45881
C	0.27872	2.96621	-0.58295
C	0.38889	4.02972	0.30797
C	0.59116	-2.03452	-0.83688
C	1.25543	-3.09017	-1.72271
C	0.45598	-4.39557	-1.61473
B	4.84266	0.61945	0.99697
H	-1.86890	1.96700	-2.21422
H	-3.88565	3.78447	-2.20784
H	-5.71191	2.84296	-0.41132
H	-5.34820	-1.35926	2.94077
H	-3.09891	-2.77154	3.57170
H	-1.29331	-2.14680	1.64783
H	0.00643	0.41912	1.62686
H	0.20751	2.29574	3.21922
H	0.45204	4.61901	2.37926
H	-0.78178	-1.67729	-2.40845

H	-2.71185	-2.91581	-1.44913
H	-1.71527	-3.40220	-0.08677
H	-1.57081	-5.13794	-1.83656
H	-1.10069	-3.94017	-3.03816
H	2.17207	-3.33021	0.69659
H	4.17838	-3.83536	2.36285
H	5.71797	-1.57237	2.40169
H	5.55930	2.77953	-0.66254
H	3.95659	3.26336	-2.82093
H	2.00480	1.37907	-2.70881
H	0.31132	3.15343	-1.65387
H	0.50123	5.04358	-0.06619
H	0.54735	-2.37701	0.20847
H	2.30258	-3.24569	-1.45509
H	1.23682	-2.71906	-2.75496
H	0.90025	-5.16302	-2.25691
H	0.52526	-4.77138	-0.58355
F	-0.02266	0.78388	-2.50697

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[2(F)]$^{\bullet 2-}$

F	6.58158	-0.21099	0.09390
F	5.43079	-1.12470	-1.63543
N	1.21472	0.64795	0.66437
N	4.62327	0.95040	-0.70827
N	4.40523	-1.12786	0.56563
C	3.11619	2.57803	-1.01642
C	4.28889	2.92150	-1.70637
C	5.18797	1.88957	-1.49128
C	4.76407	-2.19423	1.30862
C	3.72892	-2.53315	2.17027
C	2.69154	-1.61799	1.93685
C	3.12588	-0.75759	0.92641
C	2.48890	0.43653	0.39983
C	3.33541	1.34053	-0.38996
C	0.20919	-1.79156	-0.08594
C	0.05592	-3.06902	0.46109
C	0.21051	-4.21717	-0.31287
C	0.53181	-4.10708	-1.66313
C	0.57979	1.95869	0.50155
C	1.11238	3.11617	1.34618
C	0.30577	4.36719	0.95937
B	-0.02786	-0.47278	0.79669
B	5.31262	-0.41629	-0.44614
F	-6.43471	0.60261	-0.48593
F	-6.03131	-1.58863	-0.89460
N	-1.12953	0.42340	0.27480
N	-4.72170	-0.49317	0.83156
N	-4.33800	0.02184	-1.55344
C	-3.16362	-0.46913	2.46593
C	-4.41826	-0.77226	3.03819
C	-5.34459	-0.77772	2.00846
C	-4.54724	0.28331	-2.87436
C	-3.35406	0.65992	-3.46871
C	-2.36471	0.62835	-2.46158
C	-2.99957	0.22739	-1.27773
C	-2.47617	0.05136	0.03681
C	-3.37485	-0.29967	1.08942
C	0.51768	-1.70569	-1.44799
C	0.68588	-2.84392	-2.23113
C	-0.88568	1.72098	0.86180
C	-1.71903	2.90192	0.38750
C	-1.21226	4.16347	1.10376
B	-5.42910	-0.37581	-0.53645
F	-0.13821	-0.78258	2.18458
H	2.22717	3.18293	-0.97475
H	4.46053	3.81913	-2.28321
H	6.19791	1.74942	-1.85022
H	5.74468	-2.63145	1.18179
H	3.73122	-3.34456	2.88423
H	1.73643	-1.55222	2.43391
H	-0.19387	-3.15223	1.51598
H	0.08125	-5.19935	0.13626
H	0.65810	-4.99960	-2.27143
H	0.58618	2.22581	-0.56568
H	2.18242	3.28786	1.21026
H	0.95048	2.87308	2.40326
H	0.62786	5.22622	1.56037
H	0.53296	4.61690	-0.08778
H	-2.19846	-0.41317	2.94626
H	-4.62780	-0.97243	4.08144
H	-6.41015	-0.96215	2.02397
H	-5.53883	0.18389	-3.29433
H	-3.21810	0.92057	-4.51062
H	-1.30983	0.84798	-2.54487
H	0.62674	-0.72061	-1.89849
H	0.93217	-2.74825	-3.28546
H	-0.97093	1.68691	1.96805
H	-2.77674	2.72655	0.60846
H	-1.63132	2.99583	-0.70266
H	-1.74030	5.05263	0.73929
H	-1.44914	4.07298	2.17263

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[2(F)]$^{3-}$ (singlet)

F	6.23134	0.60542	0.73926
F	6.34219	-0.65372	-1.14263
N	1.19158	0.39078	0.68039
N	4.49548	0.89316	-0.93832
N	4.55800	-1.12893	0.43067

C	2.65279	1.99347	-1.59691
C	3.74916	2.44195	-2.37054
C	4.85894	1.74399	-1.93769
C	5.01576	-2.26615	1.02680
C	3.98532	-2.85725	1.73363
C	2.84267	-2.04083	1.57058
C	3.21785	-0.97065	0.75195
C	2.46821	0.16736	0.26171
C	3.13664	1.02201	-0.70368
C	-0.01098	-1.76045	-0.38693
C	-0.32410	-3.10055	-0.13755
C	-0.32547	-4.05566	-1.15317
C	0.00094	-3.68624	-2.45596
C	0.67507	1.74665	0.80891
C	1.47308	2.71699	1.67331
C	0.70955	4.05114	1.71039
B	-0.03133	-0.64350	0.78158
B	5.45215	-0.07187	-0.22132
F	-6.28421	0.87417	0.32443
F	-6.24740	-0.66620	-1.33523
N	-1.17184	0.36405	0.66429
N	-4.66826	-0.93776	0.49299
N	-4.35994	0.84761	-1.16823
C	-3.09759	-1.77051	1.88343
C	-4.31574	-2.46203	2.10109
C	-5.25319	-1.92727	1.23890
C	-4.56746	1.62361	-2.27787
C	-3.37267	2.19911	-2.66420
C	-2.38048	1.75170	-1.75493
C	-3.02039	0.91433	-0.82582
C	-2.48689	0.15829	0.26801
C	-3.33876	-0.82603	0.87594
C	0.30953	-1.41242	-1.70547
C	0.31927	-2.35656	-2.72919
C	-0.71966	1.54488	1.37972
C	-1.51027	2.84289	1.31805
C	-0.75358	3.88589	2.15819
B	-5.42707	0.03196	-0.42391
F	-0.01834	-1.28989	2.07277
H	1.62309	2.28970	-1.72069
H	3.72363	3.17958	-3.16339
H	5.88751	1.77123	-2.27029
H	6.05025	-2.55776	0.90288
H	4.04412	-3.78514	2.29027
H	1.85334	-2.18516	1.97532
H	-0.58209	-3.38597	0.87941
H	-0.58373	-5.09011	-0.93046
H	0.00538	-4.42759	-3.25387
H	0.51930	2.22533	-0.16925
H	2.48168	2.85559	1.27023
H	1.56991	2.29783	2.68368
H	1.22256	4.77334	2.36095
H	0.72092	4.47848	0.69733
H	-2.13963	-1.91306	2.36179
H	-4.48620	-3.27484	2.79908
H	-6.29912	-2.16400	1.09438
H	-5.55622	1.69064	-2.71192
H	-3.22696	2.84773	-3.52080
H	-1.31350	1.92961	-1.78331
H	0.55816	-0.37437	-1.92297
H	0.57700	-2.05695	-3.74314
H	-0.60757	1.30426	2.45910
H	-2.52617	2.68561	1.69734
H	-1.61056	3.18022	0.28121
H	-1.26559	4.85748	2.12066
H	-0.76091	3.56513	3.21051

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[2(F)]$^{\bullet\bullet 3-}$ (triplet)

F	6.25434	1.24758	0.74079
F	6.57547	-0.92809	0.19855
N	1.19826	0.52816	0.09369
N	4.78704	0.25470	-0.92456
N	4.56453	-0.35870	1.43234
C	3.11310	0.52115	-2.39924
C	4.34158	0.50591	-3.10499
C	5.34147	0.33848	-2.16937
C	4.88101	-0.76690	2.69665
C	3.72548	-0.85692	3.44899
C	2.64789	-0.48117	2.61206
C	3.19021	-0.17850	1.35847
C	2.56217	0.25066	0.13267
C	3.40933	0.36198	-1.03364
C	0.06887	-1.91349	0.09781
C	-0.70437	-2.87727	0.75906
C	-0.72562	-4.21072	0.35448
C	0.04786	-4.62244	-0.72918
C	0.70110	1.62675	-0.71744
C	1.42349	2.96850	-0.62641
C	0.68874	3.96936	-1.53169
B	-0.02594	-0.35300	0.53527
B	5.58529	0.05964	0.37305
F	-6.29122	1.04527	-0.60257
F	-6.54309	-0.77667	0.71966
N	-1.18026	0.39235	-0.20504
N	-4.66249	0.68645	1.16945
N	-4.66890	-0.75260	-0.82391
C	-2.83096	1.39875	2.27683
C	-3.97933	1.74125	3.02795
C	-5.07939	1.28830	2.32036
C	-5.08915	-1.56992	-1.83346
C	-3.99569	-1.98607	-2.57425

C	-2.85046	-1.39055	-1.99805
C	-3.29076	-0.63027	-0.90870
C	-2.55011	0.15712	0.03046
C	-3.27710	0.74336	1.12137
C	0.83858	-2.35273	-0.98838
C	0.83423	-3.68573	-1.39807
C	-0.74506	1.77463	-0.26193
C	-1.50612	2.70213	-1.20109
C	-0.81090	4.07194	-1.20753
B	-5.58308	0.05483	0.11057
F	-0.26847	-0.29760	1.95458
H	2.12491	0.59078	-2.82690
H	4.47524	0.59294	-4.17696
H	6.41370	0.25731	-2.28529
H	5.91438	-0.95363	2.95787
H	3.66287	-1.17359	4.48391
H	1.59458	-0.44709	2.84216
H	-1.30747	-2.55536	1.60497
H	-1.35005	-4.93162	0.88049
H	0.03722	-5.66326	-1.05026
H	0.64254	1.35920	-1.78926
H	2.46837	2.86818	-0.93492
H	1.41185	3.30879	0.41778
H	1.15452	4.96292	-1.47004
H	0.80335	3.63414	-2.57297
H	-1.79048	1.49851	2.54824
H	-4.00418	2.24294	3.98840
H	-6.13540	1.33794	2.55093
H	-6.14305	-1.78676	-1.94906
H	-4.02280	-2.65813	-3.42405
H	-1.81233	-1.50800	-2.27450
H	1.45939	-1.63064	-1.51634
H	1.44969	-3.99621	-2.24092
H	-0.73310	2.25963	0.73624
H	-2.54915	2.79565	-0.87828
H	-1.51216	2.26051	-2.20706
H	-1.30216	4.75547	-1.91443
H	-0.92269	4.51965	-0.20957

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[2(Cl)]$^{-}$

F	5.77008	0.91280	1.39970
F	6.61555	-0.80654	0.15844
N	1.23916	0.53642	0.03416
N	4.81139	0.47985	-0.77698
N	4.39316	-1.04337	1.06711
C	3.23714	1.08907	-2.24960
C	4.49207	1.23244	-2.85579
C	5.43576	0.84725	-1.90960
C	4.63662	-1.99734	1.97429
C	3.43348	-2.47978	2.48909
C	2.41307	-1.75604	1.87391
C	3.01868	-0.85598	0.97667
C	2.51237	0.12498	0.05374
C	3.45477	0.62304	-0.94420
C	-0.11990	-1.76984	0.00331
C	-1.01445	-2.66804	0.59870
C	-1.16451	-3.96722	0.12246
C	-0.40461	-4.40657	-0.95854
C	0.84717	1.83915	-0.54361
C	1.68199	3.06382	-0.17319
C	1.07120	4.28404	-0.87713
B	-0.06052	-0.23488	0.44765
B	5.47777	-0.09471	0.49591
F	-6.50240	0.00015	-0.75487
F	-5.79766	-1.29346	0.97658
N	-1.14043	0.70852	-0.19625
N	-4.74293	0.85054	0.67328
N	-4.31217	-0.98484	-0.91447
C	-3.20801	2.20948	1.61383
C	-4.45038	2.48741	2.17957
C	-5.36450	1.61952	1.57671
C	-4.51867	-1.88668	-1.88379
C	-3.34006	-2.08929	-2.61140
C	-2.38038	-1.25094	-2.05222
C	-2.99188	-0.57902	-0.97975
C	-2.47903	0.45747	-0.15183
C	-3.39807	1.18640	0.66473
C	0.64155	-2.23696	-1.07610
C	0.50598	-3.53802	-1.55399
C	-0.58233	2.04684	-0.03729
C	-1.22642	3.18292	-0.82386
C	-0.41977	4.46280	-0.56637
B	-5.41197	-0.39063	0.00329
Cl	-0.34647	-0.03590	2.36423
H	2.28388	1.26579	-2.72207
H	4.69195	1.56148	-3.86495
H	6.51302	0.79522	-1.97116
H	5.65756	-2.26554	2.20836
H	3.31695	-3.26926	3.21655
H	1.35781	-1.88410	2.03691
H	-1.61391	-2.33228	1.44100
H	-1.87932	-4.63583	0.59323
H	-0.51822	-5.42035	-1.33192
H	0.76851	1.75692	-1.63455
H	2.72649	2.95263	-0.46395
H	1.65166	3.18698	0.91659
H	1.62408	5.18750	-0.60038
H	1.20002	4.15742	-1.96108
H	-2.26962	2.67790	1.86511
H	-4.67170	3.22127	2.94015
H	-6.42341	1.49359	1.75571

H	-5.50053	-2.31868	-2.02021
H	-3.21506	-2.75955	-3.44873
H	-1.35552	-1.11652	-2.36029
H	1.34799	-1.56933	-1.56665
H	1.11244	-3.87321	-2.39064
H	-0.51267	2.32138	1.02567
H	-2.26961	3.32689	-0.53460
H	-1.21470	2.92579	-1.89103
H	-0.83122	5.29077	-1.15306
H	-0.53391	4.73874	0.49081

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[2(Br)]$^-$

F	6.30398	-1.00324	-0.53645
F	4.39221	-1.81583	-1.49769
N	1.21984	0.98816	0.28470
N	4.56676	0.55863	-1.13765
N	4.26057	-0.94701	0.74680
C	3.33434	2.33004	-1.74794
C	4.49496	2.30402	-2.52940
C	5.21864	1.18808	-2.12806
C	4.59067	-1.73771	1.77973
C	3.64783	-1.59636	2.79800
C	2.69200	-0.68514	2.34196
C	3.08833	-0.29096	1.05648
C	2.51358	0.67201	0.15843
C	3.38618	1.22872	-0.87043
C	0.28071	-1.55539	0.44075
C	-0.46832	-2.49108	1.16250
C	-0.32171	-3.86008	0.94909
C	0.60736	-4.33047	0.02668
C	0.67380	2.19577	-0.33313
C	1.15449	3.53307	0.22825
C	0.47938	4.64328	-0.59254
B	0.03397	0.01245	0.60168
B	4.93230	-0.86955	-0.63444
F	-5.78845	-0.44234	-2.07585
F	-5.93952	-1.83458	-0.28390
N	-1.08750	0.68358	-0.24655
N	-4.76020	0.24442	0.00320
N	-3.78150	-1.55704	-1.35976
C	-3.61425	1.74942	1.23190
C	-4.95578	1.80520	1.60079
C	-5.62389	0.85459	0.82323
C	-3.65009	-2.58149	-2.21249
C	-2.32342	-2.68076	-2.64885
C	-1.62675	-1.64459	-2.03589
C	-2.53955	-0.96033	-1.21355
C	-2.35287	0.18707	-0.39943
C	-3.49753	0.77092	0.22382
C	1.19952	-2.05545	-0.49543
C	1.37783	-3.41986	-0.69290
C	-0.83517	2.11423	-0.10330
C	-1.52675	3.10133	-1.03330
C	-1.05197	4.50811	-0.63058
B	-5.14006	-0.92559	-0.95054
Br	-0.62248	0.43047	2.62368
H	2.58029	3.09635	-1.79864
H	4.77957	3.01946	-3.28673
H	6.15554	0.78911	-2.48989
H	5.48069	-2.34891	1.72813
H	3.66362	-2.09473	3.75589
H	1.81438	-0.33366	2.86237
H	-1.17313	-2.13392	1.90714
H	-0.92916	-4.56020	1.51563
H	0.73634	-5.39846	-0.12556
H	0.85183	2.14625	-1.41798
H	2.24207	3.62942	0.19730
H	0.85449	3.58377	1.28182
H	0.75569	5.62680	-0.19881
H	0.86332	4.60039	-1.62212
H	-2.80368	2.30551	1.67461
H	-5.39905	2.43942	2.35400
H	-6.66602	0.56683	0.82016
H	-4.51505	-3.17021	-2.48660
H	-1.92887	-3.41910	-3.33072
H	-0.58478	-1.39324	-2.14766
H	1.80576	-1.37842	-1.09268
H	2.12874	-3.75867	-1.39994
H	-1.00887	2.42594	0.93379
H	-2.61407	3.03528	-0.94861
H	-1.25856	2.87816	-2.07361
H	-1.47348	5.25700	-1.30887
H	-1.45092	4.72819	0.36865

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2(PMe$_3$)

F	-6.52621	1.01386	0.61102
F	-5.18586	1.89606	-1.02336
N	-1.40267	-0.94791	-0.14947
N	-5.04087	-0.46159	-0.60269
N	-4.14936	1.16839	1.01612
C	-3.91264	-2.13344	-1.62299
C	-5.24176	-2.18656	-2.02417
C	-5.89847	-1.12762	-1.37973
C	-4.08313	2.05530	2.00988
C	-2.80994	2.01286	2.61216
C	-2.08105	1.04975	1.93266
C	-2.92790	0.52898	0.93058
C	-2.70416	-0.50797	0.00862
C	-3.79173	-1.05020	-0.72334

C	-0.24833	1.42220	-0.68370
C	0.83087	2.20598	-0.24842
C	0.82354	3.58858	-0.39659
C	-0.26588	4.21594	-0.99721
C	-1.02782	-2.35829	-0.33410
C	-1.69983	-3.41995	0.52330
C	-1.08339	-4.77441	0.13358
B	-0.25186	-0.12281	-0.47648
B	-5.30401	0.96700	-0.00950
F	6.01152	0.74437	-1.66979
F	4.57588	1.87310	-0.28298
N	0.87564	-1.04295	-0.60740
N	4.51707	-0.52447	-0.25112
N	3.64949	0.73076	-2.17944
C	3.38527	-1.95067	1.08413
C	4.71955	-1.93650	1.47997
C	5.37940	-1.03219	0.63542
C	3.61752	1.36283	-3.35396
C	2.36446	1.17642	-3.96644
C	1.61108	0.39723	-3.10188
C	2.42427	0.12625	-1.97935
C	2.17953	-0.67549	-0.84586
C	3.26500	-1.06598	-0.01115
C	-1.33004	2.07339	-1.29498
C	-1.34021	3.45559	-1.45224
C	0.47074	-2.33212	-0.02537
C	1.09739	-3.61574	-0.55343
C	0.45111	-4.78190	0.21410
B	4.76581	0.77122	-1.09917
P	1.60823	0.48047	2.83690
C	0.70475	1.83008	3.73570
C	2.10878	-0.56198	4.28658
C	3.21780	1.34817	2.55143
H	-3.12876	-2.81278	-1.92200
H	-5.69264	-2.90173	-2.69532
H	-6.92823	-0.80564	-1.45078
H	-4.94018	2.67007	2.24869
H	-2.48513	2.61220	3.44976
H	-1.06852	0.71802	2.11628
H	1.69918	1.73000	0.19890
H	1.67331	4.17040	-0.05337
H	-0.27533	5.29507	-1.11487
H	-1.13602	-2.62700	-1.39670
H	-2.78193	-3.43695	0.37361
H	-1.51672	-3.19487	1.58094
H	-1.49254	-5.56490	0.76881
H	-1.38769	-5.01108	-0.89483
H	2.59698	-2.54398	1.52226
H	5.16973	-2.51311	2.27422
H	6.41165	-0.71050	0.63253
H	4.48433	1.90649	-3.70361
H	2.06873	1.55757	-4.93192
H	0.60543	0.03125	-3.25067
H	-2.18875	1.50539	-1.64561
H	-2.19322	3.93508	-1.92098
H	0.58425	-2.27559	1.06921
H	2.18164	-3.62995	-0.42703
H	0.89425	-3.69793	-1.62814
H	0.83720	-5.73323	-0.16248
H	0.75480	-4.71564	1.26759
H	1.33003	2.29491	4.50445
H	-0.19473	1.42482	4.20908
H	0.39378	2.59396	3.01561
H	2.83639	-1.30731	3.95350
H	1.23906	-1.08532	4.69192
H	2.56281	0.03942	5.08065
H	3.59808	1.77712	3.48452
H	3.11047	2.14652	1.81417
H	3.95353	0.64183	2.15875

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[2(Py)]

F	-6.31215	1.00634	0.50682
F	-4.72069	1.89511	-0.87183
N	-1.17971	-1.05486	0.26217
N	-4.73697	-0.48750	-0.53959
N	-4.02603	0.99584	1.25922
C	-3.65521	-2.23233	-1.45651
C	-4.93983	-2.17997	-1.98737
C	-5.56767	-1.07885	-1.40237
C	-4.13320	1.76697	2.34818
C	-3.01518	1.58448	3.16688
C	-2.19658	0.66192	2.51876
C	-2.83840	0.30217	1.32019
C	-2.48329	-0.66926	0.32963
C	-3.52324	-1.15985	-0.53769
C	-0.46824	1.46304	-0.15630
C	-0.29021	2.60690	0.62622
C	-0.82710	3.83786	0.25054
C	-1.58500	3.94440	-0.90873
C	-0.80358	-2.24248	-0.50599
C	-1.20788	-3.60220	0.06118
C	-0.72717	-4.68356	-0.91898
B	-0.00219	-0.01835	0.20401
B	-5.00987	0.92613	0.06773
F	5.94599	1.67633	-0.91550
F	4.37227	2.05077	0.70544
N	0.97433	-0.77017	-0.80791
N	4.56288	-0.17097	-0.19201
N	3.61209	1.63759	-1.53956
C	3.63424	-2.15316	0.34120
C	4.92850	-2.11514	0.85789

C	5.45924	-0.86946	0.51731
C	3.54385	2.65496	-2.40518
C	2.33071	2.60487	-3.10824
C	1.63298	1.50621	-2.62279
C	2.44021	0.90790	-1.63398
C	2.25780	-0.30966	-0.93501
C	3.40316	-0.92303	-0.31506
C	-1.24876	1.59826	-1.31629
C	-1.80878	2.81185	-1.68962
C	0.71467	-2.18462	-0.58720
C	1.19930	-3.16758	-1.64699
C	0.77778	-4.57968	-1.21220
B	4.68981	1.36015	-0.47139
H	-2.93608	-2.99960	-1.68510
H	-5.37447	-2.86476	-2.69972
H	-6.55729	-0.67319	-1.55946
H	-5.00270	2.39415	2.48420
H	-2.83919	2.05698	4.12148
H	-1.26388	0.26993	2.88832
H	0.23697	2.54976	1.57491
H	-0.67092	4.70742	0.88124
H	-2.02215	4.89665	-1.19108
H	-1.18261	-2.13378	-1.53282
H	-2.28482	-3.67174	0.22943
H	-0.72020	-3.73791	1.03587
H	-0.96400	-5.67762	-0.52904
H	-1.28047	-4.57822	-1.86251
H	2.97423	-3.00397	0.38609
H	5.43926	-2.90513	1.38784
H	6.42502	-0.43764	0.74084
H	4.36075	3.35933	-2.48099
H	2.02010	3.28553	-3.88606
H	0.67993	1.12558	-2.95288
H	-1.44783	0.71657	-1.92574
H	-2.43916	2.87062	-2.57027
H	1.10470	-2.50516	0.39379
H	2.28323	-3.11153	-1.77954
H	0.73983	-2.90306	-2.60678
H	1.06018	-5.30776	-1.97790
H	1.33530	-4.84994	-0.30417
N	0.87989	-0.09973	1.60592
C	1.95973	0.69420	1.73842
C	0.70152	-1.10895	2.47933
C	2.89888	0.50326	2.74120
C	1.59459	-1.35520	3.50678
C	2.71836	-0.54193	3.63647
H	2.08323	1.48234	1.00438
H	-0.19137	-1.70508	2.32301
H	3.76313	1.15470	2.75942
H	1.40877	-2.17906	4.18494
H	3.44281	-0.72652	4.42242

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[2(Py)]$^{\bullet-}$

F	6.45899	-0.76582	0.58674
F	5.04220	-1.82403	-0.85304
N	1.22916	0.99227	0.22980
N	4.80612	0.55663	-0.56536
N	4.14843	-0.96044	1.22263
C	3.64691	2.22922	-1.51075
C	4.93495	2.22301	-2.04806
C	5.61111	1.16815	-1.44397
C	4.28115	-1.73790	2.30753
C	3.14189	-1.63160	3.10386
C	2.28118	-0.74739	2.45052
C	2.92137	-0.33616	1.27163
C	2.52561	0.64067	0.29012
C	3.56577	1.17560	-0.57197
C	0.50054	-1.52050	-0.15411
C	0.39907	-2.65862	0.65017
C	0.95730	-3.87800	0.26698
C	1.65683	-3.97907	-0.92895
C	0.80829	2.17309	-0.52755
C	1.21065	3.53999	0.02674
C	0.69632	4.60812	-0.95149
B	0.00789	-0.04565	0.24203
B	5.17135	-0.81336	0.08034
F	-6.09137	-1.54669	-0.87988
F	-4.60106	-2.01457	0.78409
N	-0.97932	0.68710	-0.74687
N	-4.62837	0.22211	-0.12782
N	-3.74162	-1.63682	-1.44294
C	-3.65444	2.17597	0.38409
C	-4.98832	2.20417	0.84274
C	-5.54926	0.98491	0.51557
C	-3.74414	-2.67271	-2.31785
C	-2.56070	-2.66443	-3.04140
C	-1.80507	-1.57274	-2.57639
C	-2.55830	-0.94293	-1.58067
C	-2.30275	0.25305	-0.82703
C	-3.43832	0.92391	-0.22337
C	1.21270	-1.65290	-1.35524
C	1.79205	-2.85408	-1.74054
C	-0.71095	2.09692	-0.56262
C	-1.22846	3.06132	-1.62461
C	-0.81305	4.48310	-1.21922
B	-4.81608	-1.28812	-0.40682
H	2.89063	2.95213	-1.75901
H	5.33318	2.90996	-2.77978
H	6.61818	0.80373	-1.59056
H	5.18452	-2.31352	2.45062
H	2.96827	-2.13401	4.04374
H	1.30970	-0.43326	2.79258

H	-0.09413	-2.59830	1.61679
H	0.86188	-4.74299	0.91700
H	2.10996	-4.92145	-1.22163
H	1.15421	2.06607	-1.56525
H	2.28921	3.62914	0.17643
H	0.73466	3.67169	1.00689
H	0.92990	5.60859	-0.57255
H	1.23567	4.50158	-1.90367
H	-2.95724	2.99451	0.45868
H	-5.48477	3.02909	1.33453
H	-6.54232	0.59550	0.68971
H	-4.59269	-3.34062	-2.36542
H	-2.28470	-3.36332	-3.81821
H	-0.84408	-1.23498	-2.92761
H	1.33366	-0.77724	-1.99251
H	2.36144	-2.91190	-2.66300
H	-1.07179	2.45163	0.41937
H	-2.31442	2.98546	-1.72175
H	-0.79012	2.78583	-2.59197
H	-1.11490	5.20273	-1.98712
H	-1.35726	4.75596	-0.30425
N	-0.80080	0.02907	1.62932
C	-1.94536	-0.70659	1.70150
C	-0.63428	1.05929	2.50146
C	-2.94676	-0.41192	2.61949
C	-1.58459	1.38923	3.43659
C	-2.78488	0.65935	3.48021
H	-2.03999	-1.53968	1.01669
H	0.30329	1.59695	2.40676
H	-3.85495	-1.00050	2.57560
H	-1.39961	2.21767	4.11021
H	-3.56952	0.93063	4.17796

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[2(Py)]$^{2-}$ (singlet)

F	5.64621	-0.71279	1.07892
F	6.51525	-0.78461	-1.03223
N	1.18574	-0.17852	0.35307
N	4.64194	0.68747	-0.63483
N	4.31814	-1.72450	-0.67620
C	3.07260	2.27594	-0.86984
C	4.33899	2.84212	-1.14575
C	5.27228	1.83657	-0.99123
C	4.51991	-2.96063	-1.20224
C	3.29460	-3.55363	-1.46136
C	2.30175	-2.62303	-1.07920
C	2.96803	-1.49865	-0.58137
C	2.43422	-0.20588	-0.19377
C	3.27920	0.92880	-0.53982
C	-0.11264	1.59739	-1.14856
C	0.02964	0.90704	-2.35876
C	0.00666	1.56828	-3.58294
C	-0.16449	2.94999	-3.62496
C	0.76600	-1.10421	1.42997
C	1.57734	-2.29292	1.93214
C	0.81824	-2.85007	3.14983
B	-0.04059	0.72819	0.19974
B	5.34599	-0.64487	-0.28399
F	-5.95331	-1.11894	0.69780
F	-6.42250	-0.51702	-1.44514
N	-1.15283	-0.31812	0.34897
N	-4.31970	-1.62691	-1.02271
N	-4.66548	0.67900	-0.29262
C	-2.31421	-2.53563	-1.45988
C	-3.31138	-3.32827	-2.06954
C	-4.52757	-2.73687	-1.77818
C	-5.28362	1.87268	-0.09750
C	-4.36147	2.81186	0.32209
C	-3.11421	2.15406	0.40616
C	-3.31847	0.81854	0.00777
C	-2.44312	-0.31183	-0.12841
C	-2.96540	-1.47819	-0.80970
C	-0.29487	2.98247	-1.21759
C	-0.31767	3.65774	-2.43607
C	-0.62638	-1.52488	0.99405
C	-1.41236	-2.05814	2.18831
C	-0.62904	-3.23118	2.79634
B	-5.39928	-0.66016	-0.50433
N	-0.04854	1.69989	1.55385
C	1.08568	2.38360	1.87718
C	-0.99141	1.53926	2.52867
C	-0.85077	2.09945	3.78638
C	0.28719	2.83836	4.10436
C	1.27369	2.96769	3.10700
H	2.11878	2.76013	-0.99697
H	4.53526	3.85931	-1.45750
H	6.34633	1.84152	-1.11167
H	5.52560	-3.31869	-1.37028
H	3.13791	-4.53052	-1.89878
H	1.22827	-2.71175	-1.18332
H	0.16743	-0.17262	-2.32843
H	0.12517	1.00624	-4.50527
H	-0.18066	3.47132	-4.57878
H	0.64678	-0.47131	2.33168
H	2.59440	-1.98340	2.19706
H	1.66791	-3.07318	1.17485
H	1.34738	-3.72428	3.54751
H	0.80310	-2.09532	3.94877
H	-1.24510	-2.66145	-1.54905
H	-3.15855	-4.21770	-2.66620
H	-5.53301	-3.01340	-2.06201
H	-6.34883	1.95593	-0.26311

H	-4.55713	3.85507	0.53089
H	-2.16594	2.61173	0.62723
H	-0.40023	3.55186	-0.29575
H	-0.45555	4.73597	-2.45768
H	-0.50989	-2.35162	0.28082
H	-2.41475	-2.36782	1.87469
H	-1.52686	-1.25860	2.93247
H	-1.14592	-3.61331	3.68498
H	-0.60815	-4.05225	2.06640
H	1.84855	2.42641	1.10646
H	-1.86007	0.95777	2.24913
H	-1.64366	1.94335	4.51057
H	0.42782	3.26086	5.09324
H	2.19558	3.50916	3.28838

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[2(Py)]$^{\bullet 2-}$ (triplet)

F	5.87582	1.32177	1.12975
F	6.62239	-0.78673	0.71675
N	1.26110	0.53508	-0.19537
N	4.91971	0.11058	-0.74227
N	4.36688	-0.53182	1.54801
C	3.47599	0.29268	-2.45098
C	4.79109	0.26053	-2.97046
C	5.64631	0.14752	-1.89211
C	4.51911	-1.08742	2.78145
C	3.27566	-1.34517	3.32397
C	2.31595	-0.92021	2.37598
C	3.01695	-0.41453	1.27106
C	2.58762	0.10808	-0.00175
C	3.57487	0.19432	-1.05178
C	0.14732	-1.83914	-0.22971
C	-0.18721	-2.86952	0.65357
C	0.03817	-4.21056	0.34190
C	0.62828	-4.55637	-0.86754
C	1.00453	1.64246	-1.10919
C	1.77216	2.94072	-0.88770
C	1.30362	3.95340	-1.94351
B	-0.02733	-0.25283	-0.00781
B	5.49895	0.04682	0.68284
F	-6.44481	-0.70866	-0.22615
F	-4.84799	-1.33848	1.27757
N	-1.03449	0.54008	-0.91634
N	-4.60016	0.80342	0.18352
N	-4.24182	-1.26776	-1.06455
C	-3.21178	2.55374	0.41183
C	-4.43971	2.86413	1.03998
C	-5.26210	1.76715	0.88268
C	-4.51450	-2.39095	-1.78374
C	-3.42604	-2.69758	-2.58270
C	-2.44209	-1.71685	-2.33606
C	-2.97018	-0.83536	-1.38841
C	-2.42003	0.36466	-0.81855
C	-3.32346	1.25517	-0.11915
C	0.77526	-2.21761	-1.42715
C	1.00942	-3.54778	-1.75135
C	-0.48695	1.88443	-0.95944
C	-0.97998	2.80936	-2.06533
C	-0.22239	4.14087	-1.94970
B	-5.08130	-0.65443	0.05665
H	2.56506	0.31268	-3.02938
H	5.07625	0.29713	-4.01391
H	6.72413	0.08161	-1.84757
H	5.51171	-1.25325	3.17605
H	3.07763	-1.80819	4.28192
H	1.24871	-1.05437	2.44378
H	-0.62233	-2.63562	1.62224
H	-0.24310	-4.98382	1.05237
H	0.80743	-5.60010	-1.11343
H	1.16501	1.34376	-2.15707
H	2.84916	2.76903	-0.96681
H	1.56540	3.31501	0.12502
H	1.79853	4.92069	-1.79482
H	1.62119	3.58682	-2.92965
H	-2.36376	3.21516	0.33331
H	-4.69679	3.79447	1.52936
H	-6.27727	1.58988	1.20890
H	-5.46791	-2.88713	-1.66834
H	-3.35343	-3.53206	-3.26731
H	-1.46483	-1.62468	-2.78402
H	1.09604	-1.43586	-2.11320
H	1.50109	-3.79900	-2.68749
H	-0.62322	2.40614	0.00860
H	-2.06014	2.96698	-1.98995
H	-0.78008	2.33341	-3.03397
H	-0.51472	4.81905	-2.76082
H	-0.52272	4.62960	-1.01112
N	-0.69349	0.06918	1.50586
C	-1.91523	-0.42513	1.79031
C	-0.20407	1.08022	2.24875
C	-2.70273	0.09619	2.80989
C	-0.92688	1.63546	3.28810
C	-2.20832	1.15178	3.55890
H	-2.27490	-1.23648	1.16800
H	0.79116	1.40799	1.96629
H	-3.70267	-0.30185	2.92963
H	-0.49414	2.44895	3.85876
H	-2.81296	1.60163	4.34052

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