Electronic Supplementary Material (ESI) for ChemComm.

Redox Switchable Catalysis Utilizing a Fluorescent Dye

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Supporting Information

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1) Synthetic Procedures and Catalytic Conditions

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. 8-methylthio-BODIPY (BoSMe),[1] bis[2-(diphenylphosphino)ethyl]ammonium chloride,[2] and KC_8 were prepared according to previously reported literature procedures.[3] $[(COD)_2Rh]BF_4$ and diphenylphosphine were purchased from Strem Chemicals and were used as received. Pinacolborane and catecholborane were purchased from Alfa Aesar and were used as received. All remaining reagents were purchased from Sigma Aldrich, Acros Organics, or Alfa Aesar and were used without further purification. All color names listed are taken in relation to a crayon of most similar color from a 120 Crayola crayon set.

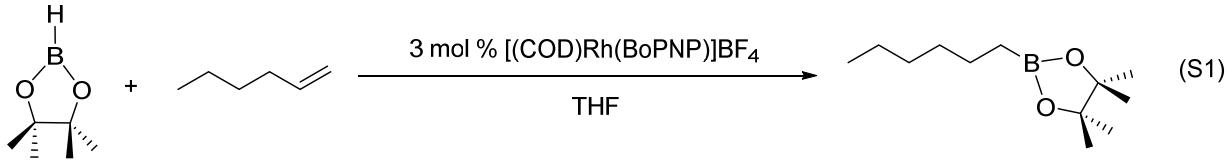
BoPNP. 1.00 g (4.2 mmol) of BoSMe in 20 mL of anhydrous acetonitrile was added to a solution containing 2.00 g (4.2 mmol) of bis[2-(diphenylphosphino)ethyl]ammonium chloride in 50 mL of acetonitrile, resulting in a burnt sienna colored solution with a white solid. 1.16 mL (8.4 mmol) of triethylamine dissolved in 10 mL of anhydrous acetonitrile at 23 °C was added under a N_2 atmosphere. The white solid dissolved upon the addition of the trimethylamine solution. The resulting brick red solution fluoresced yellow green under UV light. After stirring the solution for 18 hours a maroon colored solution containing an orange precipitate was observed. The solvent was removed under reduced pressure from the maroon solution and the resulting brick red solid was stirred in 10 mL anhydrous toluene at 23 °C under a N_2 atmosphere for one hour. The brick red solution was filtered and the solvent was removed under reduced pressure resulting in a maroon oil. The oil was triturated with 100mL of pentanes for 18 hours, resulting in a brick red solid. Yield: 1.79 g (68 %). ^{1}H NMR (600 MHz, CD_3Cl): δ = 2.48 (m, NCH_2CH_2, 4 H) 4.02 (m,

NC*H*$_2$CH$_2$, 4H) 6.24 (q, J = 0.9 Hz, BODIPY (3,5-position), 2 H) 6.66 (d, J = 3.9 Hz, BODIPY (2,6-position), 2 H) 7.36 (m, P*Ph*$_2$, 20 H). 7.49 (s, BODIPY (1,7-position), 2 H). ^{11}B NMR (192 MHz, $CDCl_3$): δ = -0.09 (t, $^1J_{BF}$ = 23 Hz). ^{19} F NMR (564 MHz, $CDCl_3$): δ = -149.1 (q, $^1J_{BF}$ = 23 Hz). ^{31}P NMR (240 MHz, $CDCl_3$): δ = -21.0 (s). λ_{abs} (CH_2Cl_2) = 340 and 428 nm. $\lambda_{emission}$ (CH_2Cl_2) = 536 nm. Quantum yield: (CH_2Cl_2) 0.042. Fluorescence lifetime: (CH_2Cl_2) 2.59 and 5.67 ns, excited at 532 nm.

[(COD)Rh(BoPNP)]BF$_4$. A brick red solution containing 0.580 g (0.918 mmol) of BoPNP dissolved in 10 mL anhydrous dichloromethane was added dropwise to a sunglow colored solution of 0.373 g (0.918 mmol) of [(COD)$_2$Rh]BF_4 dissolved in 10 mL of anhydrous dichloromethane at 23 °C under a N_2 atmosphere. The resulting black solution stirred for 18 hours, and the solvent was removed under reduced pressure. The resulting dark red solid was dissolved in a minimal amount (5 mL) of anhydrous dichloromethane, and upon the addition of 10 mL anhydrous diethyl ether a red orange immediately precipitated. The solution was filtered after five minutes and the red orange solid was collected. Yield: 0.580 g (68 %). ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.17 (d, J = 2.1 Hz, COD, 4 H) 2.42 (br s, COD, 4H) 2.77 (s, COD, 4 H) 3.99 (br s, N*CH*$_2$CH$_2$, 4 H) 4.59 (br s, NCH$_2$*CH*$_2$, 4 H) 6.38 (q, J = 2.11 Hz, BODIPY (3,5-position), 2 H) 6.72 (s, BODIPY (2,6-position), 2 H) 7.18 (m, BODIPY (1,7-position), 2 H) 7.51 (m, P*Ph*$_2$, 2 H) ^{11}B NMR (192 MHz, $CDCl_3$): δ −0.31 (s, 1B, [*B*F$_4$]$^-$), 0.24 (t, $^1J_{BF}$ = 28 Hz , 1B, *B*F$_2$ of BODIPY); ^{19}F NMR (564 MHz, $CDCl_3$): δ −152.28 (s, 4F, [*B*F$_4$]$^-$), −147.21 (q, $^1J_{BF}$ = 28 Hz ,2F, B*F*$_2$ of BODIPY); ^{31}P NMR (240 MHz, $CDCl_3$): δ 26.78 (d, $^1J_{RhP}$ = 142 Hz, 2P); λ_{abs} (CH_2Cl_2) = 344, 429, 500, 530 nm. $\lambda_{emission}$ (CH_2Cl_2) = 537 nm. Quantum yield: (CH_2Cl_2) 0.072. Fluorescence lifetime: (CH_2Cl_2) 4.36 ns and 5.46 ns, excited at 532 nm. Anal. Calcd for $C_{45}H_{46}B_2F_6N_3P_2Rh$●1.5$CH_2Cl_2$: C, 52.85; H, 4.67; N, 3.98. Found: C, 52.44; H, 4.55; N, 3.90.

(COD)Rh(BoPNP). Ten mL of anhydrous THF containing 0.480 g (0.517 mmol) [(COD)Rh(BoPNP)]BF_4, a brick red solution, was added slowly (over about two minutes) to a black slurry containing 0.062 g (0.465 mmol) of KC_8 in 10 ml of anhydrous THF under a N_2 atmosphere. The resulting black slurry was stirred at 23 °C for two hours. The slurry was filtered, and the solvent was removed from the maroon colored filtrate under reduced pressure. The resulting brown solid was recrystallized out of THF at −30 °C resulting in a mahogany colored solid. Yield: 0.326 g (83 %). 1H NMR spectroscopic analysis showed only dichloromethane and pentane multinuclear NMR spectra showed no resonances (Figures S20–S22), indicating a paramagnetic species. λ_{abs} (CH_2Cl_2) = 338, 422, 500 nm. EPR (THF, 90K): g-value = 2.005. Anal. Calcd for $C_{45}H_{46}BF_2N_3P_2Rh\bullet 3CH_2Cl_2+C_5H_{12}$: C, 54.43; H, 5.52; N, 3.59. Found: C, 54.80; H, 5.55; N, 3.70.

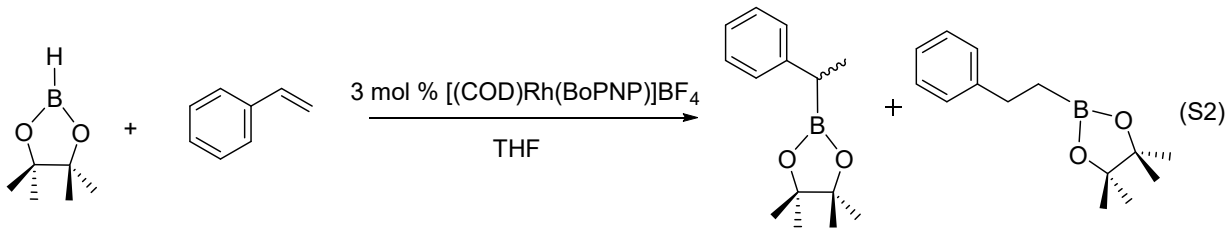
Hydroboration Reactions



(S1)

17.8 µL (0.143 mmol) of 1-hexene was added via syringe to an NMR tube containing 2.25 mg (3 mol %) [(COD)Rh(BoPNP)]BF_4 dissolved in 0.5 mL of anhydrous THF under an N_2 atmosphere. 17.2 µL mg (0.118 mmol) of pinacolborane was added to the orange colored solution by syringe, and the NMR tube was inverted 5 times. The solution went from orange to brown color upon inverting the NMR tube. An NMR spectrum was taken immediately (~3 min after inverting the NMR tube), and every half hour until the reaction had reached completion (~2 hours). Product formation and percent conversion was determined by the formation of a singlet at 34.06 ppm and disappearance of a singlet at 29.16 ppm in the $^{11}B\{^1H\}$ NMR spectra. The resonance at 29.16

ppm is attributed to pinacolborane and the resonance at 34.06 is attributed to 2-hexyl-4,4,5,5-tetramethyl-1,3,2-dioxaborolane, which matched the value previously reported by Huang and coworkers.[4]



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13.24 µL (0.115 mmol) of styrene was added via syringe to an NMR tube containing 2.25 mg (3 mol %) [(COD)Rh(BoPNP)]BF_4 dissolved in 0.5 mL of anhydrous THF under an N_2 atmosphere. 13.9 µL mg (0.096 mmol) of pinacolborane was added to the orange colored solution by syringe, and the NMR tube was inverted 5 times. The solution went from orange to brown color upon inverting the NMR tube. An NMR spectrum was taken immediately (~3 min after inverting the NMR tube), and every half hour until the reaction had reached completion (~2 hours). Product formation and percent conversion was determined by the formation of a singlet at 33.5 ppm and disappearance of a singlet at 29.16 ppm in the $^{11}B\{^1H\}$ NMR spectra. The resonance at 29.16 ppm is attributed to pinacolborane and the resonance at 33.5 is attributed to 4,4,5,5-tetramethyl-2-phenethyl-1,3,2-dioxaborolane, which matched the value previously reported by Huang and coworkers.[4] The product was hydrolozyed following the literature procedure described by Pàmies and coworkers,[5] and analyzed by GC/MS showing a 7:1 ratio of 1-phenylethanol to 2-phenylethanol. The 1-phenylethanol had a retention time of 7.04 minutes and m/z of 122. The 2-phenylethanol had a retention time of 7.58 minutes and m/z of 122. Products were assigned using EI MS library of the NIST/EPA/NIH Mass Spectral Library 2011 (NIST11).

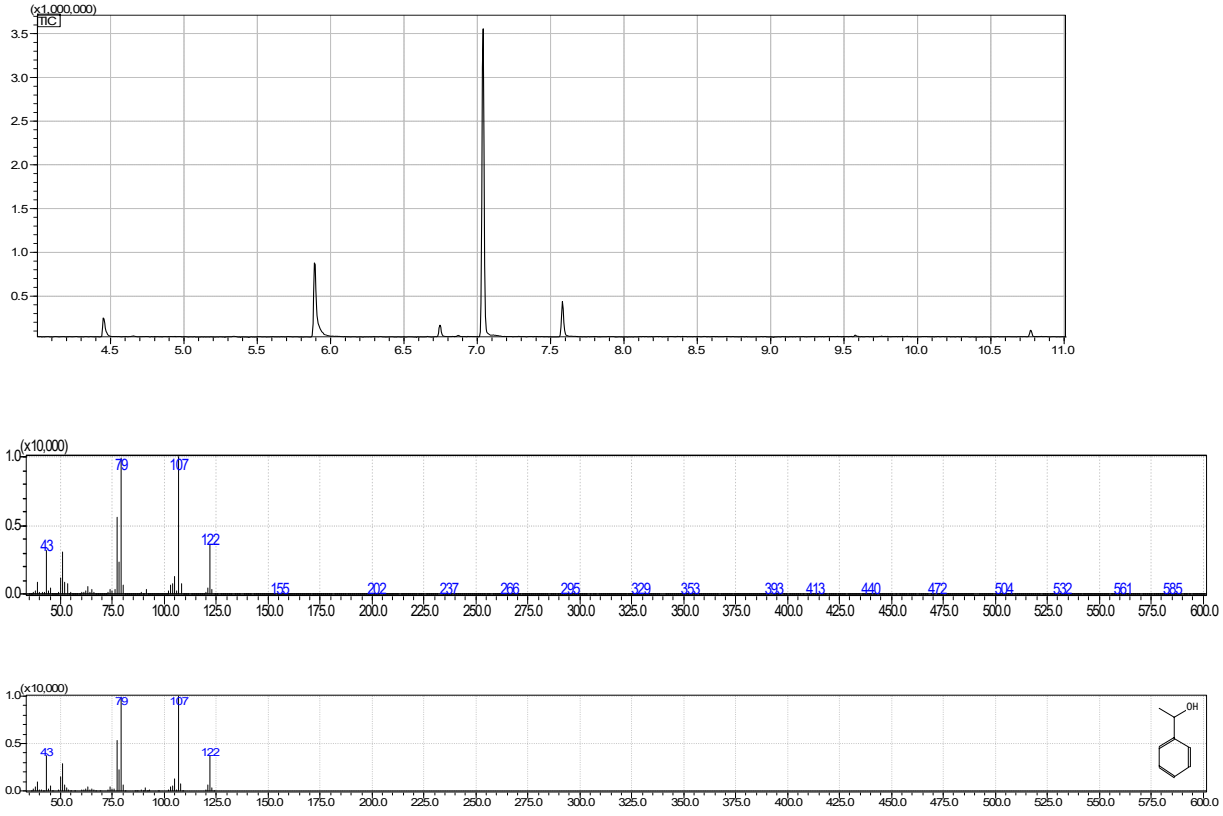


Figure S1. (top) GC trace of the hydrolyzed product from the catalytic hydroboration of styrene. (middle) ESI Mass spectra of the first hydrolyzed styrene product (retention time of 7.04 minutes) and (bottom) 1-phenylethanol.

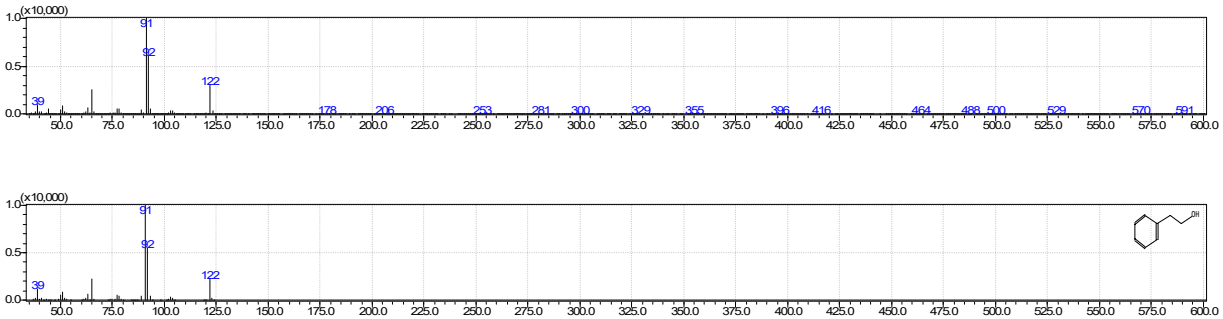
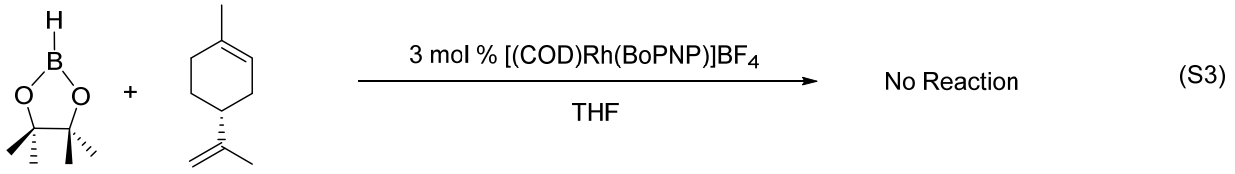
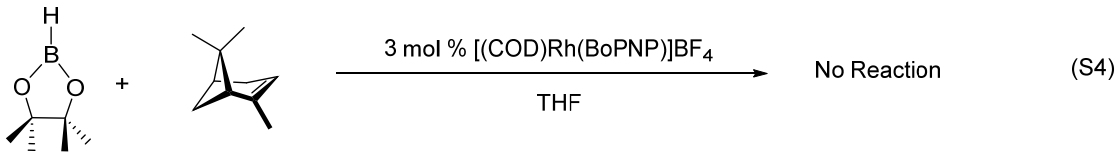


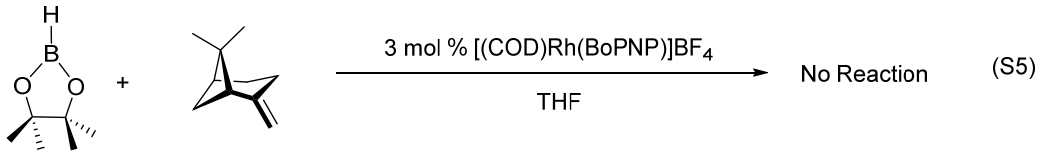
Figure S2. ESI Mass spectra of (top) the second hydrolyzed styrene product (retention time of 7.58 minutes) and (bottom) 2-phenylethanol.



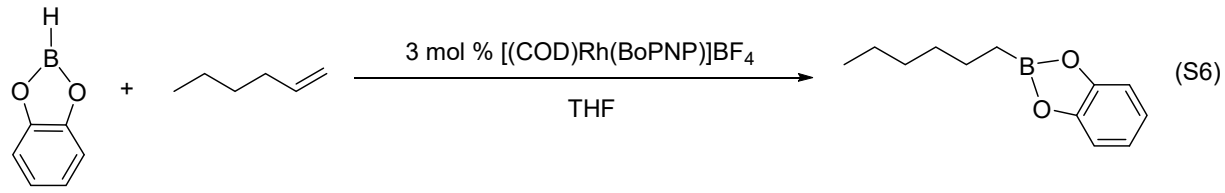
14.3 µL (0.088 mmol) of (+)-limonene was added via syringe to an NMR tube containing 2.25 mg (3 mol %) [(COD)Rh(BoPNP)]BF_4 dissolved in 0.5 mL of anhydrous THF under an N_2 atmosphere. 10.65 µL (0.0.07 mmol) of pinacolborane was added to the orange colored solution by syringe, and the NMR tube was inverted 5 times. An NMR spectrum was taken immediately (~3 min after inverting the NMR tube), and after 24 hours. No product formation was observed.



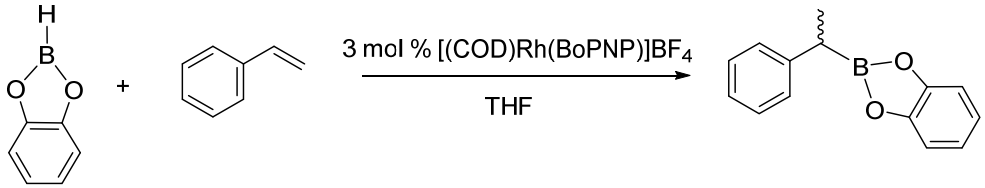
16.25 µL (0.103 mmol) of α-pinene was added via syringe to an NMR tube containing 2.40 mg (3 mol %) [(COD)Rh(BoPNP)]BF_4 dissolved in 0.5 mL of anhydrous THF under an N_2 atmosphere. 12.50 µL (0.086 mmol) of pinacolborane was added to the orange colored solution by syringe, and the NMR tube was inverted 5 times. An NMR spectrum was taken immediately (~3 min after inverting the NMR tube), and after 24 hours. No product was observed.



16.25 µL (0.103 mmol) of β-pinene was added via syringe to an NMR tube containing 2.40 mg (3 mol %) [(COD)Rh(BoPNP)]BF_4 dissolved in 0.5 mL of anhydrous THF under an N_2 atmosphere. 12.50 µL (0.086 mmol) of catecholborane was added to the orange colored solution by syringe, and the NMR tube was inverted 5 times. An NMR spectrum was taken immediately (~3 min after inverting the NMR tube), and after 24 hours. No product was observed.



12.9 µL (0.103 mmol) of 1-hexene was added via syringe to an NMR tube containing 2.40 mg (3 mol %) [(COD)Rh(BoPNP)]BF_4 dissolved in 0.5 mL of anhydrous THF under an N_2 atmosphere. 9.22 µL mg (0.086 mmol) of catecholborane was added to the orange colored solution by syringe, and the NMR tube was inverted 5 times. The solution went from orange to brown color upon inverting the NMR tube. An NMR spectrum was taken immediately (~3 min after inverting the NMR tube), and every half hour until the reaction had reached completion (~1 hour). Product formation and percent conversion was determined by the formation of a singlet at 36.37 ppm and disappearance of a singlet at 29.16 ppm in the $^{11}B\{^1H\}$ NMR spectra.



(S7)

13.24 µL (0.115 mmol) of styrene was added via syringe to an NMR tube containing 2.70 mg (3 mol %) [(COD)Rh(BoPNP)]BF_4 dissolved in 0.5 mL of anhydrous THF under an N_2 atmosphere. 10.3 µL mg (0.096 mmol) of catecholborane was added to the orange colored solution by syringe, and the NMR tube was inverted 5 times. The solution went from orange to brown color upon inverting the NMR tube. An NMR spectrum was taken immediately (~3 min after inverting the NMR tube), and every half hour until the reaction had reached completion (~3 hours). Product formation and percent conversion was determined by the formation of a singlet at 35.7 ppm and disappearance of a singlet at 29.16 ppm in the $^{11}B\{^1H\}$ NMR spectra. The product was hydrolozyed following the literature procedure described by Pàmies and coworkers,[5] and analyzed by GC/MS showing a single product, 1-phenylethanol. The 1-phenylethanol had a retention time of 7.04 minutes and m/z of 122. Products were assigned using EI MS library of the NIST/EPA/NIH Mass Spectral Library 2011 (NIST11).

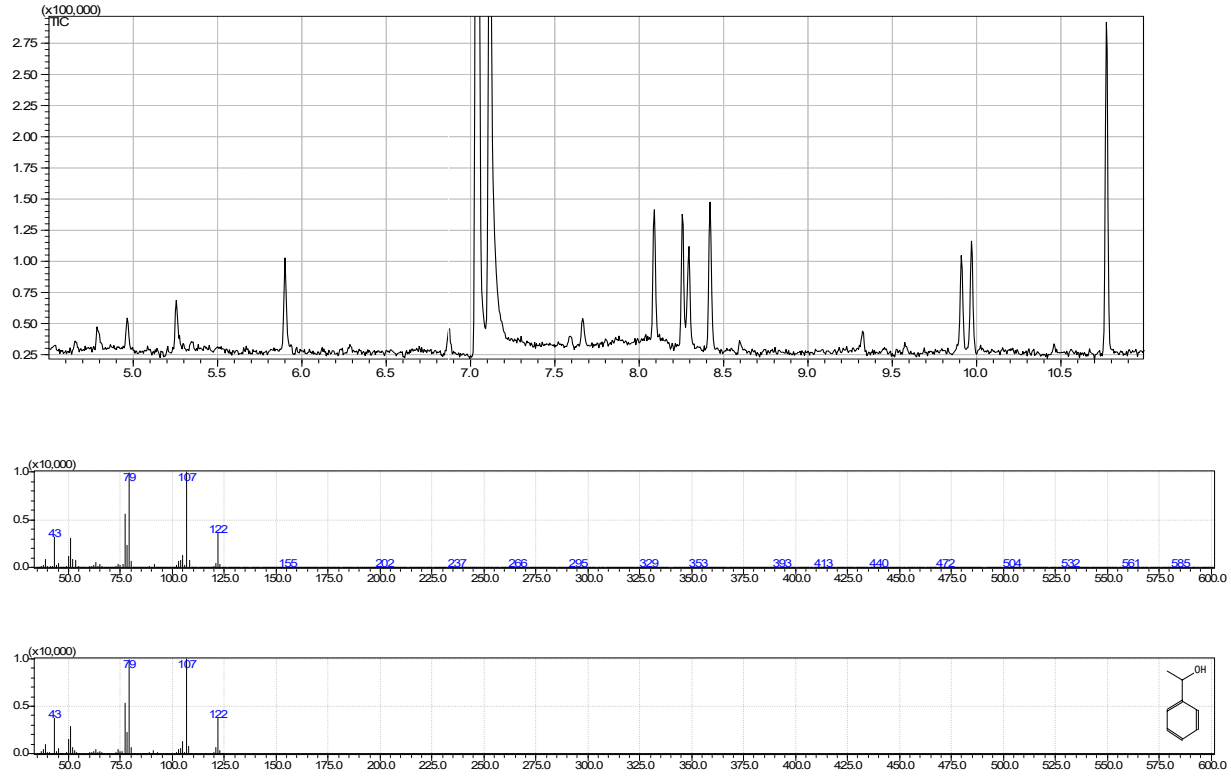
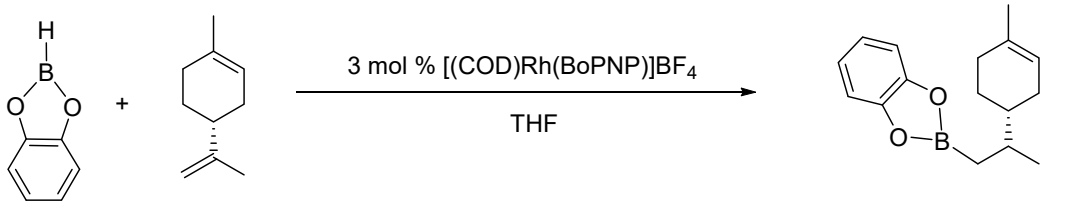


Figure S3. (top) GC trace of the hydrolyzed product from the catalytic hydroboration of styrene. (middle) ESI Mass spectra of the hydrolyzed styrene product (retention time of 7.04 minutes) and (bottom) 1-phenylethanol.



(S8)

14.3 µL (0.088 mmol) of (+)-limonene was added via syringe to an NMR tube containing 2.70 mg (3 mol %) [(COD)Rh(BoPNP)]BF_4 dissolved in 0.5 mL of anhydrous THF under an N_2 atmosphere. 7.82 µL (0.073 mmol) of catecholborane was added to the orange colored solution by syringe, and the NMR tube was inverted 5 times. The solution went from orange to brown color upon inverting the NMR tube. An NMR spectrum was taken immediately (~3 min after inverting the NMR tube), and after 24 hours. Product formation and percent conversion was determined by the

formation of a singlet at 36.8 ppm and disappearance of a singlet at 29.16 ppm in the $^{11}B\{^{1}H\}$ NMR spectra. The product was hydrolozyed following the literature procedure described by Pàmies and coworkers,[5] and analyzed by GC/MS showing the terminal hydrolysis product with a retention time of 9.20 minutes and m/z of 121. Products were assigned using EI MS library of the NIST/EPA/NIH Mass Spectral Library 2011 (NIST11).

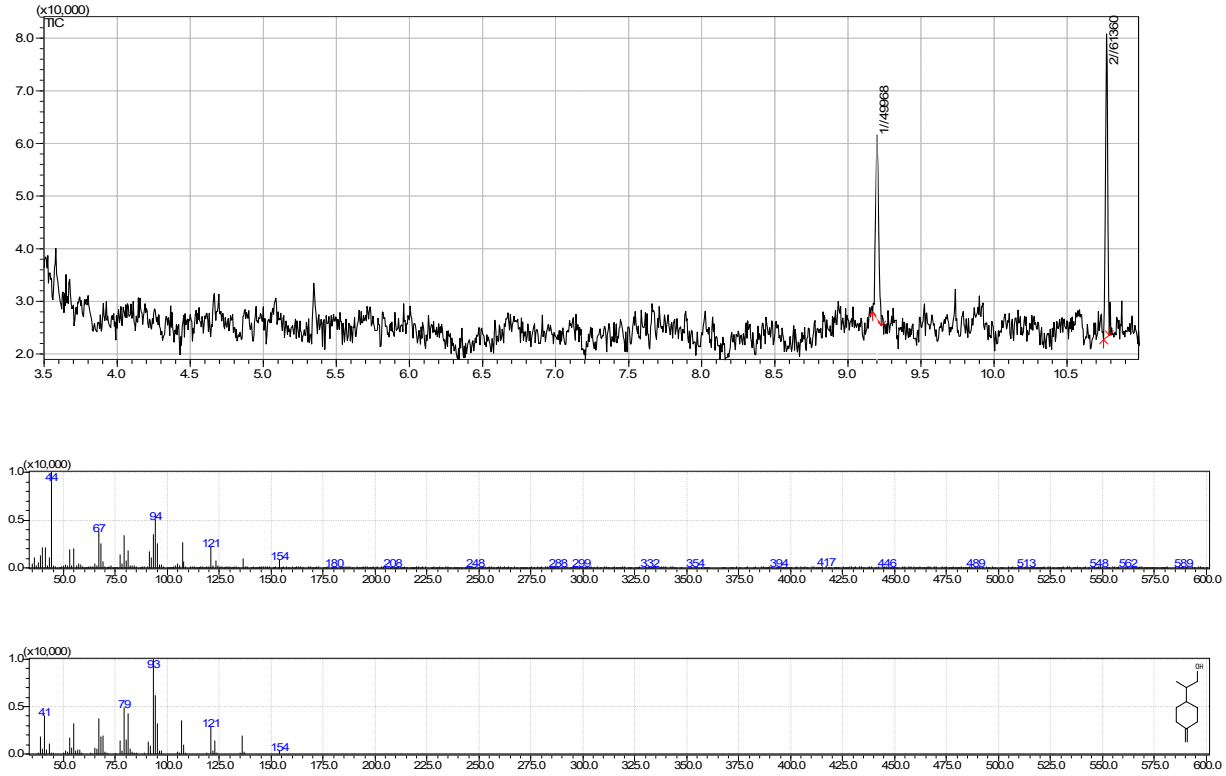
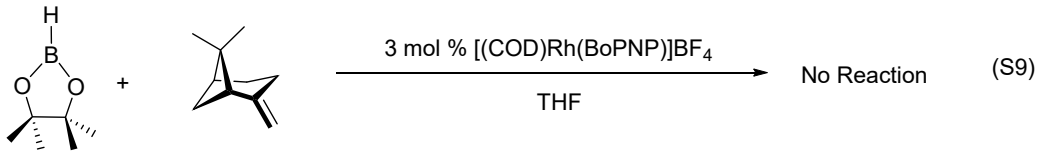
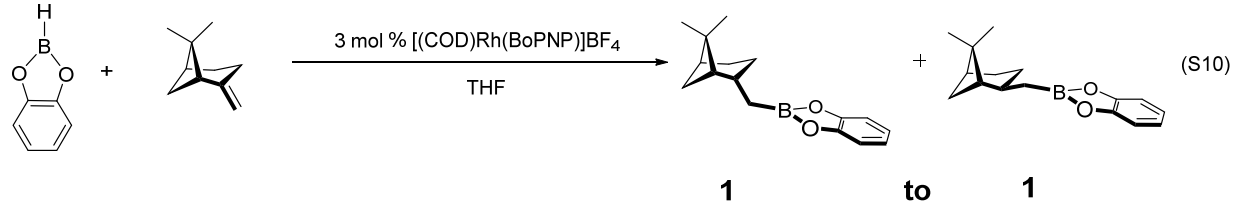


Figure S4. (top) GC trace of hydrolyzed limonene product and ESI Mass spectra of (middle) the hydrolyzed limonene product and (bottom) the assigned product.



16.25 µL (0.103 mmol) of β-pinene was added via syringe to an NMR tube containing 2.40 mg (3 mol %) [(COD)Rh(BoPNP)]BF_4 dissolved in 0.5 mL of anhydrous THF under an N_2 atmosphere. 12.50 µL (0.086 mmol) of catecholborane was added to the orange colored solution by syringe, and the NMR tube was inverted 5 times. An NMR spectrum was taken immediately (~3 min after inverting the NMR tube), and after 24 hours. No product was observed.



13.9 µL (0.088 mmol) of β-pinene was added via syringe to an NMR tube containing 2.70 mg (3 mol %) [(COD)Rh(BoPNP)]BF_4 dissolved in 0.5 mL of anhydrous THF under an N_2 atmosphere. 7.86 µL (0.073 mmol) of catecholborane was added to the orange colored solution by syringe, and the NMR tube was inverted 5 times. The solution went from orange to brown color upon inverting the NMR tube. An NMR spectrum was taken immediately (~3 min after inverting the NMR tube), and after 24 hours. Product formation and percent conversion was determined by the formation of a singlet at 36.3 ppm and disappearance of a singlet at 29.16 ppm in the $^{11}B\{^1H\}$ NMR spectra. The product was hydrolozyed following literature procedures and analyzed by GC/MS showing both (-)-cis-myrtanol and (+)-trans-myrtanol. The (+)-trans-myrtanol had a retention time of 8.87 minutes and M/Z of 123. The (-)-cis-myrtanol had a retention time of 8.94 minutes and m/z of 123 Products were assigned using EI MS library of the NIST/EPA/NIH Mass Spectral Library 2011 (NIST11).

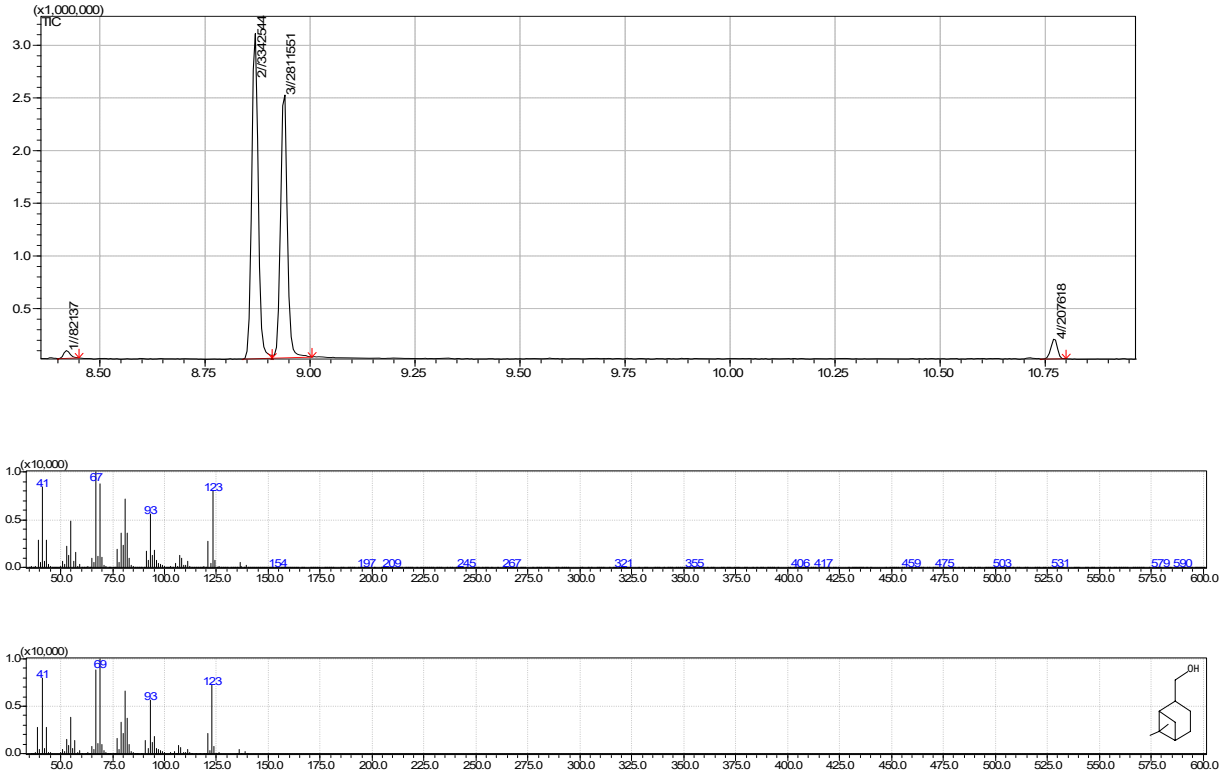


Figure S5. (top) GC trace of hydrolyzed product from the catalytic hydroboration of β-pinene and ESI Mass spectra of (middle) the hydrolyzed β-pinene product and (bottom) (+)-trans-myrtanol.

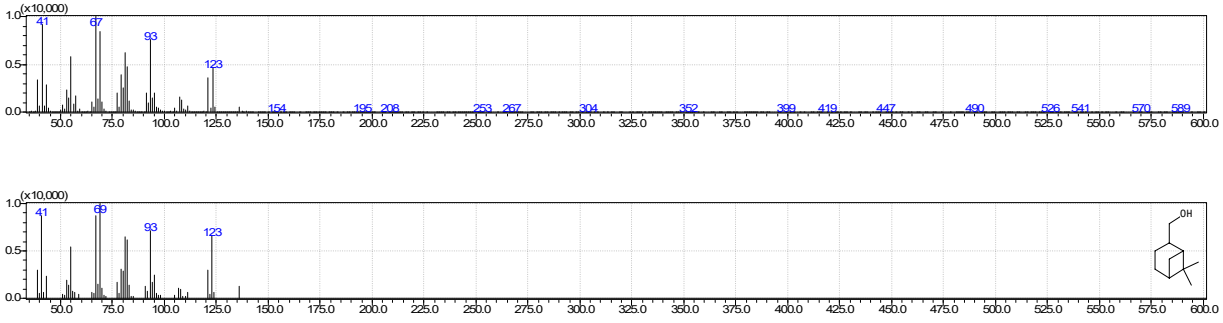


Figure S6. ESI Mass spectra of (top) the hydrolyzed β-pinene product and (bottom) (−)-cis-myrtanol.

Redox Switchable Hydroboration of Styrene. A brick red solution of 2.67 mg (3 mol %) of [(COD)Rh(BoPNP)]BF_4 in 400 µL of anhydrous THF was transferred to an NMR tube and capped with a septum under an N_2 atmosphere. 12 mg (0.115 mmol) of styrene was added by syringe, and the NMR tube was inverted 5 times. Then 12.3 mg (0.096 mmol) of pinacolborane was added by syringe, and the NMR tube was inverted 5 times. The solution darkened from sunglow to light brown, and an NMR spectra was taken immediately, and every 5 minutes for 1 hour. Then, 100 µL of a 0.029 mM slurry of Cp^*_2Co was added by syringe and the NMR tube was inverted 5 times. The solution darkened further to a mahogany colored solution and an NMR spectra was taken immediately, and every 5 minutes for 1 hour. Then, 100 µL of a 0.029 mM slurry of $[Cp_2Co][PF_6]$ was added by syringe and the NMR tube was inverted 5 times. The solution became sunglow colored and an NMR spectra was taken immediately, and every 5 minutes for 1 hour. After ten minutes the solution changed from sunglow to light brown, it remained fluorescent. The addition of an equivalent of oxidant or reductant was introduced by syringe, 60 minutes after the prior addition, and monitered by NMR spectroscopy every 5 minutes until the reaction had reached completion. Exposure of styrene to pinacolborane with sequential additions of Cp^*_2Co and $[Cp_2Co]PF_6$ (repeating the procedure without [(COD)Rh(BoPNP)]BF_4) resulted in no product formation.

Spectroscopic Techniques

NMR spectra were obtained on a Varian VNMRS 600 MHz spectrometer, and spectra were referenced to residual solvent (^1H, ^{13}C) or externally (^{11}B; $BF_3{\bullet}OEt_2$, ^{19}F; CCl_3F, ^{31}P; H_3PO4).[6] Chemical shifts are reported in parts per million (ppm). NMR solvents were purchased from Cambridge Isotope Laboratories, Inc., and vacuum distilled over CaH_2. All UV-Vis spectra were obtained on a Cary 60 UV-Vis spectrometer. Cyclic voltammetry (CV) experiments were carried out at room temperature in nitrogen-purged methylene chloride 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. Photoluminescent spectra were obtained with a Horiba FluoroMax-4 fluorometer equipped with a Xenon lamp. Luminescent lifetime measurements were obtained using a Horiba Fluorolog with a PMT detector and using a NanoLED 332 excitation source and FluoroHub-B pulse controller. 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.[7] Fitting was implemented using the Nelder/Mead downhill simplex. All GCMS spectra were determined using a Shimadzu GCMS-QP2010 SE equipped with a FID detector and a DB-5 capillary column. GCMS samples were made using a 20 µL aliquot reaction mixture diluted with 0.96 mL of dichloromethane.

2) Catalytic Hydroboration Results

Table S1. Influence of catalyst identity on the hydroboration of (0.088–0.115 mmol) alkenes with 3 mol% catalyst in THF with 0.82 equivalents of pinacolborane at 23 °C after four hours.

Olefin	$[(COD)_2Rh]BF_4$	BoPNP
1-hexene	100 %	0 %
styrene	100 %	0 %
(+)-limonene	0 %	0 %
α-pinene	0 %	0 %
β-pinene	80 %	0 %

Table S2. Influence of solvent on the hydroboration of (0.115 mmol) styrene with 3 mol% $[(COD)Rh(BoPNP)]BF_4$, 0.82 equivalents of pinacolborane after 4 hours at 23 °C.

Solvent	Conversion
Acetonitrile	0%
Acetone	75%
CH_2Cl_2	82%
THF	100%

Table S3. Hydroboration of styrene with [(COD)Rh(BoPNP)]BF_4, 0.82 equivalents of pinacolborane under various conditions.

Mol %	Solvent	Temperature (°C)	LED Exposure	Time (hours)	Conversion
0.1	THF	23	No	24	0
0.5	THF	23	No	24	20
1	THF	23	No	10	100
3	THF	23	No	4	100
5	THF	23	No	0.5	100
3	MeCN	23	No	4	0
3	Acetone	23	No	4	75
3	CH_2Cl_2	23	No	4	82
3	THF	30	No	3	98
3	THF	40	No	3	100
3	THF	23	Yes	3	94

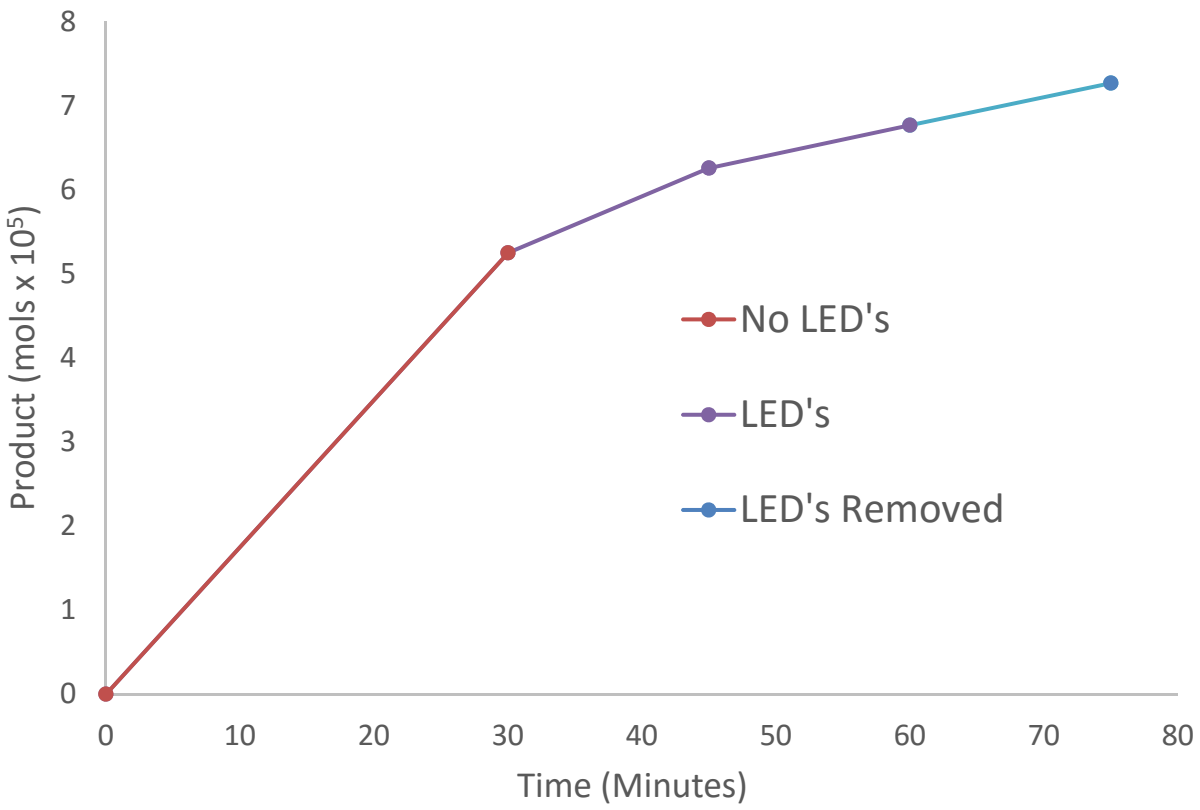


Figure S7. Plot showing the hydroboration of styrene with 3 mol % [(COD)Rh(BoPNP)]BF_4 in THF at 23 °C in the absence and presence of light.

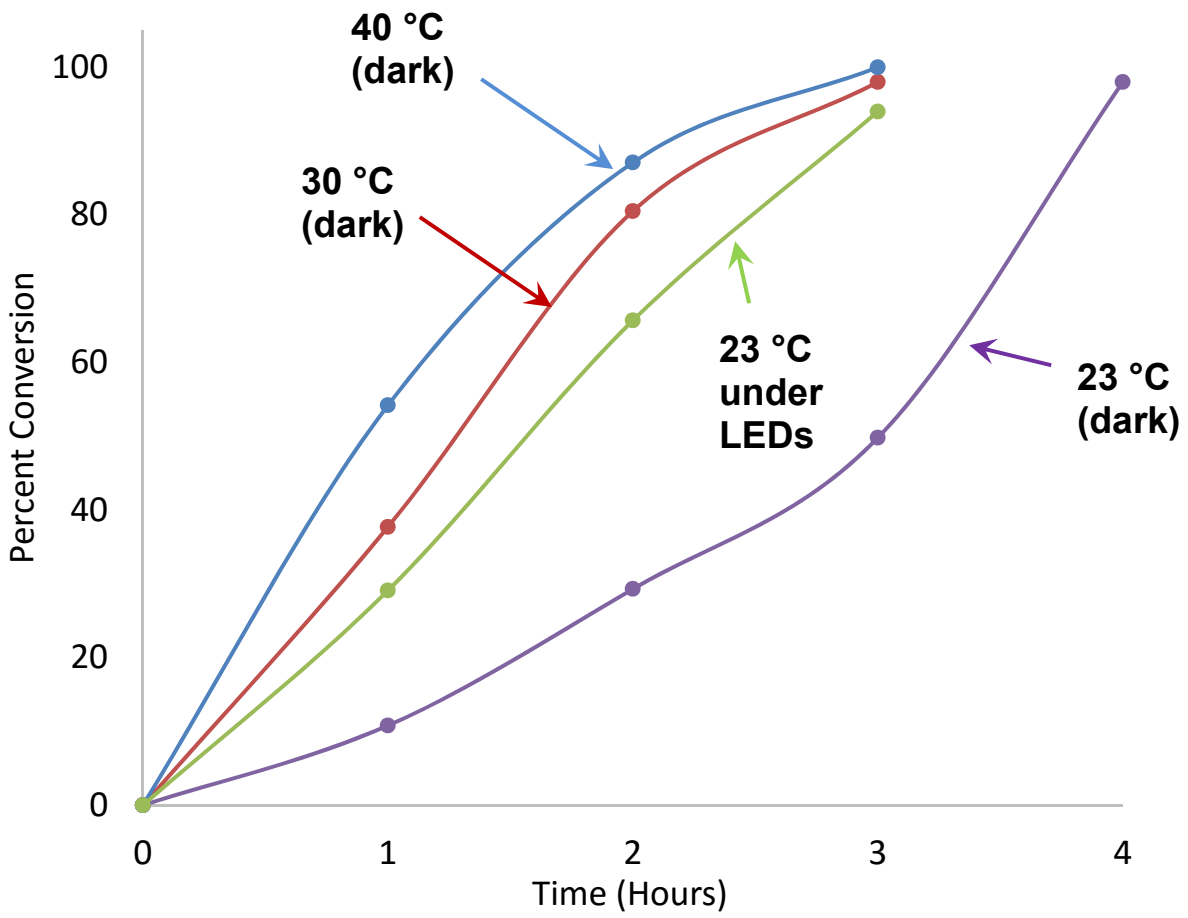


Figure S8. Plot showing the hydroboration of styrene with 3 mol % [(COD)Rh(BoPNP)]BF_4 in THF at difference temperatures in the absence and presence of light.

3) Photographs of Catalytic Reactions with [(COD)Rh(BoPNP)]BF_4

Figure S9. Photograph of the catalytic reactions with 1.5 mol % [(COD)Rh(BoPNP)]BF_4 in CH_2Cl_2 for the (far left) hydrogenation of limonene, (left middle) hydrosilylations of limonene, (right middle) hydroboration of limonene, and (far right) hydroacylation of 2,2-dimethyl-4-penenal under (top) ambient light and (bottom) UV light five minutes after the additon of [(COD)Rh(BoPNP)]BF_4.

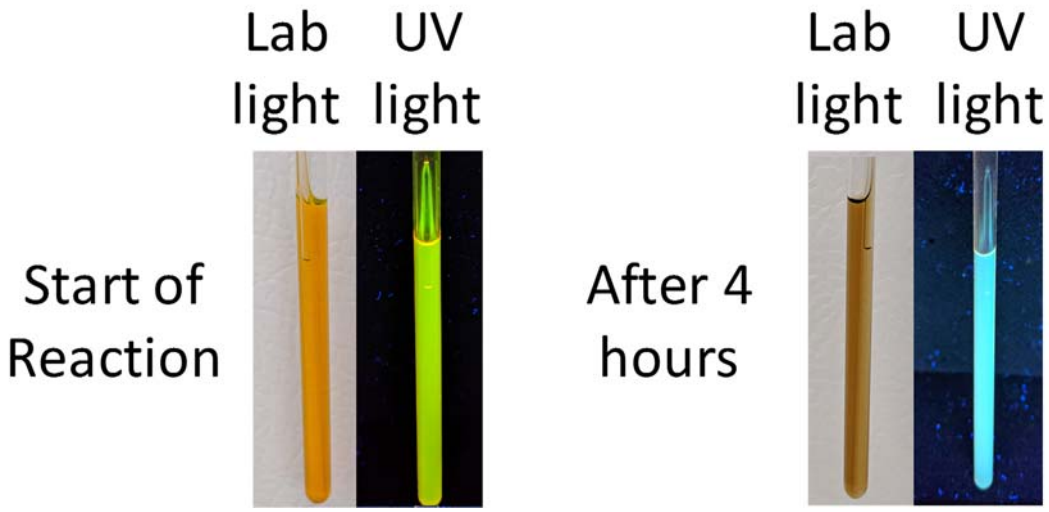


Figure S10. Photographs of the hydroboration reaction of styrene with pinacolborane and [(COD)RhBoPNP]BF_4 in tetrahydrofuran (left) at time zero and (right) after four hours under ambient (lab) light and UV light.

4) Photographs of Catalytic Reactions with (COD)Rh(BoPNP)

Figure S11. Photograph of the catalytic reactions with 1.5 mol % [(COD)Rh(BoPNP)]BF_4 in THF for the (far left) hydrogenation of limonene, (left middle) hydrosilylations of limonene, (right middle) hydroboration of limonene, and (far right) hydroacylation of 2,2-dimethyl-4-penenal under (top) ambient light, (middle) UV light 20 minutes after the additon of [(COD)Rh(BoPNP)]BF_4, and (bottom) UV light after 24 hours.

5) Multinuclear NMR Spectra of BoPNP

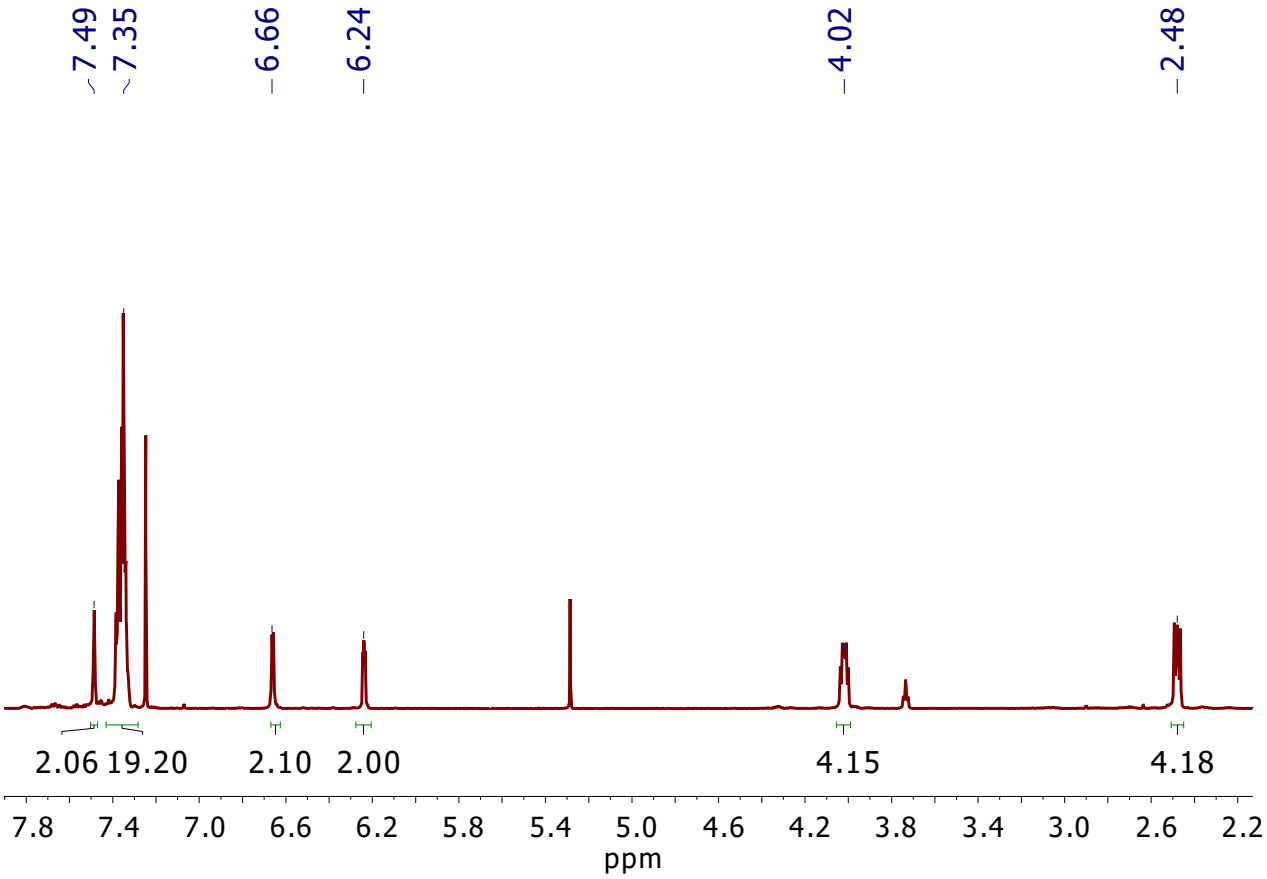


Figure S12. ^{1}H NMR Spectrum of BoPNP in $CDCl_3$.

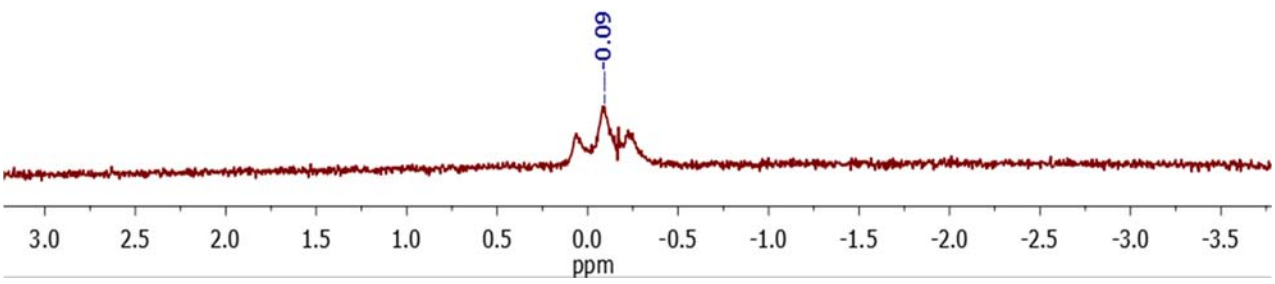


Figure S13. ^{11}B NMR Spectrum of BoPNP in $CDCl_3$.

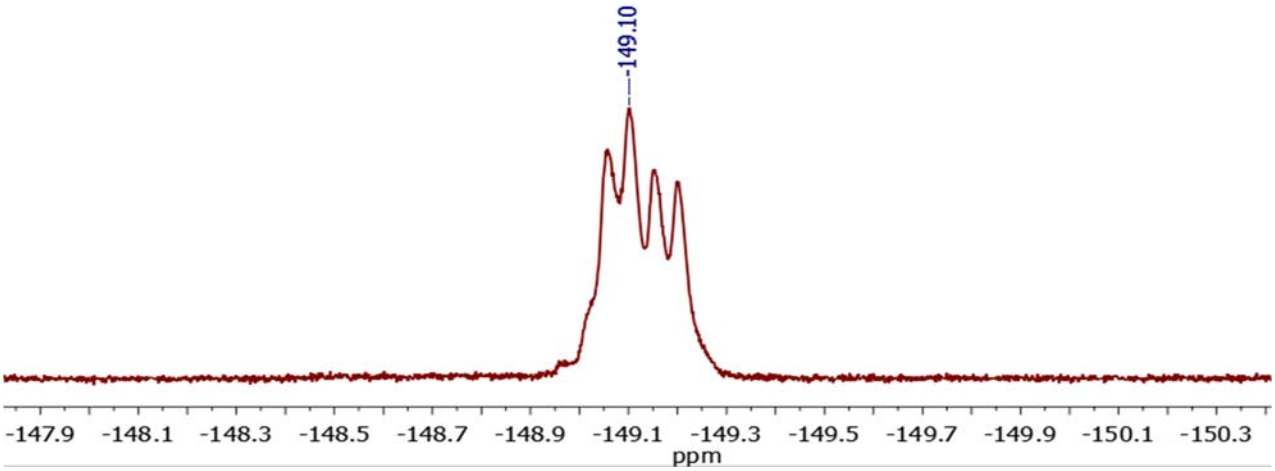


Figure S14. ^{19}F NMR Spectrum of BoPNP in $CDCl_3$.

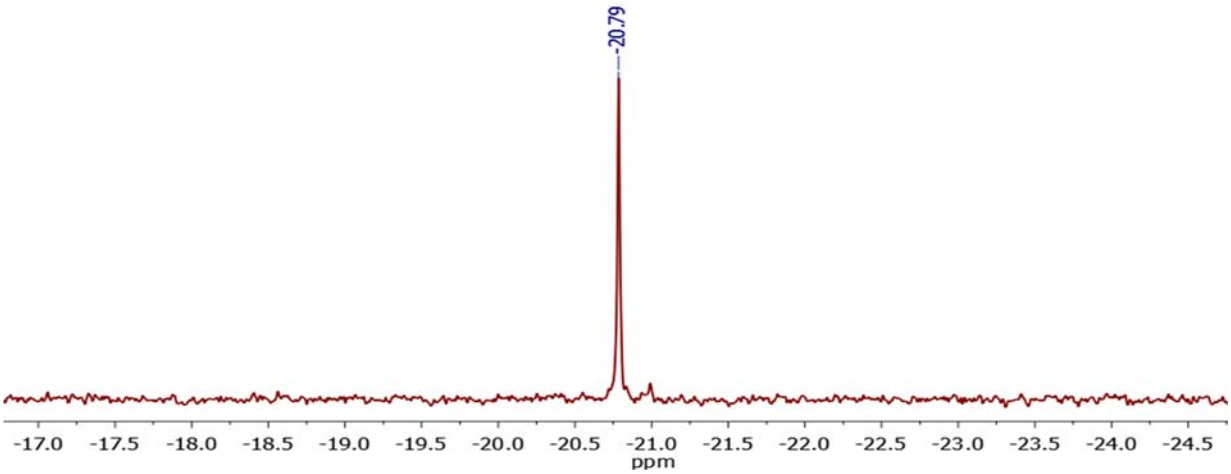


Figure S15. ^{31}P NMR Spectrum of BoPNP in $CDCl_3$.

6) Multinuclear NMR Spectra of [(COD)Rh(BoPNP)]BF_4 and (COD)Rh(BoPNP)

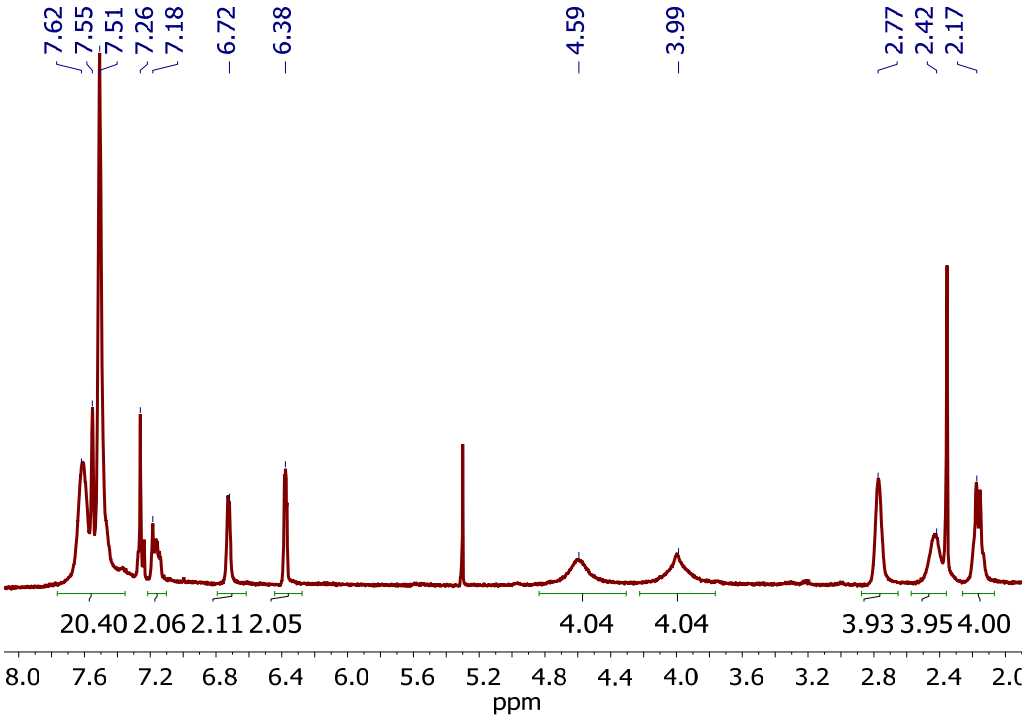


Figure S16. ^{1}H NMR Spectrum of [CODRh(BoPNP)]BF_4 in $CDCl_3$.

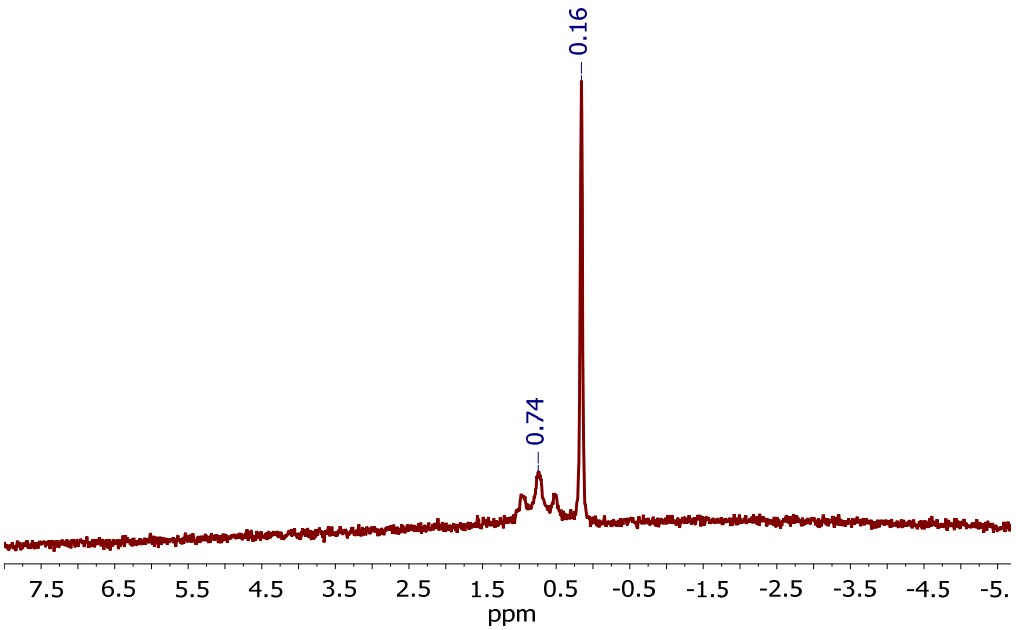


Figure S17. ^{11}B NMR Spectrum of [CODRh(BoPNP)]BF_4 in $CDCl_3$.

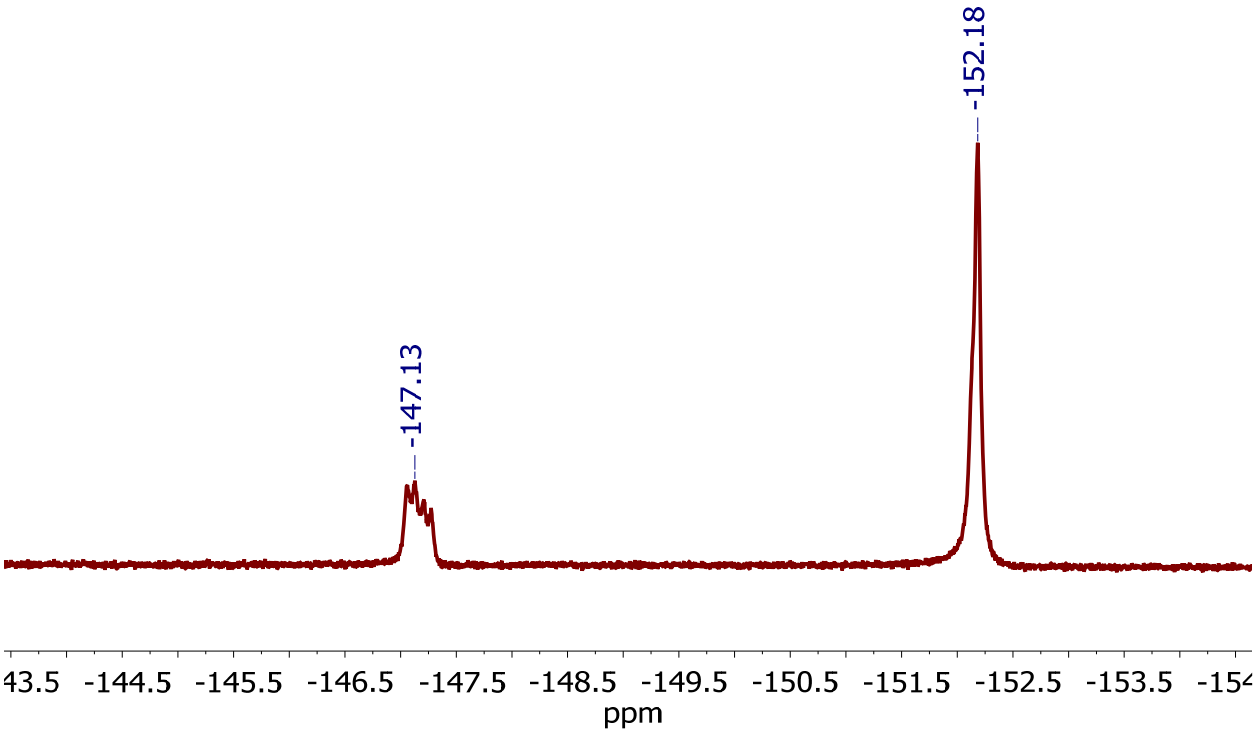


Figure S18. ^{19}F NMR Spectrum of [CODRh(BoPNP)]BF_4 in $CDCl_3$.

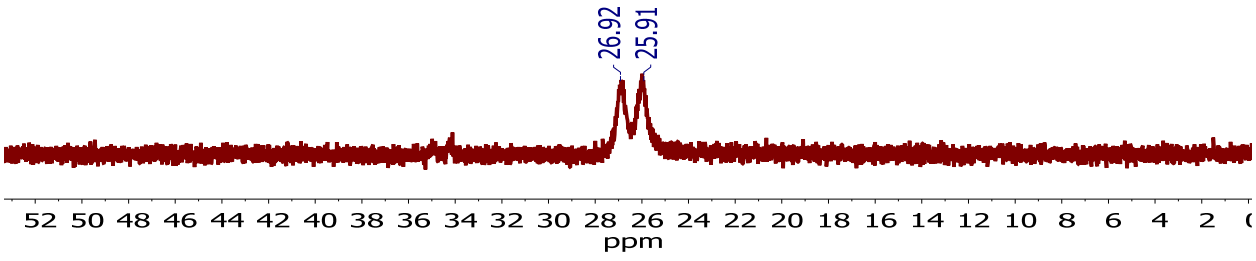


Figure S19. ^{31}P NMR Spectrum of [CODRh(BoPNP)]BF_4 in $CDCl_3$.

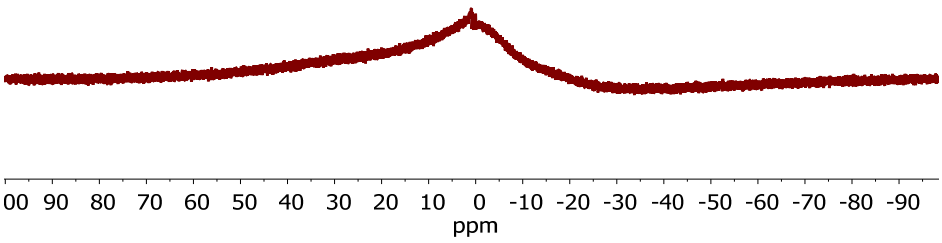


Figure S20. ^{11}B NMR Spectrum of (COD)Rh(BoPNP) in $CDCl_3$.

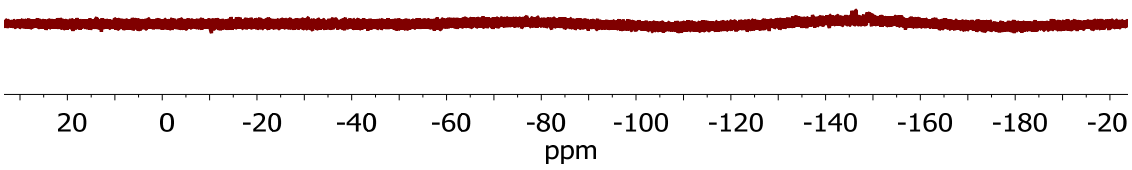


Figure S21. ^{19}F NMR Spectrum of (COD)Rh(BoPNP) in $CDCl_3$.

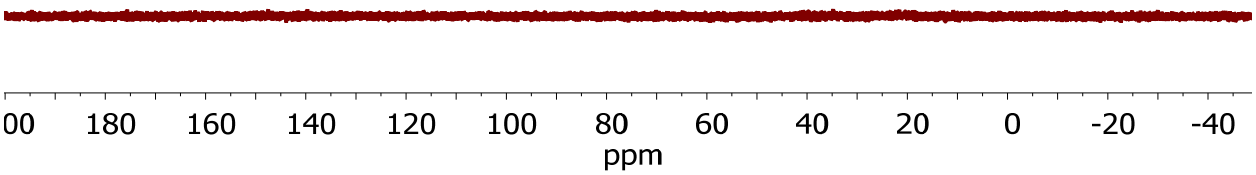


Figure S22. ^{31}P NMR Spectrum of (COD)Rh(BoPNP) in $CDCl_3$.

7) Details of Molecular Structure Analysis

X-ray diffraction data for **BoPNP** were collected at 100 K on a Bruker D8 Venture using MoKα-radiation (λ=0.71073 Å) using APEX2[8] software. The crystal selected was a yellow prism with dimensions of 0.26 mm x 0.20 mm x 0.10 mm. Data have been corrected for absorption using SADABS[9] area detector absorption correction program. Crystallogrpahic data were solved using the Olex2[10] software.

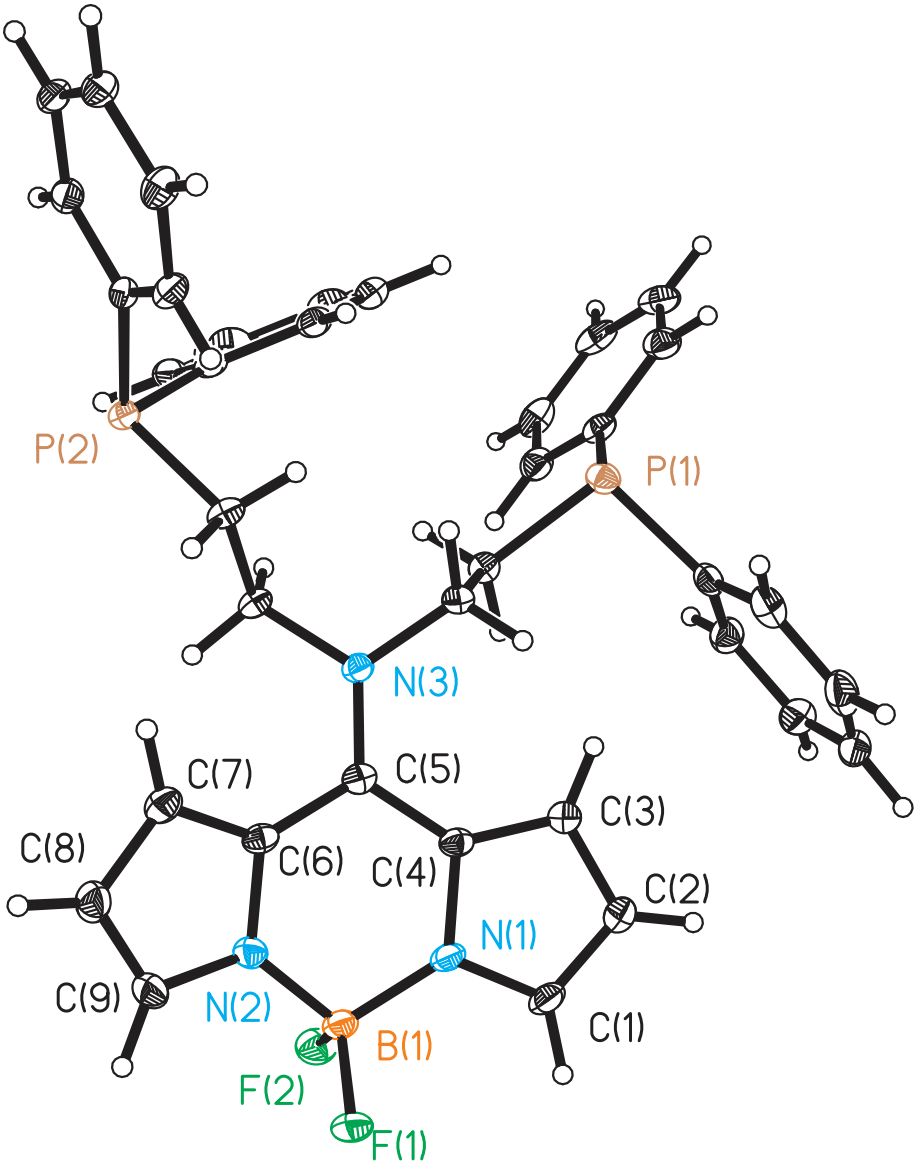


Figure S23. Molecular structure of **BoPNP**. Thermal ellipsoids are drawn at 50% probability.

X-ray diffraction data for **[(COD)Rh(BoPNP)]BF_4** were collected at 100 K on a Bruker D8 Venture using MoKα-radiation (λ=0.71073 Å) using APEX2[8] software. The crystal selected was a yellow plate with dimensions of 0.12 mm x 0.08 mm x 0.01 mm. Data have been corrected for absorption using SADABS[9] area detector absorption correction program. Crystallogrpahic data were solved using the Olex2[10] software.

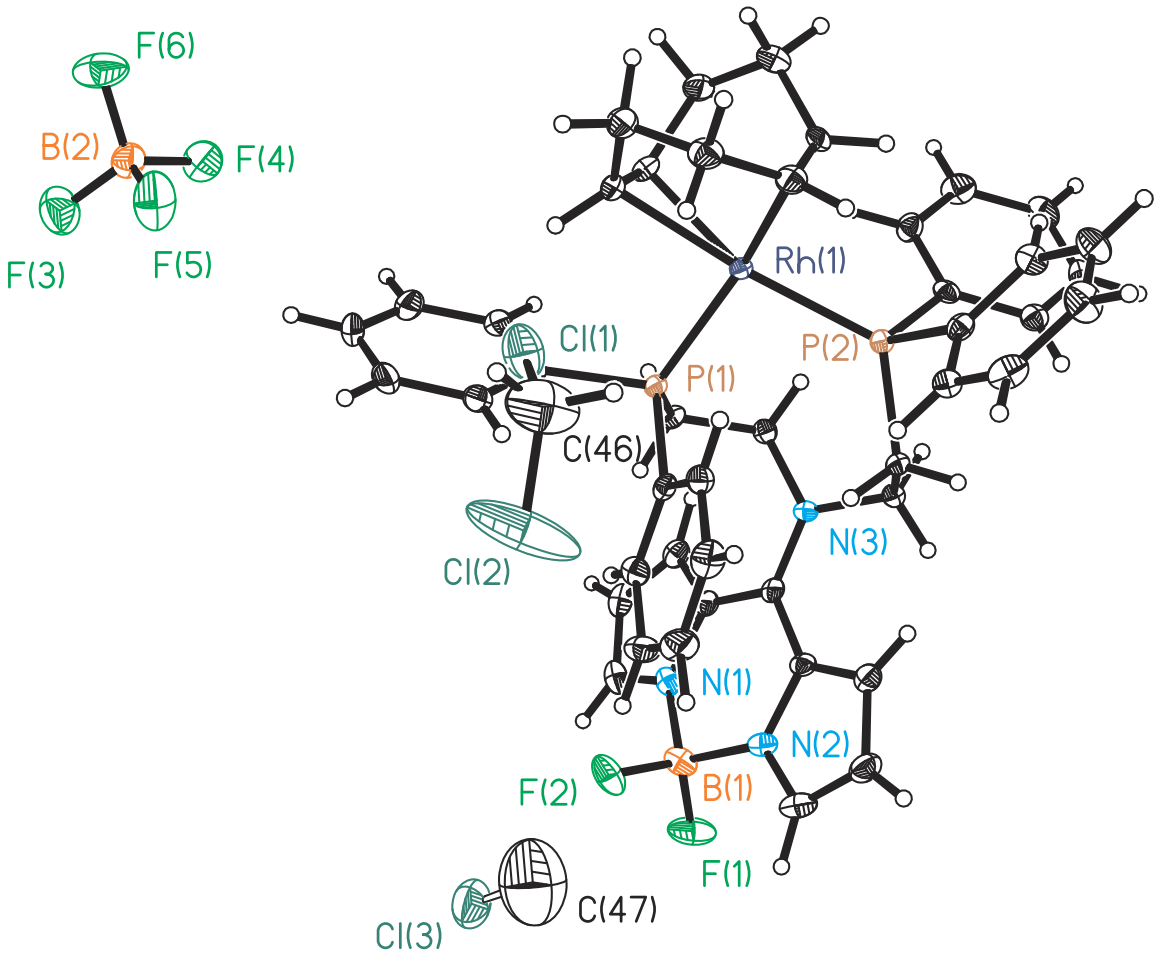


Figure S24. Molecular structure of **[(COD)RhBoPNP]BF_4** showing the 1.5 CH_2Cl_2 solvent molecules per unit cell. Thermal ellipsoids are drawn at 50% probability.

8) Cyclic Voltammograms of PNP, BoPNP, and [(COD)Rh(BoPNP)]BF_4

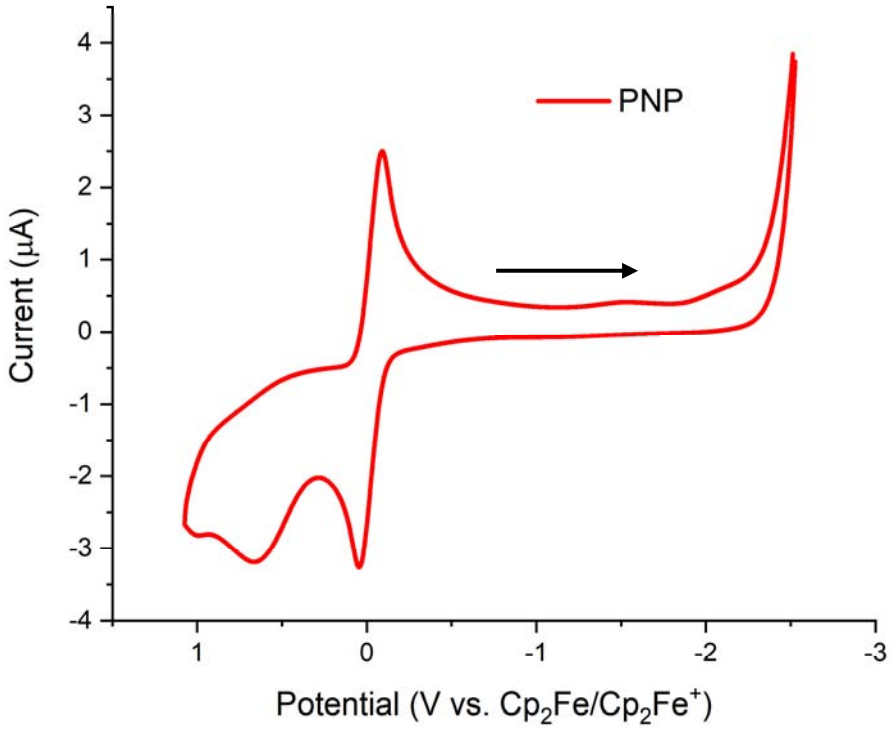


Figure S25. Cyclic voltammogram of bis[2-(diphenylphosphino)ethyl]ammonium chloride (PNP) in CH_2Cl_2. Electrolyte = Bu_4NPF_6, scan rate = 100 mV/s and potential range of scan: = 1.1 V to -2.5 V. The wave at 0.0 V vs. Cp_2Fe/Cp_2Fe^+ is attributed to the ferrocene internal standard. The arrow indicates the initial direction of the scan.

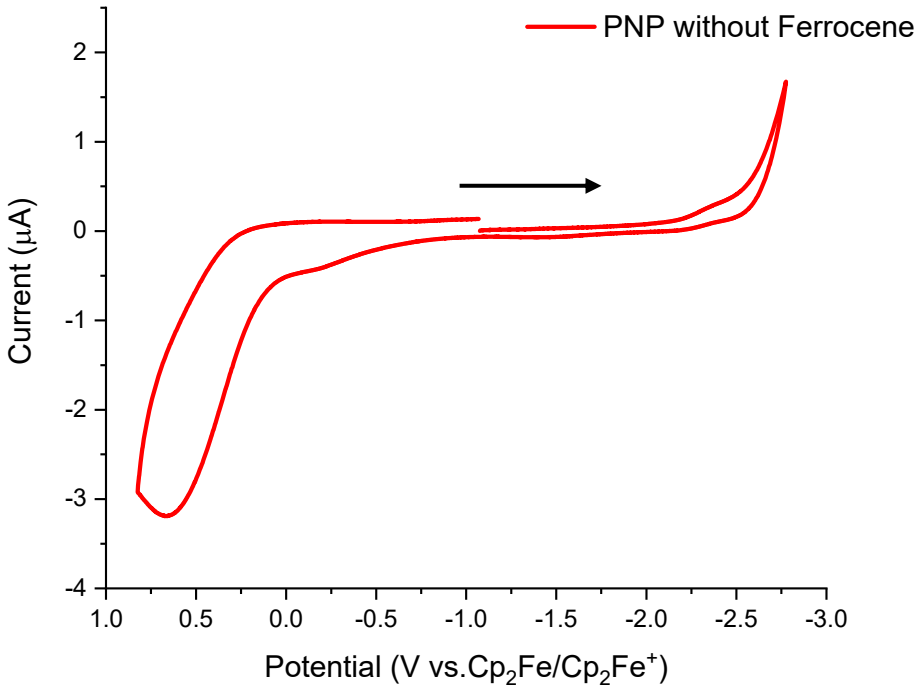


Figure S26. Cyclic voltammogram of bis[2-(diphenylphosphino)ethyl]ammonium chloride (PNP) in CH_2Cl_2 without the ferrocene internal standard. Electrolyte = Bu_4NPF_6, scan rate = 100 mV/s and potential range of scan: 1.0 V to -2.7 V. The arrow indicates the initial direction of the scan.

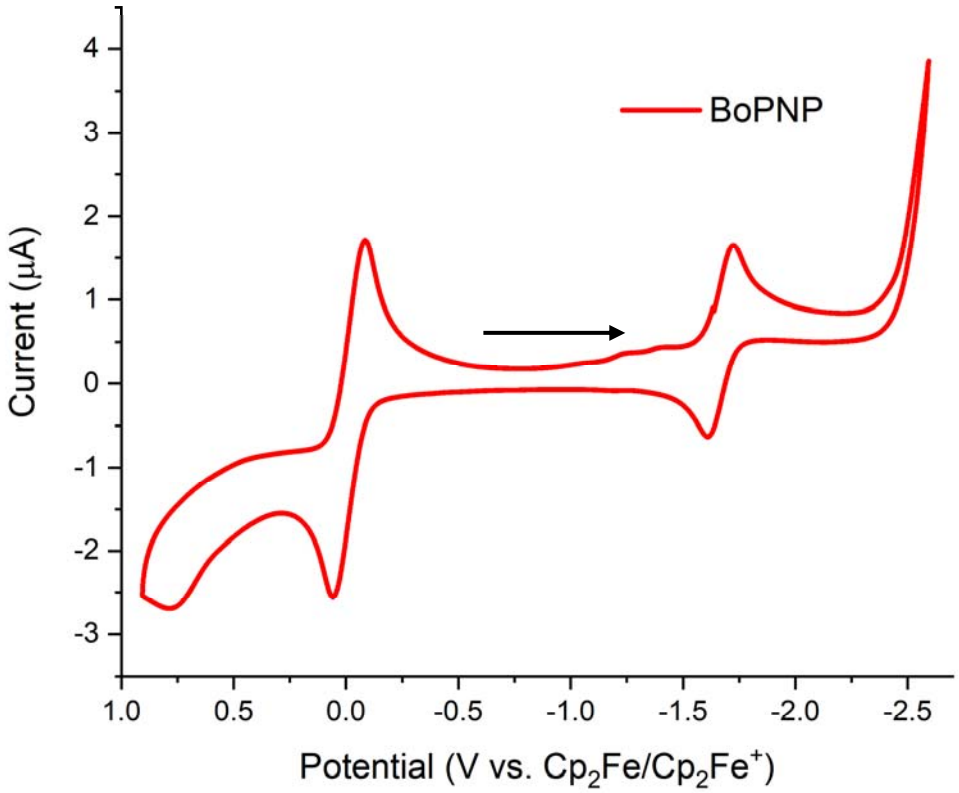


Figure S27. Cyclic voltammogram of BoPNP in CH_2Cl_2. Electrolyte = Bu_4NPF_6, scan rate = 100 mV/s and potential range of scan: 1 V to -2.7 V. The wave at 0.0 V vs. Cp_2Fe/Cp_2Fe^+ is attributed to the ferrocene internal standard. The arrow indicates the initial direction of the scan.

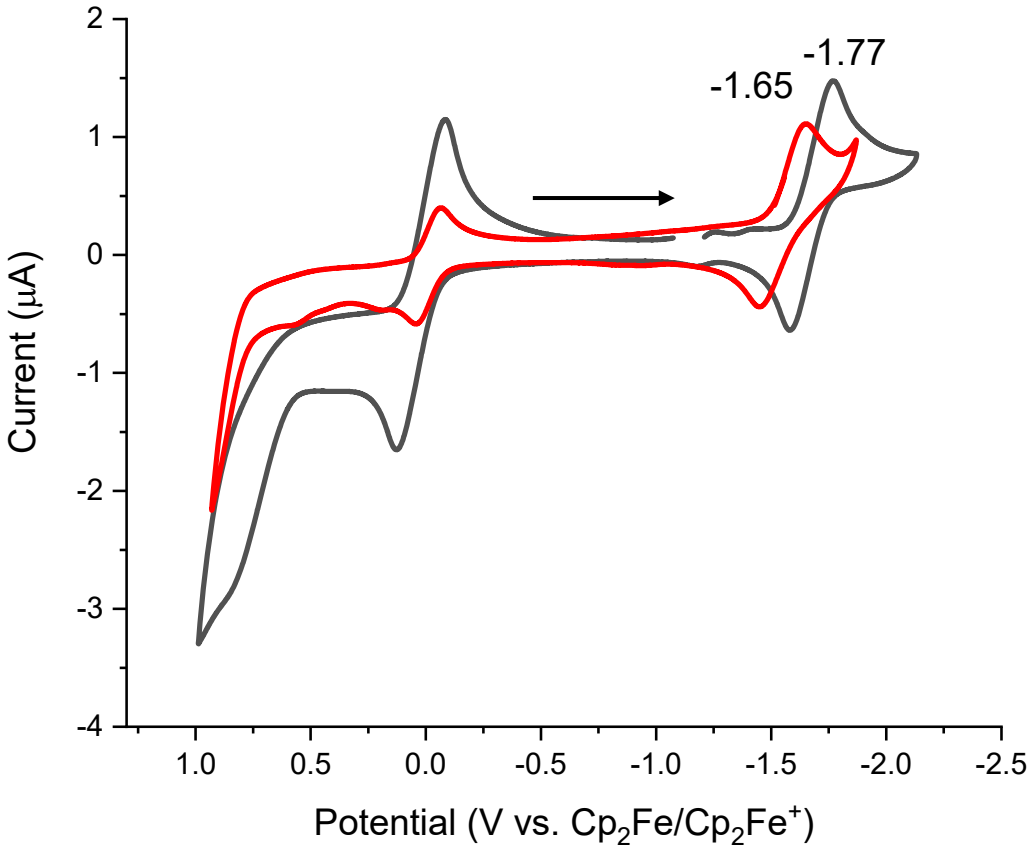


Figure S28. Cyclic voltammogram of BoPNP (black) and [(COD)Rh(BoPNP)]BF_4 (red) in THF. Electrolyte = Bu_4NPF_6, scan rate = 100 mV/s and potential range of scan: 1 V to -2.4 V. The wave at 0.0 V vs. Cp_2Fe/Cp_2Fe^+ is attributed to the ferrocene internal standard. The arrow indicates the initial direction of the scan.

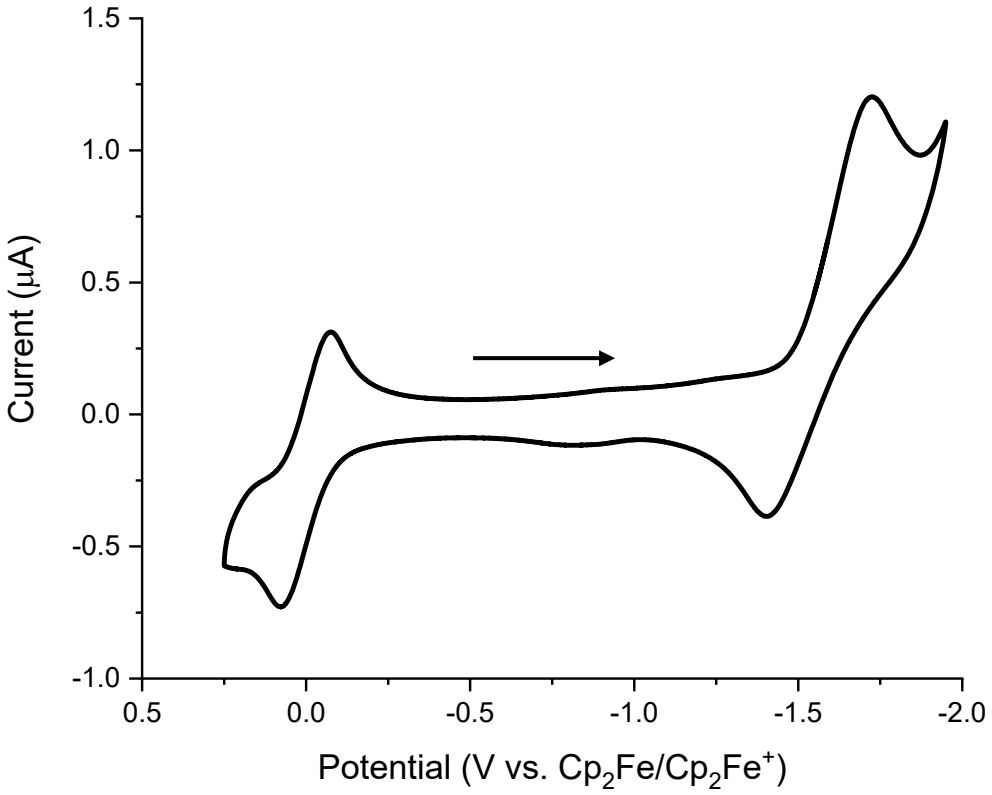


Figure S29. Cyclic voltammogram of [(COD)Rh(BoPNP)]BF_4 in THF, emphasizing the first reduction. Electrolyte = Bu_4NPF_6, scan rate = 100 mV/s and potential range of scan: 0.25 V to 2 V. The wave at 0.0 V vs. Cp_2Fe/Cp_2Fe^+ is attributed to the ferrocene internal standard. The arrow indicates the initial direction of the scan.

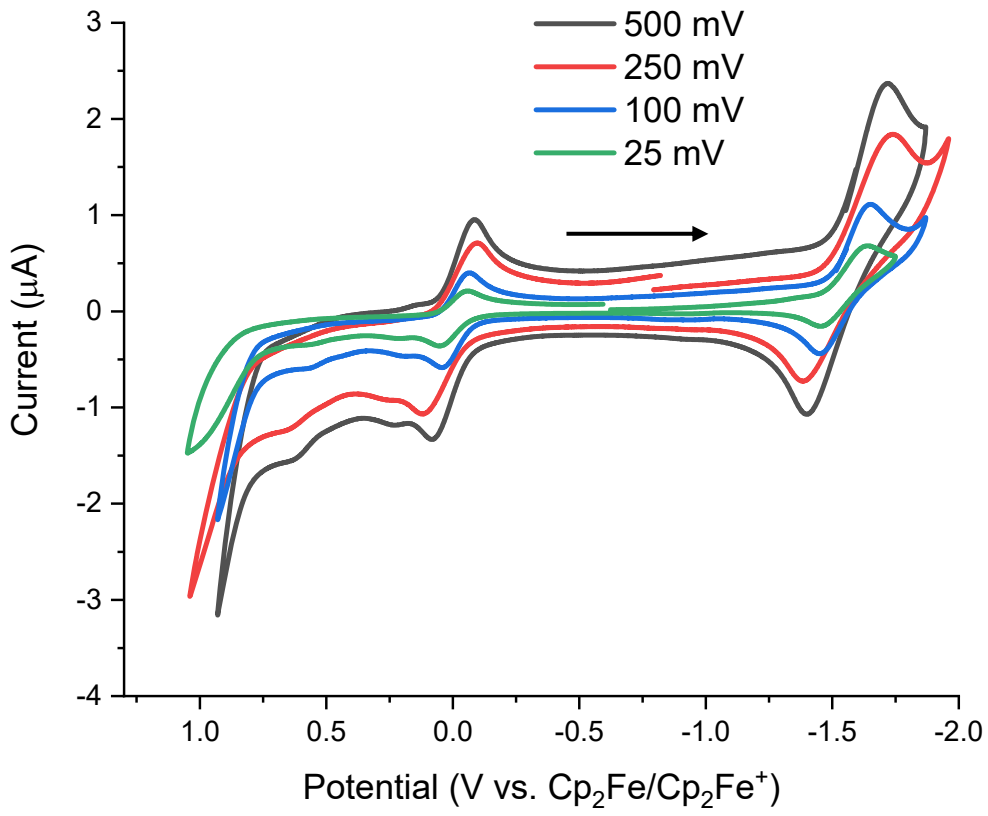


Figure S30. Cyclic voltammogram of [(COD)Rh(BoPNP)]BF_4 in THF at varying scan rates of the first reduction. Electrolyte = Bu_4NPF_6 and potential range of scan: 1.1 V to 2 V. The wave at 0.0 V vs. Cp_2Fe/Cp_2Fe^+ is attributed to the ferrocene internal standard. The arrow indicates the initial direction of the scan.

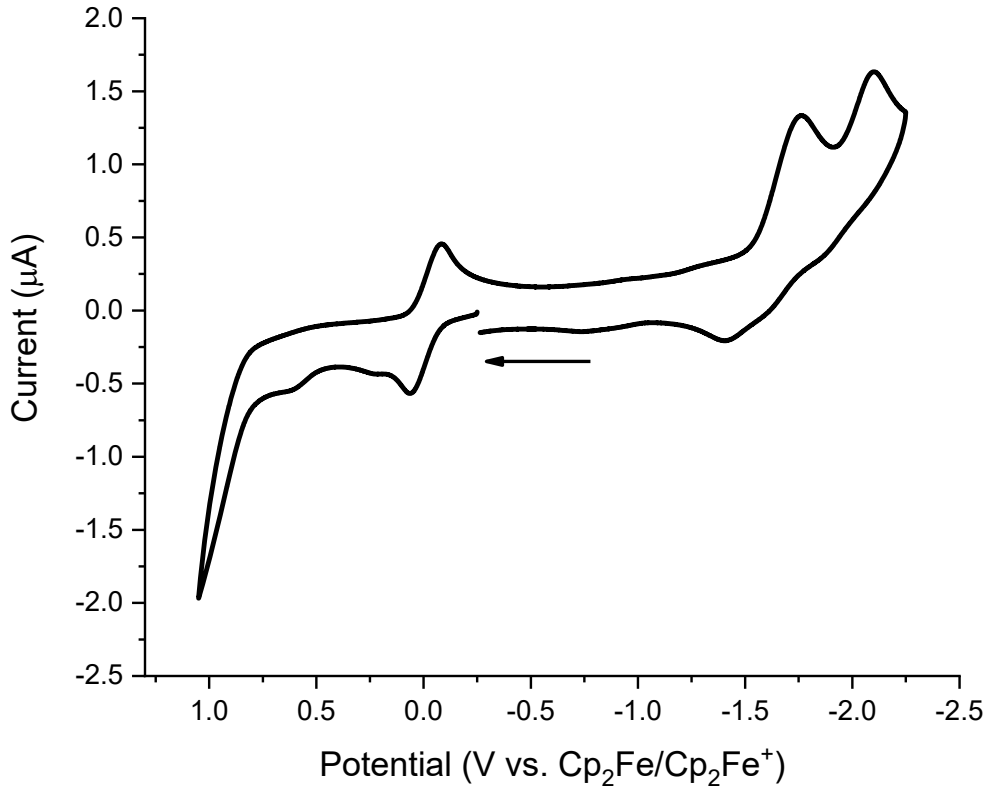


Figure S31. Full cyclic voltammogram of [(COD)Rh(BoPNP)]BF_4 in THF. Electrolyte = Bu_4NPF_6, scan rate = 100mV and potential range of scan: 1 V to 2.4 V. The wave at 0.0 V vs. Cp_2Fe/Cp_2Fe^+ is attributed to the ferrocene internal standard. The arrow indicates the initial direction of the scan.

9) Normalized Absorbance and Emission Spectra of BoPNP and [(COD)Rh(BoPNP)]BF_4

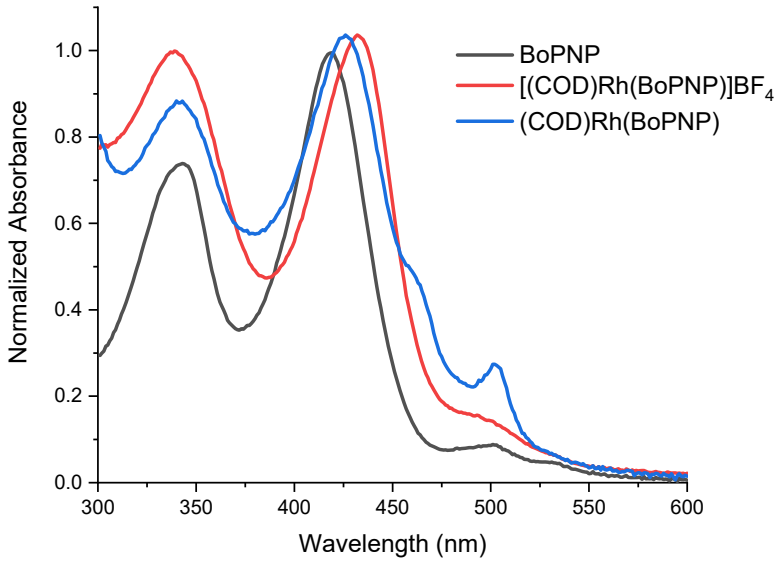


Figure S32. Normalized absorbance spectra of BoPNP, [(COD)Rh(BoPNP)]BF_4, and (COD)RhBoPNP in a 20 μM solution in CH_2Cl_2.

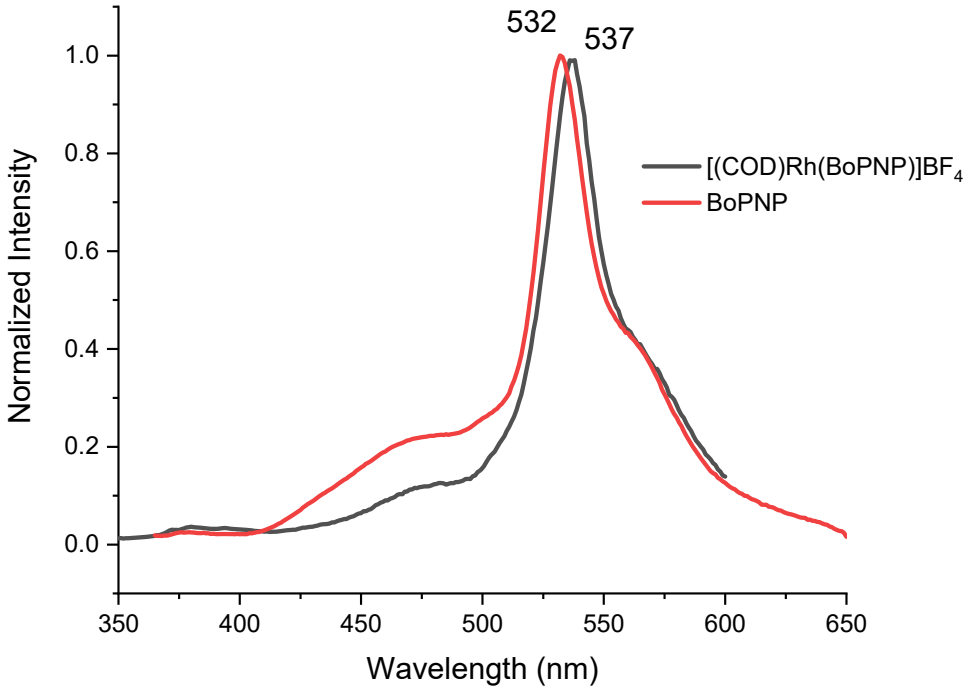


Figure S33. Normalized emission spectra of BoPNP and [(COD)Rh(BoPNP)]BF_4 in a 20 μM solution in CH_2Cl_2.

10) Sample Input File for Geometry Optimizations with Gaussian09

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%nproc=8

#p m062x/genecp opt(maxcycles=150) scf=(maxcycles = 1024) freq gfinput

CODRhBoPNP+_xtal

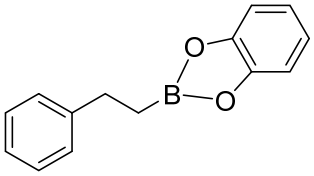
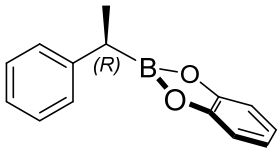
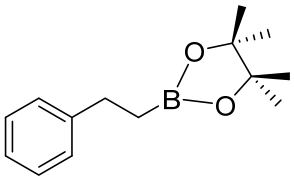
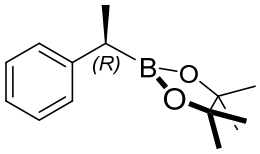
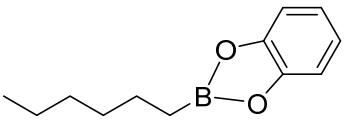
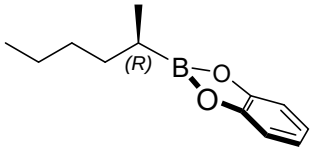
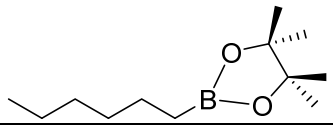
1 1
XYZ Coordinates

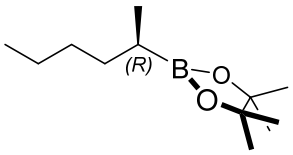
H C B F P N 0
6-31g**
****
Rh 0
SDD
****

Rh 0
SDD
```

11) Computed Energies of BoPNP and [(COD)Rh(BoPNP)]+

Table S4. Computed energies of the metal BoPNP complexes. All calculations were implemented using the M06-2X/6-31g(d,p) level of theory in the gas phase at 298K.

Complex	Energy (Hartrees)	Free Energy Correction (Hartrees)	Enthalpy Correction (Hartrees)
BoPNP	-2501.313809	0.562591	0.677991
[(COD)Rh(BoPNP)]+	-2923.552197	0.74628	0.87519
Catecholborane	-406.8806719	0.073763	0.110807
Pinacolborane	-411.7014171	0.15996	0.203031
Styrene	-309.5099302	0.103383	0.142384
	-716.445445	0.201063	0.257875
	-716.4451943	0.201147	0.257954
	-721.2651871	0.285897	0.349964
	-721.2672729	0.286551	0.349648
1-hexene	-235.7262894	0.134659	0.175686
	-642.6658186	0.233452	0.291843
	-642.6648514	0.232881	0.291615
	-647.4858844	0.319355	0.383949

Complex	Energy (Hartrees)	Free Energy Correction (Hartrees)	Enthalpy Correction (Hartrees)
	-647.4858844	0.319355	0.383949
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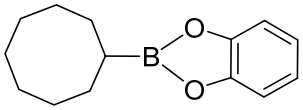
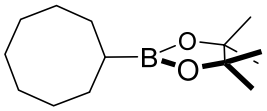
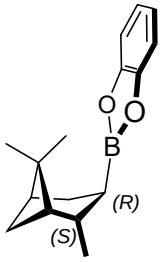
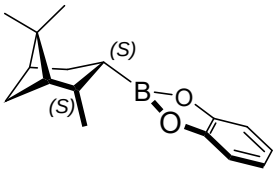
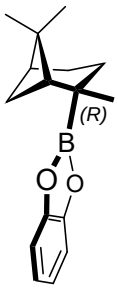
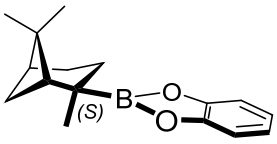
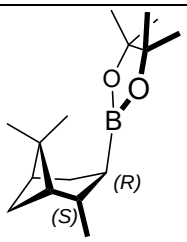
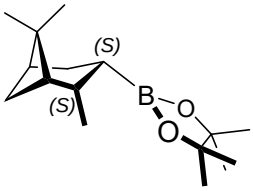
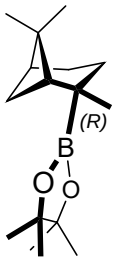
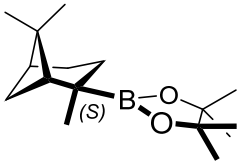
	-720.048069	0.273235	0.330491
	-724.8673976	0.358719	0.42268
α-pinene	-390.4894896	0.20423	0.248789
	-797.4207663	0.303986	0.364914
	-797.4145945	0.302341	0.365184
	-797.4126033	0.302381	0.364452
	-797.4181592	0.304276	0.364758

Complex	Energy (Hartrees)	Free Energy Correction (Hartrees)	Enthalpy Correction (Hartrees)
	-802.2424337	0.390296	0.456973
	-802.2367861	0.388606	0.456974
	-802.2342297	0.39079	0.457094
	-802.2397601	0.391496	0.45689
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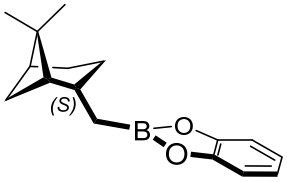
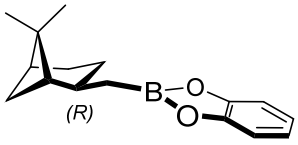
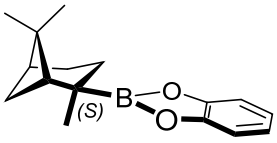
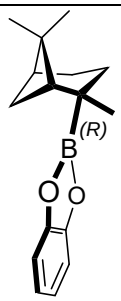
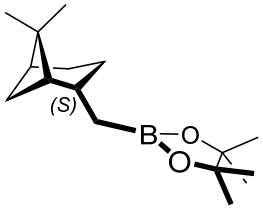
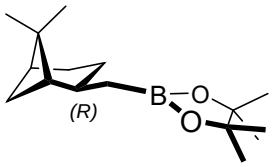
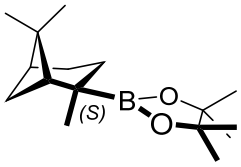
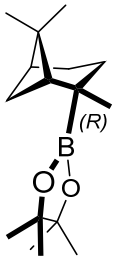
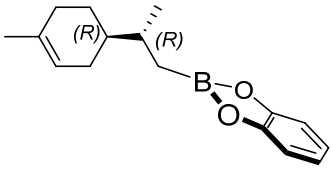
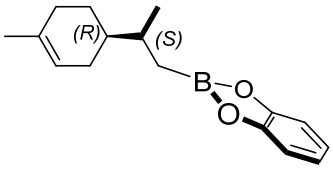
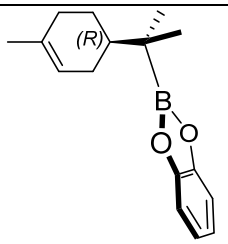
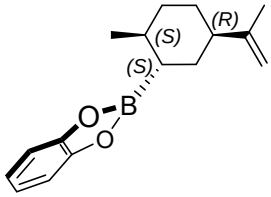
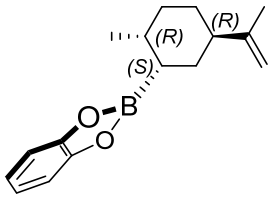
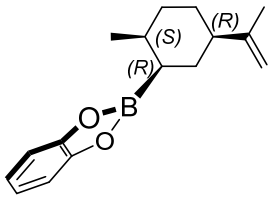
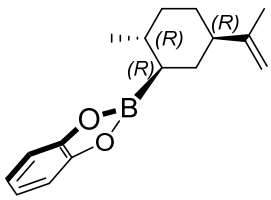
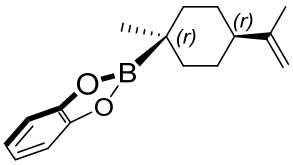
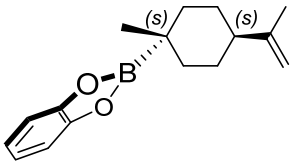
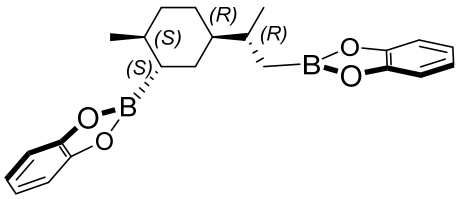
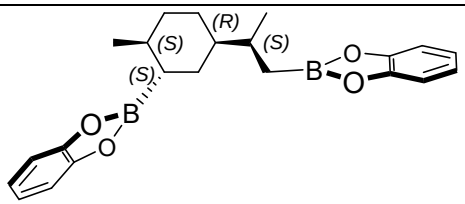
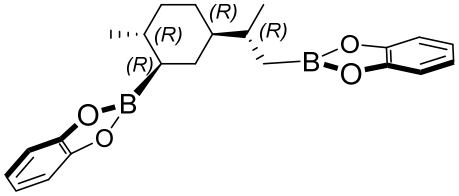
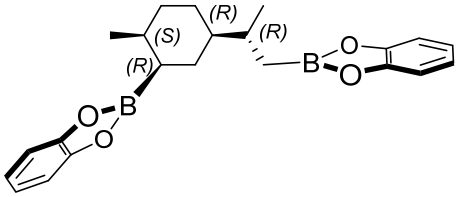
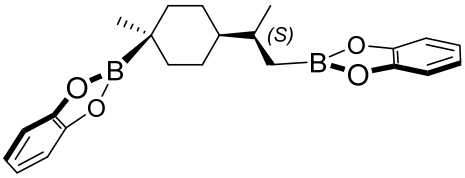
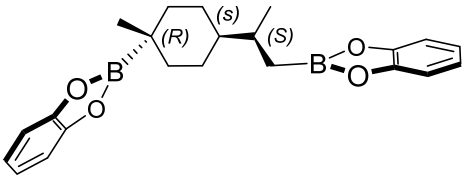
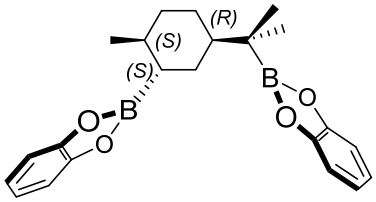
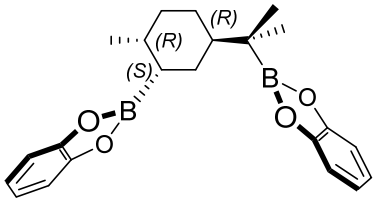
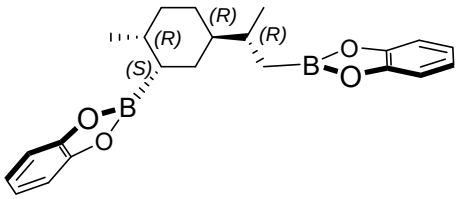
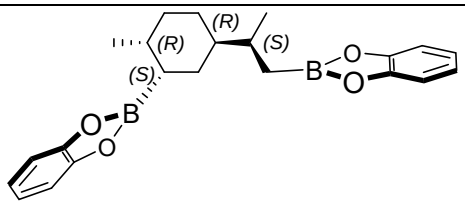
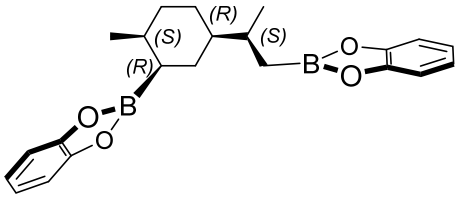
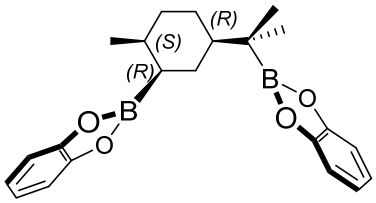
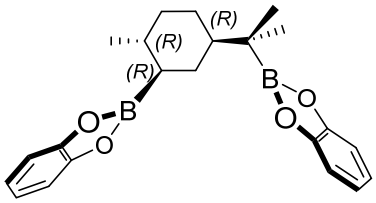
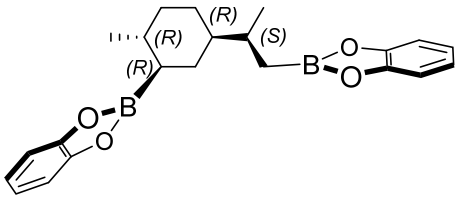
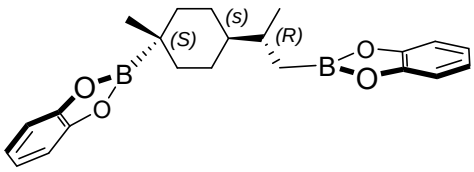
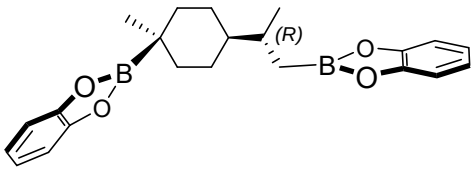
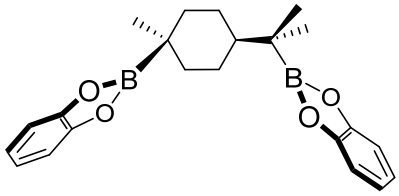
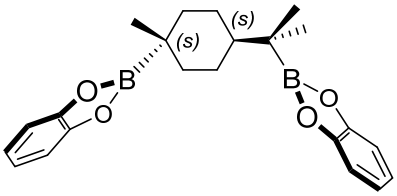
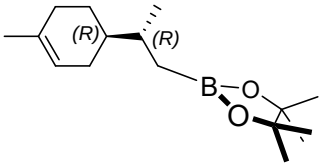
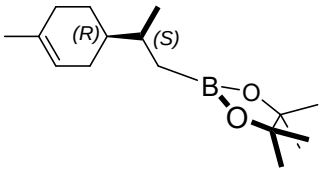
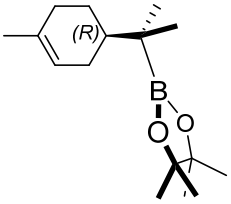
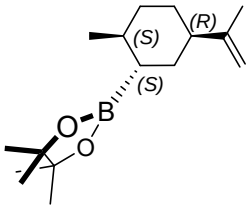
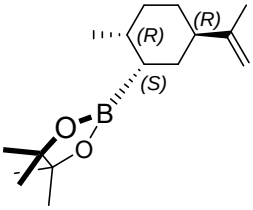
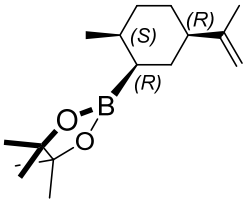
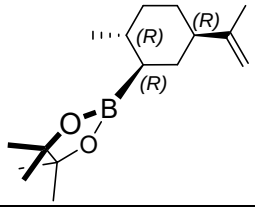
	-797.4148282	0.302733	0.365271
	-797.419471	0.303418	0.364894
	-797.4181592	0.304276	0.364758

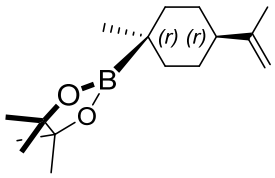
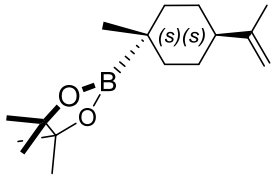
Complex	Energy (Hartrees)	Free Energy Correction (Hartrees)	Enthalpy Correction (Hartrees)
	-797.4126033	0.30238	0.364451
	-802.2396485	0.390698	0.457454
	-802.2364101	0.389498	0.457184
	-802.2397601	0.391496	0.45689
	-802.2342297	0.39079	0.457094
(+)-Limonene	-390.498353	0.201777	0.248957
	-802.254644	0.389397	0.457289
	-802.2548705	0.387713	0.4567

Complex	Energy (Hartrees)	Free Energy Correction (Hartrees)	Enthalpy Correction (Hartrees)
	-802.2526516	0.386502	0.456227
	-802.2449505	0.387287	0.456851
	-802.2412316	0.387163	0.456801
	-802.2417576	0.38614	0.45686
	-802.2414794	0.387315	0.457145
	-797.4196019	0.301141	0.364818
	-797.4204421	0.301329	0.364815
	-1204.371908	0.40412	0.479941

Complex	Energy (Hartrees)	Free Energy Correction (Hartrees)	Enthalpy Correction (Hartrees)
	-1204.357651	0.398364	0.480285
	-1204.371036	0.404057	0.480247
	-1204.37017	0.404279	0.480303
	-1204.360687	0.399591	0.480235
	-1204.35451	0.398112	0.480207
	-1204.360494	0.399712	0.480043
	-1204.358135	0.40155	0.480213
	-1204.369753	0.401605	0.479848

Complex	Energy (Hartrees)	Free Energy Correction (Hartrees)	Enthalpy Correction (Hartrees)
	-1204.363087	0.404327	0.480531
	-1204.366173	0.402456	0.480638
	-1204.356609	0.400848	0.480167
	-1204.357149	0.398787	0.479967
	-1204.363705	0.400747	0.480627
	-1204.354782	0.398246	0.480266
	-1204.354452	0.398755	0.479895
	-1204.352521	0.398528	0.479701

Complex	Energy (Hartrees)	Free Energy Correction (Hartrees)	Enthalpy Correction (Hartrees)
	-1204.352326	0.398276	0.479765
	-802.254644	0.389397	0.457289
	-802.2548705	0.387713	0.4567
	-802.2526516	0.386502	0.456227
	-802.2449505	0.387287	0.456851
	-802.2417576	0.38614	0.45686
	-802.2412316	0.387163	0.456801
	-802.2414794	0.387315	0.457145

Complex	Energy (Hartrees)	Free Energy Correction (Hartrees)	Enthalpy Correction (Hartrees)
	-802.2502898	0.387794	0.456564
	-802.2456013	0.387181	0.456824

12) Computed Free Energies for the Hydroboration of Olefins

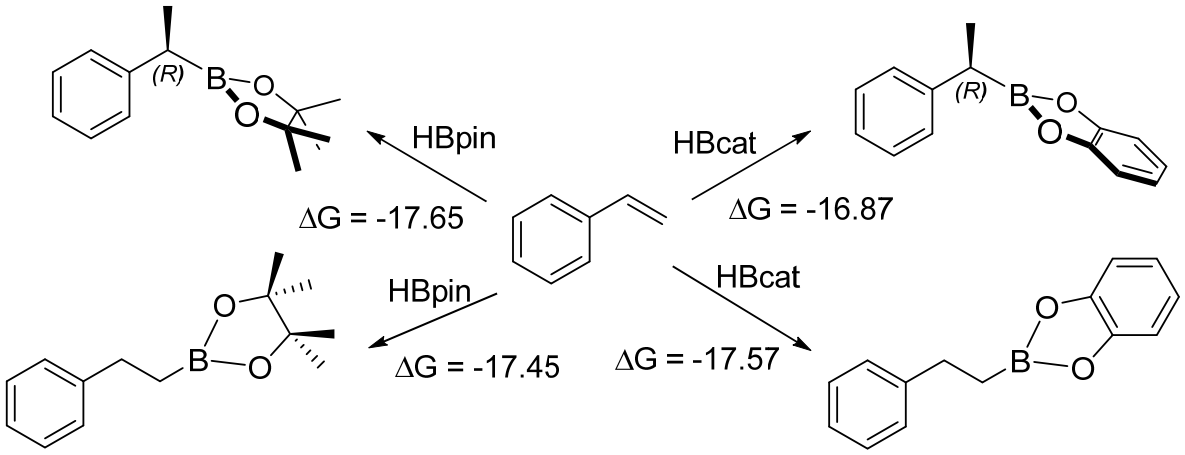


Figure 34. Computed free energies for the hydroboration of styrene with pinacolborane and catecholborane. Energies are given in units of kcal/mol at the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in THF (PCM solvation model).

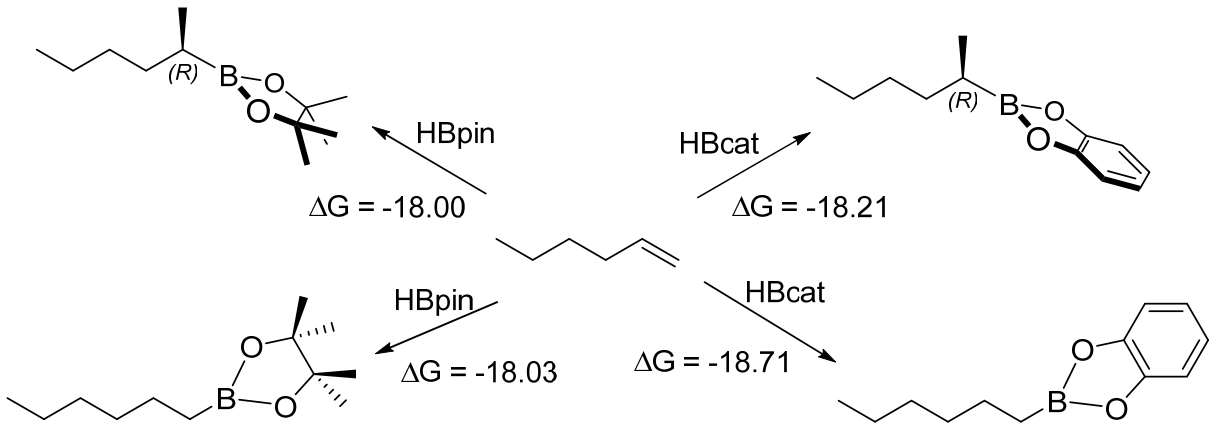


Figure 35. Computed free energies for the hydroboration of 1-hexene with pinacolborane and catecholborane. Energies are given in units of kcal/mol at the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in THF (PCM solvation model).

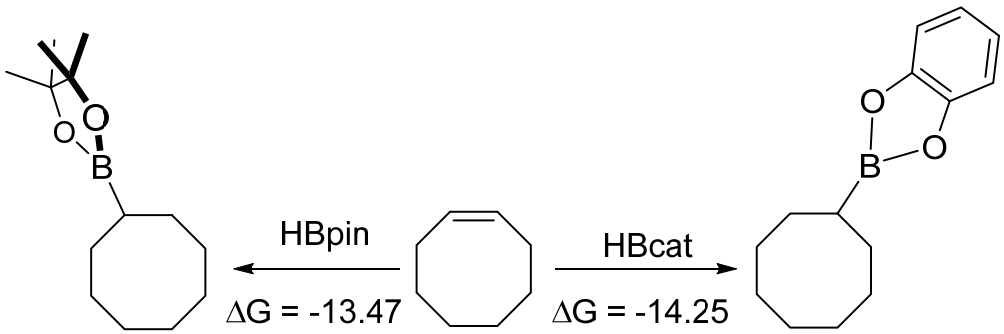


Figure 36. Computed free energies for the hydroboration of cyclooctene with pinacolborane and catecholborane. Energies are given in units of kcal/mol at the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in THF (PCM solvation model).

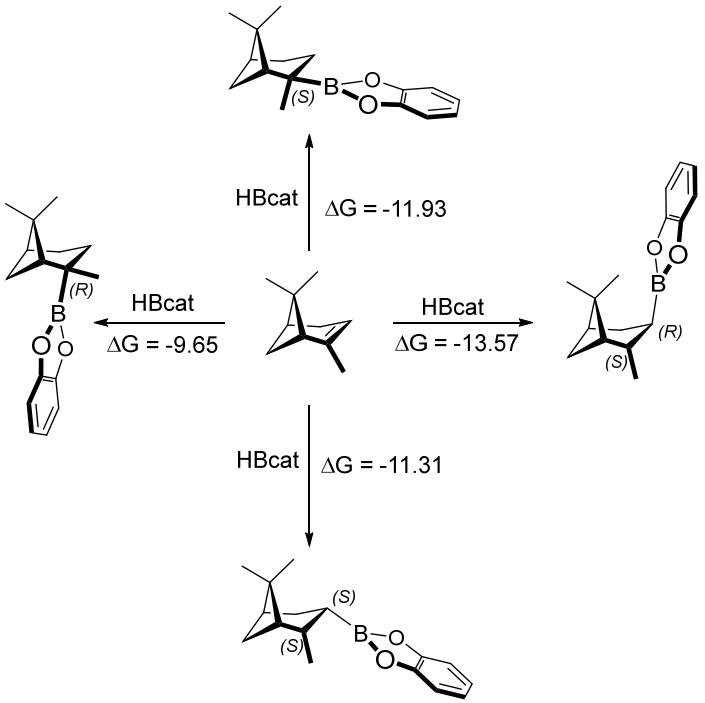


Figure 37. Computed free energies for the hydroboration of α-pinene with catecholborane. Energies are given in units of kcal/mol at the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in THF (PCM solvation model).

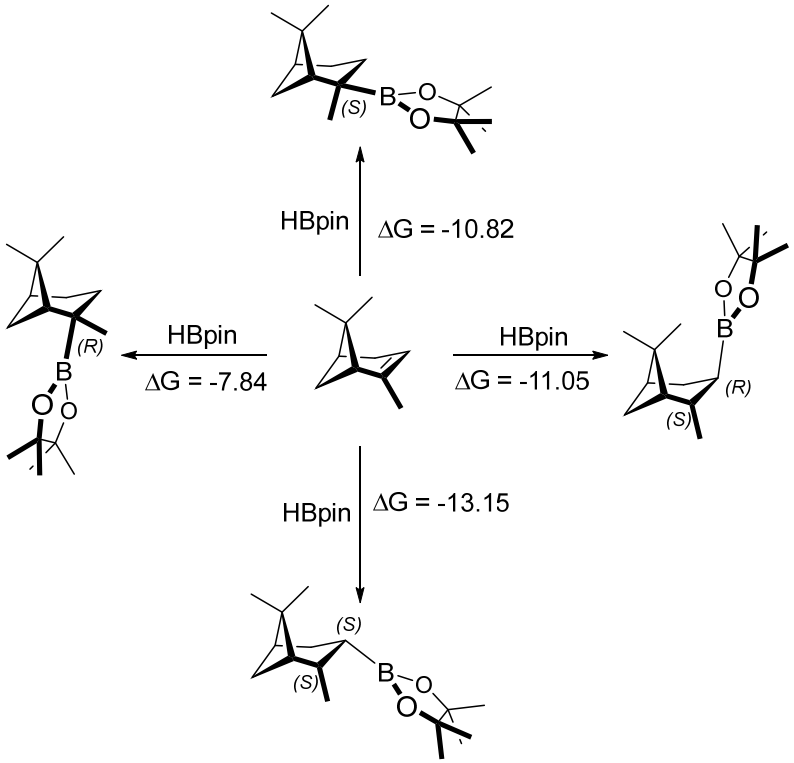


Figure 38. Computed free energies for the hydroboration of α-pinene with pinacolborane. Energies are given in units of kcal/mol at the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in THF (PCM solvation model).

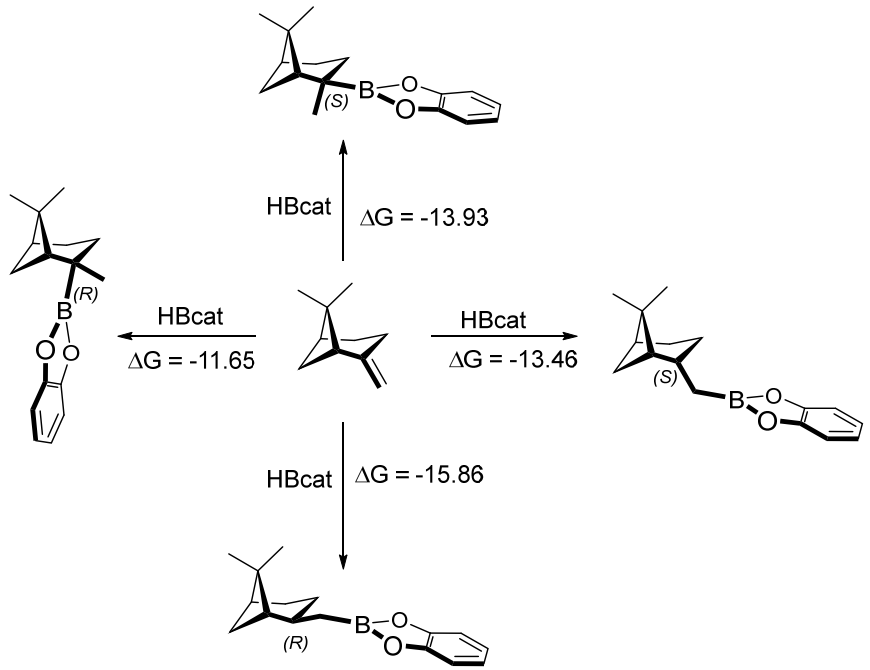


Figure 39. Computed free energies for the hydroboration of β-pinene with catecholborane. Energies are given in units of kcal/mol at the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in THF (PCM solvation model).

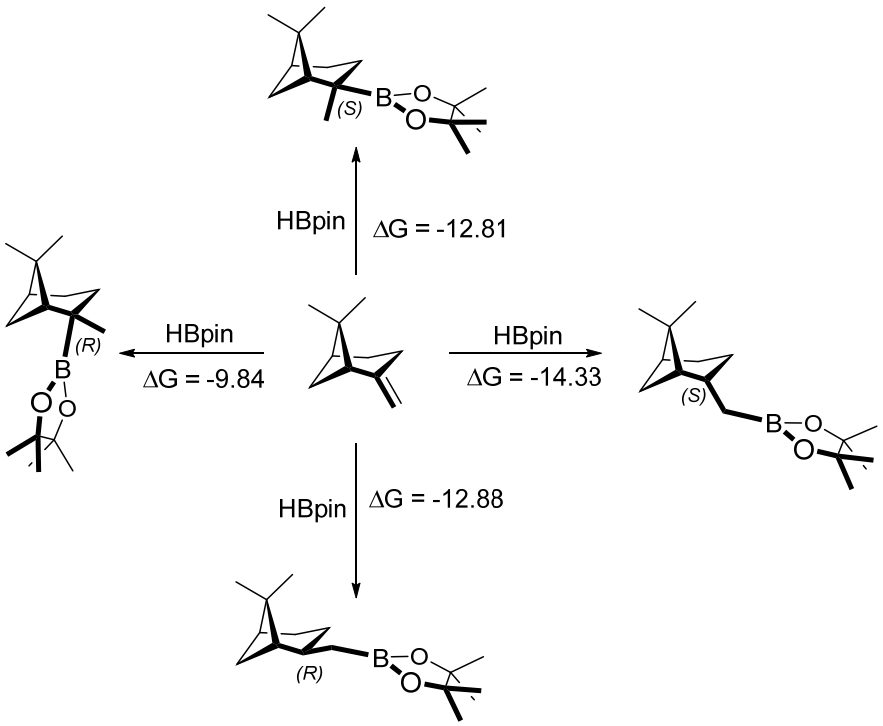


Figure 40. Computed free energies for the hydroboration of β-pinene with pinacolborane. Energies are given in units of kcal/mol at the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in THF (PCM solvation model).

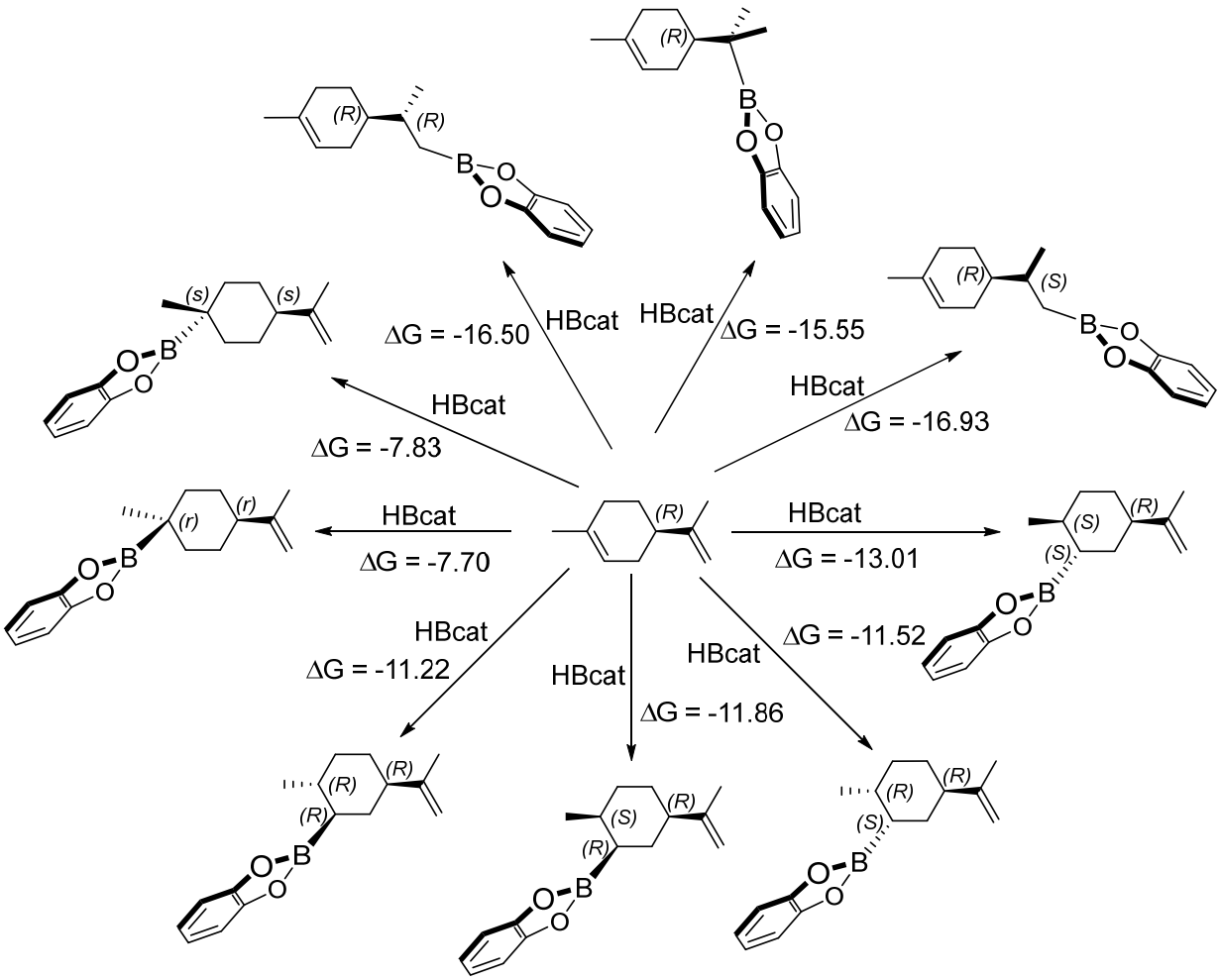


Figure 41. Computed free energies for the hydroboration of (+)-limonene with catecholborane. Energies are given in units of kcal/mol at the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in THF (PCM solvation model).

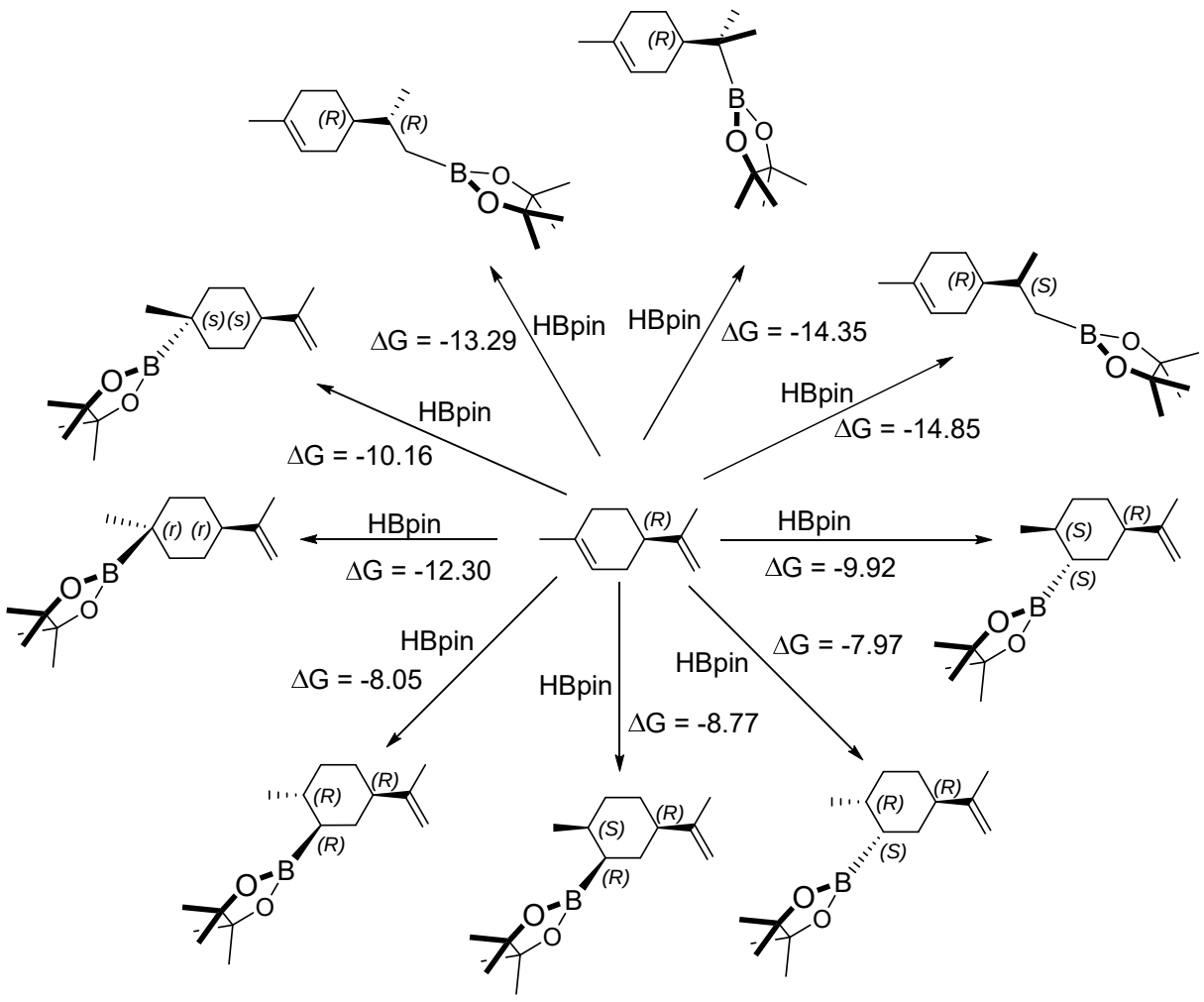


Figure 42. Computed free energies for the hydroboration of (+)-limonene with pinacolborane. Energies are given in units of kcal/mol at the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in THF (PCM solvation model).

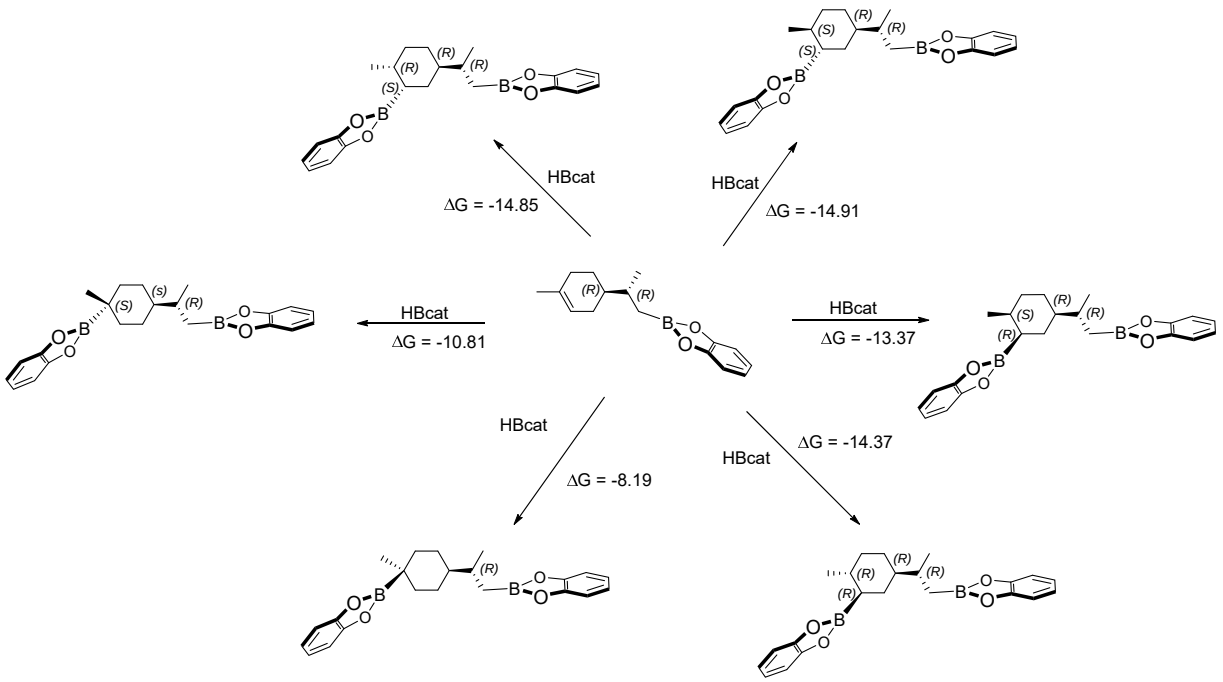


Figure 43. Computed free energies for the second hydroboration of (+)-limonene (hydroboration of 2-((*R*)-2-((*R*)-4-methylcyclohex-3-en-1-yl)propyl)benzo[d][1,3,2]dioxaborole) with catecholborane. Energies are given in units of kcal/mol at the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in THF (PCM solvation model).

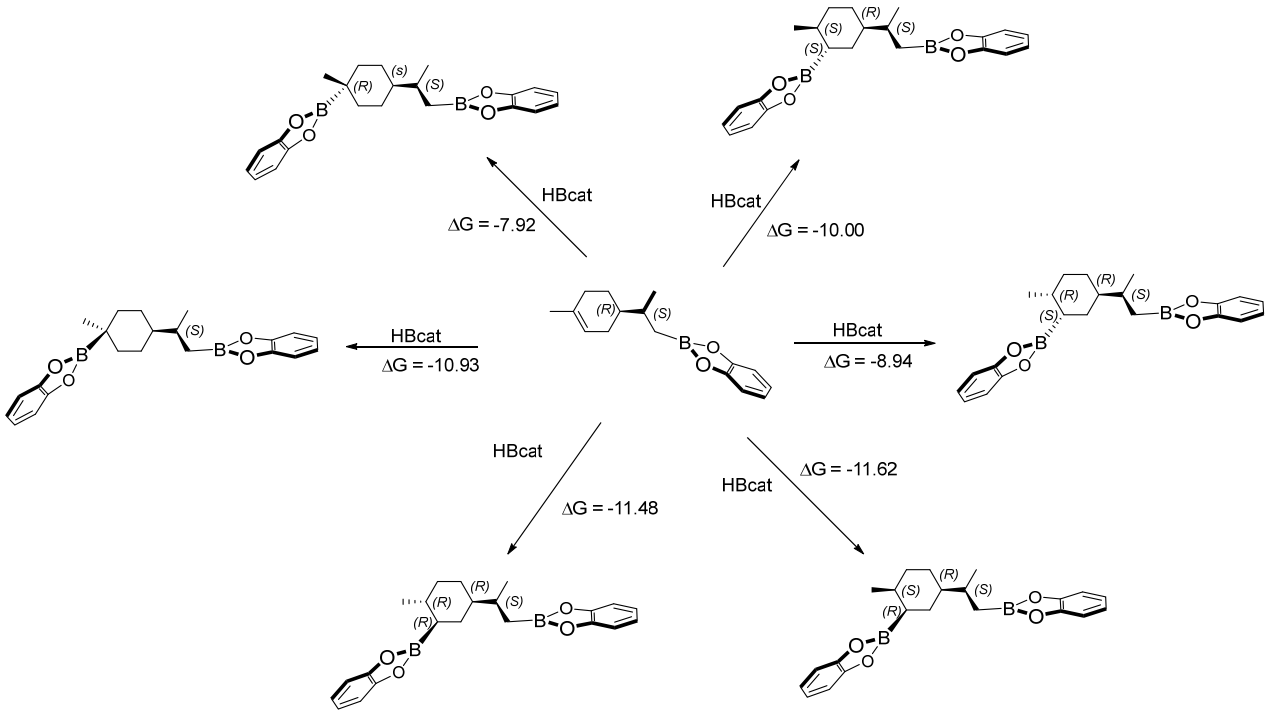


Figure 44. Computed free energies for the second hydroboration of (+)-limonene (hydroboration of 2-((*S*)-2-((*R*)-4-methylcyclohex-3-en-1-yl)propyl)benzo[d][1,3,2]dioxaborole) with catecholborane. Energies are given in units of kcal/mol at the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in THF (PCM solvation model).

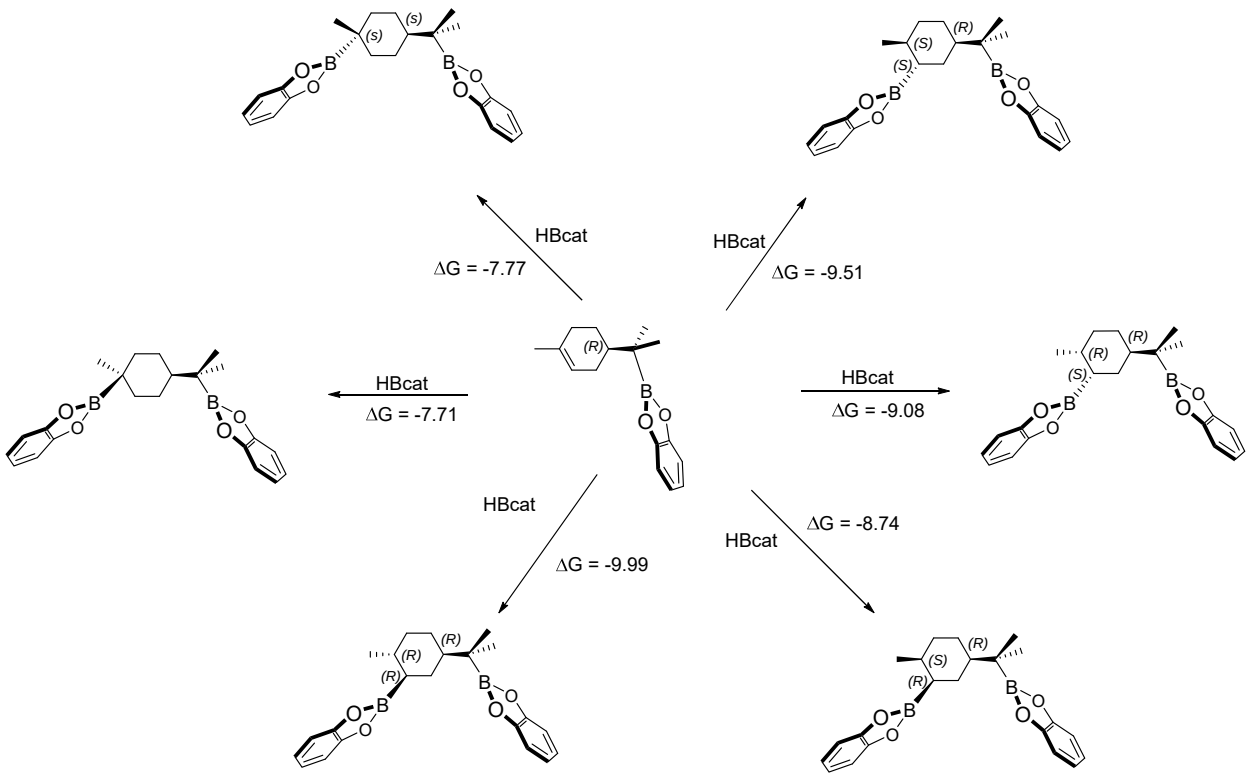


Figure 45. Computed free energies for the second hydroboration of (+)-limonene (hydroboration of (*R*)-2-(2-(4-methylcyclohex-3-en-1-yl)propan-2-yl)benzo[d][1,3,2]dioxaborole) with catecholborane. Energies are given in units of kcal/mol at the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in THF (PCM solvation model).

13) Frontier Molecular Orbitals of BoPNP and [(COD)Rh(BoPNP)]$^+$

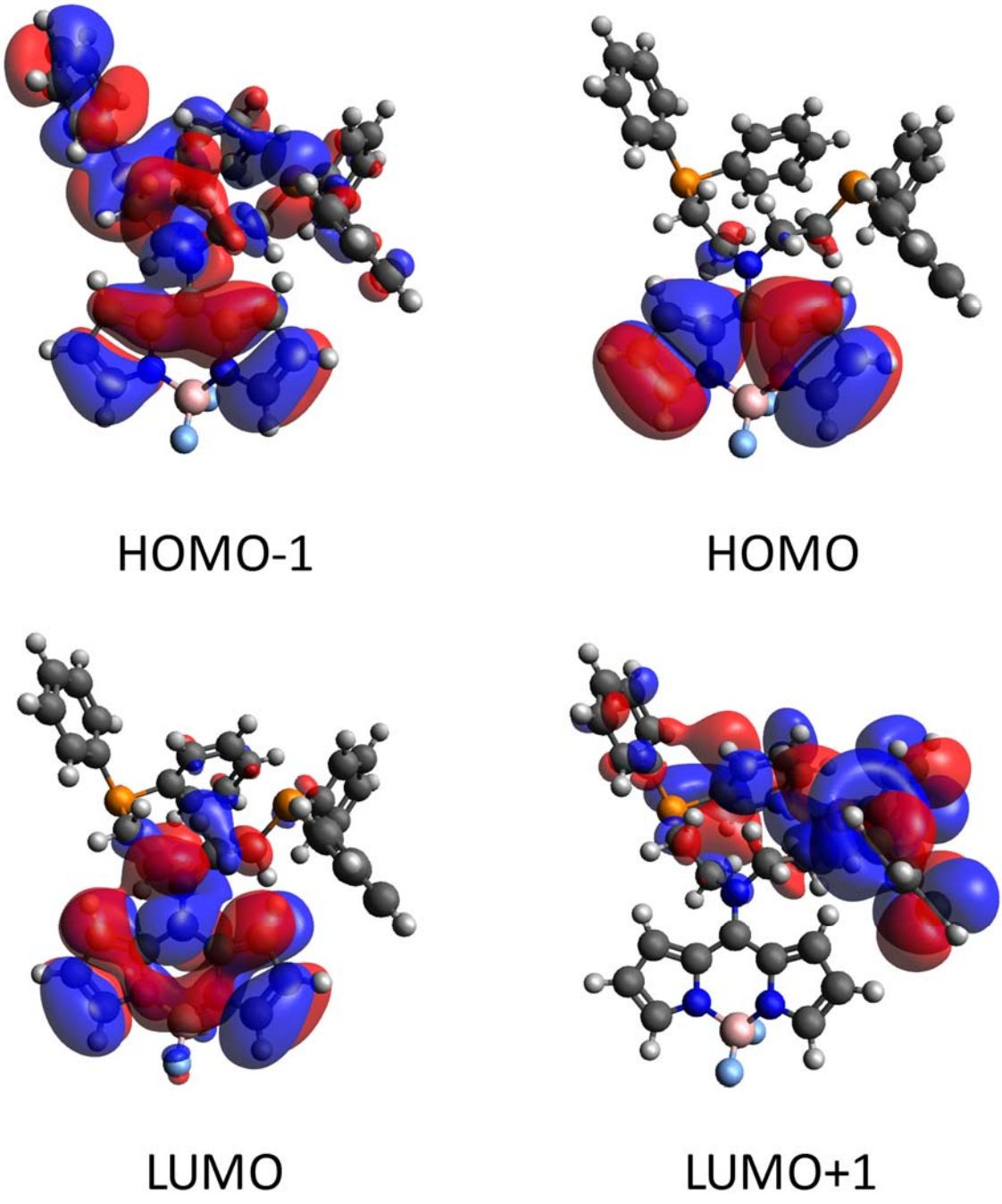


Figure S46. Frontier molecular orbitals of BoPNP. Isovalue = 0.01 e^-/a.u.

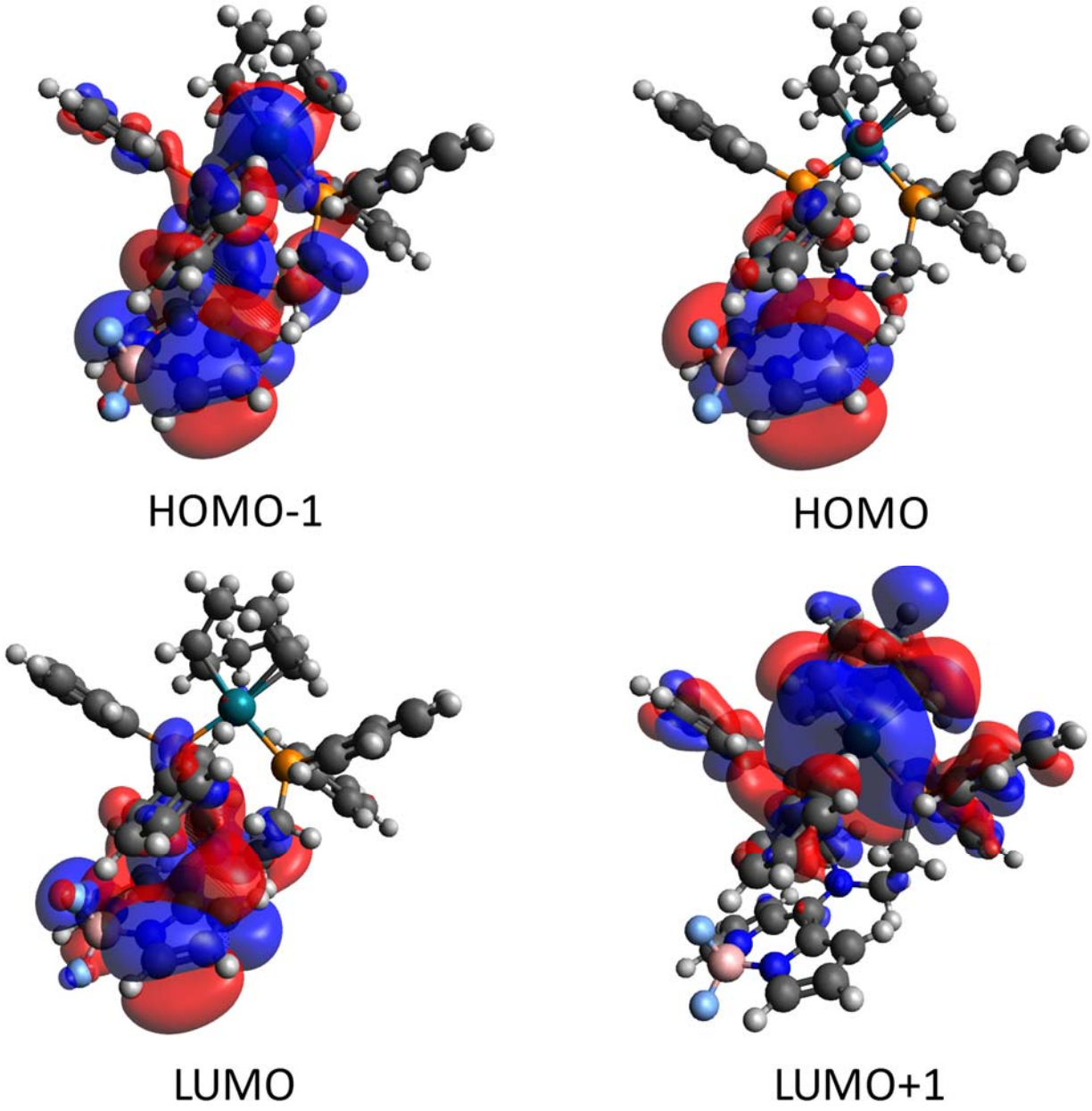


Figure S47. Frontier molecular orbitals of [(COD)Rh(BoPNP)]$^{+}$. Isovalue = 0.01 e^{-}/a.u.

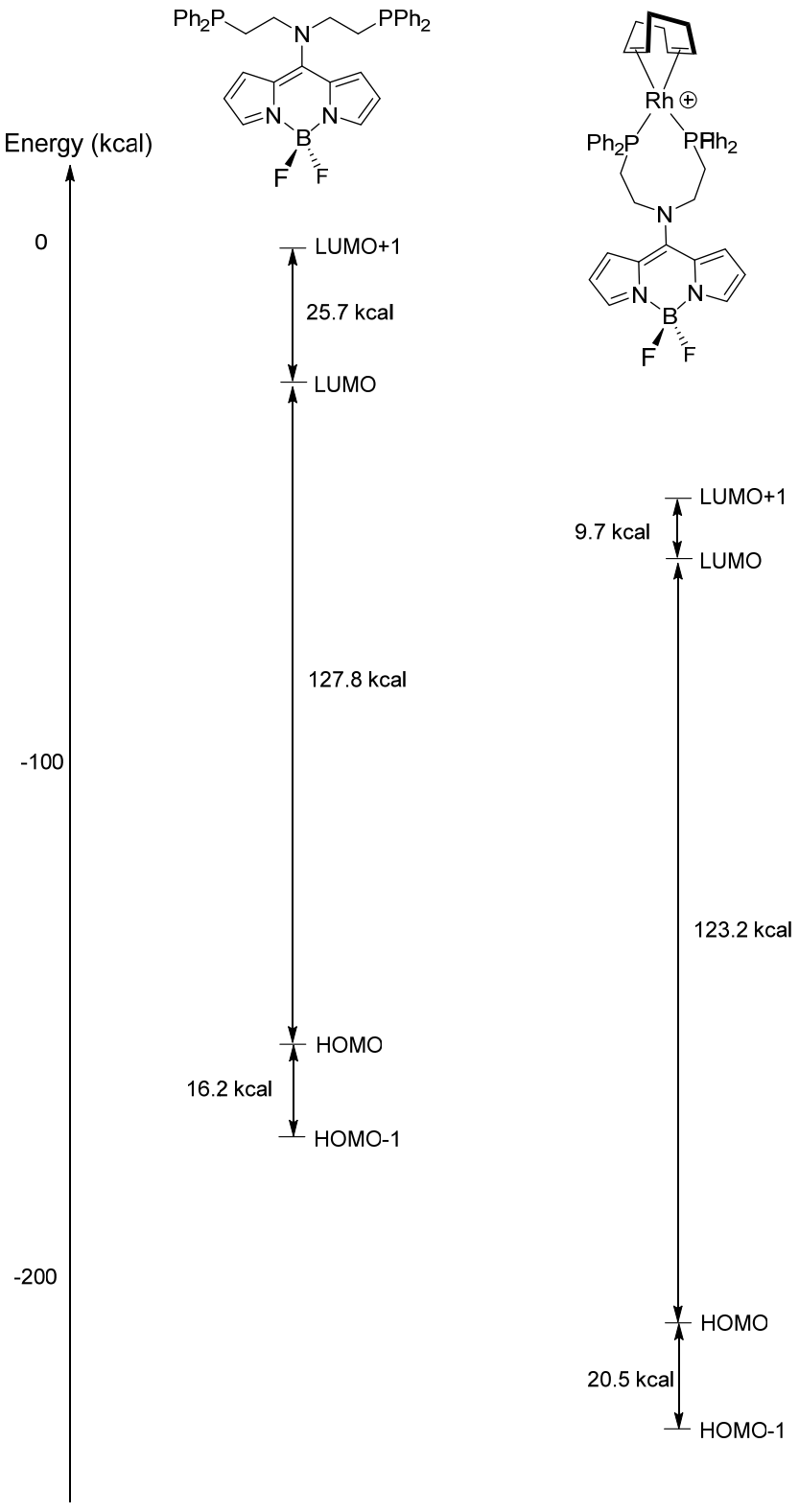


Figure S48. Energies of the frontier molecular orbitals of BoPNP and [(COD)Rh(BoPNP)]$^{+}$ at the M06-2X/6-31G(d,p) level of theory.

14) Computed UV-Vis Spectra of BoPNP and [(COD)Rh(BoPNP)]$^+$ in CH_2Cl_2.

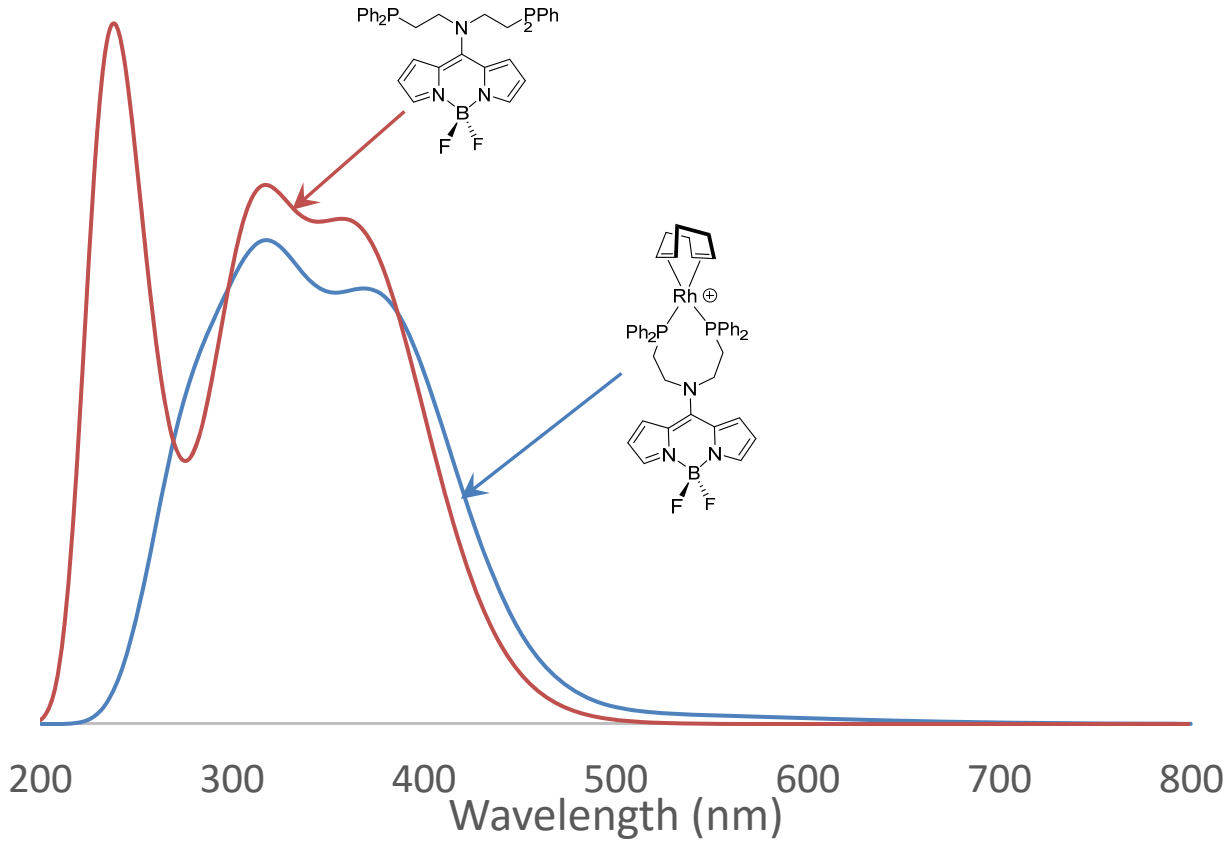


Figure 49. Computed UV-Vis spectra of BoPNP and [(COD)Rh(BoPNP)]$^+$ at the M06-2X/6-311++G(d,p) level of theory in CH_2Cl_2 (PCM solvation model).

15) 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.

79
BoPNP

P	-0.19720	2.65307	0.92659
P	-3.28650	-2.19184	-0.83352
F	5.59537	-3.58594	-0.72643
F	4.46296	-2.48115	-2.37709
N	4.26938	-1.66508	-0.12460
N	3.19634	-3.75352	-0.76524
N	0.61504	-1.34302	0.18249
C	5.26132	-0.81517	0.15299
C	4.74381	0.34662	0.72827
C	3.36244	0.18883	0.77363
C	3.06049	-1.08805	0.24013
C	1.85877	-1.85003	0.02651
C	1.99475	-3.24084	-0.33265
C	1.11798	-4.32415	-0.14014
C	1.81111	-5.48603	-0.47789
C	3.09212	-5.08572	-0.86118
C	0.33851	-0.07362	0.85838
C	0.27695	1.14348	-0.06921
C	-0.53278	-1.82783	-0.60589
C	-1.73806	-2.28832	0.21804
C	1.47090	3.10248	1.57458
C	2.48535	3.65012	0.78187
C	3.75883	3.84583	1.30538
C	4.03561	3.49047	2.62564
C	3.03153	2.95470	3.42585
C	1.75194	2.77185	2.90425
C	-0.45140	3.88819	-0.41407
C	-0.04464	3.71058	-1.74061
C	-0.36268	4.65535	-2.71296
C	-1.08692	5.79481	-2.37154
C	-1.48889	5.98866	-1.05160
C	-1.17778	5.03852	-0.08347
C	-3.29811	-0.35923	-1.08618
C	-3.05685	0.12779	-2.37518
C	-2.97014	1.49933	-2.61322
C	-3.13557	2.39832	-1.56439
C	-3.38133	1.92381	-0.27507
C	-3.45920	0.55433	-0.03670
C	-4.58064	-2.35345	0.46772
C	-4.36240	-2.97814	1.69857
C	-5.40361	-3.12461	2.61443
C	-6.67378	-2.64692	2.31394
C	-6.90312	-2.02314	1.08850
C	-5.86784	-1.88384	0.17263
B	4.45107	-2.89898	-1.06229
H	6.27983	-1.08087	-0.09408
H	5.30123	1.20269	1.07741
H	2.68954	0.92563	1.17660
H	0.11698	-4.27095	0.25736
H	1.44353	-6.49999	-0.43306
H	3.94113	-5.67166	-1.18291
H	-0.63698	-0.17547	1.34343
H	1.06400	0.05441	1.66226
H	-0.52253	1.01099	-0.80974
H	1.22779	1.27844	-0.59620
H	-0.83315	-0.98255	-1.23505
H	-0.19369	-2.61593	-1.27485
H	-1.88200	-1.66694	1.10758
H	-1.61050	-3.31975	0.55712
H	2.27710	3.91766	-0.25090
H	4.54029	4.26714	0.68062
H	5.03266	3.63522	3.02980
H	3.24181	2.68230	4.45511
H	0.96437	2.36012	3.53095
H	0.51040	2.82325	-2.02951
H	-0.04501	4.49932	-3.73923
H	-1.33726	6.52874	-3.13095
H	-2.05447	6.87390	-0.77868
H	-1.51592	5.18049	0.94029
H	-2.93322	-0.57558	-3.19488
H	-2.77514	1.86542	-3.61645
H	-3.05829	3.46716	-1.74459
H	-3.49969	2.62503	0.54549
H	-3.66096	0.18932	0.96832
H	-3.37886	-3.35671	1.95887
H	-5.21594	-3.61094	3.56654
H	-7.48175	-2.75924	3.02950
H	-7.89146	-1.64571	0.84585
H	-6.05396	-1.39327	-0.77981

100
[(COD)Rh(BoPNP)]$^{+}$

Rh	-2.050913	0.940188	0.057204
P	0.218956	1.476236	0.090518
P	-1.691848	-1.451167	0.049019
F	7.022614	-0.863924	-0.186385
F	5.431415	0.597251	-0.940640
N	5.200705	-0.293705	1.278156

N	4.814230	-1.710826	-0.667049
C	2.977963	-2.895236	-1.198514
C	-4.336083	0.546969	0.360929
N	1.702232	-1.405926	1.265013
C	-4.005051	-2.763692	-0.941858
C	-2.362793	-3.578470	1.772316
C	-3.075772	-3.298393	4.060502
C	3.521320	-1.990558	-0.253747
C	3.925773	-0.577175	1.732638
C	5.915908	0.237601	2.272072
C	-0.084140	-2.362435	-0.248567
C	-4.105775	0.737447	-0.977582
C	1.024429	-0.406622	2.095317
C	-2.272470	-2.188037	1.623626
C	-2.988404	-1.916426	3.922725
C	-2.255829	-2.308766	-2.545268
C	3.015123	-1.328968	0.918645
C	3.956689	-3.146143	-2.153884
C	-2.728135	-2.268842	-1.226250
C	5.130370	0.315498	3.427838
C	-4.325948	-3.312919	-3.272277
C	3.881314	-0.192024	3.094902
C	2.456702	0.763727	-1.489605
C	-2.622102	2.794017	1.151033
C	0.873425	-2.559971	0.934382
C	1.177049	1.032376	1.612545
C	3.050855	0.304103	-2.663228
B	5.696617	-0.530239	-0.165702
C	0.818649	3.825537	-1.322713
C	-3.928328	3.287751	-1.001898
C	-2.762529	-4.129437	2.984916
C	-2.587047	-1.363095	2.708246
C	1.040475	5.191993	-1.462126
C	0.273797	0.362658	-2.447910
C	0.643813	4.104130	1.067073
C	2.259469	-0.138032	-3.719976
C	-3.050996	-2.830383	-3.560617
C	-4.798619	-3.281804	-1.963612
C	-4.287332	2.008655	-1.767733
C	0.870912	5.470534	0.923825
C	-2.661513	3.138084	-0.183618
C	0.615976	3.266111	-0.054110
C	1.064008	0.778838	-1.367935
C	-3.807550	2.436335	2.017301
C	5.070782	-2.384165	-1.793507
C	1.066411	6.017414	-0.340611
C	-4.887253	1.577527	1.328264
C	0.869901	-0.101193	-3.617799
H	2.002987	-3.351351	-1.200939
H	-4.355772	-0.483216	0.711833
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H	-2.133849	-4.231678	0.933336
H	-3.389916	-3.730582	5.004795
H	6.945258	0.523354	2.106456
H	-0.384065	-3.352940	-0.609852
H	0.435881	-1.858566	-1.068078
H	-3.969838	-0.152875	-1.588515
H	-0.036536	-0.666028	2.079031
H	1.321727	-0.489037	3.142327
H	-3.233626	-1.269239	4.758436
H	-1.262237	-1.936413	-2.784246
H	3.882442	-3.813965	-2.998763
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H	3.068265	-0.320928	3.789814
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H	-1.720269	3.051454	1.704730
H	1.535494	-3.400958	0.730801
H	0.310394	-2.827001	1.836360
H	2.225067	1.316203	1.485110
H	0.770832	1.676583	2.399067
H	4.132610	0.291437	-2.725276
H	0.813363	3.191990	-2.204581
H	-3.779237	4.095184	-1.723351
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H	-2.832956	-5.206778	3.091365
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H	0.500346	3.706075	2.067001
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H	-2.673108	-2.863546	-4.577206
H	-5.786575	-3.666099	-1.732395
H	-3.649912	1.937201	-2.655701
H	-5.320500	2.058431	-2.137144
H	0.898792	6.104469	1.803658
H	-1.774107	3.602913	-0.604295
H	-3.426843	1.895386	2.890344
H	-4.260000	3.357159	2.409436
H	6.031167	-2.276706	-2.279185
H	1.245046	7.081585	-0.451652
H	-5.612017	2.208889	0.810067
H	-5.450418	1.051270	2.103690
H	0.250398	-0.420209	-4.450691

14

Catecholborane

C	0.27187	-0.69585	-0.00001
C	-0.89772	-1.42952	0.00000
C	-2.08925	-0.69803	0.00001
C	-2.08925	0.69803	0.00001
C	-0.89772	1.42952	0.00000

C	0.27187	0.69585	-0.00001
O	1.57186	1.14248	-0.00000
B	2.34750	0.00000	0.00001
O	1.57186	-1.14248	-0.00000
H	-0.88206	-2.51280	0.00001
H	-3.03464	-1.22951	0.00001
H	-3.03464	1.22951	0.00001
H	-0.88206	2.51280	0.00001
H	3.52723	0.00000	0.00004

22

Pinacolborane

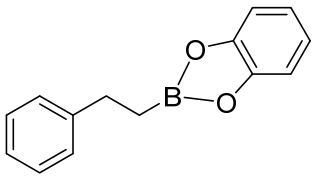
C	-0.77978	-0.18651	0.05437
C	0.77978	-0.18652	-0.05437
O	1.06140	1.18263	-0.42335
B	0.00001	1.93261	-0.00001
O	-1.06140	1.18265	0.42333
C	-1.34752	-1.11116	1.11849
C	-1.46728	-0.43039	-1.28717
C	1.34751	-1.11119	-1.11848
C	1.46728	-0.43038	1.28718
H	0.00002	3.11826	-0.00001
H	-2.43744	-1.03334	1.12447
H	-1.07882	-2.15082	0.90552
H	-0.98068	-0.84745	2.11150
H	-1.35526	-1.46852	-1.61156
H	-2.53174	-0.20870	-1.18142
H	-1.05535	0.22553	-2.05946
H	2.43743	-1.03337	-1.12446
H	1.07880	-2.15084	-0.90548
H	0.98066	-0.84750	-2.11149
H	1.35526	-1.46850	1.61158
H	2.53175	-0.20870	1.18141
H	1.05536	0.22556	2.05945

16

Styrene

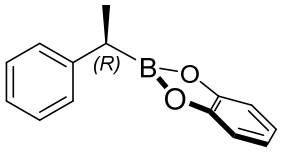
C	0.51141	-0.22361	-0.05283
C	-0.40336	-1.28090	0.00228
C	-1.77298	-1.04284	0.05402
C	-2.25278	0.26308	0.04357
C	-1.35304	1.32617	-0.02397
C	2.94931	0.33601	0.11889
C	0.01370	1.08599	-0.07507
C	1.95407	-0.52598	-0.08861
H	-0.03068	-2.30179	0.01101
H	-2.46494	-1.87764	0.10049
H	-3.32038	0.45368	0.08034
H	-1.72061	2.34723	-0.04492
H	3.98361	0.01534	0.07014
H	2.77303	1.38111	0.35388
H	0.70213	1.92203	-0.14930
H	2.19985	-1.56741	-0.29124

30



C	-2.48045	0.49081	-0.14870
C	-3.43367	-0.09977	-0.98635
C	-3.95921	-1.35370	-0.70654
C	-3.53733	-2.05116	0.42504
C	-2.59000	-1.47908	1.26434
C	-0.76562	2.34988	0.33646
B	0.47863	1.41434	0.19118
O	1.35101	1.06996	1.21496
C	2.29039	0.25131	0.63668
C	1.99057	0.10033	-0.71491
O	0.86162	0.82485	-1.00600
C	3.38260	-0.35980	1.21816
C	4.17754	-1.14602	0.37718
C	3.87585	-1.29977	-0.97620
C	2.76622	-0.67366	-1.55414
C	-2.06670	-0.21688	0.98074
C	-1.95536	1.86853	-0.50233
H	-3.76139	0.43855	-1.87278
H	-4.69615	-1.79128	-1.37292
H	-3.94407	-3.03275	0.64593
H	-2.25241	-2.01217	2.14772
H	-1.03922	2.45192	1.39159
H	-0.48340	3.35504	-0.00059
H	3.60409	-0.23028	2.27089
H	5.04748	-1.64589	0.78915
H	4.51483	-1.91899	-1.59641
H	2.52022	-0.78470	-2.60345
H	-1.33106	0.20892	1.65764
H	-1.66199	1.85820	-1.55867
H	-2.78003	2.58712	-0.42220

30



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C	-4.09675	-1.67647	0.29842
C	-3.11586	-1.40391	1.24888
C	-1.39423	2.60663	0.56502
B	0.27015	0.84896	-0.29736
O	0.96764	0.74556	0.90047
C	2.16854	0.16140	0.57666
C	2.19827	-0.08101	-0.79427
O	1.01817	0.34673	-1.35120
C	3.22733	-0.16065	1.40120
C	4.33859	-0.74777	0.78692
C	4.36826	-0.99144	-0.58650
C	3.28876	-0.65919	-1.41182
C	-2.16967	-0.41123	1.01376
C	-1.17751	1.43808	-0.41321
H	-3.20037	0.60893	-2.04812
H	-4.88170	-1.15609	-1.63680
H	-4.83497	-2.45059	0.48135
H	-3.08542	-1.96823	2.17576
H	-1.22447	2.28416	1.59588
H	-0.70476	3.42999	0.35721
H	-2.41731	2.98490	0.49113
H	3.19071	0.03617	2.46603
H	5.19592	-1.01857	1.39346
H	5.24786	-1.44852	-1.02657
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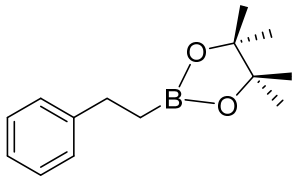
H	-1.40117	-0.20726	1.75618
H	-1.31305	1.79747	-1.43989

38



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C	5.76617	-0.18085	0.01436
C	5.22617	1.10298	0.08353
C	0.58178	-0.78834	-0.06192
B	-0.94498	-0.42769	-0.03743
O	-1.95036	-1.30682	-0.35601
C	-3.19591	-0.68333	0.02184
C	-2.82786	0.83566	-0.00879
O	-1.42046	0.81381	0.30849
C	-4.27766	-1.09839	-0.96152
C	-3.53194	-1.18153	1.42601
C	-3.55482	1.69208	1.01459
C	-2.95580	1.44708	-1.40256
C	3.84888	1.27876	0.07682
C	1.48425	0.44443	-0.00891
H	2.88109	-1.96038	-0.12563
H	5.32179	-2.27974	-0.11508
H	6.84200	-0.32357	0.01900
H	5.88133	1.96680	0.14222
H	0.78765	-1.38916	-0.95652
H	0.79386	-1.45171	0.78789
H	-5.21147	-0.56700	-0.75097
H	-4.46494	-2.17086	-0.86740
H	-3.97925	-0.89310	-1.99062
H	-3.56602	-2.27336	1.41192
H	-4.50080	-0.80532	1.76586
H	-2.76504	-0.87164	2.14207
H	-3.34249	1.36183	2.03238
H	-4.63602	1.65357	0.84761
H	-3.23003	2.73102	0.91789
H	-2.48362	2.43235	-1.39760
H	-4.00277	1.56181	-1.69652
H	-2.44824	0.82665	-2.14696
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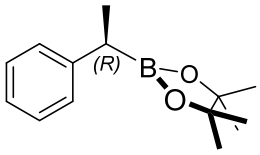
38



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C	4.06309	-1.37876	0.10828
C	3.99408	-0.43381	1.12759
C	1.07279	2.55594	-1.13158
B	-0.42865	0.85108	0.09388
O	-1.05945	0.44385	-1.05804
C	-2.05164	-0.52987	-0.66534
C	-2.34188	-0.12285	0.81603
O	-1.08144	0.44710	1.22869
C	-3.24411	-0.43064	-1.60149
C	-1.38836	-1.90097	-0.78015
C	-2.68596	-1.27897	1.74049
C	-3.38740	0.98424	0.93123
C	2.98967	0.53015	1.12115
C	0.94313	1.62311	0.08321
H	1.37139	-0.37832	-1.71204
H	3.16231	-2.08880	-1.71298

H	4.84620	-2.13033	0.11135
H	4.72436	-0.44561	1.93103
H	0.31375	3.34336	-1.10430
H	2.05881	3.02850	-1.15906
H	0.93462	1.99980	-2.06275
H	-4.04663	-1.09787	-1.27094
H	-2.94363	-0.72919	-2.60880
H	-3.62944	0.58902	-1.64775
H	-1.03029	-2.03267	-1.80448
H	-2.08968	-2.70742	-0.54898
H	-0.52807	-1.97487	-0.10738
H	-1.86961	-2.00081	1.79028
H	-3.59157	-1.78907	1.39673
H	-2.86837	-0.89790	2.74827
H	-3.38199	1.36659	1.95458
H	-4.39033	0.61438	0.70086
H	-3.15388	1.81107	0.25415
H	2.93979	1.26568	1.91973
H	1.02748	2.20840	1.00572

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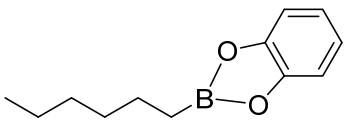
1-hexene

C	-0.76997	0.59441	0.21334
C	0.47041	-0.29626	0.08729
C	1.76582	0.50277	-0.03226
C	2.99582	-0.39069	-0.16338
C	-2.02992	-0.20060	0.39421
C	-3.06775	-0.18338	-0.43576
H	-0.63362	1.26552	1.07300
H	-0.86011	1.23203	-0.67447
H	0.35578	-0.94990	-0.78686
H	0.53207	-0.95962	0.96082
H	1.87021	1.15118	0.84698
H	1.69903	1.17115	-0.89990
H	3.91435	0.19696	-0.23894
H	2.92667	-1.02158	-1.05503
H	3.09098	-1.05237	0.70334
H	-2.06214	-0.84604	1.27289
H	-3.95023	-0.78935	-0.25924
H	-3.06950	0.44444	-1.32319

32



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C	6.71317	0.98460	-0.16412
C	1.75303	-0.14678	-0.00710
C	0.69718	-1.24379	0.16652
B	-0.77318	-0.72546	0.09311
O	-1.89679	-1.53034	-0.04911
C	-2.96781	-0.67201	-0.05606
C	-2.50378	0.63436	0.07709
O	-1.13428	0.61404	0.17009
C	-3.35953	1.71700	0.10153
C	-4.72470	1.43504	-0.01565
C	-5.18965	0.12645	-0.15012
C	-4.31208	-0.96270	-0.17319
H	3.31946	-1.15400	1.07757
H	3.33550	-1.46022	-0.65188
H	4.10001	0.89426	-1.06223
H	4.08467	1.20090	0.66710
H	5.80396	-0.59145	0.99943
H	5.81868	-0.89811	-0.72870
H	6.59661	1.76586	0.59351
H	7.72972	0.59060	-0.08627
H	6.61008	1.45792	-1.14561
H	1.61801	0.34251	-0.98011
H	1.59386	0.63613	0.74463
H	0.83611	-2.03351	-0.58258
H	0.83734	-1.74300	1.13597
H	-2.98310	2.72763	0.20610
H	-5.43604	2.25367	-0.00125
H	-6.25570	-0.05265	-0.23895
H	-4.65949	-1.98379	-0.27664

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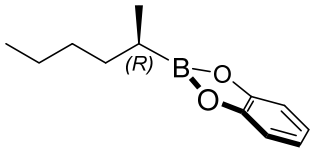

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C	4.26680	-2.41540	-0.64976
C	1.31090	1.71034	-0.13310
C	1.13194	3.03021	0.64116
B	-0.04523	0.92795	-0.11070
O	-0.31142	-0.17945	0.68695
C	-1.62321	-0.50529	0.44320
C	-2.14673	0.39132	-0.48532
O	-1.17212	1.29109	-0.83826
C	-3.45128	0.30885	-0.92824
C	-4.22650	-0.72594	-0.39497
C	-3.70216	-1.62458	0.53488
C	-2.37783	-1.53073	0.97602
H	3.36994	1.51833	0.48920

H	2.23716	0.58684	1.46106
H	1.90818	-1.01039	-0.42958
H	3.01232	-0.06957	-1.42784
H	4.86059	-0.51858	0.19546
H	3.75585	-1.43624	1.20558
H	4.50707	-2.15981	-1.68659
H	5.11111	-2.97414	-0.23766
H	3.39851	-3.08147	-0.66599
H	1.53225	1.96416	-1.17957
H	0.91038	2.83459	1.69579
H	2.04785	3.62812	0.60227
H	0.31538	3.63048	0.23077
H	-3.84424	1.01344	-1.65153
H	-5.25794	-0.83118	-0.71341
H	-4.33432	-2.41462	0.92543
H	-1.95786	-2.22235	1.69667

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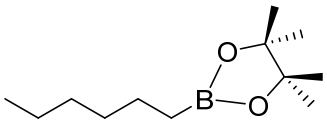

C	3.12918	-0.73799	-0.12256
C	4.23388	0.29874	0.06525
C	5.63931	-0.29097	-0.02896
C	6.73141	0.75831	0.16126
C	1.72537	-0.14537	-0.03196
C	0.61712	-1.18503	-0.21728
B	-0.83503	-0.60120	-0.11911
O	-1.10542	0.70551	0.20916
C	-2.51193	0.92322	-0.02493
C	-3.09158	-0.52419	0.08250
O	-1.97665	-1.33176	-0.34758
C	-3.04201	1.90371	1.00864
C	-2.64115	1.50812	-1.43015
C	-4.28381	-0.80451	-0.81760
C	-3.40444	-0.92888	1.52184
H	3.25357	-1.23006	-1.09738
H	3.23968	-1.52822	0.63314
H	4.11060	0.78833	1.04123
H	4.12143	1.09006	-0.68877
H	5.76034	-0.77864	-1.00445
H	5.74989	-1.08110	0.72433
H	7.73019	0.32009	0.08828
H	6.64462	1.23679	1.14189
H	6.65250	1.54333	-0.59746
H	1.60061	0.35173	0.93836
H	1.61429	0.64597	-0.78412
H	0.72580	-1.68933	-1.18724
H	0.72325	-1.98588	0.52761
H	-2.57859	2.88153	0.85597
H	-4.12622	2.01805	0.90798
H	-2.81450	1.57329	2.02320
H	-3.67821	1.76258	-1.66587
H	-2.03523	2.41528	-1.48926
H	-2.27429	0.80071	-2.17959
H	-4.61610	-1.83550	-0.67311
H	-5.11642	-0.13773	-0.57091
H	-4.02611	-0.67310	-1.86951
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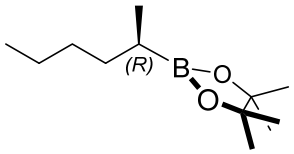

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C	2.67799	-0.07871	-0.25401
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C	4.39607	-1.92061	0.07119
C	0.93779	1.79259	-0.58074
C	0.58781	3.22564	-0.16526
B	-0.27383	0.81745	-0.34870
O	-0.54534	-0.29142	-1.11402
C	-1.53082	-1.06861	-0.40172
C	-2.22481	0.01488	0.48662
O	-1.15856	0.96428	0.69347
C	-2.44251	-1.75471	-1.40550
C	-0.76876	-2.10365	0.42371
C	-2.71700	-0.48110	1.83641
C	-3.34033	0.75314	-0.25019
H	1.90301	1.23262	1.27656
H	2.97122	2.02091	0.12663
H	2.92831	-0.02623	-1.32254
H	1.88062	-0.82933	-0.17397
H	3.64917	-0.58966	1.59873
H	4.70309	0.18729	0.43027
H	5.27070	-2.24505	0.64104
H	4.67364	-1.89917	-0.98735
H	3.61547	-2.67856	0.19223
H	1.20028	1.77245	-1.64739
H	0.30476	3.25747	0.89148
H	1.43888	3.89956	-0.30952
H	-0.25541	3.62030	-0.74006
H	-1.87095	-2.49327	-1.97320
H	-3.25859	-2.27315	-0.89188
H	-2.86732	-1.03743	-2.10925
H	-1.44992	-2.78236	0.94459

H	-0.13422	-2.69021	-0.24562
H	-0.12806	-1.61336	1.16358
H	-3.17832	0.34562	2.38227
H	-3.46756	-1.26745	1.70653
H	-1.89621	-0.87222	2.43946
H	-4.21764	0.11589	-0.39182
H	-3.63231	1.62600	0.33837
H	-2.99573	1.09903	-1.22916

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cyclooctene

C	-1.30996	0.83302	0.73653
C	-1.83873	-0.36069	-0.08079
C	-0.76392	-1.16785	-0.80846
C	0.34373	-1.75942	0.07003
C	1.33154	-0.77307	0.72000
C	1.79969	0.36644	-0.18845
C	0.86904	1.52922	-0.43239
C	-0.39269	1.74237	-0.04788
H	-2.16740	1.41739	1.08510
H	-0.81995	0.46402	1.63922
H	-2.55527	0.00840	-0.82427
H	-2.40060	-1.02017	0.59294
H	-0.31358	-0.54285	-1.58831
H	-1.25788	-1.99468	-1.33215
H	0.92795	-2.43994	-0.56206
H	-0.10532	-2.38482	0.85262
H	2.21645	-1.34734	1.01720
H	0.93473	-0.35628	1.64800
H	2.08873	-0.04863	-1.16644
H	2.72852	0.78229	0.22398
H	1.32975	2.32164	-1.02322
H	-0.83832	2.68084	-0.37411

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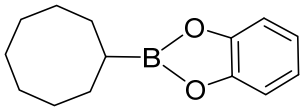

C	3.05760	-1.44655	-0.91184
C	3.98231	-1.41752	0.30655
C	4.05566	-0.10486	1.10477
C	4.11738	1.17952	0.25597
C	1.55639	-1.33389	-0.64722
C	1.05905	-0.00471	-0.03467
B	-0.50611	0.00185	-0.01807
O	-1.30864	1.12777	-0.16070
C	-2.60168	0.68027	-0.04725
C	-2.58764	-0.69763	0.15482
O	-1.28674	-1.13373	0.17033
C	-3.74946	-1.42740	0.30508
C	-4.94858	-0.70955	0.24418
C	-4.96244	0.67075	0.04115
C	-3.77793	1.39939	-0.11050
C	2.79133	1.93479	0.09540
C	1.65311	1.26676	-0.68673
H	3.36365	-0.66561	-1.61810
H	3.22962	-2.39394	-1.43649
H	4.99377	-1.64616	-0.05245
H	3.71056	-2.23563	0.98584
H	4.95179	-0.16095	1.73234
H	3.21869	-0.03265	1.80761
H	4.81968	1.87600	0.72704
H	4.54333	0.95729	-0.73133
H	1.23453	-2.16080	-0.00220
H	1.04238	-1.48847	-1.60545
H	1.33838	0.00204	1.02959
H	-3.72321	-2.49912	0.46230
H	-5.88815	-1.23930	0.35784
H	-5.91231	1.19270	-0.00065
H	-3.77352	2.47127	-0.26877
H	2.41477	2.17732	1.09940
H	3.00769	2.89692	-0.38435
H	1.98677	1.03291	-1.70609
H	0.86460	2.01837	-0.80114

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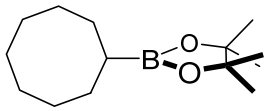

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B	0.55395	-0.00883	0.12480
O	1.34841	-0.48525	1.13859
C	2.69812	-0.54263	0.63109
C	2.66433	0.51606	-0.51788
O	1.28768	0.45871	-0.94189
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C	3.66708	-0.23232	1.75986
C	2.91420	1.93768	-0.01783
C	3.56539	0.20279	-1.70087
C	-2.70992	-1.83332	-0.62394
C	-1.52735	-0.93078	-0.99920
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H	-3.81447	1.73024	1.64327

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H	3.61558	-1.02305	2.51240
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H	3.42372	0.71524	2.24279
H	3.95892	2.08605	0.26959
H	2.66859	2.63895	-0.81888
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H	-1.77123	-0.33160	-1.88564
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α-pinene

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C	-0.32311	0.59818	-1.58270
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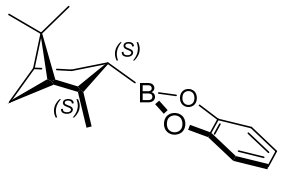

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B	-0.82022	-0.45213	0.15430
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H	1.12409	1.97264	-0.65668
H	2.80261	2.46834	-0.98699
H	2.48857	-1.38432	2.31279
H	2.23828	0.10117	3.24104
H	0.88226	-0.99233	2.93676
H	4.76926	1.72136	-0.92751
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H	5.54036	0.59737	0.19563
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H	4.45958	-1.54463	0.85764
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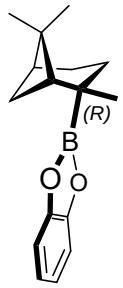

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H	0.63219	-0.25273	3.03445
H	3.20921	1.96558	-2.02283
H	4.79129	1.36255	-1.51732
H	3.92496	2.53367	-0.51205
H	3.75206	-0.64876	1.41306
H	4.20479	1.06001	1.45220
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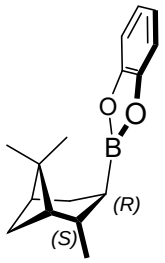

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C	-1.97562	-1.77676	-1.05996
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C	2.60392	-0.72266	0.23495
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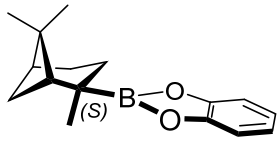

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O	1.21086	-1.22012	-0.56685
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C	3.37714	1.17600	0.94261
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H	-1.00793	-2.23896	-1.21490
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H	-4.14638	0.62204	1.25502
H	-2.12731	-2.16092	2.13363
H	-0.60964	-1.41707	2.66859
H	-0.57889	-2.83920	1.60781
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H	-1.27666	1.97646	-2.15733
H	3.68953	-1.60083	-1.83530
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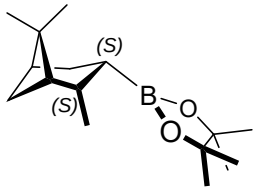

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C	-4.91629	-0.42160	0.54260
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C	2.91229	0.69337	0.18821
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O	1.52559	-1.16353	-0.12503
C	2.77397	1.02661	1.67239
C	4.06545	1.46799	-0.42703
C	3.50999	-1.19371	-1.45263
C	3.59696	-1.67852	1.00139
H	-0.78852	0.61284	-1.69053
H	-1.65873	-1.47694	-1.90021
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H	-2.92220	-1.31542	2.23231
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H	-2.83298	0.62771	-2.00674
H	-4.28960	1.40054	-1.37090
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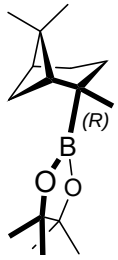

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C	-0.98365	-0.73459	-2.24142
C	-3.81877	1.89339	0.14790
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C	2.60771	0.85395	-0.28503
O	1.39072	0.67112	-1.03675
C	3.46460	-1.56685	-0.44594
C	3.40584	-0.46881	1.80378
C	2.35003	1.99856	0.69312
C	3.73568	1.21171	-1.23859
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H	-0.54676	0.12453	-2.75993
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H	-3.91395	2.37605	-0.83091
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H	-4.10767	0.15448	-1.90603
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H	3.01794	-1.59965	-1.44417
H	3.47440	-1.47692	2.21988
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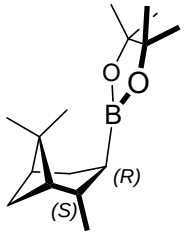

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C	1.33675	-1.05234	-0.66178
C	3.43192	-1.09327	0.73976
C	1.10468	-2.49611	-1.10229
C	4.46343	1.26136	-0.57868
C	2.05554	1.83779	-0.73332
B	-0.79680	-0.37890	0.49066
O	-1.23477	0.92486	0.54555
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C	-3.01714	-0.49978	0.03099
O	-1.78088	-1.24289	0.07151
C	-2.22630	1.34184	-1.58105
C	-3.38408	2.02429	0.53258
C	-3.72486	-0.73843	1.36304
C	-3.86518	-1.01290	-1.12089
H	0.68092	-1.78846	1.23864
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H	1.42298	-0.18682	2.68815
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H	0.03980	-2.74487	-1.06831
H	1.46849	-2.66023	-2.12141
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H	1.01514	1.60703	-0.49168
H	2.13318	1.94642	-1.82177
H	2.28638	2.81279	-0.28889
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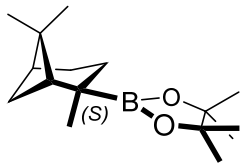

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B	-0.46823	-0.45692	-0.10641
O	-1.33799	-0.90032	0.86101
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H	-2.25522	0.55820	2.78762
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β-pinene

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C	-2.46780	-0.64902	-0.28202
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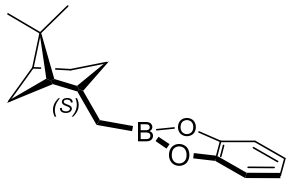

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C	2.55069	0.10953	-1.85111
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H	3.09778	-1.78216	1.43841
H	4.65959	-0.22138	0.85167
H	4.87789	-1.01027	-0.69942
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H	1.28680	-2.03901	-0.82300
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H	0.58030	-2.57383	1.38840
H	0.95779	-0.97280	2.01301
H	2.54920	3.33211	-0.18487
H	1.78263	2.61124	-1.60573
H	0.85495	2.81855	-0.11597
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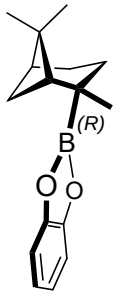

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H	-3.20916	-1.96495	-2.02346
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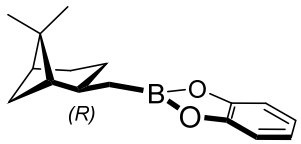

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C	3.52013	1.43796	-0.80435
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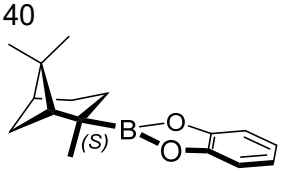

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O	1.21085	-1.22011	-0.56686
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C	4.70206	-0.03612	-0.70564
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H	-1.00793	-2.23896	-1.21490
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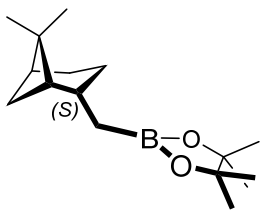

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C	-3.35371	1.52093	1.44997
C	-3.65719	1.68404	-1.02957
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H	3.46781	2.63317	-0.14322
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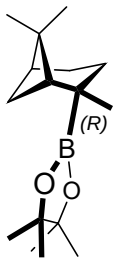

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O	1.39072	0.67113	-1.03674
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C	3.73568	1.21171	-1.23858
C	2.35003	1.99856	0.69313
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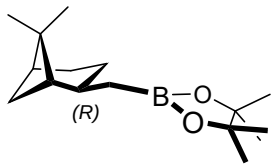

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C	-1.26566	0.15683	-0.68381
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O	1.66193	0.62234	-0.69112
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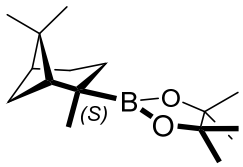

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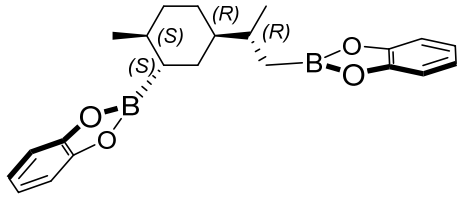

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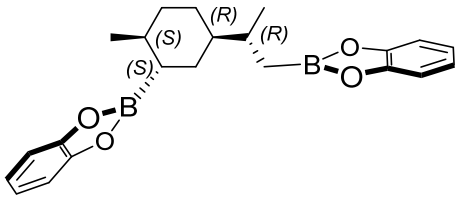

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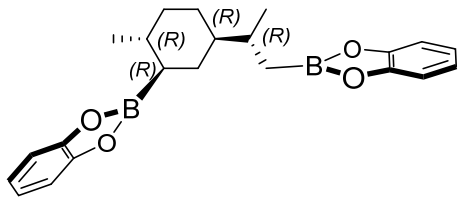

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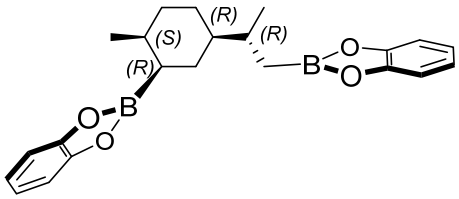

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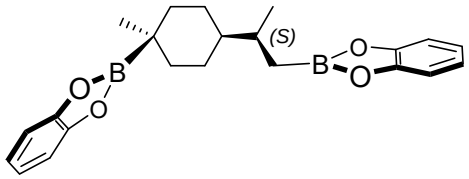

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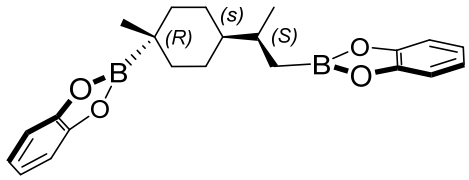

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C	4.40634	-1.13224	0.37957
O	4.39960	0.22829	0.19283
C	3.35745	-3.08686	-0.60260
C	4.06108	-3.85370	0.33190
C	4.91515	-3.26335	1.26398
C	5.10707	-1.87825	1.30564
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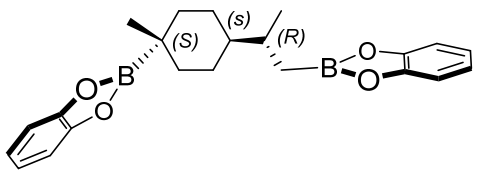

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C	-3.05868	-1.50176	-2.53173
C	-4.31453	-1.73243	-0.38520
B	1.62073	-0.63813	0.09309
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C	3.51072	0.47002	-0.10692
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C	6.06947	-0.40092	-0.57658
C	5.80136	0.95905	-0.41778
C	4.50442	1.42518	-0.17792
B	-2.56278	0.07879	-0.64682
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C	-0.98172	4.28108	-0.26105
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H	0.25484	-2.81784	-0.77643
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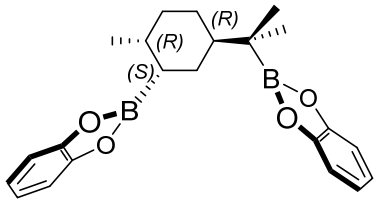

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C	0.76452	-2.89776	1.96416
C	-2.98131	-1.17784	-1.02251
C	-3.08156	-1.17612	-2.56209
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B	1.59333	-0.65929	0.12044
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O	2.40579	-0.06745	1.08163
C	3.56283	-0.38953	-0.82239
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C	4.64987	-0.35894	-1.67221
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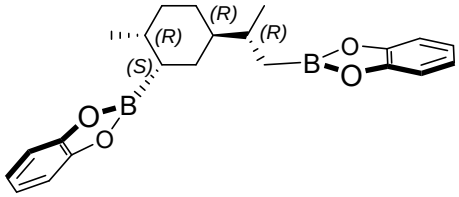

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C	1.57964	3.57607	-0.51113
C	3.60939	-0.91748	0.24689
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H	3.21587	-2.52554	-1.17581
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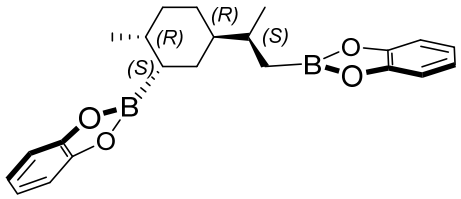

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O	0.87441	-1.83768	1.01204
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H	2.14635	4.49366	-0.35392
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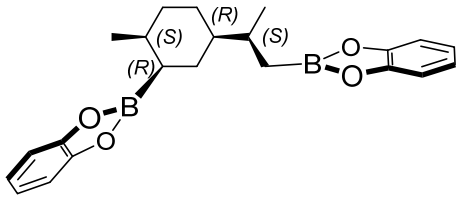

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C	3.67123	0.10566	-0.40750
C	4.19772	-0.46508	0.92401
C	4.59481	0.61462	1.92849
C	0.89897	-1.51951	-0.76448
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C	0.37357	-1.20432	-2.17015
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O	1.77946	1.58770	-1.39525
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C	0.71221	2.20697	0.48733
C	-0.29386	2.94150	-1.59309
C	-1.28102	3.56163	-0.81986
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O	-2.70140	-2.57295	0.08755
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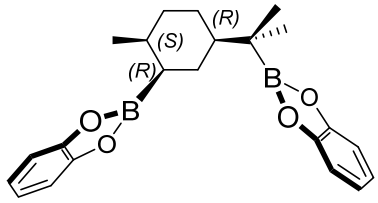

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C	-2.12529	-2.19780	-0.81572
C	-1.62550	-2.39085	-2.25722
C	-3.13446	-3.31237	-0.49655
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O	2.90339	-0.11163	-0.83712
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C	4.19550	0.34896	-0.78228
C	5.96476	0.54987	0.86511
C	6.75113	1.11479	-0.14454
C	6.26208	1.28701	-1.43975
C	4.96241	0.90306	-1.78716
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H	-5.72996	3.62380	0.95237
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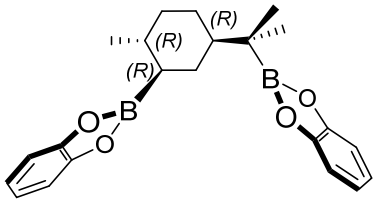

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C	1.13566	-0.17692	3.31645
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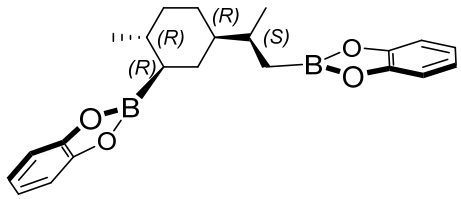

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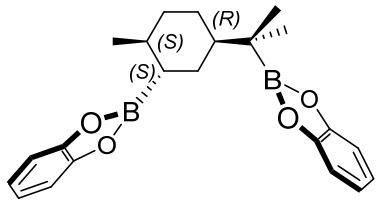

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H	2.89087	-2.03939	1.43468
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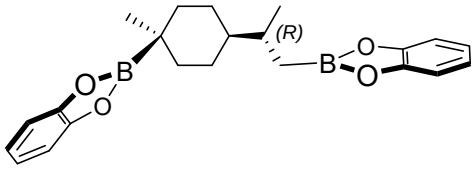

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O	4.51157	-1.28362	0.47351
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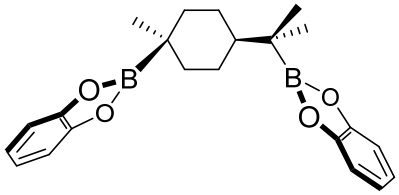

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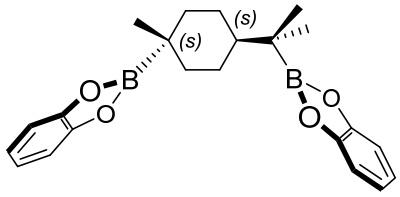

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B	3.07852	0.50126	0.18685	H	-0.02172	3.38855	-0.11622
O	3.89576	0.36847	-0.92970	H	1.51116	1.29697	-1.73068
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O	-3.68618	-0.01799	1.08237	H	-3.96054	3.13285	-0.85214
C	-4.39676	-1.10853	0.64349	H	-2.92121	2.46989	-2.12160
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O	-3.63549	-0.06987	-1.20330	H	7.17363	-2.81949	-1.49880
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H	1.21385	0.46401	2.03510	H	-4.96831	-2.14019	-2.55546
H	-0.97921	-0.01445	1.05821				

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