

Supporting Information

Dehydropolymerisation of methylamine borane using highly active rhodium(III) bis(thiophosphinite) pincer complexes: catalytic and mechanistic insights

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Experimental section

Preparation of $[(^{\text{Ph}}\text{PSCSP}^{\text{Ph}})\text{Rh}(\text{H})(\text{Cl})]$ (3b**):** Synthesis of complex **3b** was attempted in NMR scale by a procedure similar to that used for **3a**. To a suspension of 5 mg **3a** (0.008 mmol) in 0.5 mL C_6D_6 was added one drop of $\text{BF}_3\cdot\text{OEt}_2$ (48% in OEt_2). As both, precursor **2b** and the product **3b** are poorly soluble, we could only assign characteristic high-field ^1H and ^{31}P resonances (Figures S15 and S16).

Synthesis of deuterated amine boranes

Commercially available $\text{BH}_3\cdot\text{THF}$, which is a commonly used precursor for the synthesis of deuterated amine boranes was found to reproducibly contain large amounts of esters (Figure S1). We have thus followed a different route to prepare deuterated borane for the synthesis of deuterated amine boranes.

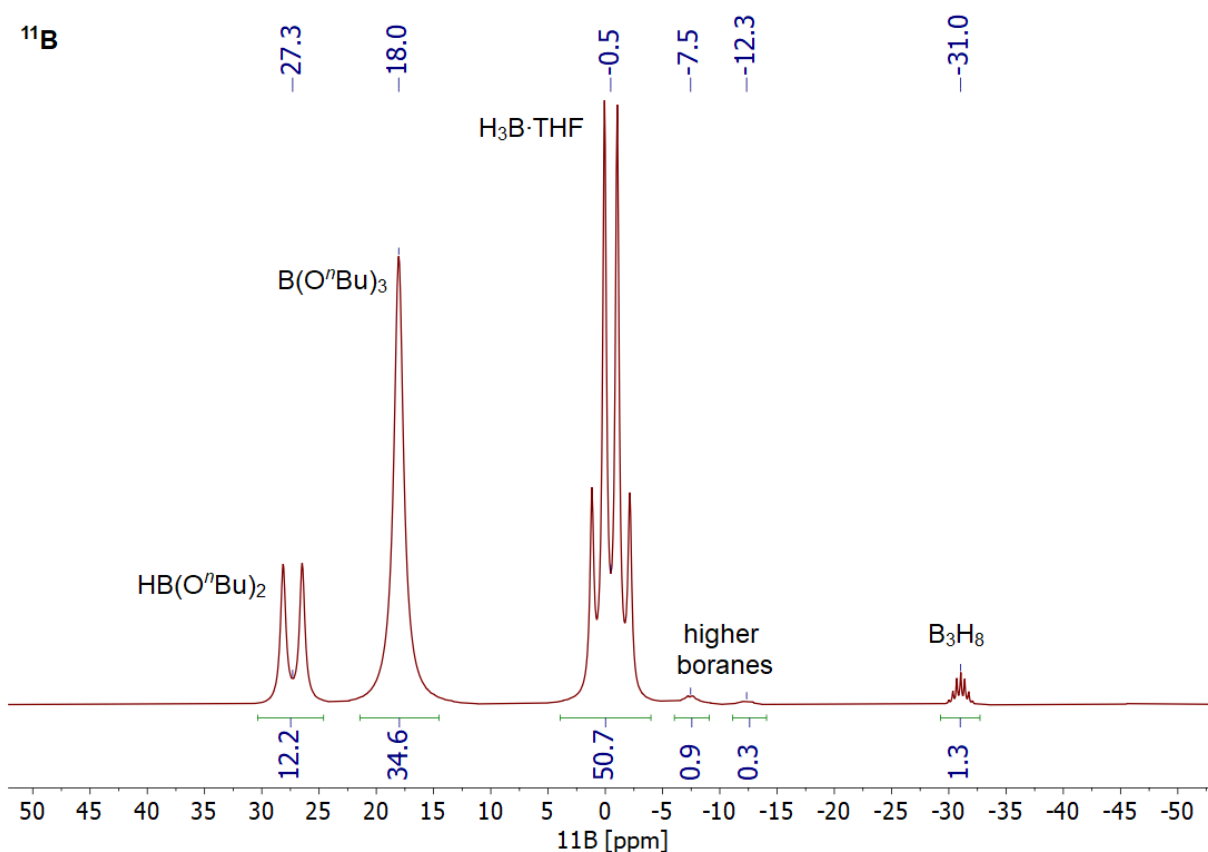
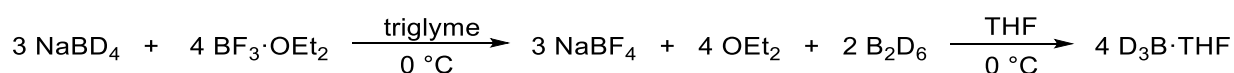


Figure S1. ^{11}B NMR spectrum ($\text{THF}-d_8$, 96 MHz, 297 K) of a freshly opened batch of commercial $\text{H}_3\text{B}\cdot\text{THF}$.

Preparation of $\text{D}_3\text{B}\cdot\text{NMeH}_2$:¹ *Method A:* $[\text{Rh}(\text{dppp})(\text{nbd})][\text{BF}_4]$ (65 mg, 94.15 μmol) and $\text{BH}_3\cdot\text{NMe}_3$ (420 mg, 5.76 mmol) were dissolved in THF (10 mL) in a J. Young flask. The solution was freeze-pump-thaw degassed three times and filled with D_2 while immersed in liquid N_2 (1.0 atm at 77 K). The solution was thawed and stirred for 50 minutes. Then the flask was freeze-pump-thaw degassed three times, refilled with D_2 and stirred for 50 minutes twice more, giving a dark brown solution. At this point, new Rh catalyst (30 mg, 43.25 μmol) was added to the reaction mixture, the flask was freeze-pump-thaw degassed three times, refilled

with D₂ and stirred for 50 minutes three more times. The solution was degassed, refilled with Argon and cannula-transferred to a Schlenk flask. The solvent was removed in an ice bath with the Schlenk flask opened under a constant Argon flow, yielding a brown solid. (Note: Exposure to vacuum will result in loss of D₃B·NMe₃ due to sublimation). White crystals of the product were isolated on a cold finger apparatus at -78 °C following sublimation under static reduced pressure at room temperature. The white solid was then transferred to a Schlenk flask, NMeH₂ (2.0 M in THF, 8.5 mL, 17.0 mmol) was added and the resulting solution was stirred for 72 h at room temperature. The solvent was again removed in an ice bath with the Schlenk flask opened under a constant Argon flow, giving a pale yellow/white solid, which was then recrystallized from a saturated Et₂O solution (5 mL) at -20 °C. The white crystals were isolated by filtration, washed with cold Et₂O and dried under an Argon flow to yield 118 mg (43%) of D₃B·NMeH₂. ¹¹B NMR (THF-*d*₈, 96 MHz): δ -18.6 (s). ¹H{¹H} NMR (THF-*d*₈, 96 MHz): δ -18.6 (s).

Method B: Preparation of D₃B·THF (≈ 1 M):²



An oven-dried three-necked flask (50 mL) was connected to a dropping funnel and a cooling trap. NaBD₄ powder (1 g, 23.89 mmol) was placed in the three-necked flask, dissolved in anhydrous triglyme (10 mL) and the mixture was cooled to 0 °C. BF₃·OEt₂ (4.02 mL, 32.01 mmol, 1.34 eq) was added to the dropping funnel. BF₃·OEt₂ was added dropwise over a period of 15 min into the flask containing NaBD₄ in triglyme. The generated diborane was passed through a cooling trap (-78 °C) with an Argon flow and bubbled slowly into a Schlenk flask containing 24 mL anhydrous THF at 0 °C for 90 minutes. The borane content was determined by hydride analysis: 1.01 M. Uncomplexed diborane was destroyed in a solution of alcohol/water. It should be noted that full conversion was not achieved by using NaBD₄ obtained from Deutero and the molarity of the D₃B·THF was only 0.6 - 0.7 M.

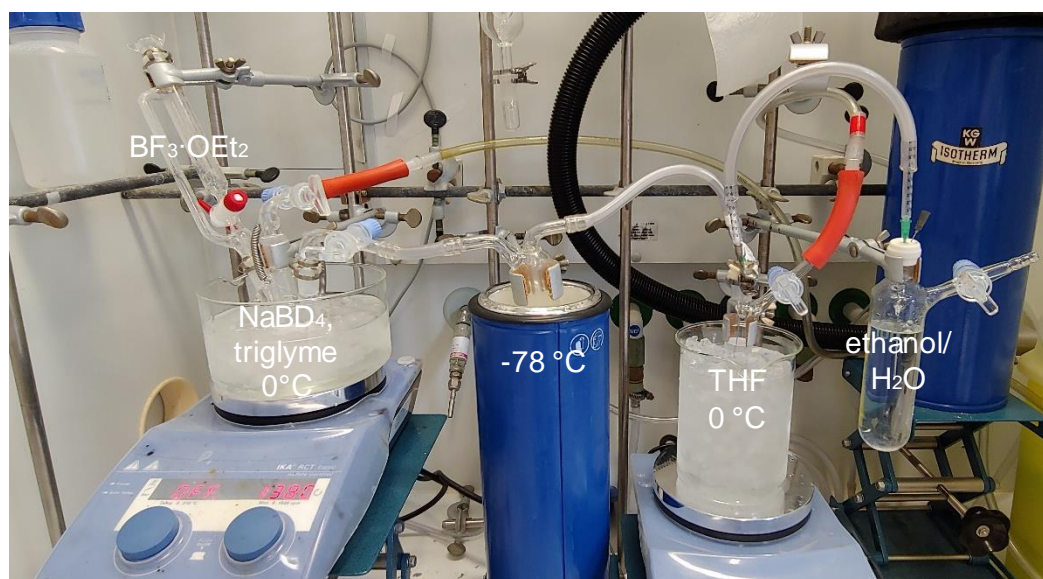
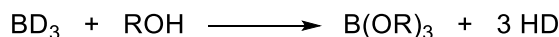


Figure S2. Setup for the generation of D₃B·THF.

Notes: Generation of diborane only occurred after 50% of BF₃·OEt₂ was added. Diborane reacts immediately with NaBD₄ to form NaBD₄·BD₃ as an intermediate. Complexation of diborane to THF is an exothermic process. The borane complexed to THF can interact with the solvent and ring-open the THF to produce dibutoxyborane or tributoxyborane. This ring

opening is minimal below 5 °C and the borane-THF solution must be stored at low temperature.³ The remaining triglyme solution, containing NaBF₄ and unreacted BF₃·OEt₂ can be neutralised by addition to an aqueous solution of NaHCO₃ salt.

Determination of the borane content:⁴ The borane content of the THF solution was determined by quantitative reaction of the borane with a mixture of *i*PrOH/ distilled water (1:1). Measurement of the volume of the hydrogen gas in an automatic gas buret is an accurate method for the determination of the borane concentration.



A reaction vessel was equipped with a magnetic stirrer, capped with a septum and attached to the gas burette. *i*PrOH (10 mL) and H₂O (10 mL) was added, data acquisition was started, and the solution was stirred for 15 minutes for the adjustment of the equilibrium between liquid and gas phase (vapour pressure). An aliquot of 0.5 mL of D₃B·THF was added via syringe to the reaction vessel. Immediately vigorously gas evolution occurred. To determine the amount of hydrogen the overall volume was corrected by the vapour pressure of THF ($p(\text{THF}) = 216$ mbar; $T = 25^\circ\text{C}$).⁵

$$n_{\text{Hydrogen}} = \frac{p^*V}{RT} \quad p^* = p(\text{atmosphere}) - p(\text{solvent})$$

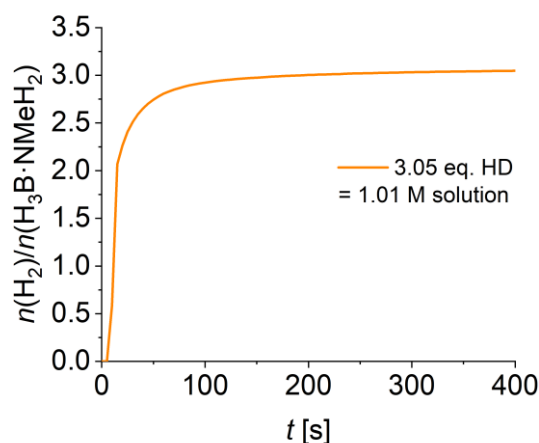


Figure S3. Hydrogen evolution from hydrolysis of borane THF adduct.

Synthesis of *B*-deuterated methylamine borane adduct D₃B·NMeH₂:

According to the synthesis protocol for non-deuterated amine boranes⁶ 1 eq. of D₃B·THF (1 M) and 2 eq. of NMeH₂ (2 M THF,) were transferred into a Schlenk flask at -78°C. The solution was warmed to room temperature and stirred overnight. The solvent was removed in vacuum at 0°C and the residue was washed with hexane. The resulting D₃B·NMeH₂ was dried in vacuum for 1 to 2 hours. The yields varied from 67 to 90 %. Isotopic purity: 87% (by ¹H NMR). If necessary, D₃B·NMeH₂ was sublimed prior to use.

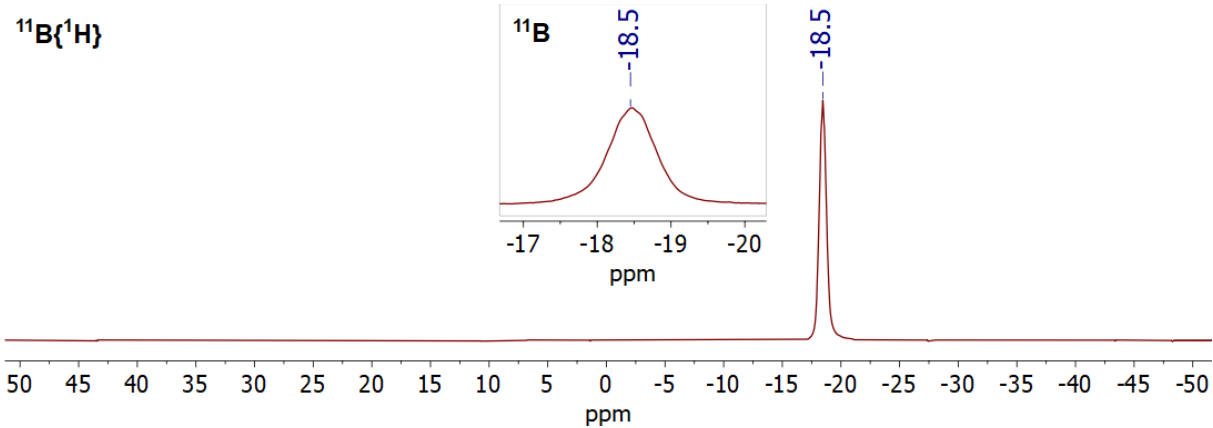


Figure S4. ^{11}B and $^{11}\text{B}\{^1\text{H}\}$ NMR spectra (CDCl_3 , 96 MHz) of $\text{D}_3\text{B}\cdot\text{NMeH}_2$.

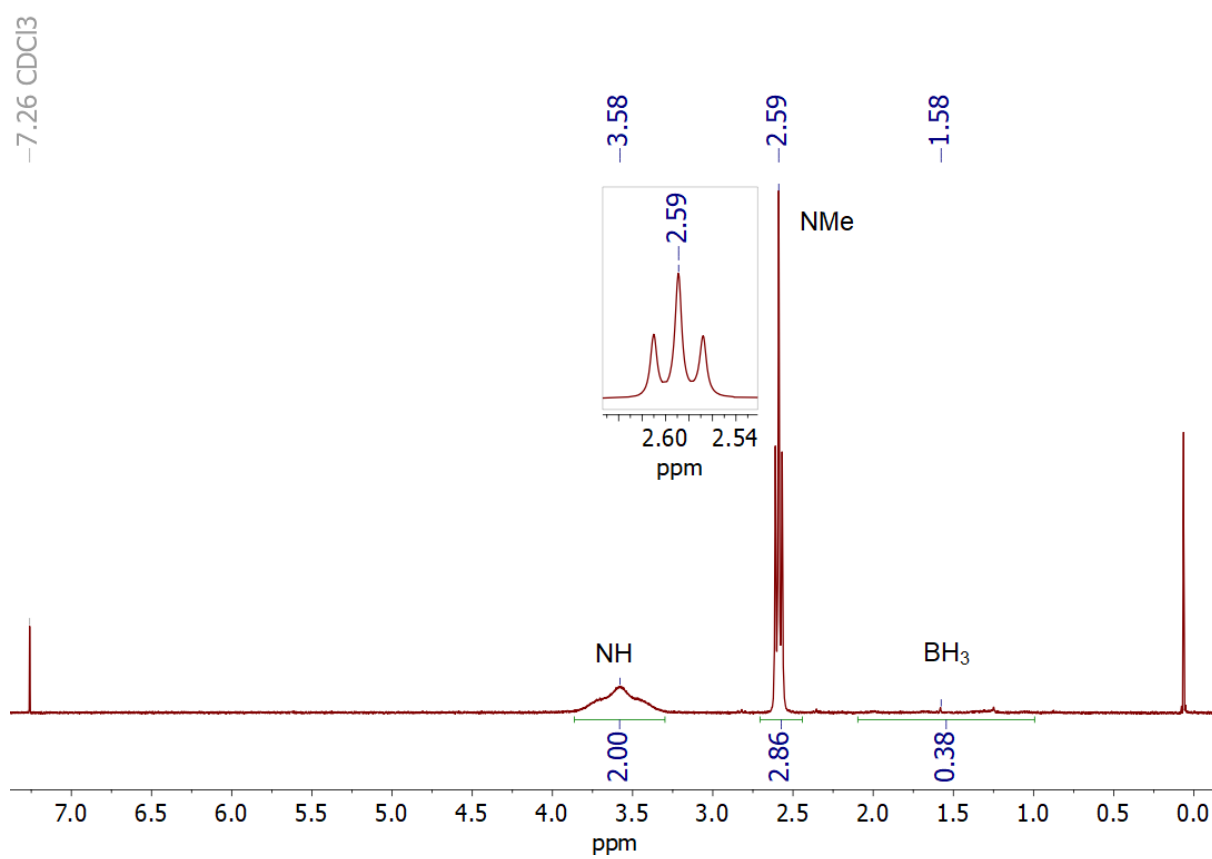


Figure S5. ^1H NMR spectrum (CDCl_3 , 300 MHz) of $\text{D}_3\text{B}\cdot\text{NMeH}_2$.

Crystallographic details

Diffraction data were collected on a Bruker Kappa APEX II Duo diffractometer using Mo-K α radiation. The structures were solved by direct methods (SHELXS-97⁷) and refined by full-matrix least-squares procedures on F^2 (SHELXL-2014⁸). XP (Bruker AXS) was used for graphical representations. CCDC 1978167 (**2a**), CCDC 1979143 (**3a**) and CCDC 2047590 (**2b**) contain the supplementary crystallographic data for this paper. These data are provided free of charge by the Cambridge Crystallographic Data Centre.

Table S1. Crystallographic details.

	2a	2b	3a
Chemical formula	C ₂₃ H ₃₇ CINP ₂ RhS ₂	C ₃₅ H ₂₉ CINP ₂ RhS ₂	C ₁₈ H ₃₂ CIP ₂ RhS ₂
Formula weight [g/mol]	591.96	729.01	512.88
Colour	brown/dark yellow	yellow	yellow
Crystal system	monoclinic	monoclinic	monoclinic
Space group	<i>P2₁/c</i>	<i>P2₁/n</i>	<i>P2₁/c</i>
a [Å]	18.4250(7)	9.2984(2)	11.1268(4)
b [Å]	8.8088(4)	15.2480(3)	11.9807(5)
c [Å]	17.9270(7)	22.7278(4)	17.1003(7)
α [deg]	90	90	90
β [deg]	113.4200(10)	100.4790(10)	92.1410(10)
γ [deg]	90	90	90
Cell volume [Å ³]	2669.89(19)	3168.65(11)	2278.00(16)
Formula units Z	4	4	4
Temperature [K]	150(2)	150(2)	150(2)
Reflections collected	73849	46248	58736
Independent reflections	5818	8196	6390
Observed reflections ($I > 2\sigma(I)$)	5250	7640	5657
Parameters	283	383	243
GOF (F^2)	1.053	1.075	1.025
R_1 ($I > 2\sigma(I)$)	0.0192	0.0210	0.0245
wR_2 (all data)	0.0505	0.0537	0.0619

NMR spectra

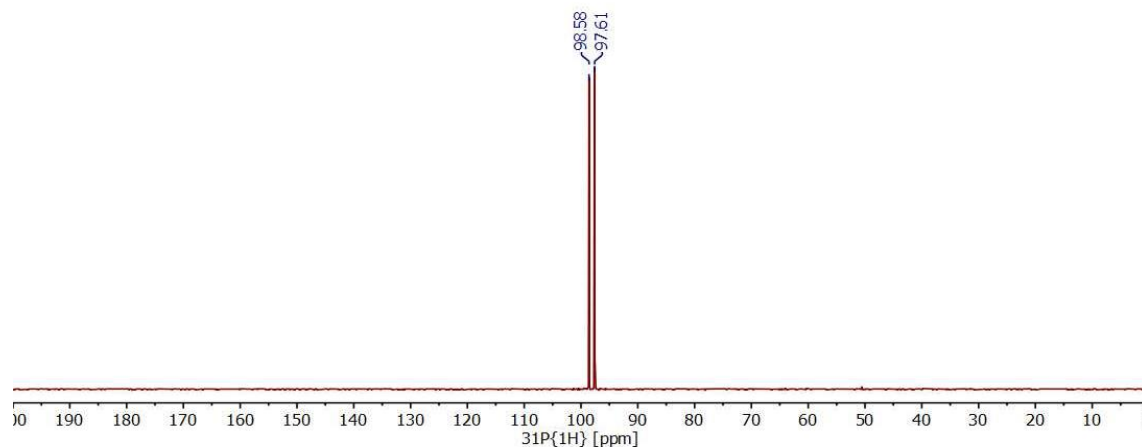


Figure S6. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (toluene- d_8 , 122 MHz, 297 K) of complex **2a**.

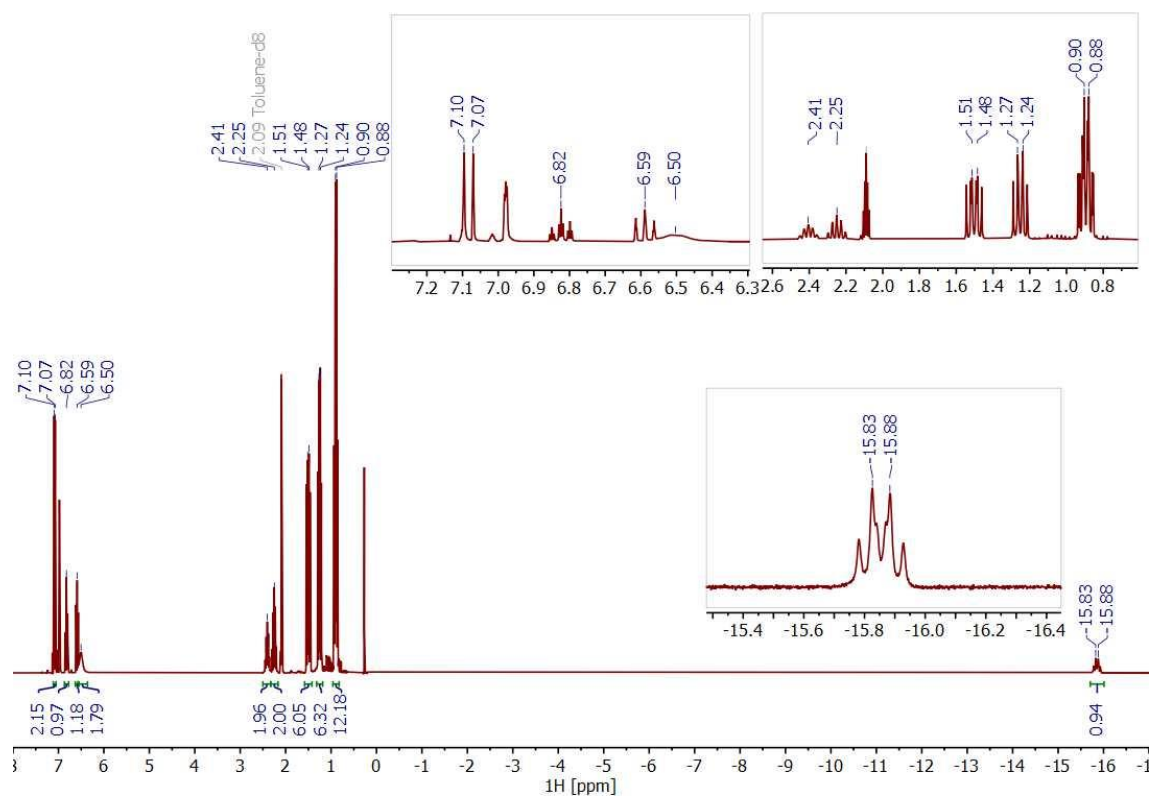


Figure S7. ^1H NMR spectrum (toluene- d_8 , 300 MHz, 297 K) of complex **2a**.

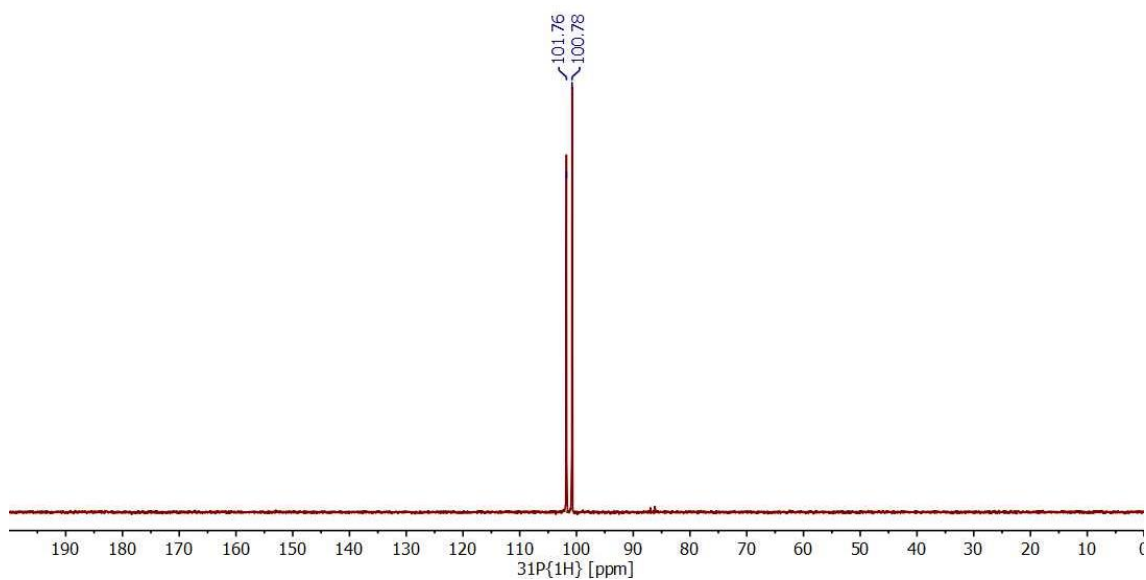


Figure S8. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 122 MHz, 297 K) of complex **3a**.

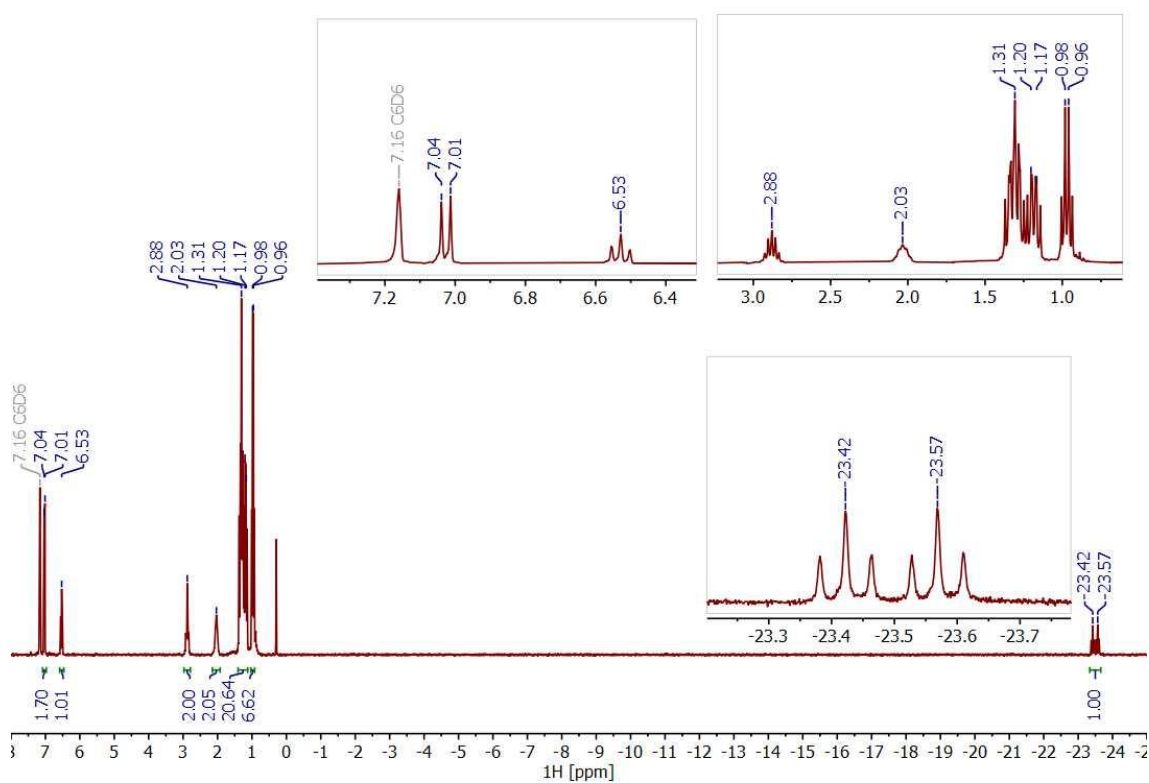


Figure S9. ^1H NMR spectrum (C_6D_6 , 300 MHz, 297 K) of complex **3a**.

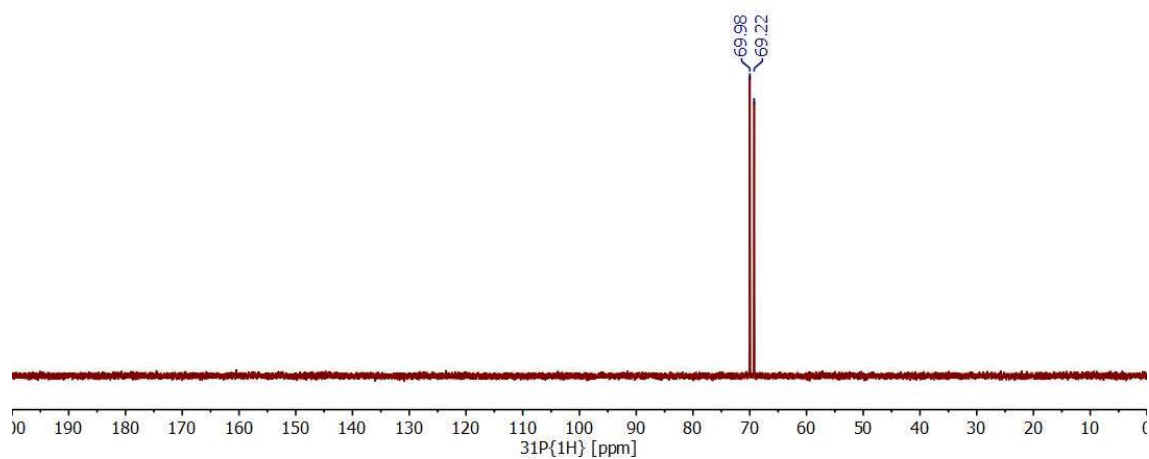


Figure S10. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 162 MHz, 297 K) of complex **2b**.

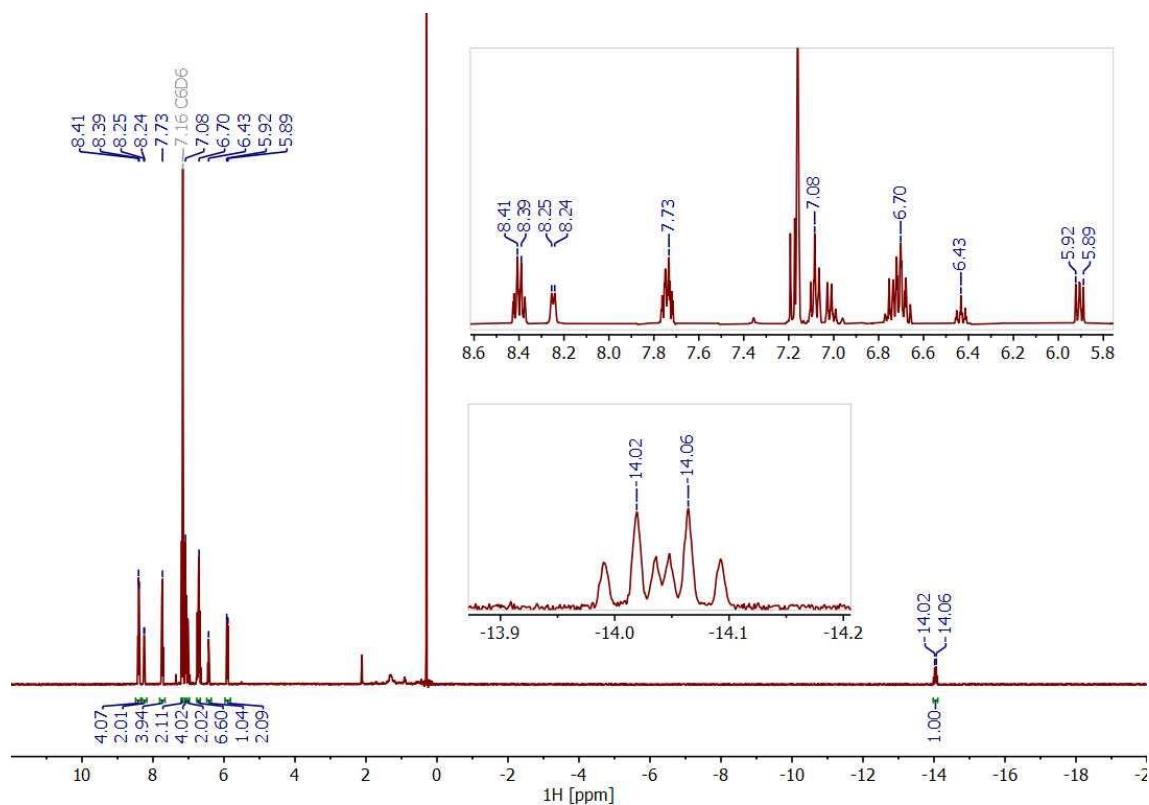


Figure S11. ^1H NMR spectrum (C_6D_6 , 400 MHz, 297 K) of complex **2b**.

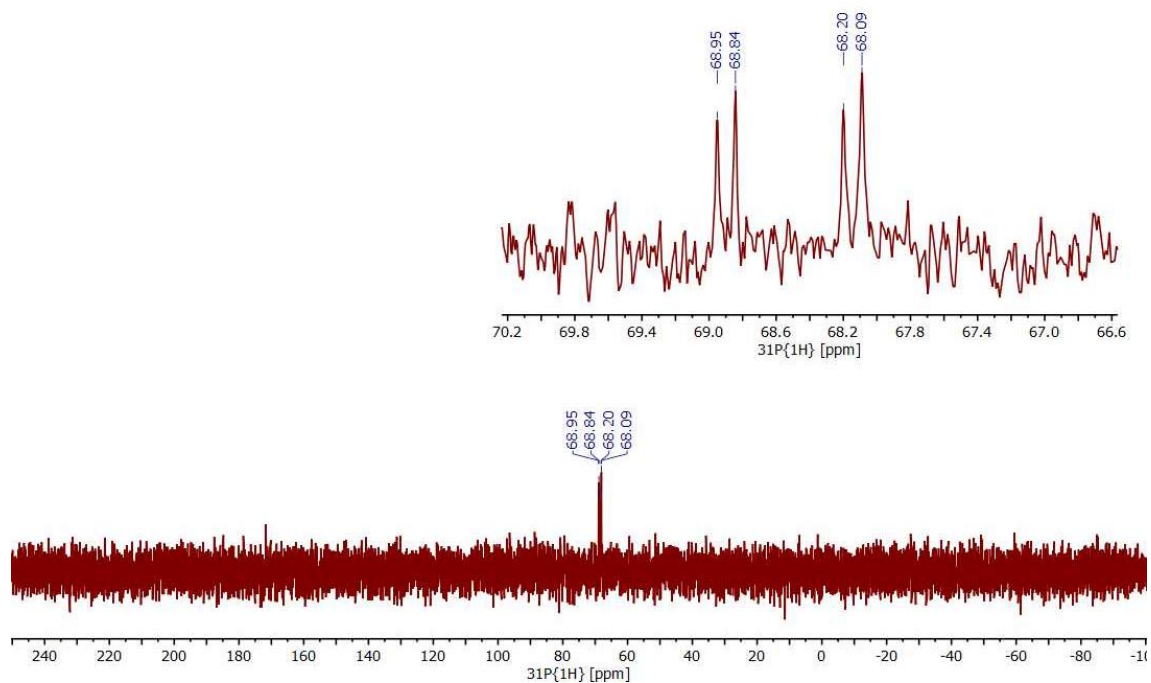


Figure S12. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 162 MHz, 297 K) of a solution of the reaction of complex **2b** and $\text{BF}_3\cdot\text{OEt}_2$ (48% in OEt_2).

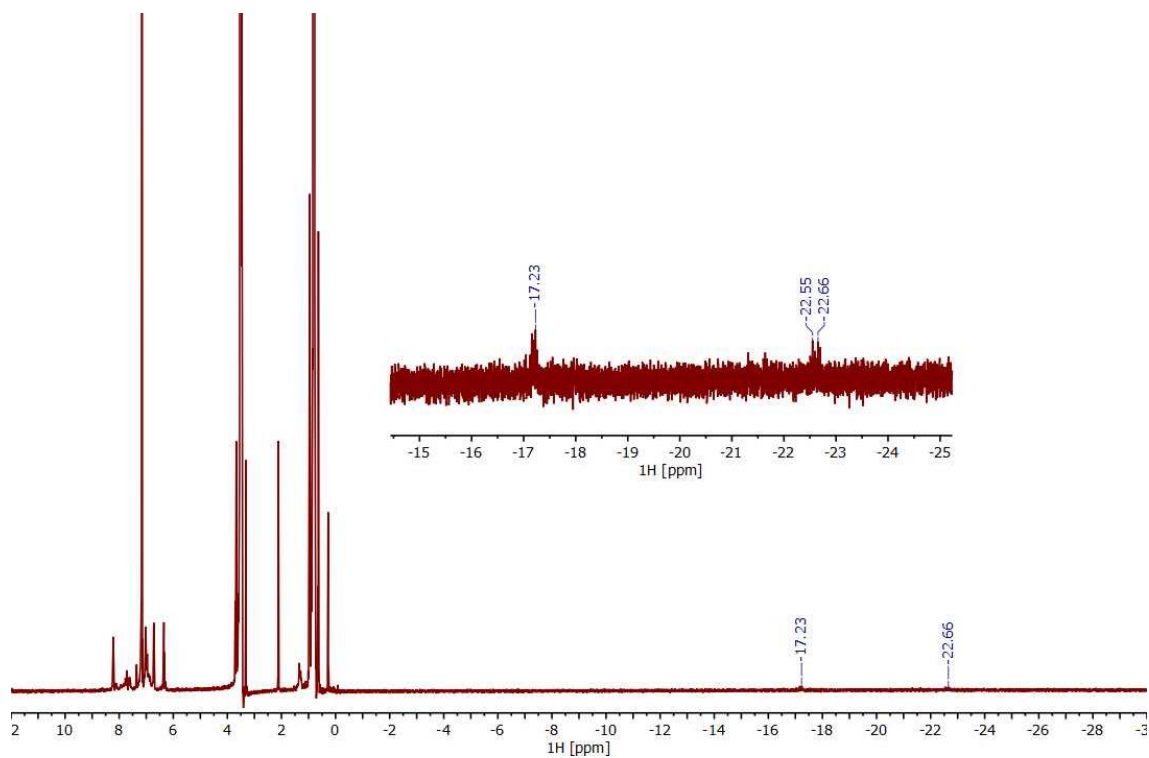


Figure S13. ^1H NMR spectrum (C_6D_6 , 400 MHz, 297 K) of a solution of the reaction of complex **2b** and $\text{BF}_3\cdot\text{OEt}_2$ (48% in OEt_2).

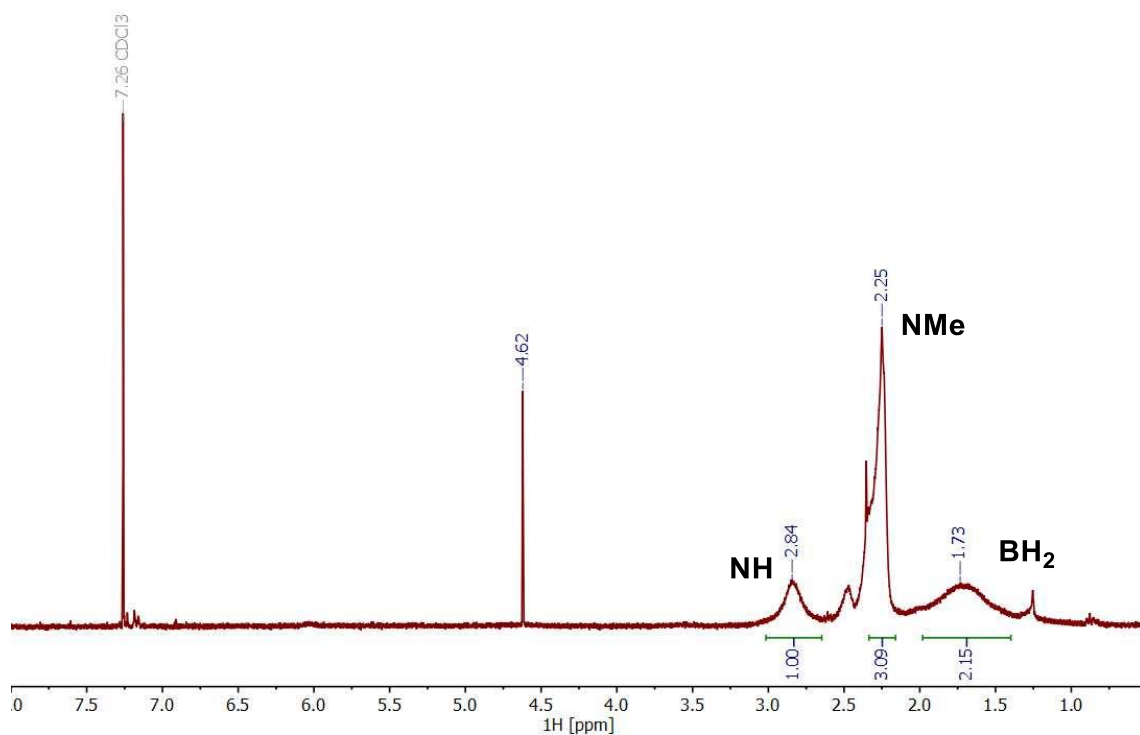


Figure S14. ^1H NMR spectrum (CDCl_3 , 300 MHz, 297 K) of the isolated poly(N-methylaminoborane) (H_2BNMeH) $_n$.

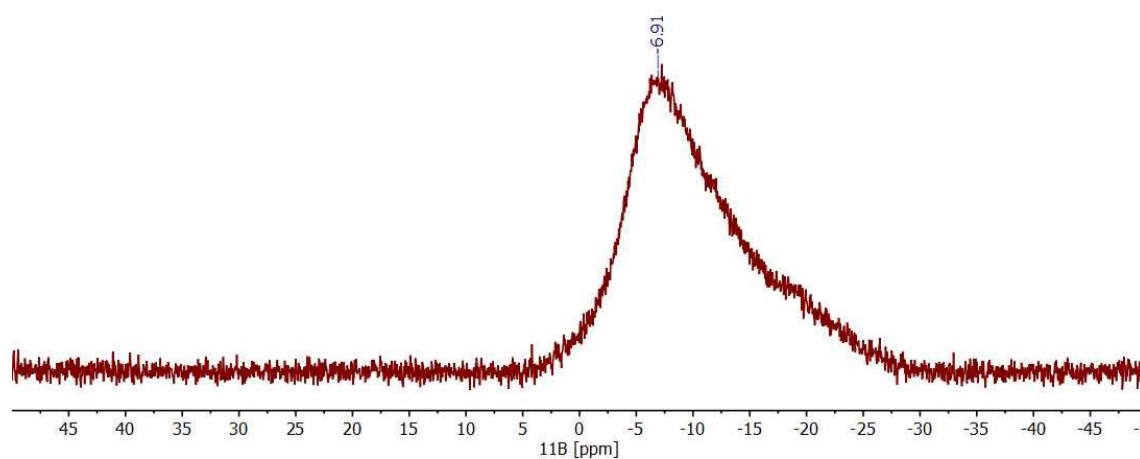


Figure S15. ^{11}B NMR spectrum (CDCl_3 , 96 MHz, 297 K) of the isolated poly(N-methylaminoborane) (H_2BNMeH) $_n$.

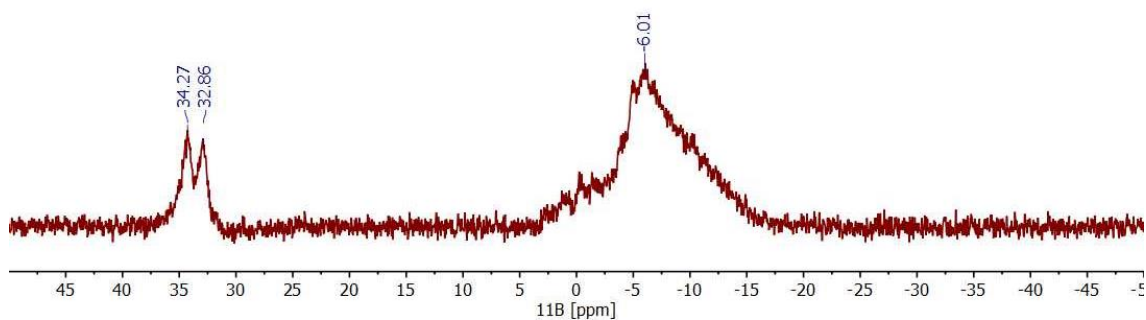


Figure S16. ^{11}B NMR spectrum (toluene- d_8 , 96 MHz, 297 K) of a reaction mixture (1 mol% **2a**) at full conversion.

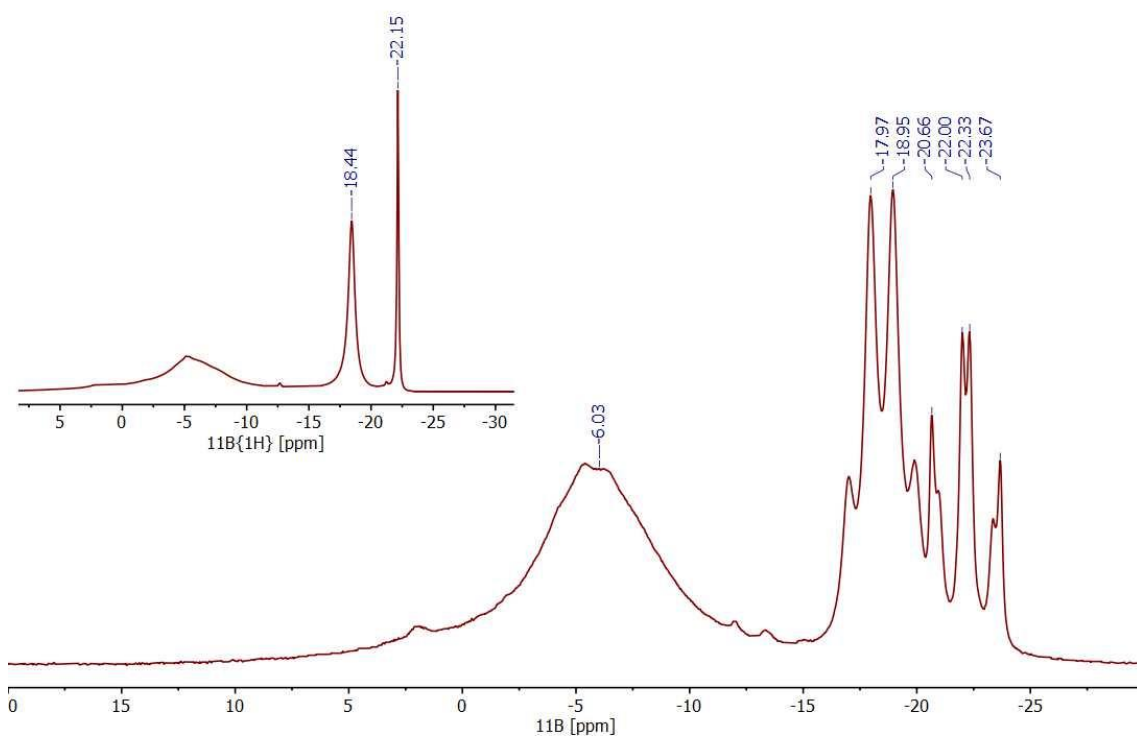


Figure S17. ^{11}B and $^{11}\text{B}\{^1\text{H}\}$ NMR spectra (CDCl_3 , 96 MHz, 297 K) of the isolated solids of a dehydropolymerisation reaction with 1 mol% **3a**.

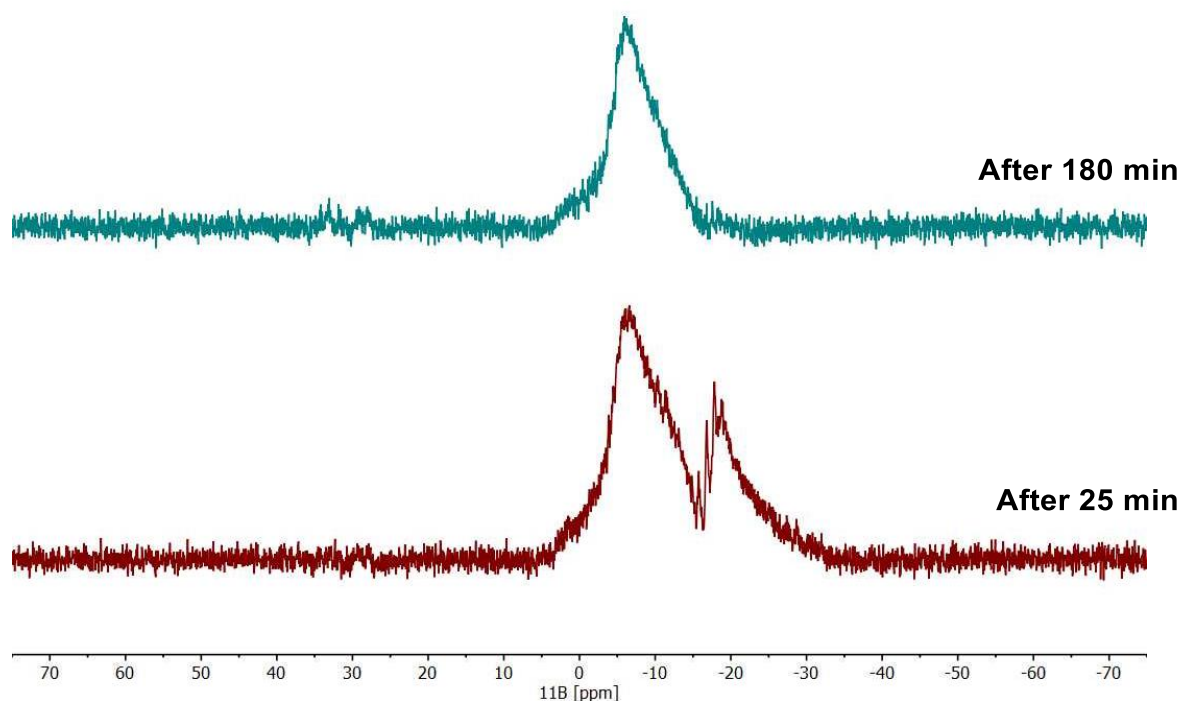


Figure S18. ^{11}B NMR spectra (toluene- d_8 , 96 MHz, 297 K) of a reaction mixture (1 mol% **2a** + 20 eq. cyclohexene) after 25 and 180 min.

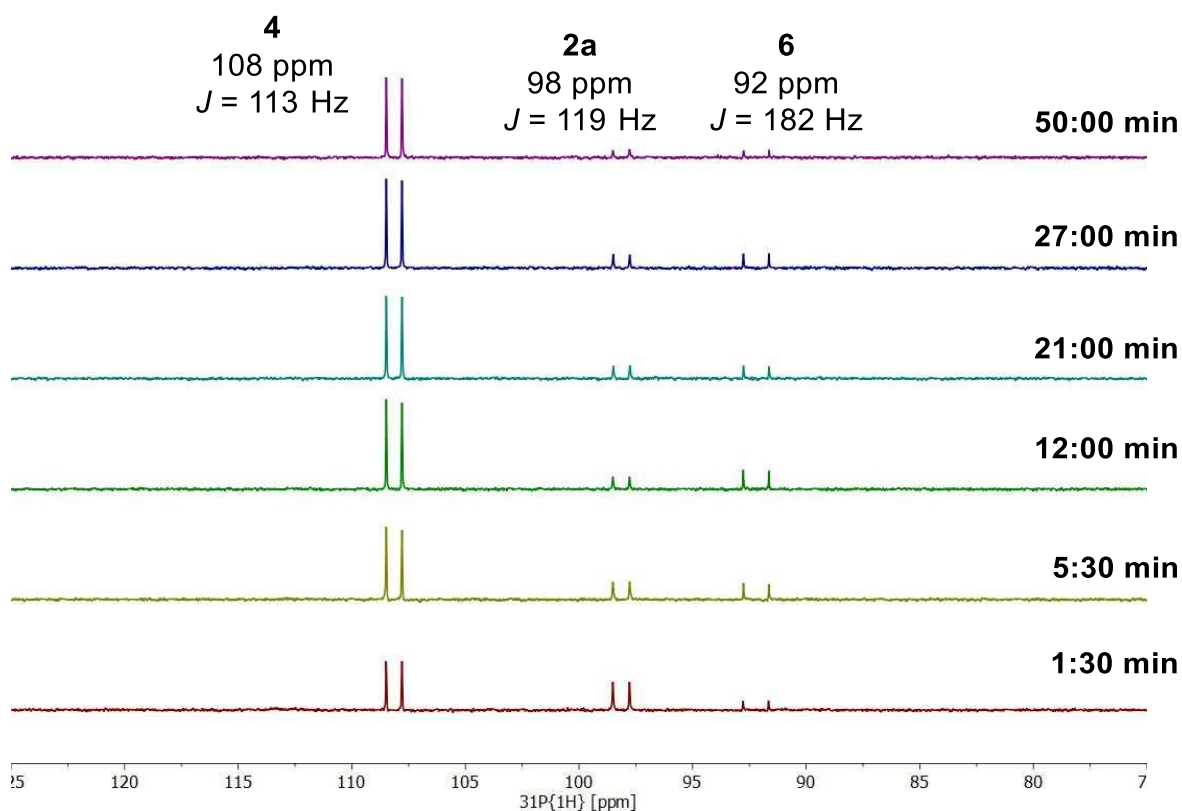


Figure S19. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra (toluene- d_8 , 162 MHz, 297 K) of monitoring a dehydropolymerisation reaction at room temperature (5 mol% **2a**). Given times indicate the time of sampling from the reaction solution.

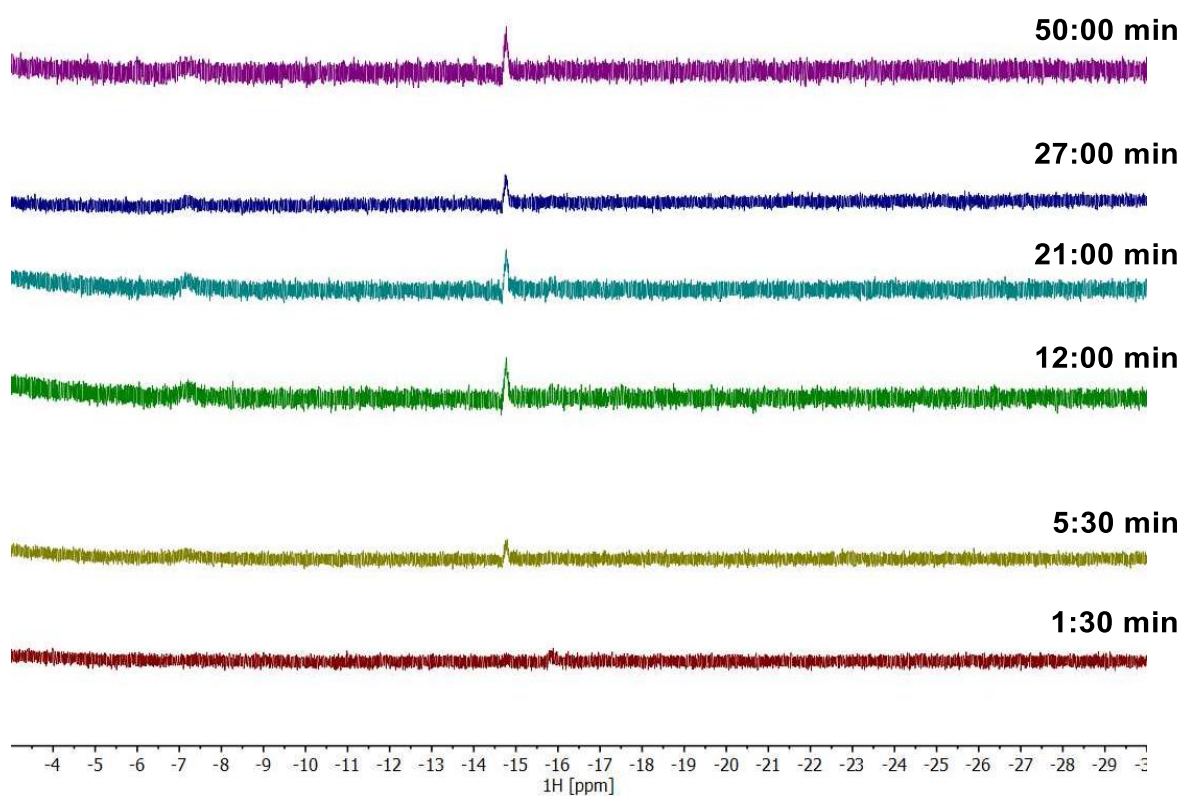


Figure S20. ^1H NMR spectra (toluene- d_6 , 400 MHz, 297 K) of monitoring a dehydropolymerisation reaction at room temperature (5 mol% **2a**). Given times indicate the time of sampling from the reaction solution.

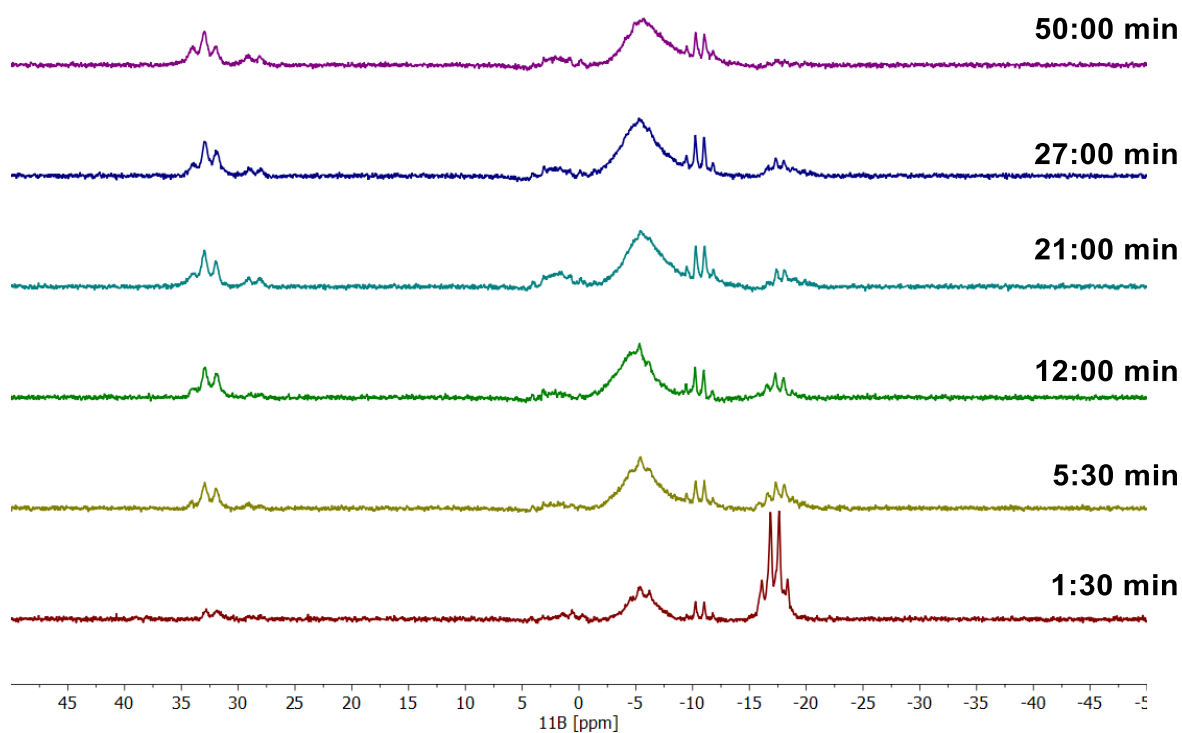


Figure S21. ^{11}B NMR spectra (toluene- d_6 , 128 MHz, 297 K) of monitoring a dehydropolymerisation reaction at room temperature (5 mol% **2a**). Given times indicate the time of sampling from the reaction solution.

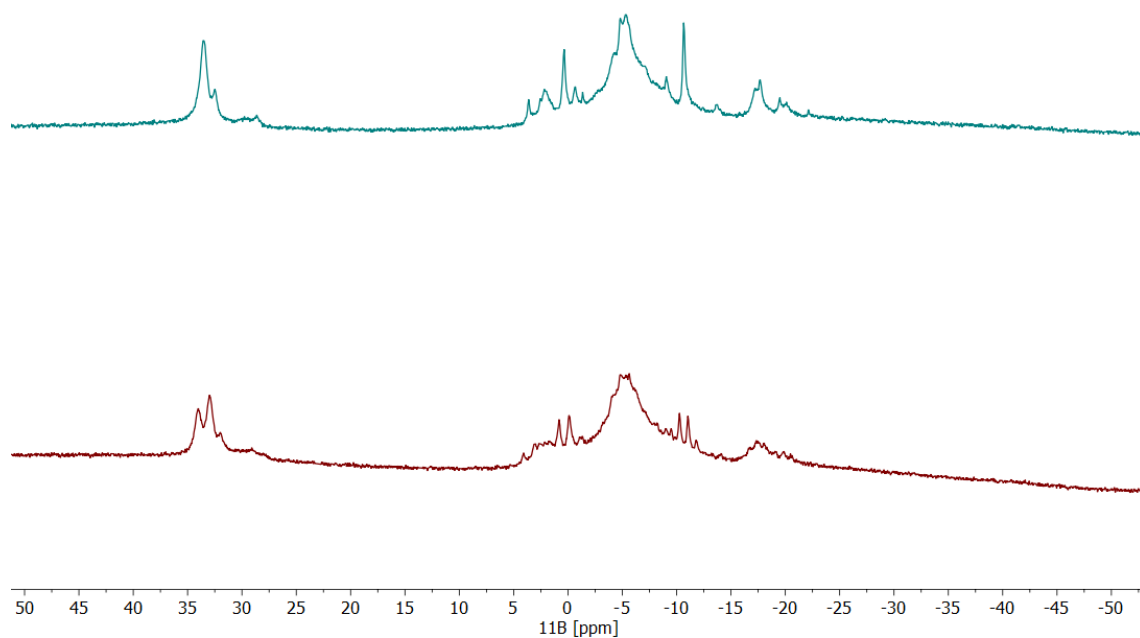


Figure S22. ^{11}B (bottom) and $^{11}\text{B}\{^1\text{H}\}$ NMR (top) spectra (toluene- d_8 , 128 MHz, 297 K) of a dehydropolymerisation reaction at room temperature (5 mol% **2a**), recorded after 30 min.

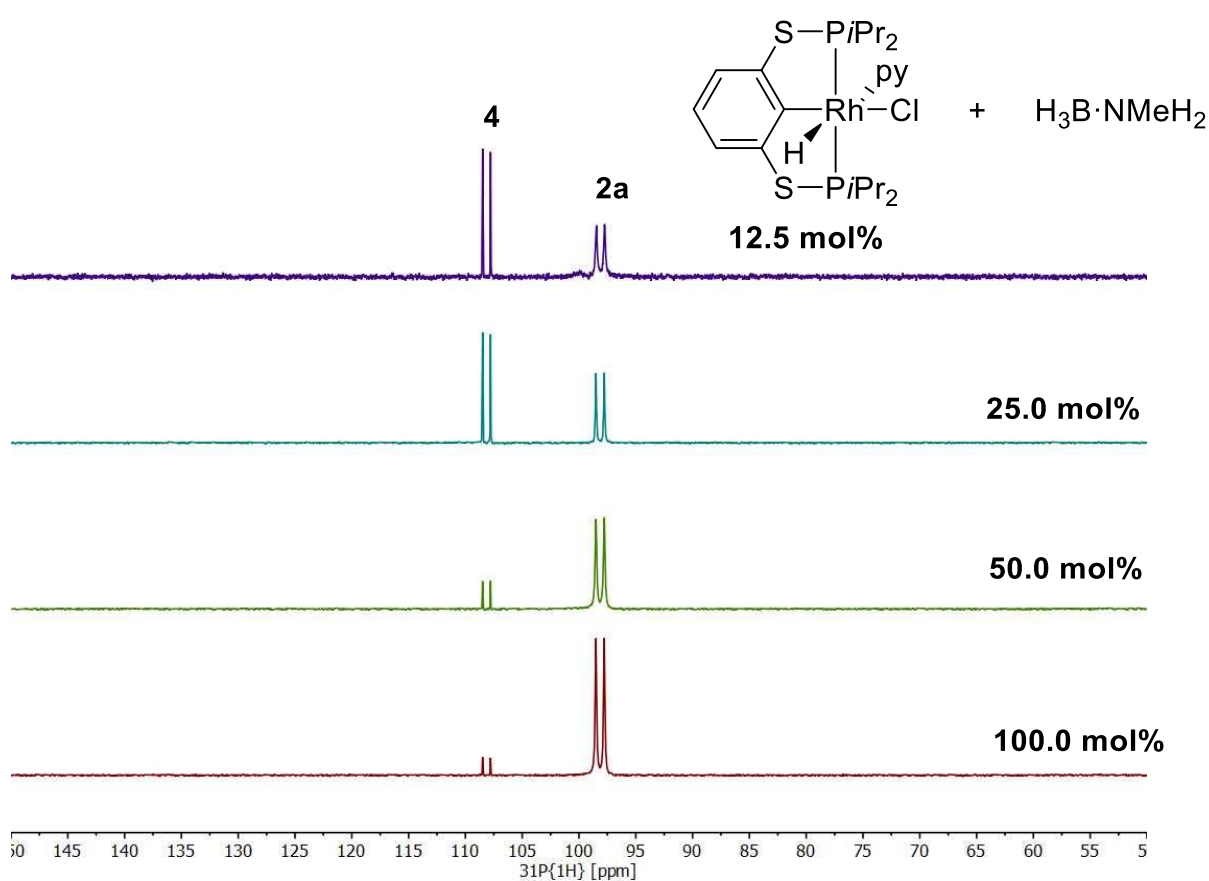


Figure S23. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra (toluene- d_8 , 162 MHz, 297 K) of complex **2a**/ $\text{H}_3\text{B}\cdot\text{NMeH}_2$. Amount of **2a** is given in relation to the amount of used $\text{H}_3\text{B}\cdot\text{NMeH}_2$ ($c = 66.8 \text{ mmol}\cdot\text{L}^{-1}$).

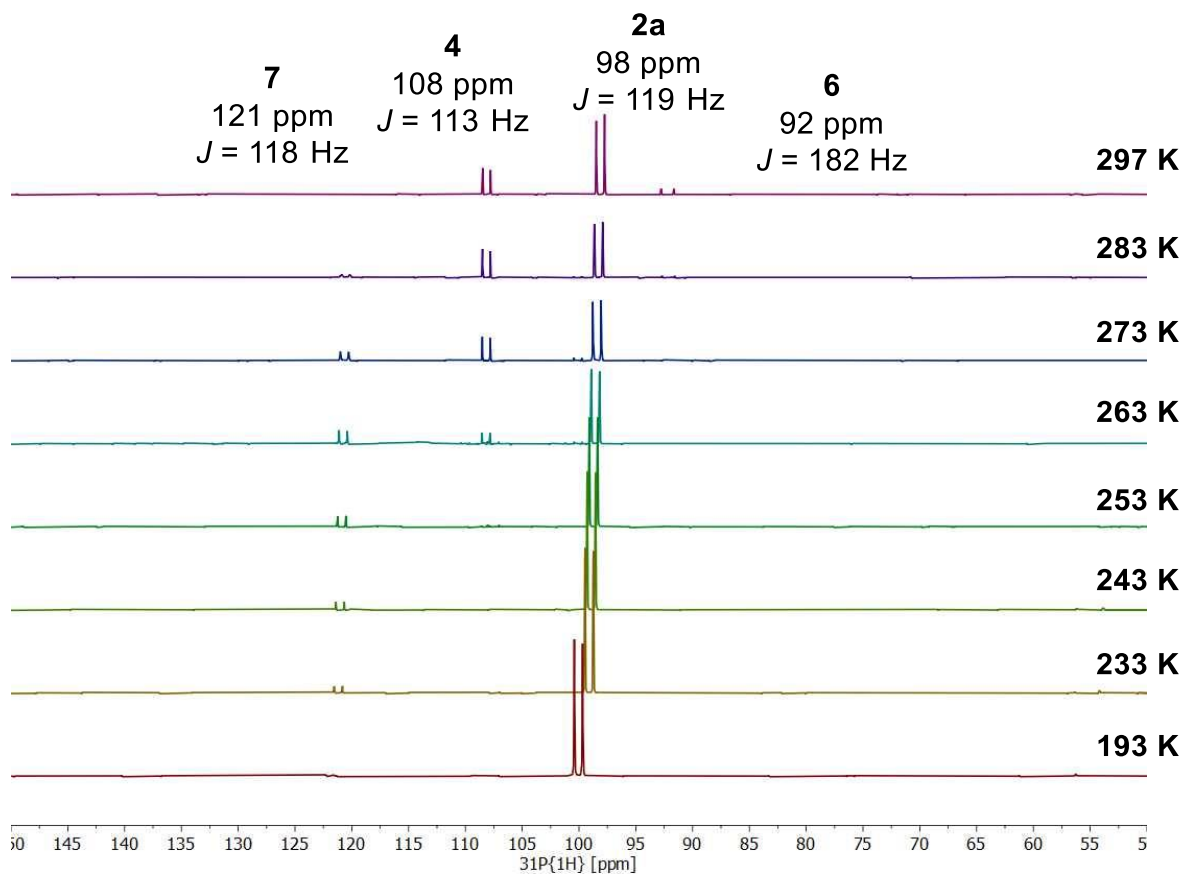


Figure S24. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra (toluene- d_8 , 162 MHz) of monitoring a dehydropolymerisation reaction at different temperatures (10 mol% **2a**).

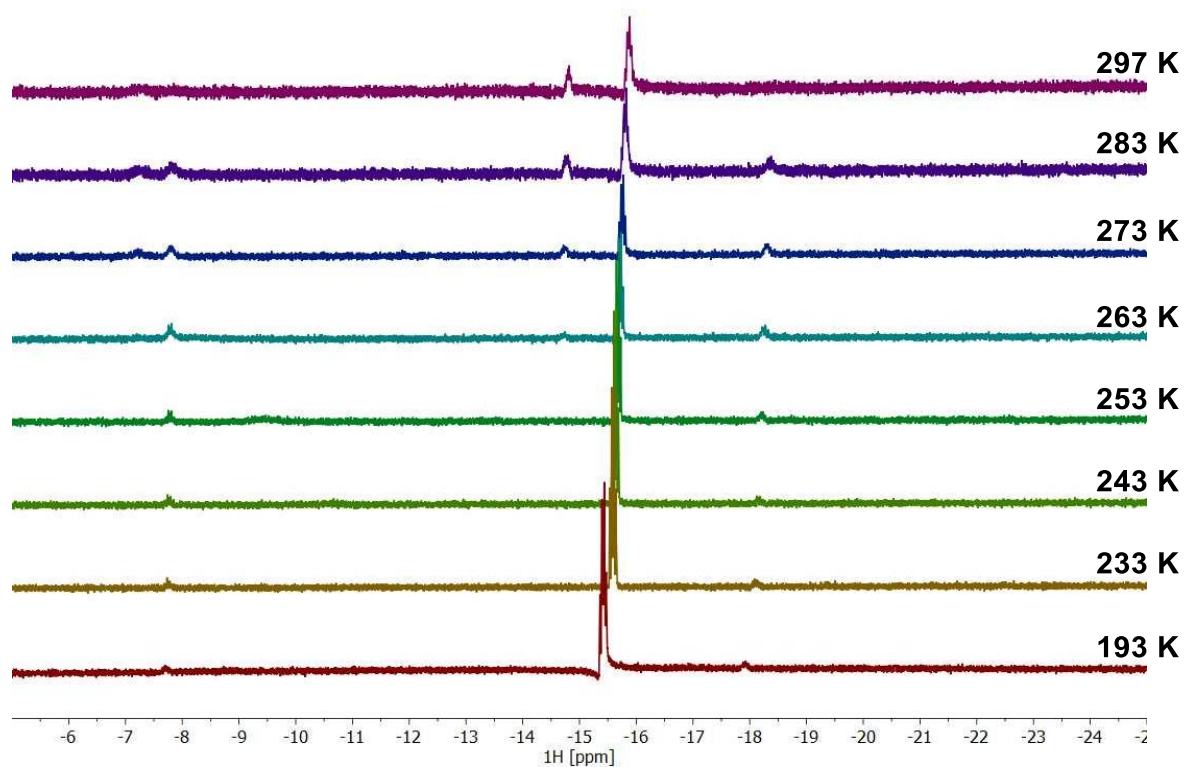


Figure S25. ^1H NMR spectra (toluene- d_8 , 400 MHz) of monitoring a dehydropolymerisation reaction at different temperatures (10 mol% **2a**).

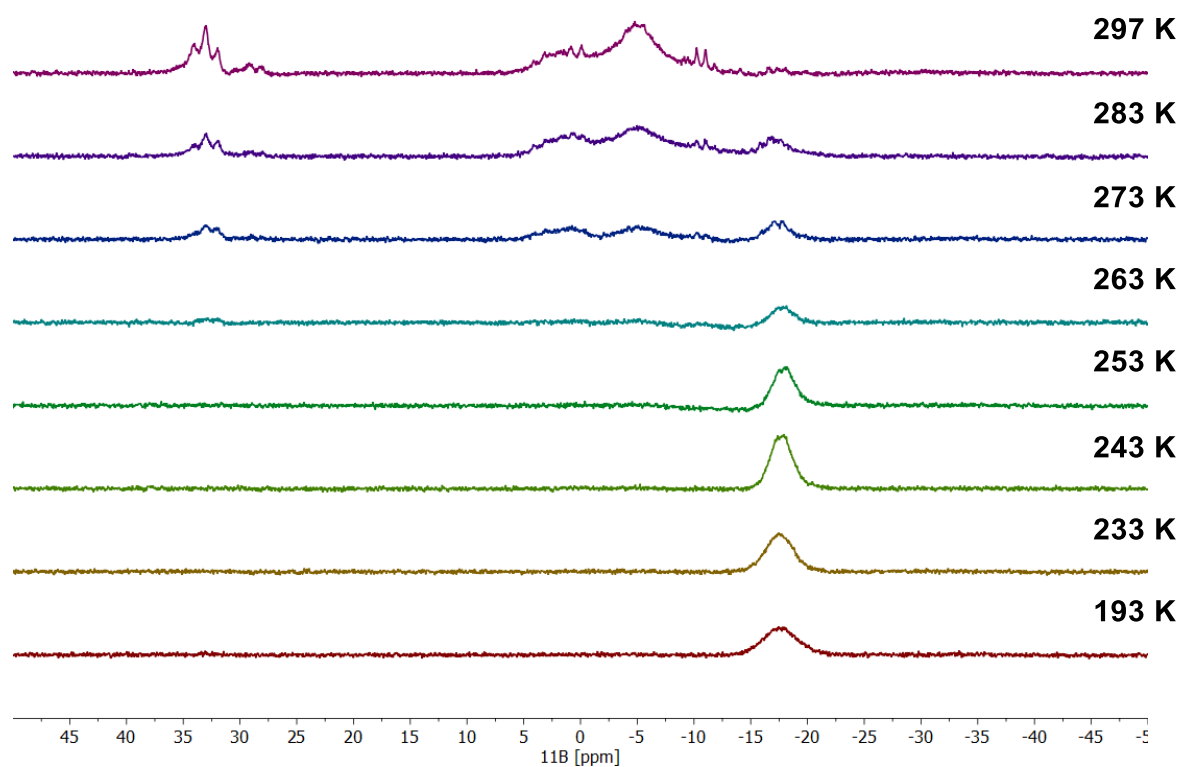


Figure S26. ^{11}B NMR spectra (toluene- d_8 , 128 MHz) of monitoring a dehydropolymerisation reaction at different temperatures (10 mol% **2a**).

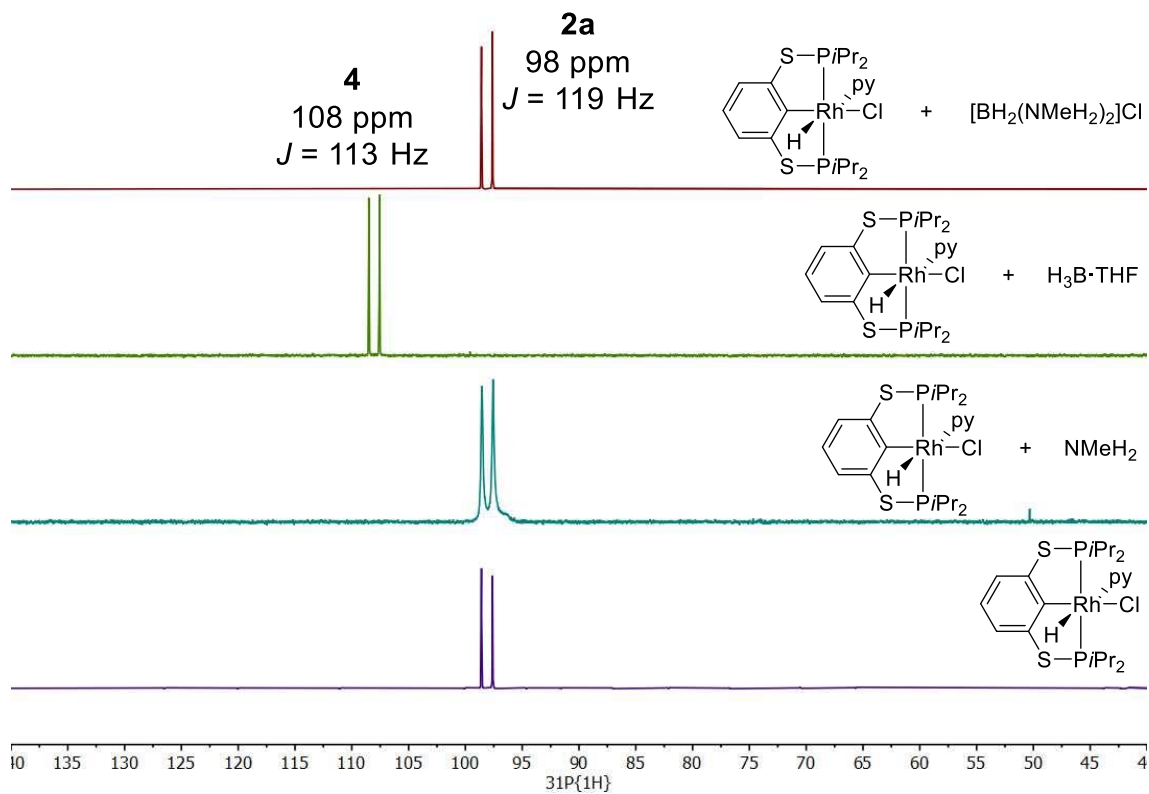


Figure S27. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra (toluene- d_8 , 122 MHz, 297 K) of complex **2a** (10 mg, 0.017 mmol) + various additives.

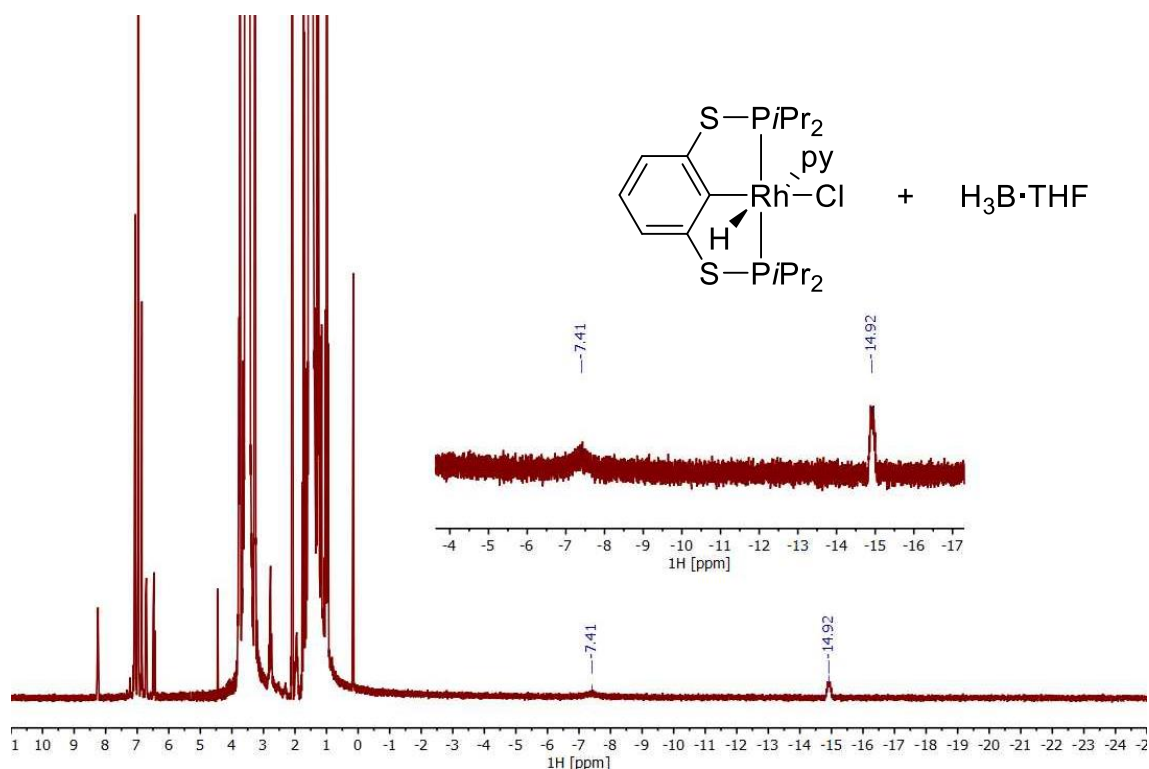


Figure S28. ^1H NMR spectrum (toluene- d_8 , 300 MHz, 297 K) of complex **2a** + 1.0 equivalent of $\text{BH}_3\cdot\text{THF}$ (0.89 M in THF).

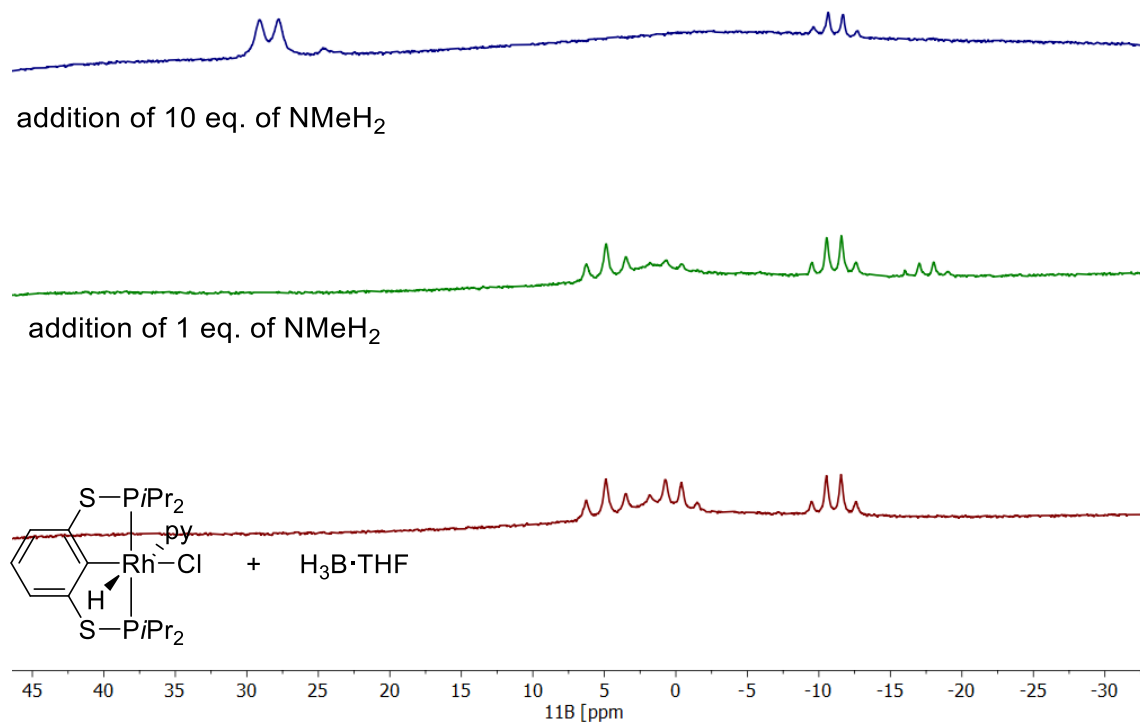


Figure S29. ^{11}B NMR spectra (toluene- d_8 , 96 MHz, 297 K) of complex **2a** after addition of 1 eq. of $\text{BH}_3\cdot\text{THF}$ (0.89 M in THF, bottom), after addition of 1 eq. of NMeH_2 to the same sample (centre), after addition of 10 eq. of NMeH_2 to the same sample (top), indicating the stepwise formation of **4** (δ 4.8 ppm), BH_3 -pyridine (δ -10.8 ppm) and the consumption of **4** to yield an amine complex **5**.

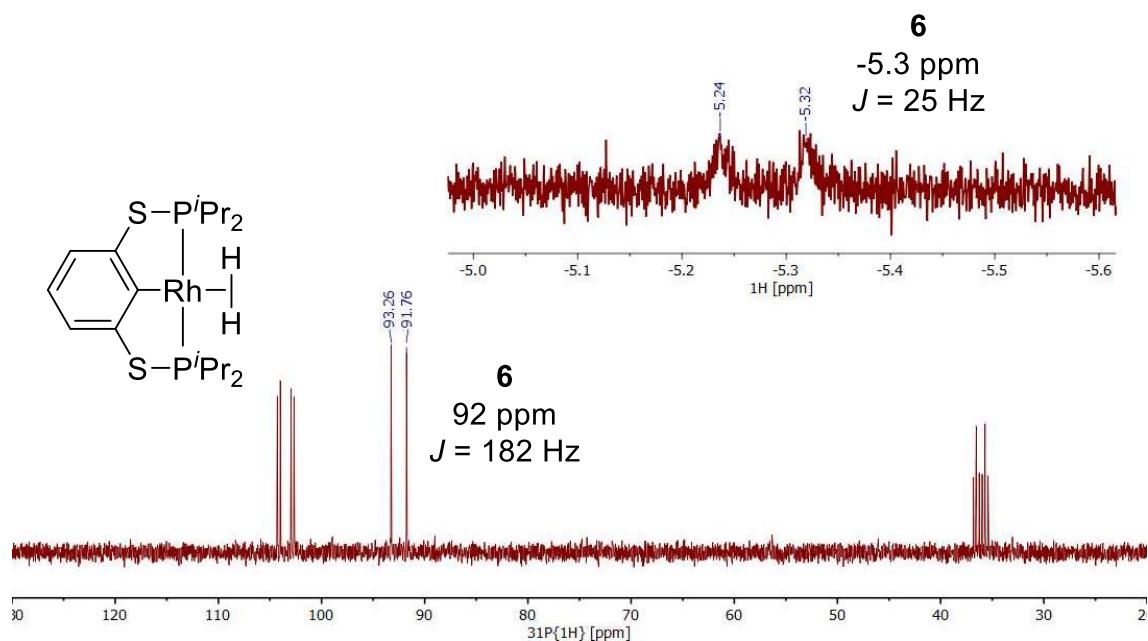


Figure S30. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra (C_6D_6 , 122 MHz, 297 K) of reaction of complex **2a** with $\text{LiN}(\text{TMS})_2$ and H_2 , showing the formation of complex **6**. The inset shows the ^1H NMR spectrum (C_6D_6 , 300 MHz, 297 K) of the dihydrogen ligand of complex **6**. Resonances at 36 and 104 ppm could not be assigned.

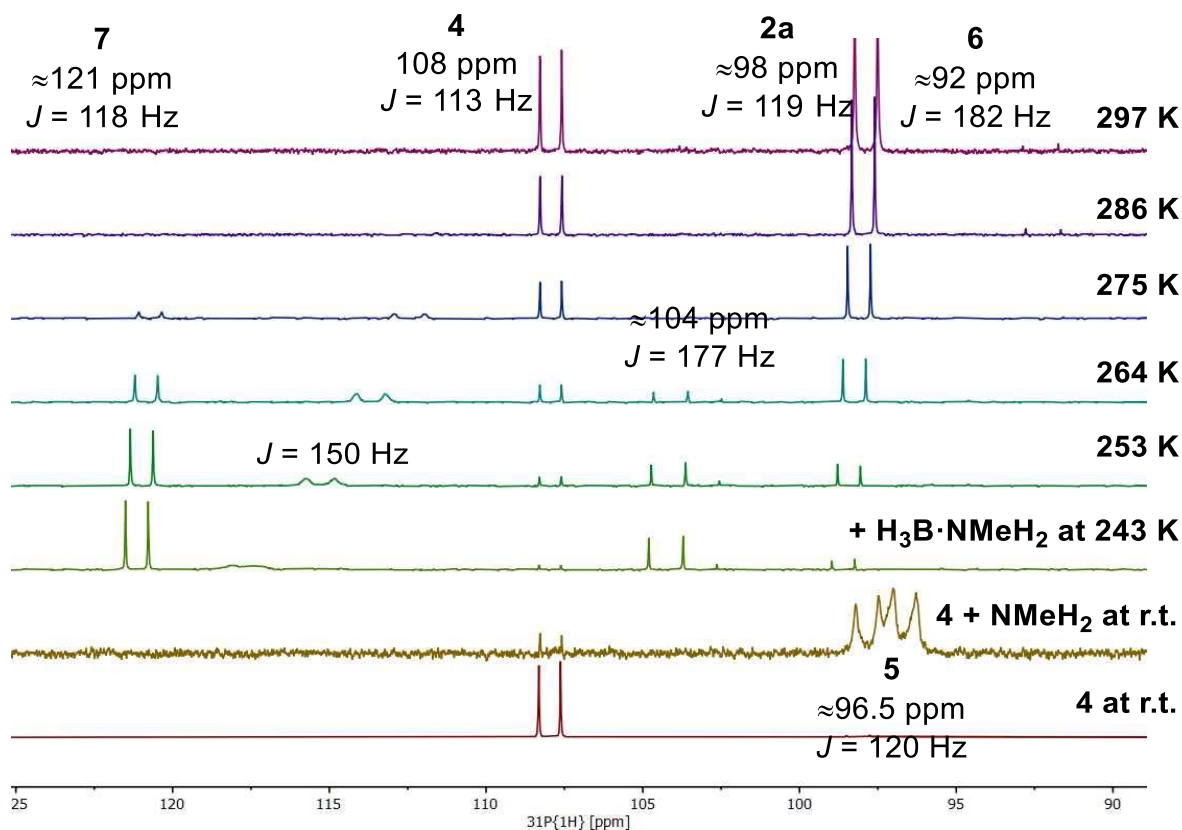


Figure S31. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra (toluene- d_8 , 162 MHz) of monitoring a dehydropolymerisation reaction at different temperatures (10 mol% **4**).

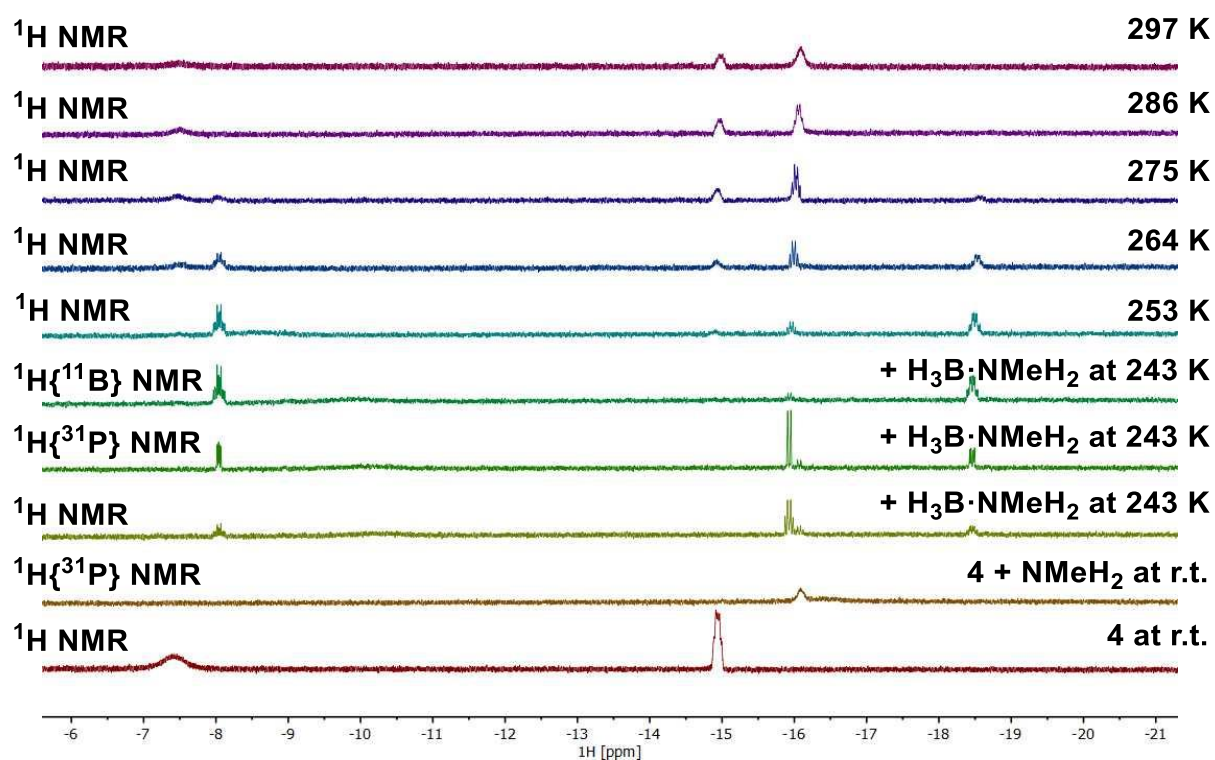


Figure S32. ¹H NMR spectra (toluene-*d*₈, 400 MHz) of monitoring a dehydropolymerisation reaction at different temperatures (10 mol% **4**).

IR spectra⁹

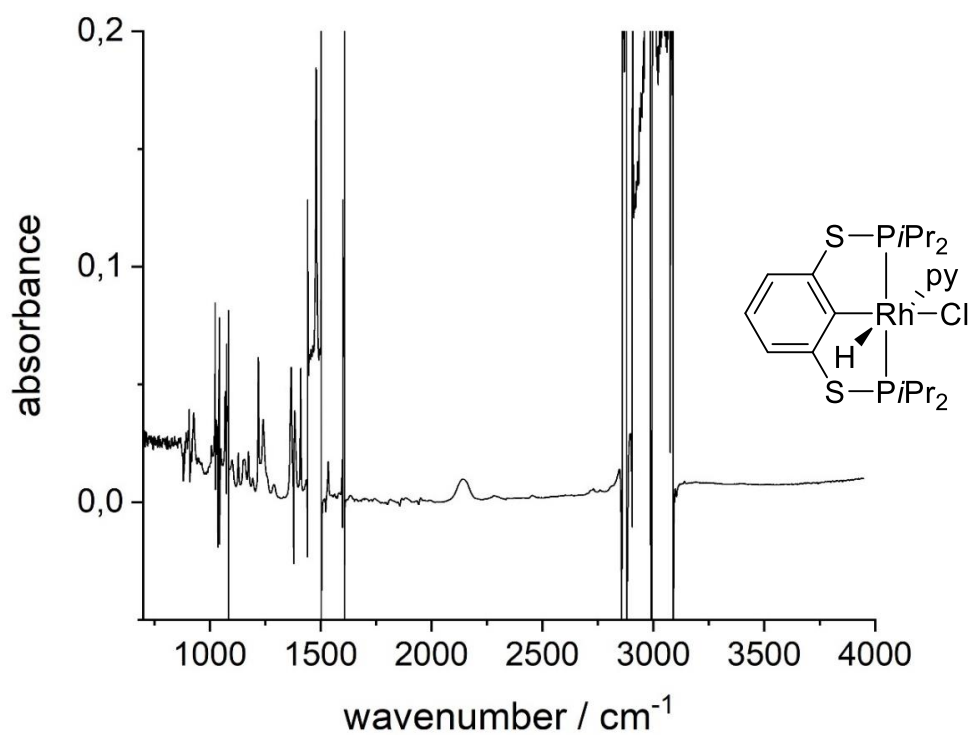


Figure S33. Absorbance IR spectrum of complex **2a** (17 mmol/L in toluene, 297 K, CaF_2 , 200 μm , NS = 32). Full spectrum.

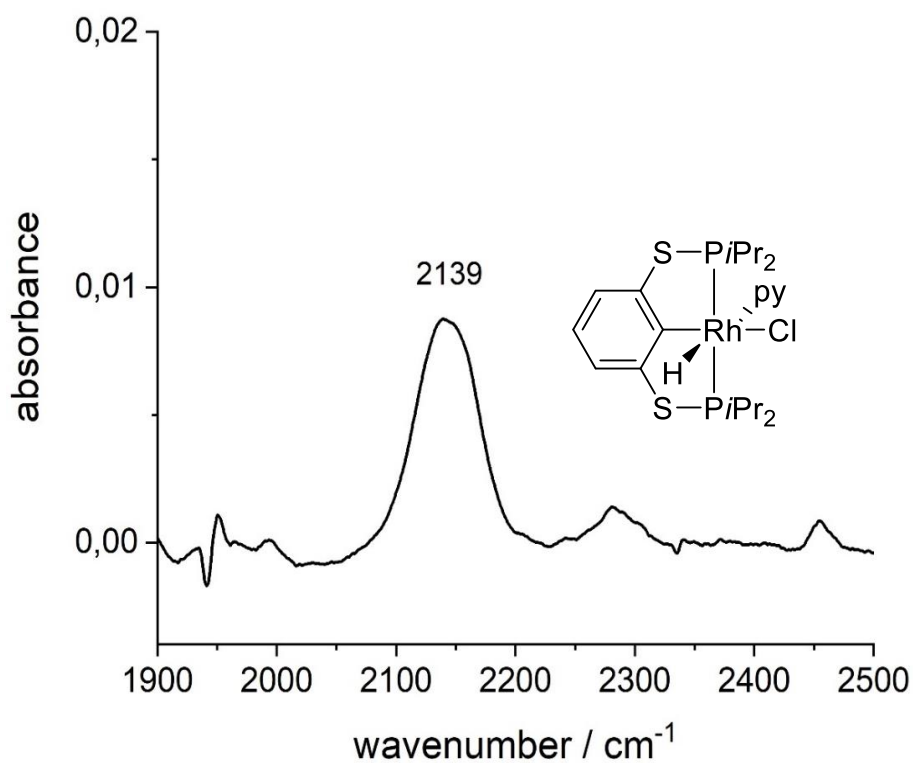


Figure S34. Absorbance IR spectrum of complex **2a** (17 mmol/L in toluene, 297 K, CaF_2 , 200 μm , NS = 32) between 1900-2500 cm^{-1} .

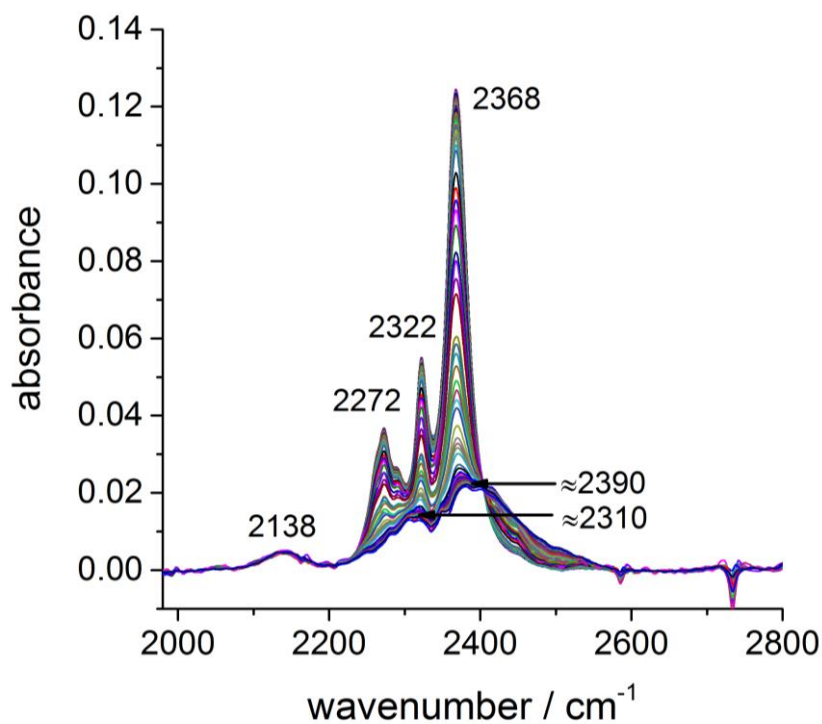


Figure S35. Absorbance IR spectra (17 mmol/L of **2a** in toluene, 297 K, CaF₂, 200 μm, NS = 32) of monitoring a dehydropolymerisation reaction (50 mol% **2a**). The band at 2138 cm⁻¹ is assigned to the Rh-H vibration of precatalyst **2a**. The bands at 2272, 2322 and 2368 cm⁻¹ are assigned to boron hydride vibrations. The product poly(N-methylaminoborane) shows vibrational bands at ≈2310 and ≈2390 cm⁻¹.

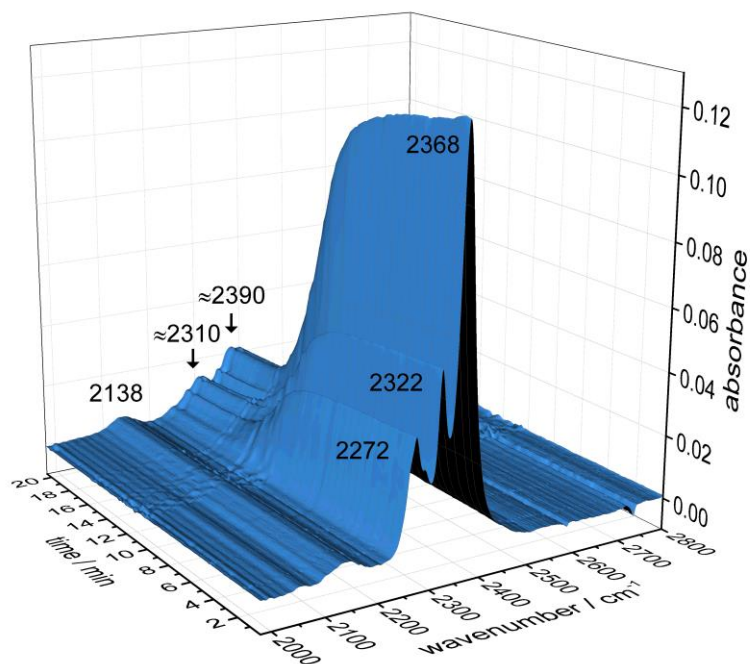


Figure S36. Absorbance IR spectra plotted over time (17 mmol/L of **2a** in toluene, 297 K, CaF₂, 200 μm, NS = 32) of monitoring a dehydropolymerisation reaction (50 mol% **2a**).

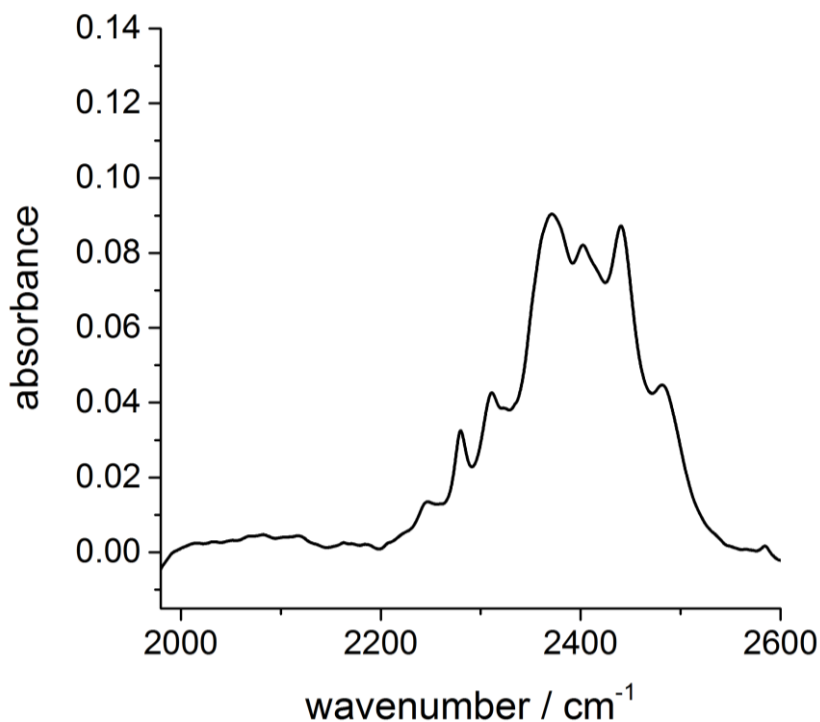


Figure S37. Absorbance IR spectrum of complex **2a** + $\text{BH}_3 \cdot \text{THF}$ (17 mmol/L of in THF/toluene, 297 K, CaF_2 , 200 μm , NS = 32). The identification of a respective rhodium hydride band was not possible with this sample. Bands in the region between 2200 – 2600 cm^{-1} are assigned to B-H vibrations.

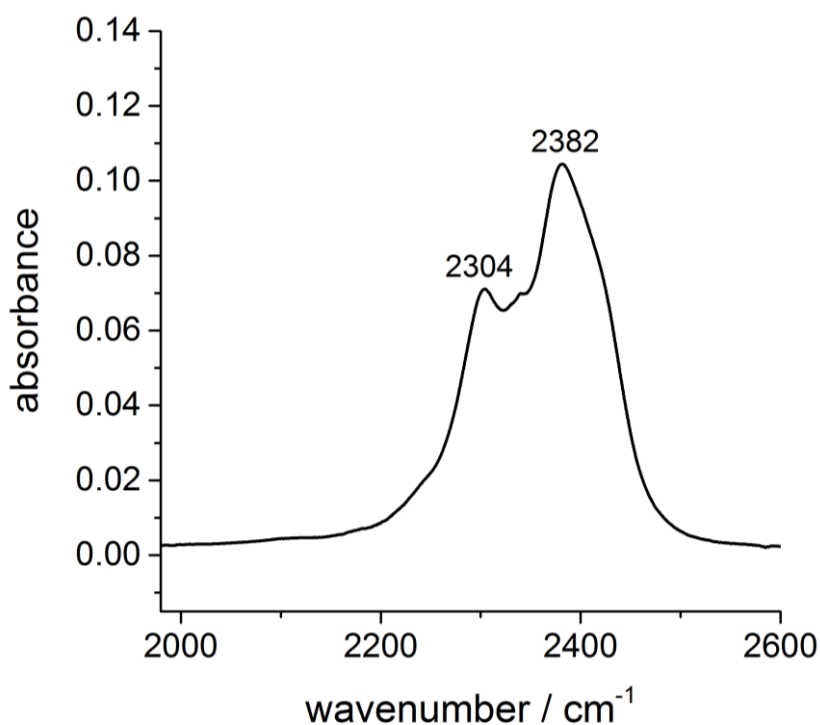


Figure S38. Absorbance IR spectrum of poly(N-methylaminoborane) (Saturated solution, ~55 mmol/L of in toluene, 297 K, CaF_2 , 200 μm , NS = 32). Bands at 2304 and 2382 cm^{-1} are assigned to boron hydride vibrations.

Volumetric data

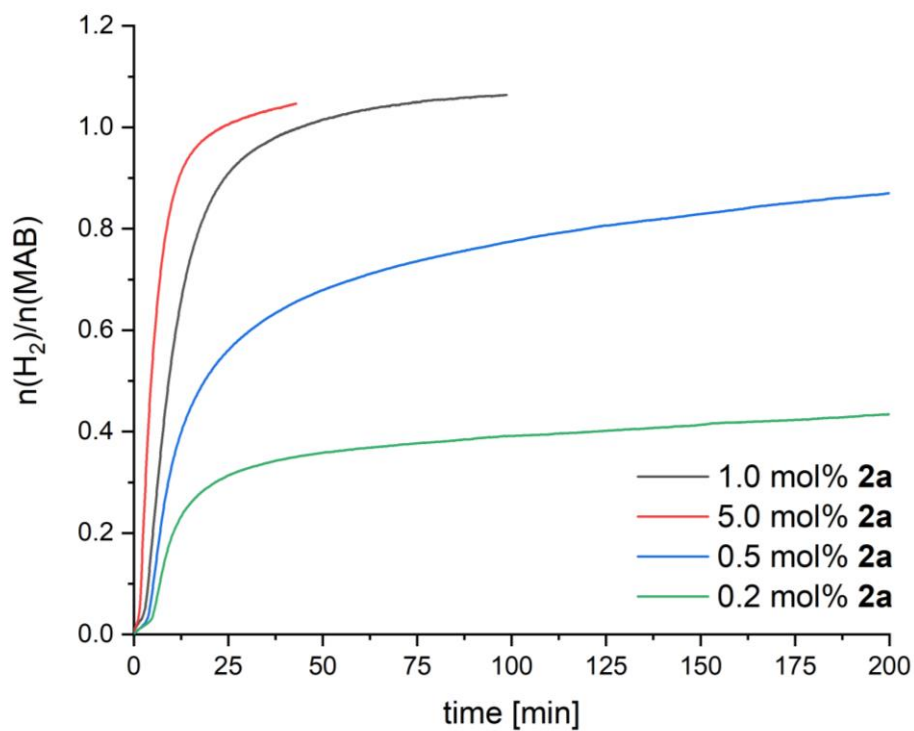


Figure S39. Volumetric data recorded during dehydropolymerisation of $\text{H}_3\text{B}\cdot\text{NMeH}_2$ using complex **2a** ($[\text{H}_3\text{B}\cdot\text{NMeH}_2] = 0.11 \text{ M}$, toluene, $T = 25 \text{ }^\circ\text{C}$).

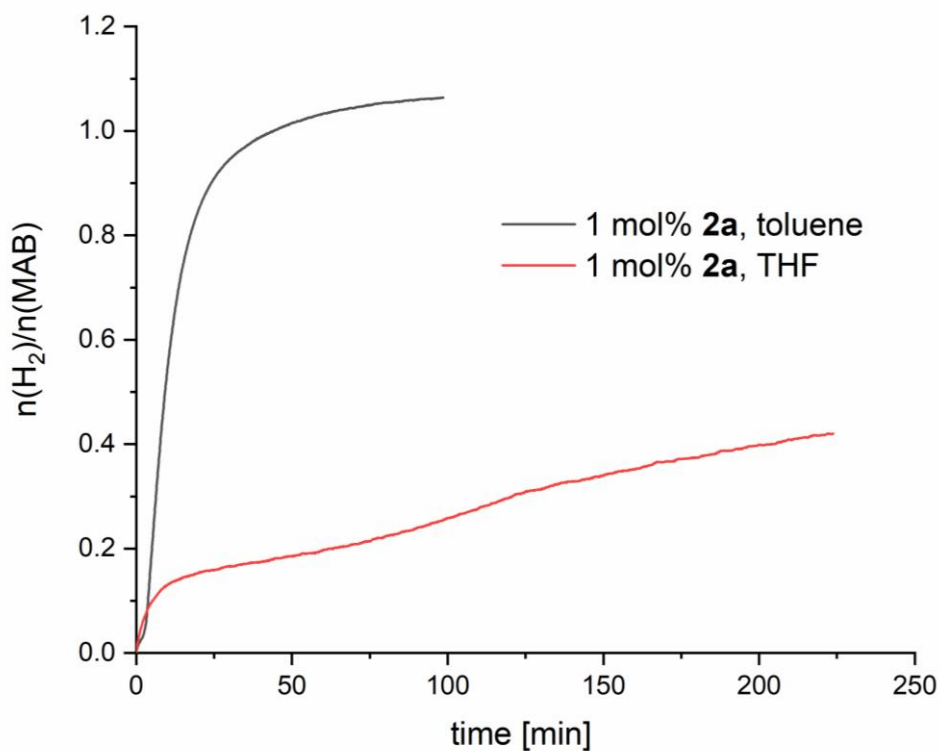


Figure S40. Volumetric data recorded during dehydropolymerisation of $\text{H}_3\text{B}\cdot\text{NMeH}_2$ using complex **2a** in THF and toluene ($[\text{H}_3\text{B}\cdot\text{NMeH}_2] = 0.11 \text{ M}$, $T = 25 \text{ }^\circ\text{C}$).

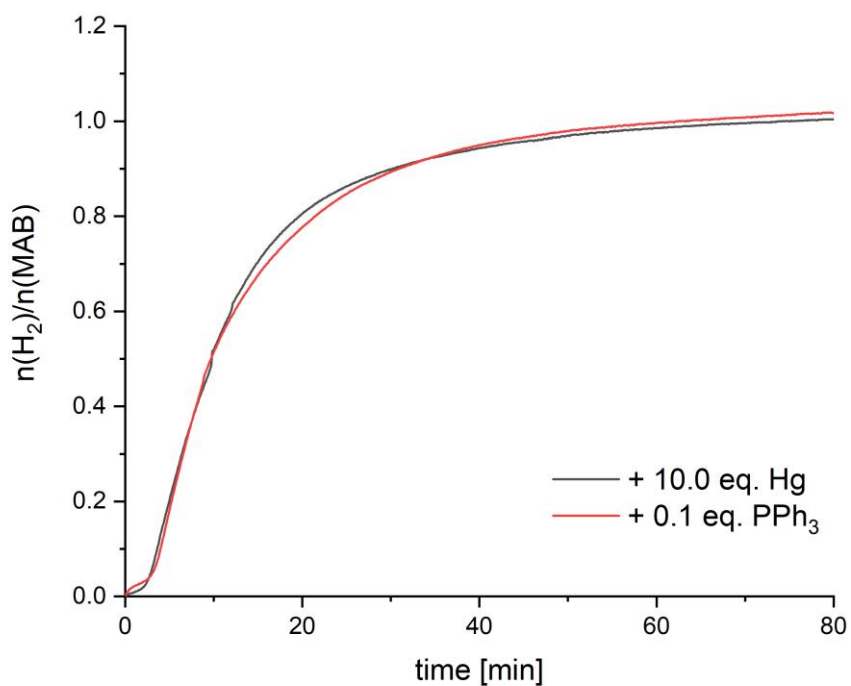


Figure S41. Volumetric data recorded during dehydropolymerisation of $\text{H}_3\text{B}\cdot\text{NMeH}_2$ with 1 mol% complex **2a** in the presence of potential catalyst poisons ($[\text{H}_3\text{B}\cdot\text{NMeH}_2] = 0.11 \text{ M}$, toluene, $T = 25 \text{ }^\circ\text{C}$).

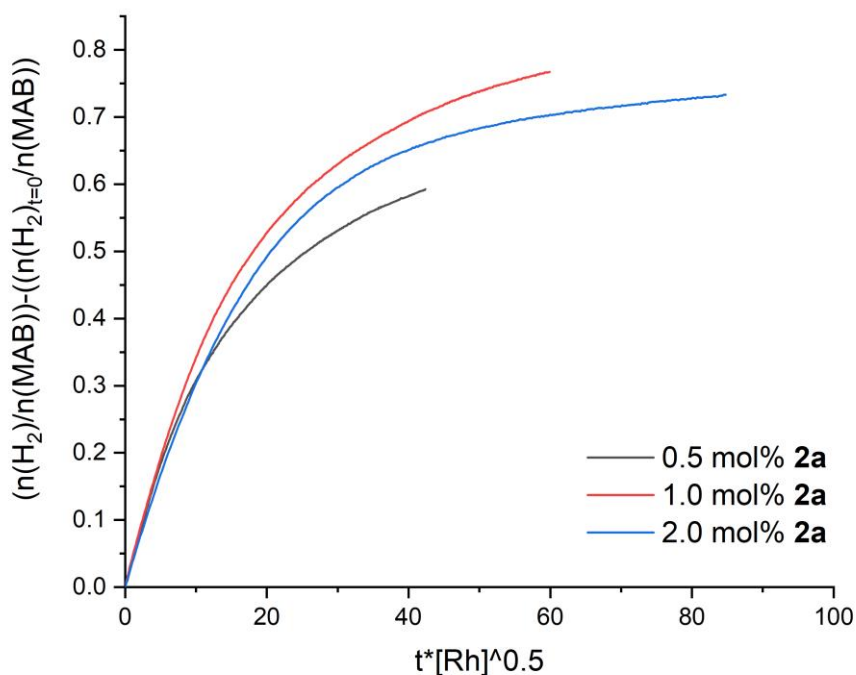


Figure S42. Time Normalisation Analysis (TNA¹⁰) for the order in $[\text{Rh}]$ (0.5 mol% - 2.0 mol% **2a**, induction periods removed). This figure shows the plots for $[\text{Rh}]^{0.5}$.

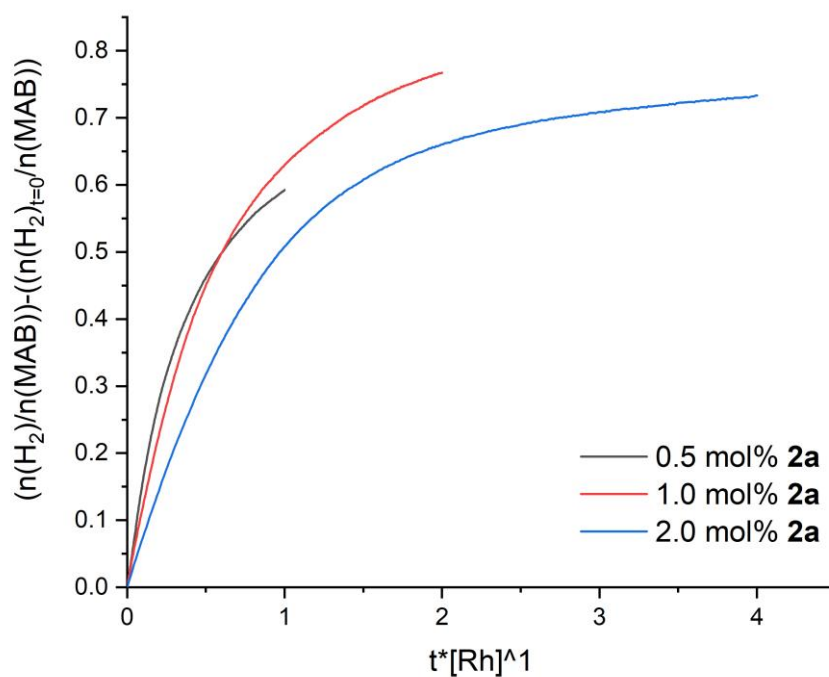


Figure S43. Time Normalisation Analysis (TNA¹⁰) for the order in [Rh] (0.5 mol% - 2.0 mol% **2a**, induction periods removed). This figure shows the plots for [Rh]¹.

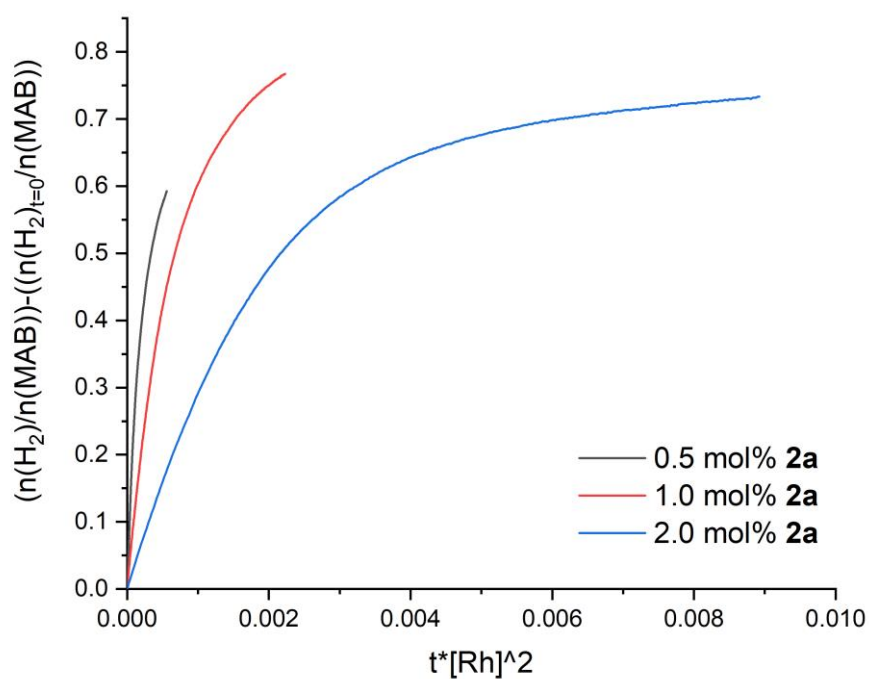


Figure S44. Time Normalisation Analysis (TNA¹⁰) for the order in [Rh] (0.5 mol% - 2.0 mol% **2a**, induction periods removed). This figure shows the plots for [Rh]².

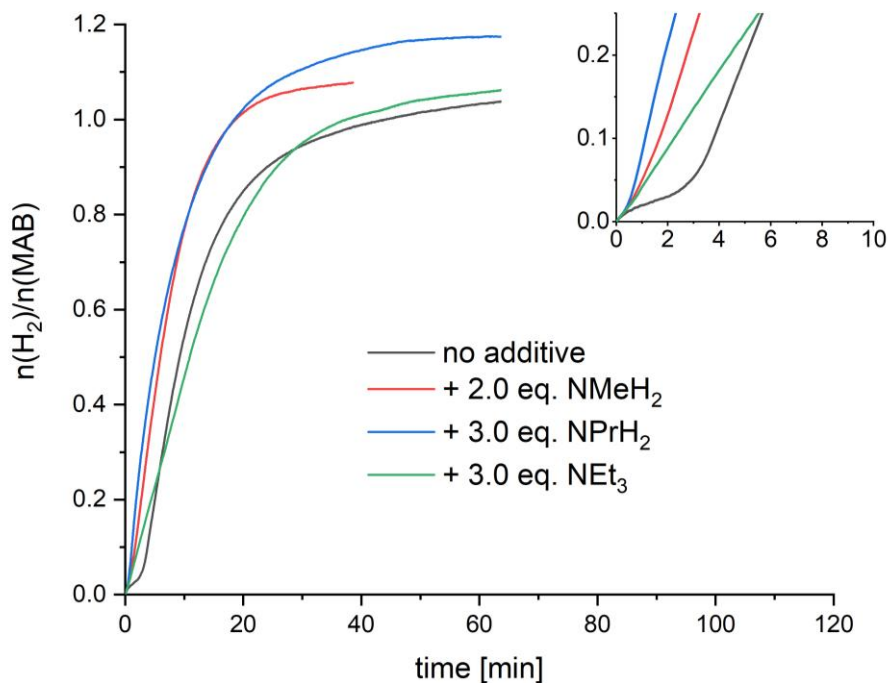


Figure S45. Volumetric data recorded during dehydropolymerisation of $\text{H}_3\text{B}\cdot\text{NMeH}_2$ with 1 mol% complex **2a** in the presence of different amines as additives ($[\text{H}_3\text{B}\cdot\text{NMeH}_2] = 0.11 \text{ M}$, toluene, $T = 25 \text{ }^\circ\text{C}$). The inset shows the volumetric profile for the first six minutes of the reaction.

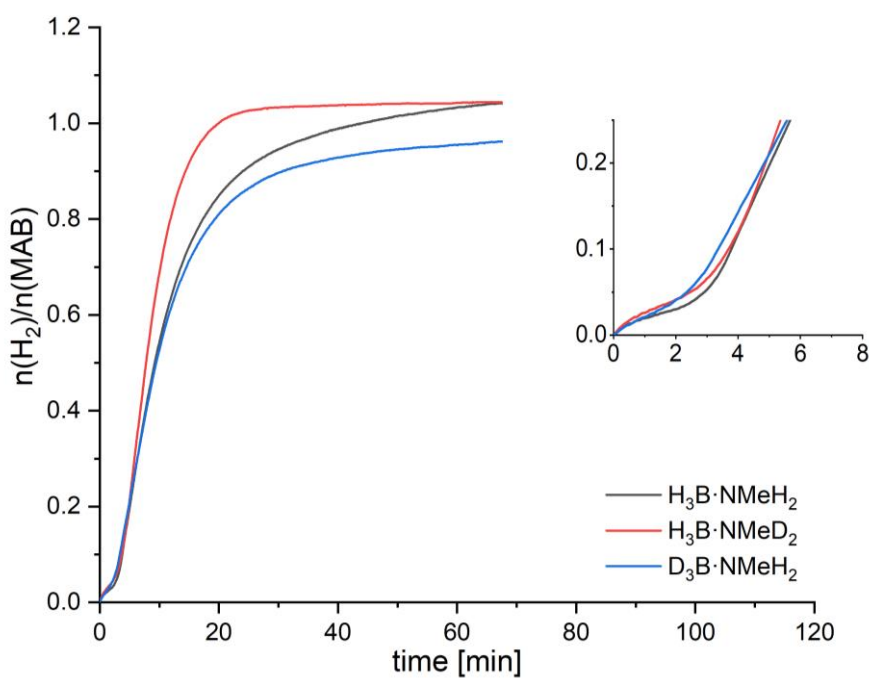


Figure S46. Volumetric data recorded during dehydropolymerisation of deuterated amine boranes (50-53 mg, 1.11 mmol) with 1 mol% complex **2a** in 10 mL toluene. The inset shows the volumetric profile for the first six minutes of the reaction.

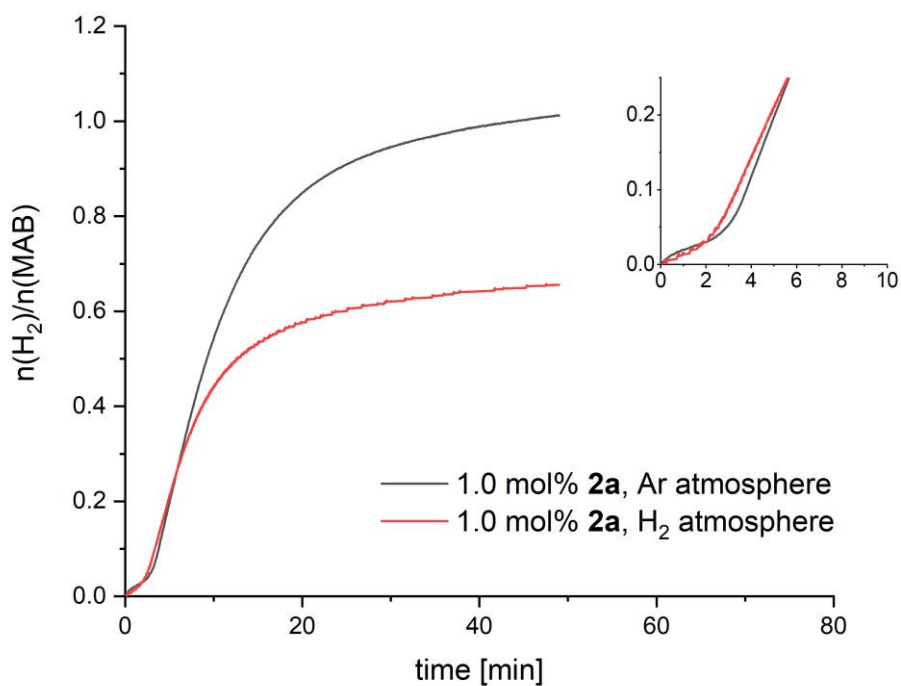


Figure S47. Volumetric data recorded during dehydropolymerisation of $\text{H}_3\text{B}\cdot\text{NMeH}_2$ using complex **2a** under H_2 and Ar atmospheres ($[\text{H}_3\text{B}\cdot\text{NMeH}_2] = 0.11 \text{ M}$, toluene, $T = 25 \text{ }^\circ\text{C}$). The inset shows the volumetric profile for the first six minutes of the reaction. **Note:** By exchanging the atmosphere to H_2 , some substrate was lost due to sublimation.

SEC analysis

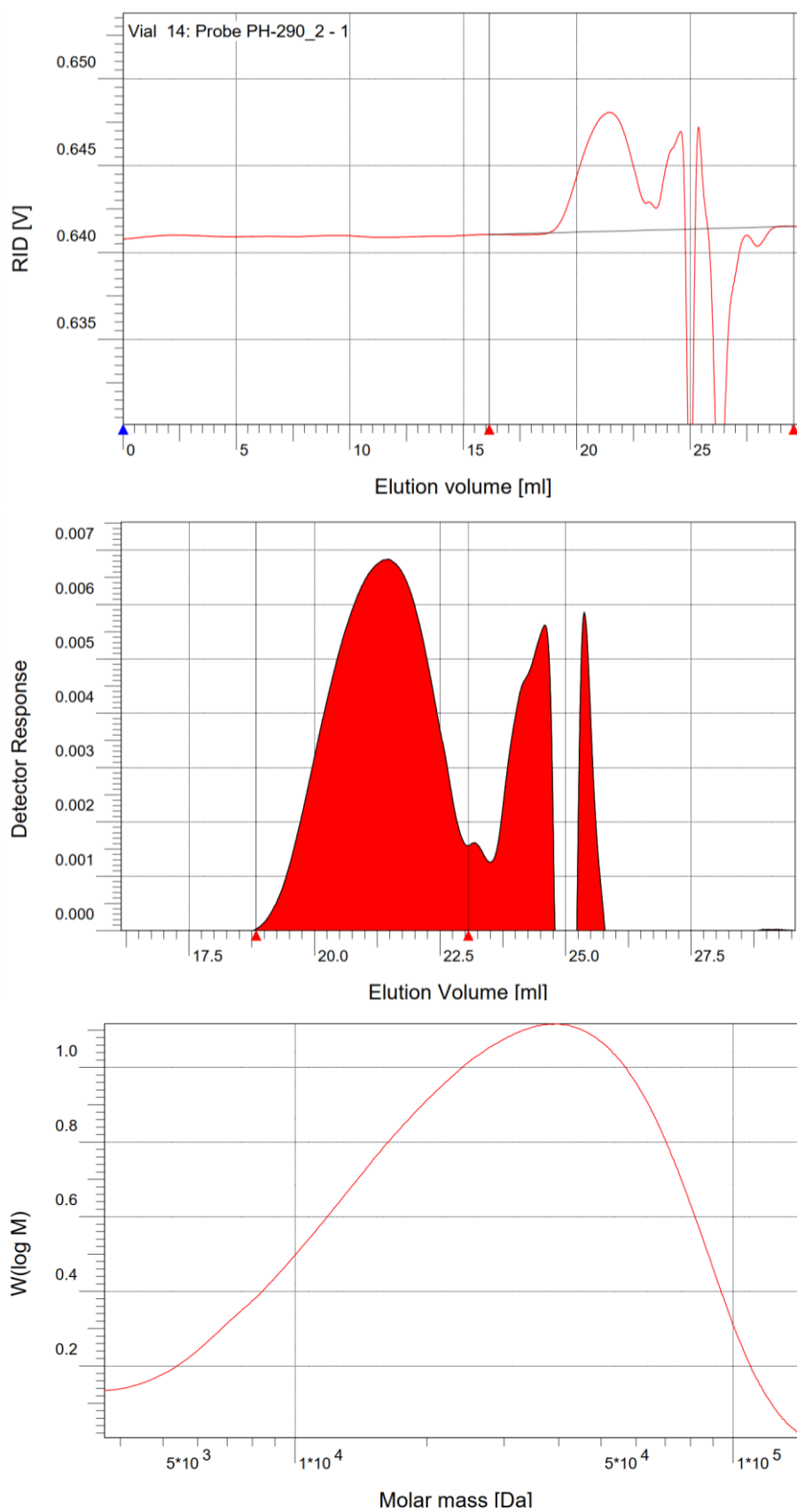


Figure S48. Gel-permeation chromatograms of isolated polymer from the dehydropolymerisation of $\text{H}_3\text{B}\cdot\text{NMeH}_2$ with 1 mol% **2a** ($[\text{H}_3\text{B}\cdot\text{NMeH}_2] = 0.11\text{M}$, toluene, $T = 25\text{ }^\circ\text{C}$).

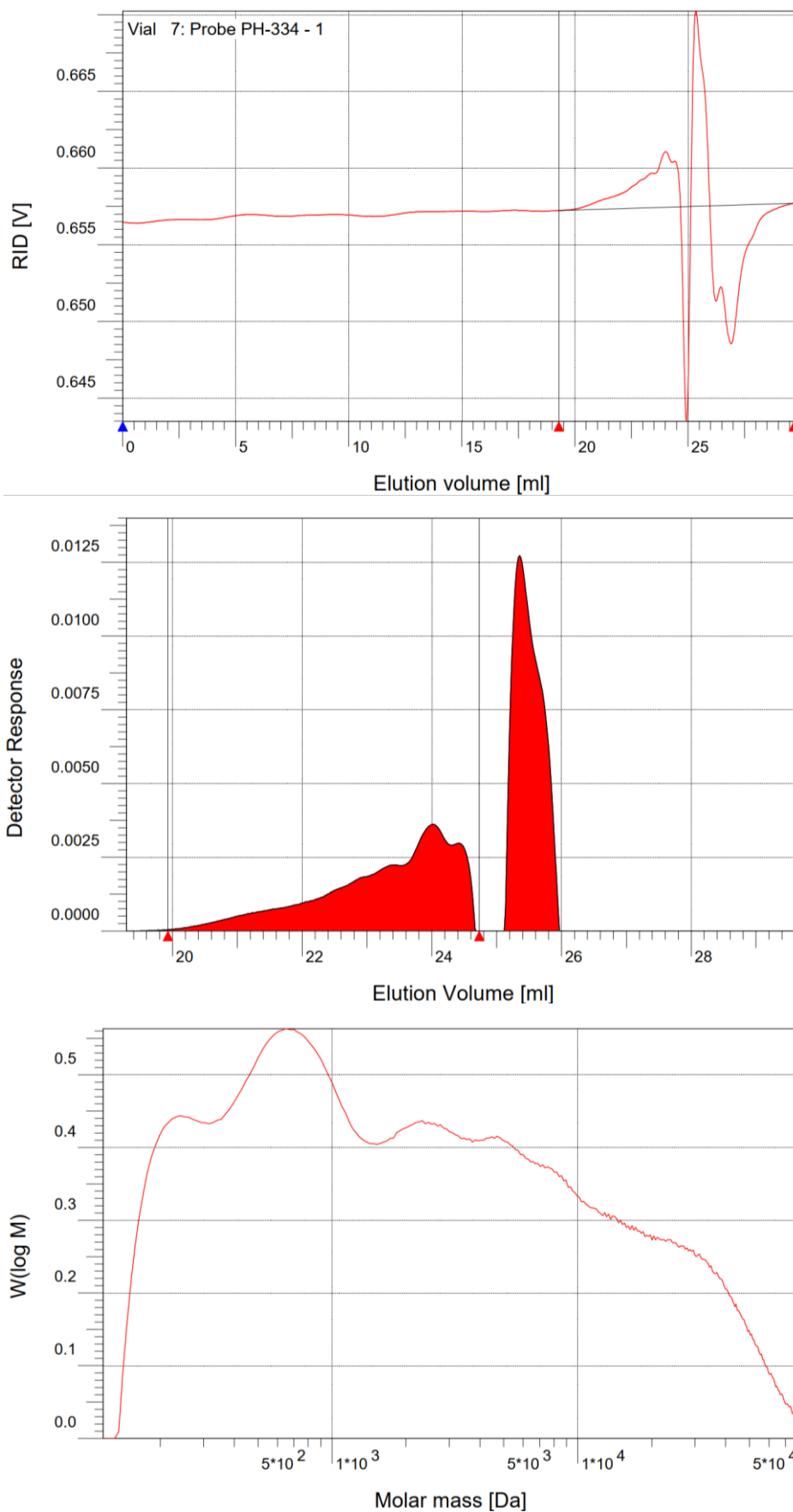


Figure S49. Gel-permeation chromatograms of isolated polymer from the dehydropolymerisation of $\text{H}_3\text{B}\cdot\text{NMeH}_2$ with 1 mol% **2a** in the presence of 50 equivalents $[\text{BH}_2(\text{NMeH}_2)_2]\text{Cl}$ ($[\text{H}_3\text{B}\cdot\text{NMeH}_2] = 0.11\text{M}$, toluene, $T = 25^\circ\text{C}$).

Computational Details

All structures have been optimised at the M06L functional¹¹ and TZVP basis set¹² (LANL2DZ for Rh¹³) in the gas phase and also under the consideration of solvation effect (SMD) of toluene using self-consistent reaction field theory.¹⁴ The corresponding frequency calculation was used to characterise the nature of the optimised structures using the same methods, i.e., energy minimums without imaginary frequencies or transition states with only one imaginary frequency; and the imaginary model connects the initial and the final states. The thermal corrections to Gibbs free energy at 298 K from the frequency analysis were added to the total electronic energies, and we therefore used the corrected Gibbs free energy (ΔG) at 298 K for our energetic discussion and comparison. All calculations were carried out by using the Gaussian 16 program.¹⁵ Although all molecular structures have been optimised and characterised in the gas phase at M06L, some of the structures could not be optimised in toluene solution. For the energetic discussion, we carried out single-point energy calculations of these structures in toluene using the corresponding gas phase geometries; and this information was labeled accordingly (marked with *).

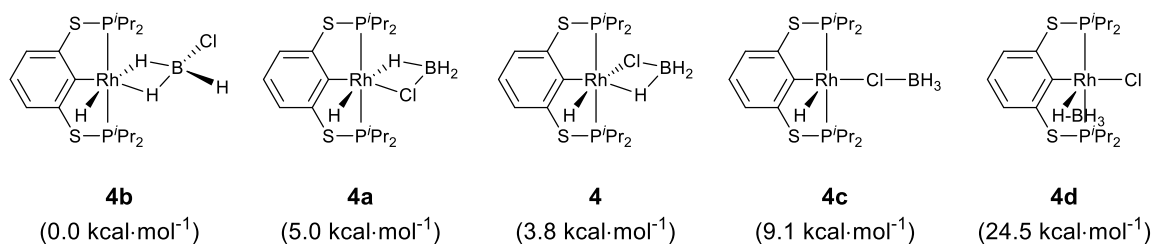


Figure S50. Thermodynamic consideration of different isomers of substitution of pyridine in **2a** by BH₃.

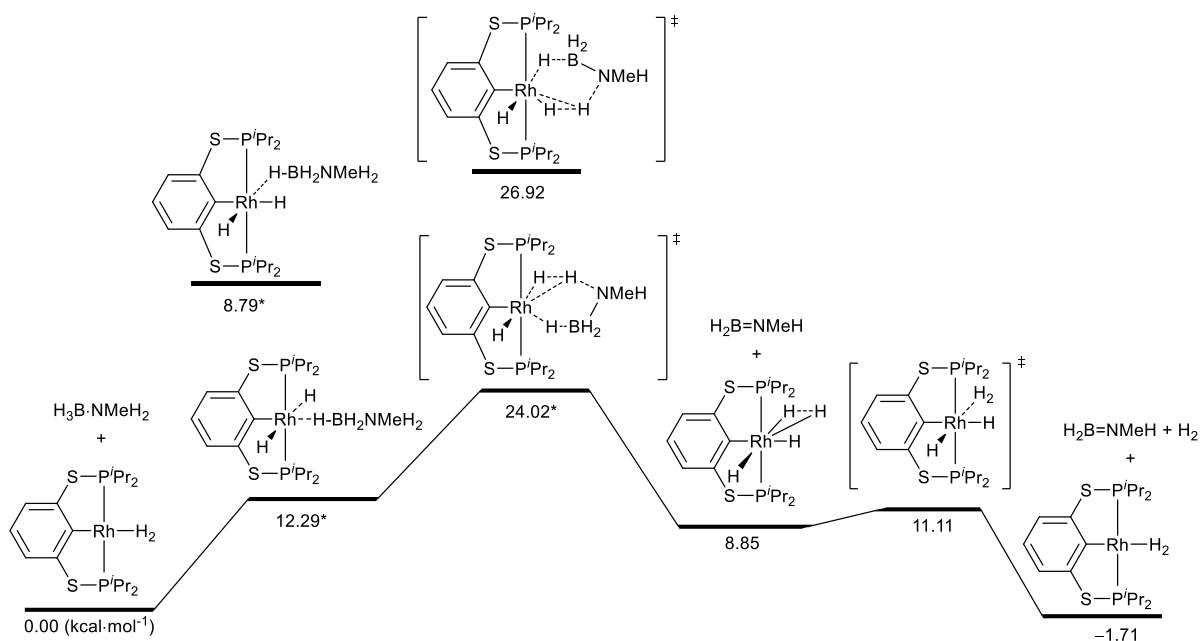


Figure S51. Proposed concerted pathway for dehydrogenation of H₃B·NMeH₂ with **2a**. Note that the computed barriers are very high and not compatible with very fast and quantitative conversion at room temperature.

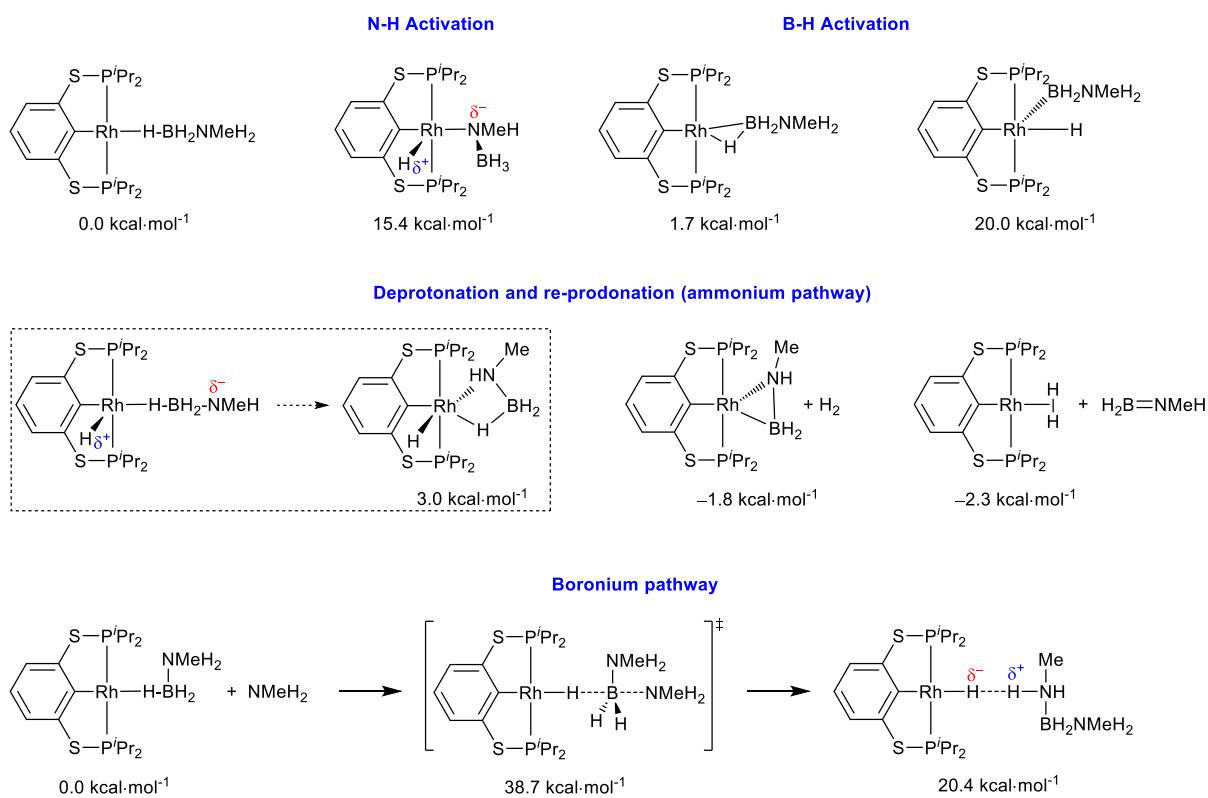
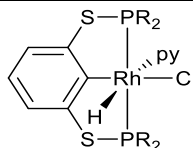
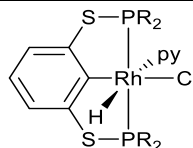
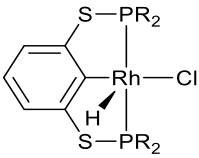
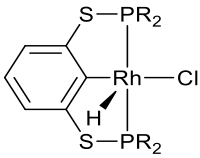
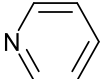
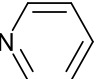
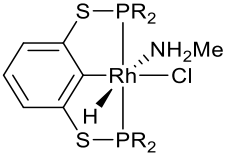
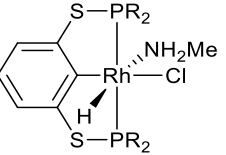


Figure S52. Proposed structures and Gibbs free energies for oxidative N-H and B-H addition at Rh(I), ammonium and boronium pathways.

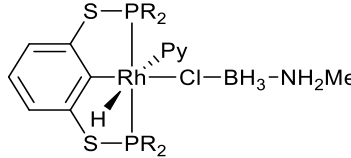
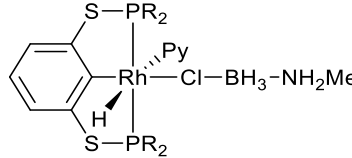
Table S2. M06L computed energetic data and optimised cartesian coordinates in the gas phase and in toluene solution (R = *i*Pr).

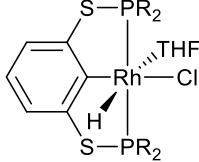
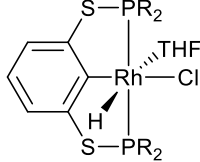
M06L/FOpt in gas phase	M06L-SCRF-SMD/FOpt in toluene solution
 <p>2a</p>	 <p>2a</p>
HF=-3002.6848583 ZPE= 0.556117 NImag=0 Htot=-3002.090796 Gtot=-3002.196171	HF=-3002.7101859 ZPE= 0.555688 NImag=0 Htot=-3002.116475 Gtot=-3002.222065
C,0,-1.8018246937,0.0963394915,-0.3875173407 C,0,-4.6464495908,0.0748415417,-0.4505827185 C,0,-2.5384200853,-0.9999111811,-0.8809539158 C,0,-2.5779782987,1.2067869025,0.0057750197 C,0,-3.9715581112,1.2025329431,-0.0199774366 C,0,-3.9316240741,-1.0251431378,-0.8898817476 H,0,-4.5187913909,2.0863022002,0.2835346162 H,0,-4.4510521944,-1.9050136929,-1.2486495358 H,0,-5.728775684,0.0598626805,-0.462667452 P,0,0.1793051177,-2.1777011791,-0.7441720766 P,0,0.0662082735,2.3871814841,-0.3458062538 S,0,-1.7480039829,-2.4398586626,-1.6001295421 S,0,-1.8305552885,2.7583946011,0.5395396197 C,0,1.3105774594,-2.8255468134,-2.0750799883 H,0,0.8629433278,-3.7695862708,-2.4076496506 C,0,0.2271069739,-3.5023380883,0.5815219647 H,0,1.1915378044,-3.3386434538,1.0779300565 C,0,-0.8970873697,-3.2853354531,1.5831654797 H,0,-0.768347612,-3.9426310997,2.4447375024 H,0,-1.8610838029,-3.5182144149,1.1279958587 H,0,-0.9453182626,-2.2605553894,1.9425992896 C,0,0.1679567574,-4.9142064908,0.0188232208 H,0,0.1525170199,-5.6405583316,0.8336023639 H,0,1.0134615283,-5.1586387542,-0.6217899874 H,0,-0.7487061106,-5.0573748491,-0.5582253375 C,0,1.3754961534,-1.8624708902,-3.2485434602 H,0,0.3837291469,-1.6024509463,-3.6206032088 H,0,1.9371231034,-2.3139918559,-4.0680614798 H,0,1.8858335713,-0.9437293178,-2.9541069074 C,0,2.6987126633,-3.0836246602,-1.5000408191 H,0,3.3561370789,-3.4601661422,-2.2854438014 H,0,2.6966939362,-3.8207197769,-0.6969601843 H,0,3.1298981972,-2.1576195154,-1.1160271427 C,0,1.2179060285,3.5017615278,0.5979445007 H,0,2.134533772,3.4467779498,0.0001772434 C,0,1.5228560447,2.9342786744,1.9731184464 H,0,2.1938428731,3.6060969566,2.51082661 H,0,2.0090816266,1.964330957,1.886515294 H,0,0.6150157257,2.8239605522,2.5712315371 C,0,0.7309273363,4.9414732437,0.6659367254 H,0,0.5532186999,5.3793252711,-0.3156638886 H,0,1.4759067303,5.5605543158,1.1685273797 H,0,-0.1940302712,5.0203589966,1.2410461361 C,0,-0.0077300932,3.142335361,-2.0496818228 H,0,-0.1753466291,4.2128130122,-1.8925498884 C,0,1.3278951144,2.9243388635,-2.7485185586 H,0,1.2928635555,3.3420847899,-3.7559486591 H,0,1.5552031874,1.8594432009,-2.8298552903 H,0,2.1613757739,3.3911246458,-2.2237198116 C,0,-1.1655737915,2.5838927597,-2.8587459889	C,0,-1.7951201984,0.1034862577,-0.3920354298 C,0,-4.6417815691,0.0749467163,-0.4408974928 C,0,-2.5327386421,-0.9943656747,-0.8818366974 C,0,-2.5727430417,1.2125005502,0.0041526023 C,0,-3.966809778,1.2038645488,-0.0137944206 C,0,-3.9263800868,-1.0230830898,-0.8839147987 H,0,-4.5160000739,2.0853503643,0.2934818423 H,0,-4.4463625409,-1.90406008,-1.2398028447 H,0,-5.7243000506,0.0573374327,-0.4469380073 P,0,0.1847991199,-2.1794283407,-0.7419920316 P,0,0.0710635163,2.3992240568,-0.35114671 S,0,-1.7437518614,-2.4338404592,-1.6028098842 S,0,-1.8290249054,2.7660660554,0.5332571783 C,0,1.3079371495,-2.8398955351,-2.0742864658 H,0,0.8575302493,-3.7868363645,-2.3939199865 C,0,0.2261018265,-3.4946228803,0.5918239972 H,0,1.1857423046,-3.3200035718,1.0934213728 C,0,-0.9057026331,-3.2758984318,1.5839907412 H,0,-0.7553504424,-3.8939780987,2.4711099029 H,0,-1.8624183473,-3.5598396827,1.1421444758 H,0,-0.9906353781,-2.2407035097,1.906167882 C,0,0.1822180353,-4.9123477686,0.0447800812 H,0,0.1624980917,-5.6274058287,0.8698972194 H,0,1.036954056,-5.1630117694,-0.5812776242 H,0,-0.726343871,-5.0741205548,-0.540477182 C,0,1.3693892221,-1.8920885723,-3.2590718894 H,0,0.3785597036,-1.6373834577,-3.6378216662 H,0,1.9308764313,-2.3530899822,-4.0739119393 H,0,1.8784094649,-0.9671092042,-2.9819678387 C,0,2.6980016103,-3.0975363492,-1.5069302562 H,0,3.345337941,-3.4976306516,-2.2895682852 H,0,2.6994164832,-3.8157996225,-0.6870062731 H,0,3.1427942122,-2.1683600702,-1.147121288 C,0,1.2177407851,3.5142923442,0.5985950141 H,0,2.1400824324,3.4540649323,0.0105045627 C,0,1.5052171566,2.9538481471,1.9796456312 H,0,2.1945898814,3.6133275981,2.5100131503 H,0,1.9650101937,1.969498833,1.9099028319 H,0,0.5963048455,2.8752004122,2.5809874808 C,0,0.7412538669,4.9571607397,0.6530602581 H,0,0.579518161,5.392530417,-0.3326527038 H,0,1.4874131141,5.5720631308,1.1597561977 H,0,-0.1880800021,5.0512770212,1.2193386094 C,0,-0.0156067905,3.1599100282,-2.0524293117 H,0,-0.2044972796,4.2255360404,-1.8886265083 C,0,1.3221487438,2.9760032605,-2.7541331239 H,0,1.2788942446,3.4098719172,-3.7548379814 H,0,1.5665054323,1.9167010085,-2.8589691906 H,0,2.1485797125,3.4511548676,-2.2249277417 C,0,-1.1589128819,2.5854300542,-2.8694318775

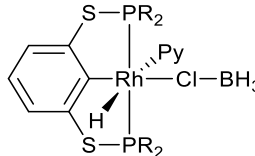
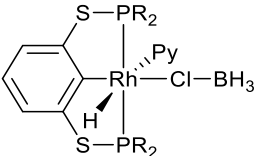
<p>H,0,-1.1943715303,3.0614535779,-3.8393364712 H,0,-2.1262953056,2.7543808146,-2.3731980164 H,0,-1.0559099476,1.5090882513,-3.0155399557 Rh,0,0.2355000051,0.102140754,-0.2908271156 H,0,0.1987943144,0.2017820732,-1.8383372638 Cl,0,2.7714837207,0.3411419643,-0.3297384211 N,0,0.3150974802,-0.1091138219,2.0161268758 C,0,0.4393888458,-0.4735897094,4.7669736727 C,0,1.4315952741,-0.5658625709,2.5977573472 C,0,-0.7376793639,0.1664475119,2.7940914186 C,0,-0.7148566162,0.0049691189,4.168860097 C,0,1.5302645597,-0.7660589941,3.9637938209 H,0,2.2652319091,-0.7404085646,1.9235454009 H,0,-1.625212913,0.5197090382,2.2827790281 H,0,-1.5927410423,0.2483785841,4.7519731729 H,0,2.4540266178,-1.1400207426,4.3846222016 H,0,0.4880773303,-0.6155999969,5.8394588152</p>	<p>H,0,-1.1967798715,3.0762985002,-3.8436046507 H,0,-2.1264272014,2.7293689302,-2.3881044474 H,0,-1.0263228802,1.5156486751,-3.0444102986 Rh,0,0.2419500591,0.1089026304,-0.2929140125 H,0,0.2126090783,0.2125684256,-1.8410097231 Cl,0,2.8010560602,0.34512247,-0.3277368542 N,0,0.3143051836,-0.1165783242,2.0165900392 C,0,0.4315011971,-0.5202816349,4.7641408395 C,0,1.4178474514,-0.6104008963,2.5931772112 C,0,-0.7301167167,0.1744374595,2.800880264 C,0,-0.7105296084,-0.0053756562,4.1731364311 C,0,1.5136151994,-0.830413963,3.9560894878 H,0,2.2462960336,-0.8044824351,1.9195804648 H,0,-1.6103822758,0.5562353797,2.2982166133 H,0,-1.5822646063,0.2521589712,4.7595647965 H,0,2.4279197364,-1.2340103372,4.3702815231 H,0,0.4773961301,-0.6774055359,5.8346283113</p>
 <p>3a</p>	 <p>3a</p>
<p>HF= -2754.3249639 ZPE= 0.464161 NImag=0</p> <p>Htot= -2753.827978 Gtot= -2753.923201</p> <p>C,0,-2.035017852,-0.0189715434,0.9969360317 C,0,-4.8367514386,-0.0900344467,1.4677708979 C,0,-2.7680028564,-1.2240635946,1.0111517144 C,0,-2.8009826047,1.1529564946,1.172228376 C,0,-4.1718193587,1.1204305877,1.4194394744 C,0,-4.1382960073,-1.2643048162,1.2590216536 H,0,-4.7128445136,2.0465757458,1.5674813709 H,0,-4.6520017414,-2.2170687125,1.2834118176 H,0,-5.9013588982,-0.1178626084,1.6610207711 P,0,0.0047017985,-2.2847299982,0.7567351173 P,0,-0.0781596195,2.3128940763,0.88340073 S,0,-2.0385679618,-2.8302832075,0.6885745692 S,0,-2.1226888014,2.8109427387,1.0630120628 Cl,0,2.4179586723,0.1060272586,1.2851577022 C,0,0.7689851416,-3.154373033,-0.6937379719 H,0,1.8408461563,-2.9958285461,-0.528344507 C,0,0.6340434846,-3.1737705544,2.2737020532 H,0,0.1193395696,-4.1409973003,2.2788344095 C,0,2.1393903807,-3.3881421072,2.232820261 H,0,2.4678136262,-3.8475857679,3.1667872785 H,0,2.6682386349,-2.4407588099,2.1204065392 H,0,2.4441236691,-4.049396084,1.42146303 C,0,0.2074978193,-2.3723745546,3.4948826145 H,0,0.4578095553,-2.9077750707,4.4117025542 H,0,-0.8660935223,-2.1767692995,3.5025280857 H,0,0.7307254044,-1.4129476464,3.5169656468 C,0,0.4643263625,-4.6440953353,-0.7065426906 H,0,0.7652245157,-5.141849362,0.2156421234 H,0,0.9897238331,-5.1311972145,-1.529485814 H,0,-0.60305751,-4.8226763816,-0.8520195518 C,0,0.3675498712,-2.4709610617,-1.9900029203 H,0,0.8274894481,-2.974252221,-2.8415030256 H,0,0.6806198644,-1.4267995704,-2.0033711483 H,0,-0.7150199871,-2.501238862,-2.130575109 C,0,0.73835428,3.0416189275,2.3835325367 H,0,1.7971061408,2.817413992,2.2095730625</p>	<p>HF=-2754.3491412 ZPE= 0.463968 NImag=0</p> <p>Htot= -2753.852322 Gtot= -2753.946721</p> <p>C,0,-2.0040817204,-0.0211806371,1.0243448936 C,0,-4.8397858181,-0.079518097,1.2823078901 C,0,-2.7597486791,-1.2008833949,0.8457813277 C,0,-2.7656640222,1.1343949115,1.3035584816 C,0,-4.1528073093,1.1098910085,1.4365587514 C,0,-4.1456980456,-1.2380428788,0.9869589283 H,0,-4.6905727338,2.0245191437,1.6541423926 H,0,-4.6765829205,-2.1734544717,0.8606287863 H,0,-5.917104004,-0.1026975536,1.3868916695 P,0,0.0034706359,-2.2951297661,0.7503271375 P,0,-0.044548942,2.3091621665,0.9976562806 S,0,-2.0297183324,-2.7810210269,0.4050910993 S,0,-2.0460615493,2.7674639526,1.5165394077 Cl,0,2.5373828361,0.0473940729,1.0389989417 C,0,0.923673628,-3.1328109787,-0.6240908273 H,0,1.9696774833,-2.9784263263,-0.3363704672 C,0,0.4351154306,-3.2310077959,2.3068415255 H,0,-0.0174148536,-4.2223217139,2.1979509935 C,0,1.9404148974,-3.366748656,2.4707904208 H,0,2.1651655951,-3.837710128,3.4296993212 H,0,2.4340696692,-2.3930869925,2.4516820949 H,0,2.389579108,-3.9840191654,1.6923272578 C,0,-0.2055510514,-2.5184430829,3.4876545121 H,0,-0.0481138725,-3.0849991118,4.4067299058 H,0,-1.2810832253,-2.3880942198,3.35803341 H,0,0.239093149,-1.5303955246,3.6360015019 C,0,0.6279713741,-4.6220396528,-0.6967995397 H,0,0.8297163288,-5.1378550296,0.2425331472 H,0,1.2460036036,-5.0898051462,-1.4650989137 H,0,-0.4144302258,-4.8074401905,-0.9655210092 C,0,0.6751812908,-2.4275893368,-1.9457901006 H,0,1.2329182439,-2.9210187464,-2.7433067178 H,0,0.993495476,-1.3854692286,-1.911852877 H,0,-0.3821170319,-2.4518196805,-2.2184160954 C,0,0.9731778884,3.0822799328,2.3436601824 H,0,1.9974962596,2.9080936287,1.9956554336</p>

<p>C,0,0.2817506917,2.2719234484,3.6125147276 H,0,0.774141593,2.6559654943,4.5067464909 H,0,0.5282782811,1.2116926001,3.5272269609 H,0,-0.7967853743,2.3629433193,3.7583753445 C,0,0.52288931,4.5386367063,2.515660039 H,0,0.8964299956,5.0930053972,1.6540348805 H,0,1.0413429371,4.9187921699,3.3974270664 H,0,-0.5371038767,4.7734557585,2.6351057017 C,0,0.5083737508,3.3154986684,-0.5681430186 H,0,0.1056215029,4.3242528581,-0.420906541 C,0,2.0301527058,3.362554518,-0.5891997515 H,0,2.3724074641,3.8700895147,-1.4923148455 H,0,2.4555479979,2.3572201616,-0.5828817024 H,0,2.4427332651,3.8985942395,0.2652688312 C,0,-0.0592873071,2.7345224073,-1.8528921667 H,0,0.1889667878,3.3748561192,-2.7002636557 H,0,-1.1444289714,2.6343049523,-1.8113203353 H,0,0.363783698,1.7465748391,-2.0457724673 Rh,0,-0.0088105711,0.0206248764,0.8133681302 H,0,-0.6348472356,0.0435903404,-0.5856551349</p>	<p>C,0,0.7712493876,2.3042100975,3.6327317345 H,0,1.3874021922,2.7230789236,4.4297218652 H,0,1.0611872567,1.2583726377,3.5127458066 H,0,-0.2688926094,2.3403350693,3.9642165868 C,0,0.7238032078,4.5704451828,2.5104400288 H,0,0.9151009633,5.13400538,1.5966931357 H,0,1.3774756112,4.97607451,3.2848426684 H,0,-0.3046262256,4.7696918169,2.82055232 C,0,0.2877871806,3.3060701307,-0.5375330567 H,0,-0.0579416604,4.3201389467,-0.3087047481 C,0,1.7790221117,3.3240269928,-0.8372283029 H,0,1.9618129739,3.850373677,-1.775751761 H,0,2.1740827887,2.3111709436,-0.9393655733 H,0,2.3574034943,3.8269225439,-0.0620483607 C,0,-0.5176937744,2.7604213246,-1.7035221815 H,0,-0.427143506,3.4236021979,-2.5652131033 H,0,-1.5783355311,2.6648936095,-1.4667539105 H,0,-0.1503049648,1.7774157756,-2.0051489465 Rh,0,0.0275907703,0.006903736,0.9203000745 H,0,-0.2891360269,0.0685267201,-0.5680951226</p>
 <p>Pyridine</p>	 <p>Pyridine</p>
<p>HF=-248.3244139 ZPE= 0.088474 NImag=0</p> <p>Htot= -248.230683 Gtot= -248.263353</p> <p>N,0,1.4403521216,-0.0770720414,1.8566881441 C,0,3.533232968,-0.7800776878,3.5636365391 C,0,1.9356624704,-1.313627091,1.8792528959 C,0,1.9901044333,0.8084425715,2.6864749639 C,0,3.0310582193,0.5111011182,3.5541191449 C,0,2.9739547451,-1.7147104373,2.7074343077 H,0,1.4754010553,-2.0220406805,1.1962783638 H,0,1.5737464403,1.8113214304,2.6544654089 H,0,3.435815797,1.2753505452,4.2050671379 H,0,3.3329170986,-2.735493195,2.6793671878 H,0,4.3455449906,-1.052935062,4.2261537277</p>	<p>HF=-248.3316262 ZPE= 0.088554 NImag=0</p> <p>Htot= -248.237821 Gtot= -248.270482</p> <p>N,0,1.4417676533,-0.0775307768,1.8577986243 C,0,3.5324030796,-0.7797883486,3.5629318789 C,0,1.9356834601,-1.3152670552,1.8786654366 C,0,1.9902088777,0.8100555505,2.6871249039 C,0,3.030790452,0.5115931945,3.5540184299 C,0,2.9736669576,-1.7149987205,2.7070367488 H,0,1.4758104046,-2.0239947645,1.1960190141 H,0,1.5742472787,1.8129334591,2.6555625862 H,0,3.4357002356,1.2755782102,4.205061872 H,0,3.3327915608,-2.7356543992,2.6792139984 H,0,4.3447203795,-1.0526668792,4.2255043287</p>
 <p>2a-NMeH₂</p>	 <p>2a-NMeH₂</p>
<p>HF=-2850.2312163 ZPE= 0.532837 NImag=0</p> <p>Htot= -2849.662191 Gtot= -2849.762579</p> <p>C,0,1.6220184214,-0.0793202858,-0.0064547876 Rh,0,-0.4019234031,-0.266340029,-0.094343411 P,0,-0.125549344,-0.0486806049,-2.3536808332 P,0,-0.4412540934,0.0924141064,2.2004214184 H,0,-0.517986698,1.2809594482,-0.0857615978 N,0,-0.1375322928,-2.6000757505,-0.171270998 Cl,0,-2.9122140839,-0.4934094032,-0.3820255256 C,0,4.4546528983,0.0429480085,0.136438982 C,0,2.2952774383,0.4291652379,1.1209211939 C,0,2.448922096,-0.4717125155,-1.0768724608 C,0,3.8392878939,-0.4154603684,-1.0153466216</p>	<p>HF=-2850.254266 ZPE= 0.532562 NImag=0</p> <p>Htot= -2849.685451 Gtot= -2849.785795</p> <p>C,0,1.6102525221,-0.0701342521,-0.0117085298 Rh,0,-0.4136076857,-0.2665676678,-0.0934307931 P,0,-0.1424957358,-0.0410348002,-2.3607096173 P,0,-0.4490881679,0.0913767228,2.2095703527 H,0,-0.5485331045,1.2811000264,-0.0826932715 N,0,-0.1093065959,-2.5915630808,-0.1756410619 Cl,0,-2.9469935988,-0.5482732637,-0.3344460289 C,0,4.446166455,0.0302829376,0.1354671389 C,0,2.2874018872,0.4267149107,1.1191731646 C,0,2.4368866495,-0.463938749,-1.082604214 C,0,3.8280058303,-0.4189987908,-1.0182915532</p>

<p>C,0,3.685547254,0.4724464217,1.2040834216 H,0,4.4314738941,-0.71378739,-1.8713888801 H,0,4.1603191464,0.8455329864,2.1030208922 H,0,5.5348395981,0.0801907046,0.1963709459 S,0,1.4065463438,1.1041949608,2.5249391635 S,0,1.7567705246,-1.0029109025,-2.6599760854 C,0,-1.6940640578,1.301883785,2.862449897 H,0,-1.2902866068,1.648673209,3.8210029303 C,0,-0.396336941,-1.2555690578,3.5043566524 H,0,-1.3287453324,-1.8088560437,3.3378677057 C,0,0.788467019,-2.1766550121,3.2598593531 H,0,0.7474987611,-3.039254367,3.9265047589 H,0,1.7269285809,-1.6527427837,3.4483891518 H,0,0.8244010639,-2.5461853864,2.2367059888 C,0,-0.3665725239,-0.7177474884,4.9261976408 H,0,-0.2954752799,-1.5421801818,5.63814841 H,0,-1.2535670273,-0.1406378191,5.1818541994 H,0,0.5088689092,-0.0821017501,5.0774555444 C,0,-1.8554768213,2.4905362131,1.9301070912 H,0,-0.8992615682,2.9596351253,1.6945688826 H,0,-2.4954280843,3.2415707579,2.3963316444 H,0,-2.3254353887,2.1765033742,0.9964015947 C,0,-3.0261360893,0.5944811643,3.0859504704 H,0,-3.7632102413,1.3105517441,3.4529012332 H,0,-2.9619584514,-0.2098863548,3.8189256662 H,0,-3.3992485336,0.1778970224,2.1484119804 C,0,-1.2635603403,-0.8832458412,-3.5647385773 H,0,-2.2021556622,-0.3424786849,-3.3977943746 C,0,-1.5031799819,-2.332323981,-3.1783690593 H,0,-2.2194862835,-2.7883783692,-3.862929425 H,0,-1.9219789486,-2.3929177425,-2.1736479697 H,0,-0.5823477991,-2.9197202841,-3.2376365682 C,0,-0.8251514591,-0.7360603757,-5.0134328783 H,0,-0.7678637066,0.3033483858,-5.3337698253 H,0,-1.5379918254,-1.2383822127,-5.6694964724 H,0,0.151179881,-1.1943984047,-5.1853608613 C,0,0.0507899979,1.6876111284,-3.0037930352 H,0,0.340477833,1.5849086198,-4.0543239773 C,0,-1.3001973757,2.3846888557,-2.9009031117 H,0,-1.2089720016,3.423536462,-3.2213003292 H,0,-1.6630793824,2.3814846568,-1.8704408323 H,0,-2.0652145149,1.9141072522,-3.5186907876 C,0,1.1398998023,2.4529494953,-2.2720535643 H,0,1.2235520686,3.4586599915,-2.6869203406 H,0,2.1130251721,1.9707860277,-2.3625606063 H,0,0.9111239146,2.547475675,-1.2087965226 C,0,-1.2102922767,-3.4212069632,0.3947208392 H,0,-0.0036970055,-2.8263892894,-1.1518708619 H,0,0.7524875473,-2.8142765602,0.2667790617 H,0,-1.0632488568,-4.4937165834,0.2407373847 H,0,-1.2789727867,-3.2301304333,1.4647018294 H,0,-2.158240891,-3.1105394999,-0.0417129463</p>	<p>C,0,3.6784870533,0.45991167,1.2038287983 H,0,4.419756595,-0.7192019646,-1.8742831408 H,0,4.1556685228,0.8244959734,2.1052089518 H,0,5.5267375529,0.0590410501,0.1968815129 S,0,1.4054466961,1.0963625906,2.5284938947 S,0,1.7465143717,-0.9880402159,-2.666094119 C,0,-1.6780221219,1.3189421354,2.8879001833 H,0,-1.2579855248,1.6468337733,3.8459372683 C,0,-0.4136437527,-1.2614302465,3.5068826288 H,0,-1.3484001062,-1.8076688058,3.3303184684 C,0,0.7651191886,-2.1901002274,3.2661665359 H,0,0.7002465539,-3.0640092981,3.916512719 H,0,1.7074967448,-1.6847262011,3.485284736 H,0,0.8191334114,-2.5457641338,2.238899882 C,0,-0.3899840933,-0.7338413801,4.9319450253 H,0,-0.3338898387,-1.5661855735,5.6365487747 H,0,-1.2726393053,-0.1504697342,5.1888503543 H,0,0.4906762451,-0.109525648,5.1010035235 C,0,-1.8258800618,2.52302426,1.9750566294 H,0,-0.8650616848,2.9768857521,1.7027820463 H,0,-2.4392574237,3.283112461,2.4628460562 H,0,-2.3206475114,2.2403010457,1.0442929232 C,0,-3.0215635642,0.6409227172,3.1232798878 H,0,-3.7325287629,1.3661490862,3.5235489205 H,0,-2.9653016093,-0.1838583171,3.8338487053 C,0,-3.4264877915,0.2555095552,2.1859573182 C,0,-1.2653518988,-0.887733603,-3.578281849 H,0,-2.2072281809,-0.3471213628,-3.4325611935 C,0,-1.5035264945,-2.334248319,-3.1843801933 H,0,-2.2295455927,-2.7896885119,-3.8596617259 H,0,-1.9089794548,-2.3969525625,-2.1743915746 H,0,-0.5872506624,-2.9272414701,-3.2517856451 C,0,-0.8136230887,-0.7514832668,-5.0232088158 H,0,-0.7508577814,0.2846999021,-5.3535240617 H,0,-1.524291927,-1.256332845,-5.680275777 H,0,0.1613146328,-1.2162521079,-5.1873688369 C,0,0.0414506938,1.6922682687,-3.0198053477 H,0,0.3523693787,1.5777502209,-4.0628449475 C,0,-1.3081579568,2.3933144091,-2.9565225353 H,0,-1.2118083352,3.4176463149,-3.320588289 H,0,-1.6783730839,2.4413726174,-1.9297262627 H,0,-2.0709921553,1.9007873849,-3.5601369869 C,0,1.1129015058,2.4696041066,-2.2766347393 H,0,1.203189834,3.4693556632,-2.7053858874 H,0,2.0910753393,1.9927172961,-2.3406230549 H,0,0.8627216912,2.583302413,-1.2196541051 C,0,-1.152647825,-3.4585607725,0.3736612448 H,0,0.0468511833,-2.8212303997,-1.1526705947 H,0,0.7804301025,-2.7823721979,0.2745571419 H,0,-0.9364017348,-4.5231889663,0.2479431983 H,0,-1.2732493769,-3.2518376979,1.4362901285 H,0,-2.1016349514,-3.2227467306,-0.104241561</p>
<p>H₂N-CH₃ Methylamine HF=-95.8737154 ZPE= 0.064226 NImag=0 Htot= -95.805130 Gtot= -95.832389 H,0,0.2368203267,0.1859868723,0.0611995244 N,0,0.0062560567,0.0085674907,1.0303647046 H,0,-0.9971255207,-0.119335759,1.0583796095 C,0,0.675816495,-1.1977185857,1.4895544642 H,0,1.7550466275,-1.0501604186,1.4534451133 H,0,0.44967731,-2.115226662,0.928793678 H,0,0.4193054855,-1.3806708709,2.5328883226</p>	<p>H₂N-CH₃ Methylamine HF=-95.8762499 ZPE= 0.064238 NImag=0 Htot= -95.807665 Gtot= -95.834904 H,0,0.2357190965,0.180932334,0.0607074557 N,0,0.0073669111,0.0121370821,1.0328322742 H,0,-0.9959467915,-0.1238261533,1.056045053 C,0,0.6765048572,-1.1950171771,1.4912334015 H,0,1.7567503146,-1.0516542317,1.4533748493 H,0,0.446015872,-2.1085636006,0.9263030219 H,0,0.4193865207,-1.3825661866,2.534129361</p>

<p>H₃B-NH₂Me Methylamine borane</p>	<p>H₃B-NH₂Me Methylamine borane</p>
<p>HF=-122.545698 ZPE= 0.099196 NImag=0</p> <p>Htot= -122.440713 Gtot= -122.472487</p> <p>H,0,-0.0549461567,0.0090507934,-0.2412962499 B,0,-0.132065113,0.0019460224,0.9620279567 H,0,-0.5973400259,-1.0140522003,1.4128845654 H,0,-0.6216994221,1.0050127494,1.4182103129 N,0,1.4304015913,0.027179864,1.4804960242 H,0,1.8967147614,-0.816852554,1.162541542 H,0,1.4417195632,-0.0172870213,2.4948100327 C,0,2.1877371437,1.2084337475,1.0302046257 H,0,3.2170504693,1.1990652356,1.3873573983 H,0,1.678082276,2.0973279008,1.3913379163 H,0,2.1723456836,1.2287531962,-0.0559115635</p>	<p>HF=-122.5560258 ZPE= 0.099280 NImag=0</p> <p>Htot= -122.450984 Gtot= -122.482722</p> <p>H,0,-0.0732079544,0.0023047759,-0.2393568214 B,0,-0.1220729743,-0.0010917834,0.9672636192 H,0,-0.598804902,-1.0164573152,1.4138277251 H,0,-0.6380522178,0.9949120209,1.4145600049 N,0,1.4248648282,0.0323805972,1.4754838651 H,0,1.8984601748,-0.8097990722,1.160849293 H,0,1.4443652278,-0.0118128598,2.4904817639 C,0,2.1887103418,1.2109681939,1.0290159296 H,0,3.2143296105,1.1859490576,1.3942999189 H,0,1.6919190297,2.1060466082,1.3936571203 H,0,2.1874896017,1.2351748086,-0.0574198591</p>
 <p>2a+BH₃NH₂Me-Eq</p>	 <p>2a+BH₃NH₂Me-Eq*</p>
<p>HF=-3125.2008883 ZPE= 0.652527 NImag=1 (-165)</p> <p>Htot= -3124.505290 Gtot= -3124.621028</p> <p>C,0,-1.3743003745,0.1633680453,-0.5001757877 Rh,0,0.4812659623,-0.1091097759,0.2958672649 H,0,1.0711479345,0.0630607831,-1.1244504921 P,0,0.6367202914,2.1959930672,0.3094233565 P,0,0.4025156512,-2.3163941331,-0.4077836564 N,0,-0.4309362051,-0.3833326246,2.4521621715 B,0,4.325069406,0.3695440238,-0.186964402 C,0,-4.030041408,0.524859811,-1.4604236717 C,0,-2.0642132353,-0.8407011287,-1.2090706579 C,0,-2.0904923223,1.3665816443,-0.3209844309 C,0,-3.3886967542,1.5521263475,-0.7927058627 C,0,-3.3702797241,-0.6715222554,-1.6687137256 H,0,-3.8849971202,2.5021951518,-0.6394071507 H,0,-3.8634974272,-1.4816229694,-2.1913363414 H,0,-5.0405956108,0.6591522671,-1.8244636276 S,0,-1.339434456,-2.4259533576,-1.6155274229 S,0,-1.3979534753,2.775884722,0.5568528655 C,0,1.7145038419,-2.9020966975,-1.600676067 H,0,1.3172479855,-3.8503572923,-1.9824079209 C,0,0.200506306,-3.7403324682,0.7921852615 H,0,1.0238649962,-3.58025794,1.4994850613 C,0,-1.1260978433,-3.6217796764,1.5290270342 H,0,-1.1392711945,-4.2860220604,2.3946925854 H,0,-1.949938988,-3.9073983062,0.8739851538 H,0,-1.3237400787,-2.6099243704,1.8751419394 C,0,0.3315064153,-5.1139112767,0.1526235021 H,0,0.1476582502,-5.8897021892,0.8983015918 H,0,1.3164984484,-5.2969338668,-0.2729341833 H,0,-0.4114899966,-5.2471171255,-0.637629542 C,0,1.8891666834,-1.9458590892,-2.7682067495 H,0,0.9398310969,-1.6935004709,-3.2414358449 H,0,2.5326101761,-2.4020744266,-3.523008032 H,0,2.3722286564,-1.0240479283,-2.4404104009</p>	<p>HF=-3125.2277501 ZPE= 0.652570 NImag=1 (-194)</p> <p>Htot= -3124.530367 Gtot= -3124.654763</p> <p>*Single-Point Energy using Gas Phase Geometry</p>

<p>C,0,3.0387469815,-3.1489981476,-0.8903861338 H,0,3.7450194089,-3.6090749727,-1.5842796997 H,0,2.9463791555,-3.8102211155,-0.0281770764 H,0,3.4719514253,-2.2119958082,-0.5414291 C,0,1.5378169409,3.0920999339,1.6634930432 H,0,2.5836061505,2.8426991348,1.4432184912 C,0,1.1887827748,2.5014113866,3.0194062741 H,0,1.7281846077,3.0320032961,3.8054251524 H,0,1.4712258075,1.4510992895,3.0654606833 H,0,0.1201563682,2.5856347236,3.2321393063 C,0,1.3468808993,4.6002111002,1.6167068537 H,0,1.6702727383,5.0361988484,0.6719316097 H,0,1.9281945454,5.0728694326,2.4101464089 H,0,0.3016384032,4.8753416777,1.7741171597 C,0,1.1043636391,3.112720871,-1.2555544431 H,0,0.7025110299,4.117694239,-1.0845233048 C,0,2.6083233114,3.1929240184,-1.4597366525 H,0,2.8190870804,3.7688892384,-2.363743989 H,0,3.0536960829,2.2056667041,-1.5777759104 H,0,3.1235320898,3.6800885613,-0.6314275427 C,0,0.4068072616,2.5200071207,-2.4682156348 H,0,0.6168582164,3.1311113767,-3.3476362469 H,0,-0.6748776686,2.4714636549,-2.3447957183 H,0,0.7655309494,1.5089108134,-2.6731507806 Cl,0,2.7805121588,-0.4329598213,1.3992233097 N,0,5.8060672767,1.1609790744,-2.2440151306 C,0,-1.5221827945,-0.7834151926,4.9846197509 C,0,0.2863637508,-0.9449889129,3.4355794778 C,0,-1.691207454,-0.0260527668,2.7283421656 C,0,-2.2698758757,-0.2043349364,3.9734523334 C,0,-0.2192061925,-1.1616578014,4.7053273233 H,0,1.3044423058,-1.2108688396,3.1762935236 H,0,-2.2530719029,0.4081677096,1.912109137 H,0,-3.2926994993,0.1076189697,4.1362212062 H,0,0.4081600832,-1.6200881859,5.4579541927 H,0,-1.9462292126,-0.9379989387,5.9690044035 H,0,4.4227491398,1.4575222885,0.2859817545 H,0,5.1785875502,-0.4376723477,0.0152301867 H,0,3.5805465771,0.1930418209,-1.0978909293 H,0,5.8771666509,2.1236573832,-2.5484143305 H,0,6.738134584,0.8680266174,-1.9830297743 C,0,5.2740447203,0.3190438362,-3.3015831343 H,0,5.8599052699,0.2941844333,-4.2300168799 H,0,5.181129035,-0.7024061492,-2.9298286105 H,0,4.2640687421,0.6504039483,-3.5505985432</p>	
 <p>2a-THF</p>	 <p>2a-THF</p>
<p>HF=-2986.8367392 ZPE=0.584725 NImag=0</p> <p>Htot=-2986.213436 Gtot=-2986.319948</p> <p>H,0,0.0084684777,-0.104583097,-0.0941241912 Rh,0,1.5307999774,-0.0168120958,-0.01614599 Cl,0,1.585825252,2.4958546209,-0.2444656351 C,0,1.5695849469,-2.0568245104,0.0334349915 C,0,1.8751474225,-4.8866267288,0.1473827782 C,0,1.8846023036,-2.8347508137,-1.1015459225 C,0,1.3616630597,-2.7950679373,1.2166702803 C,0,1.5323163995,-4.1775145421,1.2831866524 C,0,2.0380494649,-4.2185644515,-1.0524536228</p>	<p>HF=-2986.8578043 ZPE=0.583539 NImag=0</p> <p>H=-2986.235282 G=-2986.345084</p> <p>H,0,0.0280725539,-0.149752381,-0.0280124752 Rh,0,1.553578474,-0.0427987633,-0.0198375051 Cl,0,1.5796074912,2.49306671,-0.2523684812 C,0,1.5704599825,-2.0889437383,-0.0162642045 C,0,1.7056068985,-4.9423541374,-0.0344948532 C,0,1.4530052389,-2.8523184345,-1.1985797578 C,0,1.7326784073,-2.8560795039,1.1572682404 C,0,1.7995776021,-4.2485829991,1.1570870074 C,0,1.5320363277,-4.2450323799,-1.2142855755</p>

<p>H,0,1.388055015,-4.6927904566,2.224661137 H,0,2.2791131687,-4.7664451252,-1.9549281937 H,0,2.0028694993,-5.9605592445,0.1941418053 P,0,1.3607980295,-0.204327835,-2.2940678475 O,0,1.1007469546,0.0010847026,2.2648828175 O,0,3.9553385537,-0.0132923835,0.2136195454 C,0,4.6981033212,-1.2089987456,-0.1091365799 H,0,4.4275204921,-1.5108249724,-1.1265357046 H,0,4.3873710985,-2.0043408511,0.5726169437 C,0,4.861922704,1.0947425304,0.3729141382 H,0,5.036942665,1.2594028491,1.4437745486 H,0,4.3723097629,1.981933328,-0.0329109888 C,0,6.1608129622,-0.827300393,0.0083770771 H,0,6.7946299298,-1.4095068762,-0.6583183989 H,0,6.5175377,-0.9850762482,1.0290425288 C,0,6.1366688767,0.6616933186,-0.3140264897 H,0,6.0679947786,0.821881283,-1.3916969643 H,0,7.0101961294,1.1985863475,0.0522357891 S,0,2.1362483944,-2.126423742,-2.7391730713 S,0,0.8245951379,-2.0474514867,2.7529080183 C,0,-0.5441283108,0.6866607633,2.843026923 H,0,-0.6914450095,0.2259536253,3.8275512413 C,0,-1.6674372954,0.2372182356,1.9228917272 H,0,-2.6324519178,0.4515075482,2.3848936181 H,0,-1.6257658075,-0.831494659,1.7088790394 H,0,-1.6279126651,0.7804956538,0.976791316 C,0,-0.5369420375,2.2016715272,2.989938782 H,0,0.0689282911,2.5347665014,3.8306597285 H,0,-1.5546430031,2.5536159716,3.1674143898 H,0,-0.1692439617,2.686228925,2.0824921327 C,0,2.3494678551,0.6217942327,3.519969568 H,0,1.8311868755,0.6358515271,4.4868106472 C,0,2.8049608494,2.0307705652,3.1536359484 H,0,3.6372614247,2.3257327809,3.79590573 H,0,2.0234673841,2.7777302863,3.2575696719 H,0,3.1346102868,2.0801246331,2.1169455787 C,0,3.5387897708,-0.3245890439,3.5986709375 H,0,4.2933714322,0.0843663844,4.2729245102 H,0,3.9971850212,-0.4452169079,2.6156869449 H,0,3.2592222202,-1.3132186141,3.9570747136 C,0,-0.3804583267,-0.2113363414,-2.961829906 H,0,-0.2807465071,-0.4307664002,-4.0299119722 C,0,2.2852721681,0.9352015413,-3.4328894443 H,0,1.7975175302,1.8978593656,-3.2418617747 C,0,-1.2208365287,-1.305209754,-2.3261742988 H,0,-2.2020625486,-1.3410534502,-2.8018406855 H,0,-1.3775575558,-1.1196460338,-1.2621749849 C,0,-0.7607499919,-2.2880358037,-2.4287282751 H,0,-0.9989029921,1.1669613828,-2.7697565656 H,0,-2.0359294821,1.1626581939,-3.1092463595 H,0,-0.472453574,1.9454939112,-3.3219004504 H,0,-0.986964071,1.4577022469,-1.7168742189 C,0,2.1626594336,0.564567687,-4.9018372516 H,0,1.1331098912,0.5775087563,-5.2576448174 H,0,2.5750207249,-0.4277107561,-5.0983502706 H,0,2.7250020813,1.2734527011,-5.5119978609 C,0,3.7283844991,1.0479836562,-2.9792837469 H,0,4.2699521207,1.7582680681,-3.6061003692 H,0,4.2405533467,0.084643546,-3.0450092452 H,0,3.7697614018,1.398474803,-1.9496388015</p>	<p>H,0,1.9221015318,-4.7826044446,2.0914679815 H,0,1.4488274437,-4.7780965547,-2.153483622 H,0,1.759223028,-6.0236884648,-0.0426579379 P,0,1.2178414661,-0.0806054637,-2.3044099923 O,0,1.3565467873,-0.1364336845,2.2951113948 O,0,3.9470292274,0.0612924208,0.2185296954 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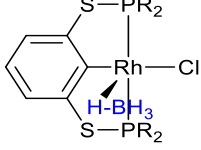
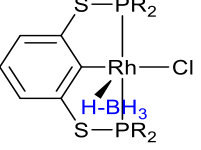
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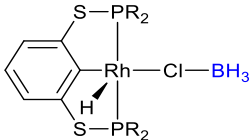
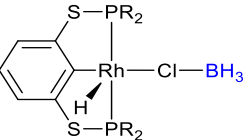
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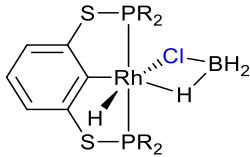
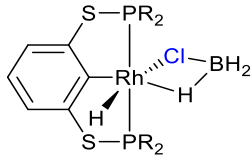
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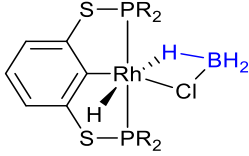
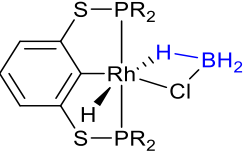
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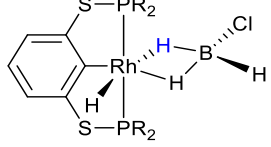
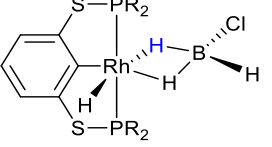
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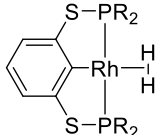
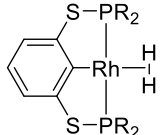
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 <p>4d</p>	 <p>4d</p>
<p>HF=-2780.9464434 ZPE= 0.495635 NImag=0</p> <p>Htot=-2780.415979 Gtot=-2780.513849</p>	<p>HF=-2780.9698676 ZPE= 0.495406 NImag=0</p> <p>Htot=-2780.439690 Gtot=-2780.536832</p>
<p>C,0,-1.8708295076,-0.0304297069,-0.0442356207 C,0,-4.705611082,0.0683415174,-0.0994974269 C,0,-2.6558764144,-0.4414516271,1.048893902 C,0,-2.5851377018,0.3867025321,-1.1846607106 C,0,-3.9778855054,0.4331277434,-1.2159287622 C,0,-4.0476994877,-0.3827948213,1.0294494784 H,0,-4.4826345495,0.7447850484,-2.1213310071 H,0,-4.6074826695,-0.695325688,1.9019773976 H,0,-5.7866473736,0.1188366424,-0.1148188938 P,0,0.0211145924,-0.4300132875,2.3256566079 P,0,0.0406395007,-0.1822959825,-2.339533087 S,0,-1.9590195466,-1.1604282841,2.5328532641 S,0,-1.78408792,0.8205829156,-2.726791004 C,0,1.0012294503,-1.7778549426,3.1531327212 H,0,0.515009327,-1.9319891781,4.1237191307 C,0,0.0696727582,1.0181992974,3.5045478928 H,0,1.0644537983,1.4484835606,3.3492052684 C,0,-0.9827337591,2.0437828472,3.1126838353 H,0,-0.8660121415,2.9430921322,3.7184582099 H,0,-1.9859405871,1.6521716385,3.2889998081 H,0,-0.9099374628,2.337965207,2.0674501374 C,0,-0.0948721475,0.5932411396,4.9550776365 H,0,-0.1190221324,1.476454791,5.5952989835 H,0,0.7148253832,-0.0435693596,5.3084311387 H,0,-1.0383564874,0.0623599603,5.1026664763 C,0,0.934388713,-3.0700412225,2.3541201436 H,0,-0.0939516876,-3.3888476258,2.1814431176 H,0,1.4444748255,-3.866570905,2.8976724292 H,0,1.4310927932,-2.9525266249,1.3904066072 C,0,2.4342400592,-1.3059681893,3.3658818965 H,0,3.008843795,-2.0878357288,3.8645895445 H,0,2.4927630955,-0.410924729,3.985941944 H,0,2.9145954594,-1.0939829734,2.4101385586 C,0,1.2117866224,0.6009685875,-3.5585005905 H,0,2.1844427058,0.2184035018,-3.2274654199 C,0,1.2113974422,2.1196142476,-3.4640966217 H,0,2.0128716078,2.518424585,-4.087291734 H,0,1.3611055234,2.4767726595,-2.449896854 H,0,0.2714916089,2.5326766919,-3.8327538219 C,0,0.9332816566,0.1601892115,-4.9909691656 H,0,1.0352905893,-0.9119549525,-5.1445493274 H,0,1.6367647222,0.6548594999,-5.6622824924 H,0,-0.0705540116,0.4529733802,-5.306320203 C,0,-0.2105898818,-1.9344738872,-2.9497583285 H,0,-0.6395972636,-1.8224081847,-3.9510850549</p>	<p>C,0,-1.8876553747,-0.0671551449,-0.0276355809 C,0,-4.7236776185,0.0506772839,-0.0539890485 C,0,-2.6653370366,-0.4622321425,1.0776905571 C,0,-2.6120991205,0.3578400879,-1.1591875907 C,0,-4.0051116065,0.4116351187,-1.1775732559 C,0,-4.0572037818,-0.3971949437,1.0713574243 H,0,-4.5189756205,0.7284783843,-2.076277181 H,0,-4.6120904505,-0.6986668075,1.9510684153 H,0,-5.8047785507,0.1056959927,-0.0592774111 P,0,0.0262049998,-0.4392046511,2.3388011045 P,0,0.0103337801,-0.1868437966,-2.3440299299 S,0,-1.9588911043,-1.1567066581,2.571027147 S,0,-1.8234396914,0.8130515444,-2.7024282921 C,0,1.006891931,-1.792485329,3.1575442014 H,0,0.513112039,-1.9684341598,4.1204082634 C,0,0.1049349448,1.0197084238,3.4988186608 H,0,1.1113199754,1.4212719865,3.339842399 C,0,-0.9200252551,2.0657623726,3.0925556194 H,0,-0.7759219654,2.9725923848,3.6816202977 H,0,-1.9346706236,1.7092416669,3.2800214521 H,0,-0.8454202278,2.3408167112,2.0418202287 C,0,-0.068975863,0.6168553456,4.9537718567 H,0,-0.0511661788,1.507925195,5.5838264615 H,0,0.7150869184,-0.0491293199,5.3116962706 H,0,-1.0326773896,0.1281228923,5.1161465582 C,0,0.9539432726,-3.0663367703,2.3301922875 H,0,-0.0700198489,-3.3933523691,2.1442085911 H,0,1.4676915576,-3.8727804045,2.855921194 H,0,1.455300722,-2.925360146,1.3709416599 C,0,2.4357586332,-1.3229426828,3.3930902731 H,0,3.0080189403,-2.1164144225,3.8767801376 H,0,2.4899310828,-0.443618826,4.0353908927 H,0,2.9258191069,-1.0858929082,2.4478793498 C,0,1.1996289162,0.6500677827,-3.5128748786 H,0,2.1719088457,0.3846902549,-3.0823058414 C,0,1.0430190817,2.1640464256,-3.5004431904 H,0,1.9013283114,2.6177533077,-3.9982194058 H,0,0.9811214058,2.5791530585,-2.4984551866 H,0,0.1495880478,2.4681735256,-4.0479477103 C,0,1.1031403872,0.1252916165,-4.9389664653 H,0,1.3256321155,-0.935747482,-5.0313893662 H,0,1.8199438282,0.6613173436,-5.5634828783 H,0,0.1131241589,0.3036286519,-5.3645259206 C,0,-0.225351534,-1.9255639104,-2.9901965612 H,0,-0.5338859571,-1.8001833813,-4.0331160418</p>

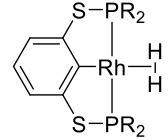
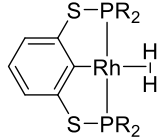
<p>C,0,1.1050232153,-2.6963639225,-3.0296654251 H,0,0.9264776149,-3.6771772043,-3.4739754662 H,0,1.5355354135,-2.8412374787,-2.0396836479 H,0,1.8575847857,-2.1912063997,-3.6342330162 C,0,-1.2094337652,-2.661473393,-2.0615599503 H,0,-1.3687369035,-3.6745721907,-2.4339336215 H,0,-2.1761421149,-2.1609879133,-2.0217004327 H,0,-0.8353084499,-2.7475388936,-1.0358654426 Rh,0,0.1795807159,-0.1889694366,-0.0165513087 Cl,0,2.4648831246,-1.0894813149,-0.2393093188 H,0,-0.2689141951,1.3477638365,0.0426637669 B,0,1.0079715969,2.1219074187,0.1930150888 H,0,0.1390147396,2.9039058179,-0.1392660439 H,0,1.3127414181,2.1267165047,1.3417960427 H,0,1.8638160955,1.9240451324,-0.6030022283</p>	<p>C,0,1.0750357495,-2.7135602089,-2.9260101767 H,0,0.9418544389,-3.6730231082,-3.4294532683 H,0,1.3650336224,-2.9112837918,-1.8940520832 H,0,1.9156209149,-2.2057811326,-3.3980708785 C,0,-1.3304875815,-2.6385648679,-2.2287845617 H,0,-1.4773022703,-3.6377946569,-2.6423798481 H,0,-2.2844220457,-2.1144432692,-2.2794910018 H,0,-1.0724924761,-2.7620557644,-1.1723907363 Rh,0,0.1622982739,-0.2334554349,-0.0198766789 Cl,0,2.5425185697,-0.9618033272,-0.2239436176 H,0,-0.2209421552,1.3222683719,0.0302736117 B,0,1.0459362655,2.0638952841,0.1557472627 H,0,0.1617174965,2.8665386425,-0.0785466943 H,0,1.4298038636,2.0299535644,1.2810605008 H,0,1.845809131,1.9282105979,-0.7085223969</p>
 <p>4c</p>	 <p>4c</p>
<p>HF=-2780.9846109 ZPE= 0.497452 NImag=0</p> <p>Htot= -2780.452819 Gtot= -2780.549269</p> <p>C,0,-1.6779919819,-0.0968422719,0.0054798107 C,0,-4.5154851956,-0.0272645649,-0.0523797295 C,0,-2.3961081359,0.3492079535,-1.1194206359 C,0,-2.4619189976,-0.449314189,1.1195479626 C,0,-3.8544936831,-0.4193653576,1.0970992758 C,0,-3.7888309305,0.3644604372,-1.1619193228 H,0,-4.4128671209,-0.6915283356,1.9838775782 H,0,-4.2961248625,0.6824376756,-2.0639524025 H,0,-5.5974809077,-0.0126316028,-0.0788396802 P,0,0.27378094,-0.019880244,-2.2897241402 P,0,0.1359843875,0.0097888682,2.3195161441 S,0,-1.5823305716,0.9604736807,-2.5970416765 S,0,-1.7303694446,-0.9159519679,2.6943128888 Cl,0,1.1919487751,-2.6932810225,0.0054719894 B,0,2.6620205794,-1.4247574789,0.0625840544 C,0,1.5091178961,1.1192203777,-3.0900864182 H,0,2.4416116114,0.5463158606,-3.0228382103 C,0,0.1679164217,-1.4886861471,-3.4375668727 H,0,-0.1483475125,-1.060249886,-4.3954517885 C,0,1.5226024197,-2.1616795357,-3.6006935226 H,0,1.4298889893,-3.0149354094,-4.2746221047 H,0,1.8996095905,-2.5330945672,-2.6480826092 H,0,2.2732403828,-1.4932224224,-4.0238602698 C,0,-0.9090771229,-2.4504786806,-2.9616439961 H,0,-1.0151303825,-3.2690542059,-3.6750094118 H,0,-1.8785899815,-1.9602968008,-2.8712819723 H,0,-0.6528589887,-2.8810444069,-1.9941715614 C,0,1.1938486469,1.4032413388,-4.5512120668 H,0,1.1618973638,0.4997602237,-5.1589460322 H,0,1.9560628421,2.0566749087,-4.9782358696 H,0,0.2344991146,1.9144030517,-4.65655507 C,0,1.6704396212,2.3993153564,-2.2863485041 H,0,2.4001103708,3.0527083666,-2.766592609 H,0,2.0128470786,2.1977825108,-1.2721064952 H,0,0.726485685,2.9443246936,-2.220769037 C,0,1.2909177231,-0.7702023875,3.5643218561 H,0,2.2763161101,-0.4754091161,3.1846310018 C,0,1.2046595541,-2.288574203,3.5351468944 H,0,2.012360719,-2.7084610295,4.1362133971 H,0,1.2857461368,-2.6911741226,2.5289450138</p>	<p>HF=-2780.9930633 ZPE= 0.495293 NImag=0</p> <p>Htot= -2780.462487 Gtot= -2780.561408</p> <p>C,0,-2.0009848007,0.0175026589,0.0106070306 C,0,-4.8433246832,0.1366666541,-0.0578507931 C,0,-2.7331091104,-0.0576718605,-1.193775215 C,0,-2.7808319164,0.1919914263,1.1756040406 C,0,-4.1735140273,0.2381747696,1.1461566854 C,0,-4.1258775303,-0.0086379569,-1.2291177163 H,0,-4.7272241591,0.3591822162,2.0689334537 H,0,-4.6420234769,-0.0798068082,-2.1785552012 H,0,-5.9248403749,0.1758777457,-0.083628518 P,0,0.0598484005,-0.2658608799,-2.2547131259 P,0,-0.0477792848,0.1378039054,2.3529062956 S,0,-1.9829910161,-0.2306367865,-2.8107299351 S,0,-2.0934623462,0.3851158398,2.8203772441 Cl,0,2.5082172166,-0.8434584389,0.3398102567 B,0,3.4247391164,0.7944896962,-0.4558993827 C,0,0.8222675056,1.140436366,-3.2016095601 H,0,1.892216199,1.0255887138,-2.9953376927 C,0,0.6733527903,-1.8314391975,-3.0635458649 H,0,0.1932992135,-1.8659345228,-4.0477148204 C,0,2.1845084728,-1.8231630719,-3.2309255536 H,0,2.5061663637,-2.7640663575,-3.6812968532 H,0,2.6925951178,-1.7262745883,-2.2707006647 H,0,2.5342050303,-1.017292169,-3.8756697232 C,0,0.2027341357,-3.0155253469,-2.2341560096 H,0,0.4431174397,-3.9545933494,-2.7346233944 H,0,-0.8753281703,-2.9978529905,-2.0633755809 H,0,0.7055151503,-3.0277256635,-1.2632433017 C,0,0.5658723111,1.0261603531,-4.6957955072 H,0,0.9141704915,0.0827634011,-5.1166851605 H,0,1.085369726,1.8283509337,-5.2224361135 H,0,-0.4976719113,1.1261082265,-4.9237748599 C,0,0.3596171077,2.4758398589,-2.6465928068 H,0,0.7869261464,3.2897242734,-3.2342408741 H,0,0.6768985598,2.6167085972,-1.6132966291 H,0,-0.7278669642,2.5731252438,-2.6897316526 C,0,0.513474565,-1.3033616395,3.3830441832 H,0,1.5918473972,-1.3332331138,3.1913046383 C,0,-0.1146083637,-2.5758652888,2.8403343217 H,0,0.2319810556,-3.4431015802,3.4039199342 H,0,0.1459914795,-2.7441089787,1.7930173994</p>

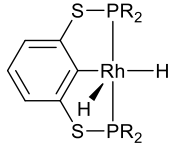
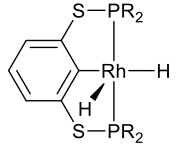
<p>H,0,0.2610537087,-2.6342462154,3.9598597125 C,0,1.1133684877,-0.2410776541,4.9810333627 H,0,1.3479788348,0.817814486,5.0781529257 H,0,1.7798362479,-0.7827401508,5.6540402363 H,0,0.0947826077,-0.3975535648,5.3424269435 C,0,-0.0316846031,1.7775769676,2.8925657745 H,0,-0.2529408091,1.715454072,3.9620221082 C,0,1.3004384018,2.4855190482,2.6822460267 H,0,1.2465708382,3.5112585658,3.0499655015 H,0,1.5516269976,2.5279747601,1.6199812649 H,0,2.1268682929,1.9933005505,3.1972852727 C,0,-1.1742548496,2.5072266696,2.2092485265 H,0,-1.2398855987,3.5265760902,2.5933100489 H,0,-2.1332954334,2.0208706299,2.3845980554 H,0,-1.02415921,2.5685801714,1.1298456038 Rh,0,0.3702314264,-0.2164207531,0.0251737899 H,0,0.2740524376,1.3206272573,-0.0114878414 H,0,3.3023313478,-1.5494913481,-0.9390797903 H,0,2.2151290669,-0.225451188,0.0586062883 H,0,3.2343664687,-1.5726459425,1.1017370688</p>	<p>H,0,-1.2037781599,-2.5460339216,2.9158431 C,0,0.2608556069,-1.1142117828,4.8677906147 H,0,0.7527499967,-0.2260100999,5.2653327542 H,0,0.6398085045,-1.9727876342,5.4250751355 H,0,-0.8073402854,-1.0353446506,5.0816377569 C,0,0.7532311981,1.6483156567,3.0870506366 H,0,0.3046081401,1.7397100373,4.083231688 C,0,2.2574028589,1.4677753614,3.2186921524 H,0,2.6943718002,2.3675040391,3.655124513 H,0,2.7266109543,1.3159047179,2.2453923714 H,0,2.529111782,0.6295728004,3.8605275048 C,0,0.4040532308,2.8813540102,2.2713895936 H,0,0.7291528033,3.7805969803,2.7966120365 H,0,-0.6682475684,2.9711617084,2.0908033109 H,0,0.9151623437,2.8634135603,1.3064151703 Rh,0,0.0077646585,-0.2070697056,0.0780091469 H,0,0.0058282136,1.3084908414,-0.0461733725 H,0,3.6315055652,0.4811146321,-1.5969536303 H,0,2.613673851,1.6734335187,-0.3220745775 H,0,4.4083034497,0.9170044875,0.2186074217</p>
 <p>4</p>	 <p>4</p>
<p>HF=-2780.9846109 ZPE= 0.497452 NImag=0</p> <p>Htot= -2780.452818 Gtot= -2780.549267</p> <p>C,0,-1.820090849,-0.1487963425,0.00073766 Rh,0,0.2109682021,-0.4255560224,0.0904645727 H,0,0.2346422529,1.1143944848,0.0558206778 P,0,-0.0842186764,-0.1839472057,2.3761689334 P,0,0.2099505069,-0.2204736754,-2.225698953 H,0,2.0473091892,-0.576484999,0.1871079877 B,0,2.4010993228,-1.8062461631,0.202314822 Cl,0,0.8408629479,-2.958147962,0.0902573909 H,0,3.0641148416,-1.9788552189,-0.7772375255 H,0,2.9242378234,-1.9985187786,1.2599630769 C,0,-4.6401534145,0.1386636397,-0.1545130802 C,0,-2.4625032944,0.3519830749,-1.1466985551 C,0,-2.666802596,-0.440817699,1.0859637026 C,0,-4.0513666551,-0.3039187368,1.0156910502 C,0,-3.8476336419,0.4742164666,-1.2370563094 H,0,-4.6592936408,-0.5329919919,1.8818217364 H,0,-4.2975088368,0.830904394,-2.1549390684 H,0,-5.7162718699,0.2363834025,-0.2181731558 S,0,-1.5535468184,0.9001193622,-2.5933057681 S,0,-2.0281117852,-0.9634863722,2.6833379184 C,0,1.5561353948,0.8206882527,-2.9792399066 H,0,2.4389453445,0.1777037636,-2.8817419124 C,0,0.0310420129,-1.6759017437,-3.3815029345 H,0,-0.2183466372,-1.2235786154,-4.3481207727 C,0,1.3347809639,-2.4509870294,-3.5007744665 H,0,1.1999385367,-3.2938494712,-4.180644287 H,0,1.6492149926,-2.851358286,-2.5372500622 H,0,2.1486678187,-1.8418275477,-3.895575727 C,0,-1.1324151475,-2.5523660947,-2.9460456692 H,0,-1.2763189815,-3.3599481728,-3.6652826597 H,0,-2.0639453501,-1.9891451653,-2.8874986415 H,0,-0.9436538253,-3.0019353405,-1.9717277628 C,0,1.3144093755,1.1290039424,-4.4494362481 H,0,1.2341010092,0.2310440779,-5.0608812858</p>	<p>HF=-2781.0045868 ZPE= 0.496963 NImag=0</p> <p>Htot= -2780.473148 Gtot= -2780.569842</p> <p>C,0,-1.8238569372,-0.1569933117,0.0035579016 Rh,0,0.2044882283,-0.4365815114,0.0927955067 H,0,0.2238333615,1.101517917,0.0619358292 P,0,-0.0871431994,-0.1813057632,2.3832873666 P,0,0.2096348155,-0.2257261928,-2.2300629277 H,0,2.0532353121,-0.5938333909,0.1922270934 B,0,2.4132686562,-1.8147893424,0.1933304062 Cl,0,0.8669894576,-2.9829051419,0.0863248204 H,0,3.0730685907,-1.9822193981,-0.7908606908 H,0,2.9518604448,-2.0172742925,1.2425619272 C,0,-4.6443877692,0.1310344111,-0.1523415376 C,0,-2.4657491005,0.3477182855,-1.1431176442 C,0,-2.6712629958,-0.4505366059,1.0883080737 C,0,-4.0562578005,-0.3153214776,1.0168355817 C,0,-3.8511256306,0.4708028833,-1.2331914783 H,0,-4.6660997676,-0.5468570349,1.8811586533 H,0,-4.3018193316,0.8316439502,-2.1493194965 H,0,-5.7206664035,0.2286974511,-0.2164308598 S,0,-1.5554482774,0.9025621734,-2.5858928417 S,0,-2.031482071,-0.9723916759,2.6856379835 C,0,1.5590478012,0.8173013234,-2.9746198415 H,0,2.4379375116,0.1680730726,-2.8848920301 C,0,0.0211911026,-1.674202618,-3.3943545621 H,0,-0.2293722105,-1.216854762,-4.3579150866 C,0,1.321006457,-2.4522736687,-3.5257341225 H,0,1.1805082354,-3.2855285174,-4.2168520682 H,0,1.6364089486,-2.8701330711,-2.5695747681 H,0,2.137729163,-1.8433967303,-3.9150254801 C,0,-1.1412755715,-2.5519303832,-2.962062649 H,0,-1.2855375158,-3.3566445768,-3.6851679505 H,0,-2.0754784655,-1.9927256398,-2.9019554924 H,0,-0.9563592505,-3.0084790773,-1.9898533213 C,0,1.3201796586,1.1403715949,-4.4410808199 H,0,1.2224256866,0.2495522346,-5.0607023158</p>

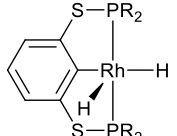
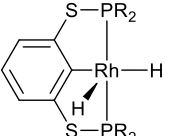
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 <p>4a</p>	 <p>4a</p>
<p>HF=-2780.9833875 ZPE= 0.497918 NImag=0</p> <p>Htot= -2780.451391 Gtot= -2780.547104</p> <p>C,0,-1.9548098099,-0.1497824291,-0.0045547878 Rh,0,0.0741033097,-0.3268138533,0.0925166848 H,0,-0.0873377844,1.20781005,-0.0157878803 P,0,-0.1199659159,-0.0405366341,2.378134771 P,0,0.1460465656,-0.254607693,-2.2333884193 Cl,0,2.6089504675,-0.781801742,0.1987752486 B,0,1.6450294611,-2.4930601595,0.3413495039 H,0,0.4096291566,-2.2457048419,0.276789667 H,0,1.9552447609,-3.1580798187,-0.5982774644 H,0,1.9042668055,-2.942275015,1.4143672358 C,0,-4.7922046616,0.0198603762,-0.1695299891 C,0,-2.6309212811,0.0743361988,-1.2208408995 C,0,-2.7844715023,-0.2023612876,1.1338858865 C,0,-4.1740564274,-0.128781758,1.0564751184 C,0,-4.0206746993,0.1318872834,-1.3096874566 H,0,-4.7633091172,-0.180561366,1.9633909379 H,0,-4.4889577796,0.2730218671,-2.2756430748 H,0,-5.8714683628,0.0672938189,-0.234212583 S,0,-1.7983823716,0.3620152062,-2.7795106264 S,0,-2.1606259326,-0.347350973,2.8077599528 C,0,1.2601974275,1.034260545,-2.9892138804 H,0,2.2587954016,0.608454946,-2.8386246885 C,0,0.4088302254,-1.760705397,-3.3065783185 H,0,0.014186752,-1.4642546739,-4.285356573 C,0,1.8853891149,-2.1053705464,-3.4389583722 H,0,1.9972791767,-3.0374506765,-3.9952034939 H,0,2.3540746263,-2.248626995,-2.4654686943 H,0,2.443379576,-1.3375633407,-3.9751707034</p>	<p>HF=-2781.0038493 ZPE= 0.497587 NImag=0</p> <p>Htot= -2780.472121 Gtot= -2780.567901</p> <p>C,0,-1.9505186267,-0.1472281375,-0.0027438419 Rh,0,0.0789788048,-0.3514831967,0.0930007262 H,0,-0.0666231183,1.1822048631,-0.0067365 P,0,-0.1112851175,-0.0515753196,2.3833929099 P,0,0.1542104427,-0.2536239103,-2.2397442471 Cl,0,2.6267724457,-0.8599338996,0.2143800521 B,0,1.6431581057,-2.559968727,0.3465976347 H,0,0.4181176959,-2.3005365703,0.2724344875 H,0,1.9608338281,-3.2268197532,-0.5912258754 H,0,1.8954306424,-3.0151918822,1.4203536016 C,0,-4.7873460515,0.043057223,-0.1627334854 C,0,-2.6265154289,0.087090945,-1.2174153932 C,0,-2.7792951743,-0.2031395054,1.1368054956 C,0,-4.1687834287,-0.1187771686,1.0615312222 C,0,-4.0165438032,0.1557139465,-1.3033478864 H,0,-4.7586051894,-0.1735975603,1.968168897 H,0,-4.4869144741,0.3049992108,-2.2672957625 H,0,-5.866524593,0.0984283527,-0.2257993984 S,0,-1.7948870306,0.3686210505,-2.777009594 S,0,-2.1544772762,-0.375268872,2.807197712 C,0,1.2593331979,1.0480169983,-2.9884800476 H,0,2.2625101394,0.6354468732,-2.8320310234 C,0,0.4090522194,-1.7536815683,-3.3240504571 H,0,0.0222322866,-1.4490351376,-4.3031077131 C,0,1.8825892806,-2.1081030066,-3.452358703 H,0,1.990203124,-3.0293064659,-4.0279973671 H,0,2.3441410016,-2.278453444,-2.4793918288 H,0,2.4538788223,-1.3355446673,-3.9676389982</p>

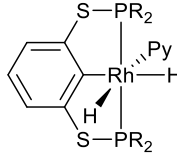
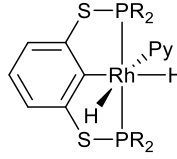
<p>C,0,-0.4232358942,-2.9189403685,-2.7818698022 H,0,-0.3791740345,-3.7564989025,-3.4793124746 H,0,-1.4709908366,-2.6404850422,-2.6610460988 H,0,-0.0481672129,-3.2645311678,-1.8194149408 C,0,1.0054882953,1.2174337054,-4.4782410071 H,0,1.1200175268,0.293130195,-5.0438286371 H,0,1.7077702729,1.9426251507,-4.89203034 H,0,-0.0004813761,1.601771838,-4.6596507466 C,0,1.175933704,2.351729144,-2.2377178646 H,0,1.8081637067,3.0981834675,-2.72083149 H,0,1.5051533991,2.2481386701,-1.2044351589 H,0,0.1537807476,2.7365449784,-2.2298154731 C,0,0.7650446335,-1.2168738023,3.5279420316 H,0,1.7522133973,-1.3063732878,3.059289947 C,0,0.0988451434,-2.5855521584,3.5171917356 H,0,0.7811279135,-3.3281535238,3.9322924567 H,0,-0.1703368787,-2.9087116858,2.5138121544 H,0,-0.8079267166,-2.5799185332,4.1227035068 C,0,0.9184634011,-0.6972623065,4.9498289407 H,0,1.5188721441,0.2091480045,5.0130868078 H,0,1.4099846741,-1.4548964995,5.5621596213 H,0,-0.0518660776,-0.4946549594,5.40903551 C,0,0.2973706244,1.6688501096,2.9908066712 H,0,0.1289860194,1.6455460429,4.0720252558 C,0,1.7669721706,1.9437537061,2.6993105671 H,0,2.0579641098,2.914776823,3.1026993198 H,0,1.9462251654,1.9608867698,1.6221456896 H,0,2.433842049,1.1923997787,3.1243317227 C,0,-0.6051633474,2.7251085321,2.3798984351 H,0,-0.3728505294,3.7027303647,2.8047190611 H,0,-1.6591656148,2.5181935739,2.5635397078 H,0,-0.4596797607,2.7920039925,1.3001033904</p>	<p>C,0,-0.4296177296,-2.9118614891,-2.8124684926 H,0,-0.3857456187,-3.7437795106,-3.5172523028 H,0,-1.4783672953,-2.6349885844,-2.6936867435 H,0,-0.0625218722,-3.2709631963,-1.8513190933 C,0,1.0165644528,1.2274255351,-4.4792743702 H,0,1.1372906913,0.3033158139,-5.0441218352 H,0,1.7238907607,1.951762258,-4.8866935722 H,0,0.0136983176,1.6140385898,-4.6742479227 C,0,1.1558659477,2.365957378,-2.2412970641 H,0,1.7899704814,3.1144835483,-2.7193786752 H,0,1.4748252509,2.2729787523,-1.2035169994 H,0,0.1328191898,2.7489519661,-2.2469453133 C,0,0.7747926956,-1.2128419135,3.5489370234 H,0,1.7648842054,-1.3000713181,3.0860641409 C,0,0.1182231521,-2.5857798094,3.5524886636 H,0,0.8118288118,-3.3226431555,3.9600032714 H,0,-0.1686838353,-2.9185859315,2.5566435029 H,0,-0.7768824053,-2.5872200643,4.1757356744 C,0,0.9232417943,-0.6785214498,4.9652983969 H,0,1.5158656768,0.2335989568,5.0215484327 H,0,1.4242420778,-1.4267371313,5.5823005047 H,0,-0.047352728,-0.482279207,5.4267700803 C,0,0.2840223561,1.6682710883,2.9805388106 H,0,0.1096251597,1.6518340886,4.060742984 C,0,1.7516919309,1.9582205113,2.6979592006 H,0,2.0254641632,2.9362354224,3.0973918597 H,0,1.9419636985,1.9740241349,1.6224778012 H,0,2.4259024107,1.2215520767,3.1372191674 C,0,-0.6239710751,2.711396491,2.3569182278 H,0,-0.3996533207,3.6937820267,2.7759904911 H,0,-1.6783406274,2.5038858454,2.539931813 H,0,-0.4772614428,2.7756013064,1.2766533219</p>
 <p>4b</p>	 <p>4b</p>
<p>HF=-2780.9878349 ZPE= 0.497274 NImag=0</p> <p>Htot= -2780.456500 Gtot= -2780.553317</p> <p>C,0,-0.0168959659,1.8074244746,-0.3946475773 C,0,-0.0869872059,4.3082975146,-1.7577460515 C,0,1.1511727744,2.5062898307,-0.7616900624 C,0,-1.2175178261,2.4996893355,-0.6498501265 C,0,-1.2596042935,3.710812129,-1.3390074359 C,0,1.1232942517,3.7164120235,-1.4526353142 H,0,-2.214176525,4.1828470228,-1.5343492318 H,0,2.0528329487,4.1923229717,-1.7382034748 H,0,-0.1150690982,5.2443702447,-2.3002631257 P,0,2.3422179428,0.0133841657,0.295447219 P,0,-2.2866253737,0.0180607009,0.5884182066 S,0,2.7991014884,1.9826367057,-0.2948530196 S,0,-2.8099081715,1.964829128,-0.03571291 C,0,3.341121713,-0.2205016617,1.8467891212 H,0,4.3482584741,0.1401468376,1.608904594 C,0,3.1678128023,-1.0364681743,-1.0050904518 H,0,2.9230958017,-2.0599811855,-0.7041381795 C,0,2.5372126334,-0.7593416219,-2.3607965403 H,0,2.9476440861,-1.4377558572,-3.1094153628 H,0,2.7449486464,0.2618930432,-2.6855406101 H,0,1.4557152061,-0.8942122,-2.3436539331 C,0,4.6755808296,-0.8471669738,-1.0357928521</p>	<p>HF=-2781.010176 ZPE= 0.497020 NImag=0</p> <p>Htot= -2780.479004 Gtot= -2780.575896</p> <p>C,0,-0.016838515,1.817222555,-0.3942533688 C,0,-0.070048748,4.3358860774,-1.7280336811 C,0,1.1562973035,2.5224430714,-0.7361100746 C,0,-1.2150501567,2.5099479746,-0.6631044028 C,0,-1.2481707416,3.7305960621,-1.3367690221 C,0,1.1364270384,3.7412753944,-1.4127265333 H,0,-2.1997259061,4.2048830373,-1.5424507928 H,0,2.0686666878,4.2228068724,-1.6802485157 H,0,-0.0911836515,5.2790610167,-2.2588739106 P,0,2.345323487,0.0089483101,0.2951340324 P,0,-2.2959415951,0.0245238788,0.5734049625 S,0,2.7994067815,1.9928678804,-0.2593995014 S,0,-2.8200367582,1.9589005009,-0.0964798385 C,0,3.3349988576,-0.2434684635,1.8497891726 H,0,4.3410871244,0.1251758692,1.6202951235 C,0,3.174375703,-1.0184187806,-1.0208936662 H,0,2.9305702574,-2.0462505945,-0.7336336839 C,0,2.5445566412,-0.7251298541,-2.372632051 H,0,2.9475996767,-1.4024508563,-3.1268005812 H,0,2.7606221912,0.2953839979,-2.6950960017 H,0,1.4612614007,-0.8512529108,-2.3585888497 C,0,4.6818725775,-0.8337846506,-1.047562559</p>

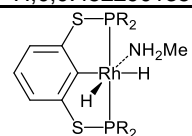
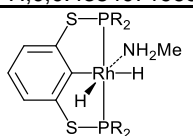
<p>H,0,5.1115234453,-1.4623273722,-1.8244495635 H,0,5.1570649064,-1.129688944,-0.0997321028 H,0,4.9368362376,0.1909066449,-1.2538139683 C,0,2.7647050051,0.6177581904,2.9755967772 H,0,2.6703285141,1.667641618,2.6979875607 H,0,3.4059772549,0.5559672506,3.8557736087 H,0,1.7743557469,0.2549356791,3.257555348 C,0,3.398531806,-1.6967772712,2.2132656438 H,0,3.9756342248,-1.8297817561,3.1293424781 H,0,3.8626350064,-2.307498972,1.4389583314 H,0,2.398752726,-2.095999431,2.3899902345 C,0,-3.3003504966,-1.0734268259,-0.5274779197 H,0,-3.0660904042,-2.0833220856,-0.1786910768 C,0,-2.8165853037,-0.9322879819,-1.9613730941 H,0,-3.3575407808,-1.6253281763,-2.6064698007 H,0,-1.7534143962,-1.1544737466,-2.054095046 H,0,-2.9871543867,0.0785825802,-2.3375020414 C,0,-4.7914237186,-0.808494728,-0.3990545687 H,0,-5.167352834,-0.9951728004,0.6070446453 H,0,-5.342018488,-1.4625916524,-1.076888854 H,0,-5.0377453041,0.2205046489,-0.6708319155 C,0,-3.0635325803,-0.1258785485,2.2725508406 H,0,-4.0904581318,0.2385758182,2.1570196951 C,0,-3.0815429323,-1.583505071,2.7105270324 H,0,-3.5033559112,-1.6647783556,3.7133370486 H,0,-2.0728544443,-1.9998605197,2.7395808676 H,0,-3.6719480891,-2.2169011018,2.0492025871 C,0,-2.3340426382,0.756167685,3.2713643189 H,0,-2.8587686078,0.7551535246,4.2276629795 H,0,-2.2586694697,1.7880907553,2.9275803087 H,0,-1.3221751271,0.3852686274,3.4458043029 Rh,0,0.028744819,-0.079100294,0.4528681278 H,0,0.0840798271,0.9704478957,1.5903016888 H,0,0.1144817963,-1.7173212033,1.3470676465 H,0,0.0183735199,-1.6831041339,-0.7364938825 B,0,0.1907726485,-2.4202144136,0.2710648528 H,0,1.2608260322,-2.9495096603,0.2376391956 Cl,0,-1.1564045108,-3.6937965151,0.3470162319</p>	<p>H,0,5.1146856451,-1.4423601702,-1.8436260594 H,0,5.1627333254,-1.1312349635,-0.1156694133 H,0,4.9517120132,0.2046544691,-1.2539134193 C,0,2.751268474,0.5734744913,2.9894389145 H,0,2.6454059426,1.6276639413,2.731675996 H,0,3.3963835209,0.5067264412,3.8668958046 H,0,1.766730915,0.1959556758,3.2731828922 C,0,3.4018748857,-1.7228091794,2.1988699382 H,0,3.9986327107,-1.8614715487,3.1019189731 H,0,3.8531571062,-2.3269687234,1.4116696697 H,0,2.4077588649,-2.1267660669,2.3966909688 C,0,-3.3066585359,-1.0936967917,-0.517043632 H,0,-3.0612498755,-2.0934811805,-0.1467124354 C,0,-2.8318038796,-0.981305589,-1.9555601874 H,0,-3.3489192954,-1.7137169265,-2.5770128219 H,0,-1.7610319278,-1.1673777557,-2.0491826583 H,0,-3.0394945944,0.0091767465,-2.3659769814 C,0,-4.7998589814,-0.8467179765,-0.3869795028 H,0,-5.1692103608,-1.0143605687,0.6249981192 H,0,-5.3441257512,-1.5255989002,-1.0460053925 H,0,-5.0661087101,0.1707439038,-0.683264199 C,0,-3.0675504475,-0.0844510014,2.2627464848 H,0,-4.0957691857,0.2735047461,2.1413282504 C,0,-3.0819560515,-1.5315253136,2.7322441861 H,0,-3.5067559493,-1.5908381289,3.7357354086 H,0,-2.0716634042,-1.9435495052,2.7783690392 H,0,-3.6720396546,-2.1813653766,2.0862818448 C,0,-2.3409950255,0.8186398678,3.2434592881 H,0,-2.8734547008,0.8430134414,4.1955842855 H,0,-2.259621665,1.8437176269,2.879913841 H,0,-1.3319076222,0.4498160577,3.4381721293 Rh,0,0.0209040813,-0.0792420259,0.4268237701 H,0,0.075296337,0.9294027307,1.5944554677 H,0,0.1009427673,-1.7388117122,1.3143931474 H,0,0.0335147301,-1.7437354182,-0.7620309891 B,0,0.2028081161,-2.4467632253,0.2551182295 H,0,1.276624559,-2.970543977,0.2466842746 Cl,0,-1.1329079317,-3.754117203,0.3367613088</p>
 <p>6-(singlet)</p>	 <p>6-(singlet)</p>
<p>HF=-2294.6581015 ZPE= 0.470457 NImag=0</p> <p>Htot= -2294.155983 Gtot= -2294.248776</p> <p>C,0,1.5990858833,-0.0001377847,-0.0025530717 C,0,2.3783210495,-0.2903773947,1.1425279613 S,0,1.6599773999,-0.7142030828,2.7313254707 P,0,-0.35526567,-0.2783996071,2.2620003924 Rh,0,-0.4853537036,-0.0004701032,0.0003027593 C,0,2.3750838015,0.2903547941,-1.1497671053 S,0,1.6522514709,0.7139998645,-2.7365745522 P,0,-0.361566446,0.2775795799,-2.2617322353 H,0,-2.185047609,-0.4262586815,-0.0477733628 H,0,-2.185076819,0.4246563555,0.0530281748 C,0,4.4667862606,0.0003106308,-0.0064898501 C,0,3.7722753222,-0.2860487058,1.1528454167 C,0,3.7690057465,0.2864586847,-1.1639125323 H,0,4.3076098233,-0.5064754909,2.0679386773 H,0,4.3017571774,0.507057907,-2.0804704298 H,0,5.5495543838,0.0004788013,-0.0079765508 C,0,-0.7646712154,-1.2073170807,-3.3219189377</p>	<p>HF=-2294.6772002 ZPE= 0.470101 NImag=0</p> <p>Htot= -2294.175359 Gtot= -2294.267686</p> <p>C,0,1.6204322766,-0.0004453643,-0.0018109078 C,0,2.3999765039,-0.2612210439,1.1512038323 S,0,1.679926763,-0.6424004676,2.7508596447 P,0,-0.3486692724,-0.2608383482,2.2671311755 Rh,0,-0.4633700503,-0.0001920804,0.0002107541 C,0,2.397792892,0.2601291889,-1.1563444709 S,0,1.6747279568,0.6413500705,-2.7546292805 P,0,-0.3530039153,0.2601854193,-2.266968099 H,0,-2.1650172212,-0.4252576639,-0.0370116411 H,0,-2.1647619914,0.4255203651,0.0407875053 C,0,4.4896452666,-0.0007762883,-0.0046004606 C,0,3.7945639396,-0.2579973939,1.161644592 C,0,3.7923568135,0.2565922499,-1.1694941313 H,0,4.331497,-0.4566166144,2.0811359856 H,0,4.3275471472,0.4550707156,-2.0900314995 H,0,5.5726740804,-0.0009024453,-0.005653549 C,0,-0.8034017901,-1.2125334936,-3.3236441286</p>

<p>H,0,-1.8331133751,-1.3700839856,-3.1343936968 C,0,-1.2629398946,1.6958184789,-3.0744623791 H,0,-0.8343391143,1.8106106146,-4.0762274312 C,0,-2.7467593797,1.3818657117,-3.1940863291 H,0,-3.2827473339,2.2364601809,-3.6099930402 H,0,-3.1846742999,1.1711766928,-2.2155674748 H,0,-2.9450522057,0.5257948559,-3.8393337667 C,0,-1.018995857,2.9671472205,-2.2769735183 H,0,-1.4941405645,3.821912535,-2.7613932719 H,0,0.0449320633,3.1806927281,-2.1761781086 H,0,-1.4328152827,2.8743792439,-1.2699561675 C,0,-0.5355246315,-0.9808361399,-4.8056668984 H,0,-1.1443907756,-0.1695764173,-5.2062797359 H,0,-0.7781021952,-1.8818974323,-5.3720500044 H,0,0.5124007933,-0.7446103998,-5.0025598697 C,0,0.0092995495,-2.4068978201,-2.7971922047 H,0,-0.2695635308,-3.3117908031,-3.3394692246 H,0,-0.1746610582,-2.5664328356,-1.7329752733 H,0,1.0834303681,-2.2582872038,-2.9253798471 C,0,-0.7558829186,1.2064544014,3.3231959299 H,0,-1.8248863305,1.3688957603,3.1386123333 C,0,0.0162793292,2.4062266121,2.7962479102 H,0,-0.2613363371,3.3110707677,3.3392461748 H,0,-0.1706885481,2.5656426651,1.732537754 H,0,1.090805647,2.257934668,2.921456726 C,0,-0.5225685734,0.9801527584,4.8063227155 H,0,-1.130083796,0.168741883,5.2086752563 H,0,-0.7638493124,1.8811836147,5.3733077376 H,0,0.5259673386,0.744254473,5.0003362322 C,0,-1.2539851522,-1.6968481365,3.0772996181 H,0,-0.8226034563,-1.8114416203,4.0778928217 C,0,-2.7375645338,-1.3833253979,3.2009743757 H,0,-3.2721547382,-2.2380478431,3.6184144521 H,0,-3.1782271226,-1.1728384752,2.2236468368 H,0,-2.9343352984,-0.5272666094,3.8467024767 C,0,-1.0118589749,-2.96816449,2.2792388845 H,0,-1.4854362296,-3.8230301954,2.765014361 H,0,0.0518500067,-3.1814143675,2.1755542992 H,0,-1.4284530305,-2.8755879794,1.2733485226</p>	<p>H,0,-1.8752760434,-1.3389359181,-3.1285222616 C,0,-1.2253803651,1.7039114166,-3.0675843113 H,0,-0.80187637,1.8150342813,-4.0716804349 C,0,-2.716322598,1.4249559308,-3.1784280466 H,0,-3.2338671488,2.2966445553,-3.5831247284 H,0,-3.1547630253,1.2158843984,-2.1993979046 H,0,-2.9407842436,0.5814563193,-3.8317729746 C,0,-0.9502797678,2.9650518198,-2.2655948846 H,0,-1.3993593067,3.8338336675,-2.7507581767 H,0,0.118101488,3.1547131947,-2.1579779131 H,0,-1.3722401766,2.8848772767,-1.2605341168 C,0,-0.5804433444,-0.9955764407,-4.8089995442 H,0,-1.156527582,-0.1579858607,-5.2039983631 H,0,-0.8714724859,-1.884776605,-5.3720601142 H,0,0.4742970848,-0.8088160592,-5.0231839954 C,0,-0.0692588787,-2.4381607993,-2.8050433273 H,0,-0.3870716923,-3.3327746196,-3.3437289545 H,0,-0.2505840799,-2.5942158803,-1.7394194149 H,0,1.009346135,-2.3348821119,-2.9421968539 C,0,-0.7968101572,1.2118197581,3.3248465902 H,0,-1.8690363942,1.3384067038,3.1317865312 C,0,-0.0634786401,2.437395113,2.8049776735 H,0,-0.3801052174,3.3319966029,3.344381641 H,0,-0.2468387064,2.5936022967,1.7397237621 H,0,1.0153739273,2.3339300452,2.9400298913 C,0,-0.5710441924,0.9946543191,4.809745171 H,0,-1.1464904865,0.1570968537,5.205743503 H,0,-0.8608705375,1.8838264755,5.3734692685 H,0,0.4840771806,0.8077157759,5.0218905723 C,0,-1.2197461358,-1.7045283521,3.0692319331 H,0,-0.7942774262,-1.8158978114,4.072470208 C,0,-2.710411936,-1.4253008495,3.1830766509 H,0,-3.2273232887,-2.2969561205,3.5886541883 H,0,-3.1507495599,-1.2159804593,2.2049514308 H,0,-2.9334130956,-0.5818685469,3.837008527 C,0,-0.9464870788,-2.9655916973,2.2664959323 H,0,-1.3947809472,-3.8343619784,2.7524062136 H,0,0.121640547,-3.155449393,2.1567318158 H,0,-1.3704237527,-2.8851677066,1.2622868957</p>
 <p>6-(triplet)</p>	 <p>6-(triplet)</p>
<p>HF=-2294.5937903 ZPE= 0.465719 NImag=0</p> <p>Htot= -2294.094464 Gtot= -2294.192002</p> <p>C,0,1.714455998,-0.0539409056,-0.0215090909 C,0,2.4635764575,-0.3599702107,1.1235057832 S,0,1.7019322835,-0.7571831429,2.7124626914 P,0,-0.3572177872,-0.4145472316,2.2562133356 Rh,0,-0.3915582675,-0.0391142396,-0.0154628384 C,0,2.4607116025,0.2425472719,-1.1712648392 S,0,1.6918128094,0.7123801073,-2.735678333 P,0,-0.3626687405,0.3252620524,-2.2881756274 H,0,-3.0818069603,1.1956936964,0.5938966523 H,0,-3.6656974872,1.6339365067,0.7827052233 C,0,4.5460502479,-0.0955248472,-0.0366676922 C,0,3.8571236708,-0.3839623121,1.1292280339 C,0,3.8542564732,0.2193634098,-1.1937127012 H,0,4.3991738157,-0.6245067766,2.035786235 H,0,4.3932800037,0.4479523451,-2.105113689 H,0,5.6288155134,-0.1141373101,-0.0427489728</p>	<p>HF=-2294.6180687 ZPE= 0.466048 NImag=0</p> <p>Htot= -2294.118783 Gtot= -2294.214677</p> <p>C,0,1.723224304,-0.0402783157,-0.0215545243 C,0,2.477087473,-0.3231130452,1.1280054849 S,0,1.7170680013,-0.7070613035,2.721696973 P,0,-0.3539439286,-0.3920955341,2.2693260895 Rh,0,-0.3868285532,-0.0329536471,-0.0148031048 C,0,2.4723994147,0.2336693115,-1.1764520034 S,0,1.7038578166,0.6505537345,-2.7569611916 P,0,-0.3640965394,0.3053814156,-2.3045410329 H,0,-3.0424859475,1.1349113921,0.5359009301 H,0,-3.6449561272,1.5587389421,0.7022465261 C,0,4.5606407785,-0.0650785025,-0.0334598272 C,0,3.8715044784,-0.3373164573,1.1364827249 C,0,3.8667988346,0.221603562,-1.1970917356 H,0,4.4153526315,-0.5589601401,2.0471935359 H,0,4.4066636894,0.4343105419,-2.1122704072 H,0,5.6438124181,-0.0762796416,-0.0382635355</p>

<p>C,0,-0.7533199943,-1.1920664478,-3.3025177709 H,0,-1.8377105451,-1.3025799682,-3.186525609 C,0,-1.1885243555,1.7526548294,-3.1593506461 H,0,-0.6948891447,1.8747801459,-4.1295614943 C,0,-2.6648092217,1.4514408849,-3.3682818546 H,0,-3.1739619663,2.3221235105,-3.7846482718 H,0,-3.150873376,1.2085888238,-2.4196216103 H,0,-2.8297138211,0.6179548768,-4.0511900098 C,0,-0.9849903229,3.0091227941,-2.3268615472 H,0,-1.4099861697,3.8789413428,-2.8299301229 H,0,0.0715270466,3.2058833426,-2.1432535908 H,0,-1.4827149124,2.9099902632,-1.3581814486 C,0,-0.4067818206,-1.0645141354,-4.7742078793 H,0,-0.9314381308,-0.2369456492,-5.2538567874 H,0,-0.6735273455,-1.9763669713,-5.312026321 H,0,0.6648141045,-0.9042879928,-4.9064363224 C,0,-0.0693345097,-2.381044308,-2.6435457613 H,0,-0.3277534292,-3.311231356,-3.1518772829 H,0,-0.3592907791,-2.4800972449,-1.592388372 H,0,1.0166032514,-2.2714970842,-2.6749829667 C,0,-0.7936618967,1.0971003095,3.2584237307 H,0,-1.8832142557,1.1632292795,3.1568120789 C,0,-0.1688306623,2.3014412007,2.5691257166 H,0,-0.4528363054,3.2295593063,3.0676062554 H,0,-0.4848547888,2.3727014505,1.5221818941 H,0,0.9210419733,2.2339272459,2.5777820583 C,0,-0.4229953324,1.0045879077,4.7265745222 H,0,-0.9079437429,0.1629802235,5.2233877146 H,0,-0.719064552,1.9119878034,5.2565089759 H,0,0.6556732683,0.8886709637,4.8462595321 C,0,-1.1623705858,-1.8564083267,3.1226203123 H,0,-0.6856018695,-1.9560317729,4.1038214202 C,0,-2.6501572665,-1.592302873,3.2984557143 H,0,-3.145285418,-2.4723921086,3.7119503144 H,0,-3.1221259155,-1.3692805902,2.3377345578 H,0,-2.8510410233,-0.757727549,3.9703903116 C,0,-0.9073121022,-3.1146895763,2.3076913532 H,0,-1.3217415169,-3.9904415428,2.8092301637 H,0,0.1580214515,-3.2856577033,2.1514477525 H,0,-1.3833055496,-3.0371053167,1.3264645199</p>	<p>C,0,-0.7880447042,-1.2004419578,-3.3215392117 H,0,-1.8761606383,-1.2758423912,-3.2112968878 C,0,-1.155208296,1.7525753116,-3.1786829274 H,0,-0.6493039407,1.8707366795,-4.1427975431 C,0,-2.6332929832,1.4809603447,-3.4086290643 H,0,-3.119674812,2.3658662236,-3.8234093521 H,0,-3.1404046575,1.2391320142,-2.4703974791 H,0,-2.8060577482,0.6584594757,-4.1029430116 C,0,-0.9402392766,3.0011184237,-2.3387863038 H,0,-1.3343103671,3.8822177343,-2.8481922475 H,0,0.1161699809,3.1781840692,-2.13237955 H,0,-1.4594095178,2.9145255896,-1.3799666124 C,0,-0.4349519739,-1.0845023332,-4.7917700831 H,0,-0.9162252345,-0.2292832661,-5.2688939419 H,0,-0.7488532354,-1.9794436046,-5.3333555965 H,0,0.6432710743,-0.9806509619,-4.9280770791 C,0,-0.1497004446,-2.4118461942,-2.6601777442 H,0,-0.4454796225,-3.3334240943,-3.1646702229 H,0,-0.4430794532,-2.4977401196,-1.6083341048 H,0,0.9402846689,-2.3497467989,-2.6925362455 C,0,-0.8110845696,1.0981703836,3.2933231771 H,0,-1.9018640936,1.1432303819,3.1922953374 C,0,-0.2128642085,2.3278359876,2.6286662819 H,0,-0.5257985038,3.2402350684,3.1395134243 H,0,-0.5224171824,2.4100750741,1.5807724851 H,0,0.8787531797,2.2941475074,2.6458729561 C,0,-0.4455351015,0.9880259564,4.7608191595 H,0,-0.9025286369,0.1193524792,5.2375884972 H,0,-0.7788829211,1.8729136476,5.3073296922 H,0,0.6357223062,0.9112933647,4.8904316663 C,0,-1.1312062066,-1.8556797686,3.1278215849 H,0,-0.6316993898,-1.9723709141,4.0954363964 C,0,-2.6147237489,-1.6046884121,3.3467566624 H,0,-3.0932423212,-2.4978104648,3.7529808052 H,0,-3.1167594307,-1.3646156961,2.4050516446 H,0,-2.8037809688,-0.787913438,4.0437879989 C,0,-0.8927847733,-3.0962546389,2.2830195162 H,0,-1.2776229215,-3.9858238101,2.7846887775 H,0,0.1673844729,-3.2571323193,2.0825710712 H,0,-1.4065344429,-3.0106304453,1.3213405724</p>
 <p>6a (singlet)</p>	 <p>6a (singlet)</p>
<p>HF=-2294.6403636 ZPE= 0.469303 NImag=0</p> <p>Htot= -2294.139594 Gtot= -2294.231206</p> <p>C,0,1.6385209947,-0.0183071607,0.0050780242 C,0,4.4897108474,0.0274528066,0.007884844 C,0,2.4010233909,0.2800421594,-1.141216716 C,0,2.4083204831,-0.300524106,1.1508675198 C,0,3.8016014626,-0.2724186429,1.1704346284 C,0,3.7940753048,0.3032178074,-1.1564714847 H,0,4.3442159216,-0.4868802054,2.0827866974 H,0,4.3312460952,0.5320243956,-2.0685930436 H,0,5.572475275,0.044720651,0.0086846098 P,0,-0.384637912,0.21450917,-2.258826793 P,0,-0.3754789378,-0.328004569,2.2563668286 S,0,1.6376155499,0.6852465232,-2.7246410598 S,0,1.6548670014,-0.7483019734,2.7254746083 H,0,-2.1457818425,-0.0214427482,0.0087312535</p>	<p>HF=-2294.6643795 ZPE= 0.469009 NImag=0</p> <p>Htot= -2294.163944 Gtot= -2294.255657</p> <p>C,0,1.6704006348,0.0005740816,-0.0029253604 C,0,4.520505374,0.0706924981,0.00011393 C,0,2.4309225458,0.2121949879,-1.1694726868 C,0,2.4387510575,-0.1965366776,1.1615264625 C,0,3.8323647586,-0.1548256364,1.1796136622 C,0,3.8246271968,0.2520955317,-1.1824067688 H,0,4.376178349,-0.3015295933,2.1049209019 H,0,4.3626594417,0.4197398801,-2.1075880815 H,0,5.603185623,0.1009660348,0.001700829 P,0,-0.3774610391,0.1672531842,-2.2781916976 P,0,-0.3641005885,-0.268742812,2.2645422507 S,0,1.6723758657,0.4616911363,-2.7863414478 S,0,1.6894365718,-0.5477876518,2.7623139684 H,0,-2.1195965114,-0.0400266764,0.0006267856</p>

<p>C,0,-0.7845928761,-1.2189304431,-3.3787376676 H,0,-1.8448820992,-1.409942651,-3.1759884741 C,0,-1.3036287445,1.6741583376,-2.9636988394 H,0,-0.8717715043,1.8885582322,-3.9471395769 C,0,-2.7827795461,1.3474068089,-3.1040526522 H,0,-3.3350620947,2.2315768064,-3.4263919844 H,0,-3.197604394,1.0253201224,-2.1462925153 H,0,-2.9711242311,0.5599448428,-3.8339904174 C,0,-1.0804314713,2.8627653209,-2.0405198004 H,0,-1.5436928899,3.7629262652,-2.4470230688 H,0,-0.0193826521,3.0669506408,-1.8905635034 H,0,-1.5350340424,2.6702750544,-1.0643629696 C,0,-0.5897448772,-0.8870261486,-4.8488157825 H,0,-1.2140467946,-0.0572342454,-5.1806041426 H,0,-0.8365234536,-1.750906828,-5.4682222777 H,0,0.4517578422,-0.6281341328,-5.051197131 C,0,0.0270516118,-2.4358709784,-2.9656369932 H,0,-0.2445371616,-3.2980493697,-3.5762334055 H,0,-0.1307563653,-2.6957135693,-1.9191706395 H,0,1.0944061631,-2.2518846828,-3.1025448466 C,0,-0.765194746,1.2221955846,3.2193473525 H,0,-1.8405292015,1.3566823961,3.0570347836 C,0,-0.0251153248,2.3841238371,2.5731012586 H,0,-0.2624558711,3.3224099316,3.0764957524 H,0,-0.290121582,2.4972430064,1.5186748896 H,0,1.0556030444,2.2385769155,2.6275481184 C,0,-0.4786296088,1.1095307256,4.7052917928 H,0,-1.0562294922,0.3163682899,5.1814496304 H,0,-0.7256506536,2.0433759877,5.213665046 H,0,0.5798588539,0.9083059212,4.8815552489 C,0,-1.2751437653,-1.6950285371,3.1392588325 H,0,-0.8256502056,-1.7576258707,4.1367979691 C,0,-2.7530554721,-1.3540432422,3.2624047882 H,0,-3.2967881212,-2.1940297085,3.697221283 H,0,-3.186292511,-1.1489897835,2.2810488235 H,0,-2.9311600308,-0.4856589778,3.8968276376 C,0,-1.060010349,-3.0127748347,2.413483899 H,0,-1.4949954906,-3.8349388125,2.9835467895 H,0,-0.0017156654,-3.2262796232,2.2633563276 H,0,-1.5432966008,-2.9938567585,1.435141109 Rh,0,-0.4949008257,-0.0197735808,0.0097144875 H,0,-0.7664794345,-1.5057203568,-0.1567330484</p>	<p>C,0,-0.9192444303,-1.2331782505,-3.3765106539 H,0,-1.9969237325,-1.2923412336,-3.1856034059 C,0,-1.1891707973,1.6953712145,-2.9746038639 H,0,-0.7370648805,1.8825631802,-3.9541123181 C,0,-2.6872706614,1.4878762236,-3.1297167037 H,0,-3.1629533077,2.419060838,-3.4432281034 H,0,-3.1417693801,1.1876999092,-2.1827428553 H,0,-2.9329459518,0.7307248633,-3.8743942118 C,0,-0.8819184046,2.8585101434,-2.0443251808 H,0,-1.2528293994,3.7965076073,-2.4607279743 H,0,0.1890199828,2.9735397573,-1.8676501458 H,0,-1.3759433698,2.7138747676,-1.0791595054 C,0,-0.6742385857,-0.9518548222,-4.849435216 H,0,-1.1662503109,-0.042210455,-5.1950048333 H,0,-1.0495957723,-1.7767825851,-5.4577982918 H,0,0.393585281,-0.8567563437,-5.0581657074 C,0,-0.2690125232,-2.5320758851,-2.9340499514 H,0,-0.6085564592,-3.3574140707,-3.5620328538 H,0,-0.5097138007,-2.7765365939,-1.8993484751 H,0,0.8184488798,-2.4768379378,-3.0193146002 C,0,-0.8763857082,1.228620603,3.2502659808 H,0,-1.9554702269,1.2854850198,3.0679166765 C,0,-0.2152328428,2.4603390163,2.6538036112 H,0,-0.5398965272,3.3621553328,3.1753489502 H,0,-0.4627444775,2.5852454608,1.5971472283 H,0,0.8723489396,2.40386552,2.7356917831 C,0,-0.6152890173,1.1003723722,4.7393442059 H,0,-1.1279134499,0.2459288711,5.1826317975 H,0,-0.9604334579,1.9941554442,5.2630132696 H,0,0.4524213526,0.9958609395,4.9434202893 C,0,-1.1794087815,-1.7142363194,3.1066243918 H,0,-0.7318510498,-1.7704874531,4.1051481695 C,0,-2.6764127858,-1.4771014105,3.2319633357 H,0,-3.1593692445,-2.3600763308,3.6542936082 H,0,-3.1266535478,-1.2903266592,2.2545069086 H,0,-2.9163172463,-0.6336993674,3.8798055801 C,0,-0.8754836789,-2.9975364169,2.3531694544 H,0,-1.2427009754,-3.8599384617,2.9121119759 H,0,0.1941063158,-3.1352752121,2.1899764361 H,0,-1.3683211111,-2.9988464103,1.3790714882 Rh,0,-0.4481522874,0.0003756842,0.003371931 H,0,-0.429300848,-1.5127628365,-0.1275288624</p>
 <p>6a-(triplet)</p>	 <p>6a-(triplet)</p>
<p>HF=-2294.601122 ZPE=0.468708 NImag=0</p> <p>Htot= -2294.100492 Gtot= -2294.193673</p> <p>C,0,1.6155922477,-0.1574291984,-0.0079723524 C,0,4.4040637168,0.3054954579,0.0668780601 C,0,2.3371784292,0.2099437145,-1.1504433904 C,0,2.3593124282,-0.2820900969,1.1735987126 C,0,3.7323007986,-0.0492951744,1.224478801 C,0,3.7124298422,0.4418137479,-1.1238484591 H,0,4.2688688185,-0.1430314173,2.1606858339 H,0,4.2361814574,0.7281578348,-2.0278357727 H,0,5.4714190624,0.4860374814,0.0949341543 P,0,-0.4803103624,0.0418960866,-2.3207669016 P,0,-0.4483075387,-0.395357526,2.2693125201 S,0,1.5758845647,0.4268403272,-2.7688845223</p>	<p>HF=-2294.6121009 ZPE= 0.466796 NImag=1 (-14)</p> <p>Htot= -2294.114659 Gtot= -2294.204919</p> <p>C,0,1.6203482144,-0.0036866035,-0.021085308 C,0,4.453012544,0.0301337975,-0.0518510259 C,0,2.3525451215,0.3396380463,-1.1746062984 C,0,2.3854056055,-0.3290569209,1.116194247 C,0,3.7787012423,-0.3091022426,1.108186474 C,0,3.7457651418,0.3529260583,-1.1968700281 H,0,4.331692953,-0.5574218881,2.0058917706 H,0,4.2730456359,0.6142243955,-2.1062853689 H,0,5.5357560651,0.0430593542,-0.0636086903 P,0,-0.4354719353,0.2625262848,-2.2734046635 P,0,-0.3792053699,-0.3180525783,2.2755471118 S,0,1.5746962173,0.8147951396,-2.720245564</p>

<p>S,0,1.6066644179,-0.7694019215,2.7375520279 H,0,-0.8204826071,-2.2764072519,-0.1930197548 C,0,-0.9511235627,-1.1300965522,-3.700461231 H,0,-2.0333117942,-1.2472826174,-3.5708378667 C,0,-1.2795536941,1.6624606748,-2.8087274266 H,0,-0.8331893101,1.9661567625,-3.7610339904 C,0,-2.7803288756,1.4804540422,-2.9724898274 H,0,-3.2624639375,2.4409068136,-3.1626623666 H,0,-3.2213033861,1.0661973238,-2.0612259729 H,0,-3.0353066666,0.8165782207,-3.7989927463 C,0,-0.9569320698,2.7041075302,-1.750788661 H,0,-1.3319772112,3.685393376,-2.0459719214 H,0,0.1172282087,2.7886633215,-1.5777602892 H,0,-1.4299495852,2.4371962633,-0.8009254978 C,0,-0.6675695142,-0.57656688,-5.0873032908 H,0,-1.1892033941,0.3609768921,-5.2800111635 H,0,-0.9829230232,-1.2892482298,-5.8517798421 H,0,0.4013165179,-0.4026379888,-5.2267099719 C,0,-0.2865459247,-2.479563857,-3.486417667 H,0,-0.5871632343,-3.1798274971,-4.2671615273 H,0,-0.5521129085,-2.9158381883,-2.5244018709 H,0,0.8005003463,-2.3859672735,-3.5227389484 C,0,-0.7682221153,1.2694819579,3.0659172191 H,0,-1.8377206156,1.433596868,2.8860815644 C,0,0.0219432683,2.3332694623,2.3193191518 H,0,-0.221477856,3.3275947442,2.6966430184 H,0,-0.1830836675,2.3153710075,1.2472005559 H,0,1.0952359034,2.1803328828,2.448886972 C,0,-0.4871292622,1.3027402955,4.5575133109 H,0,-1.1088180338,0.6052375908,5.1194225362 H,0,-0.6744948332,2.3011503735,4.9572680896 H,0,0.558494917,1.0598015746,4.7571879903 C,0,-1.2738358358,-1.6218073871,3.4107172099 H,0,-0.7838025395,-1.5270363449,4.3859007218 C,0,-2.7500185563,-1.2775618726,3.5463121761 H,0,-3.2594787696,-2.0259509138,4.1554293094 H,0,-3.235826912,-1.2630190062,2.567176845 H,0,-2.9148953156,-0.3067119768,4.0136709583 C,0,-1.0802746916,-3.0358856062,2.8897423222 H,0,-1.4877451159,-3.7608742164,3.5959060044 H,0,-0.0279569556,-3.2715257267,2.7309082403 H,0,-1.6027087907,-3.1700839451,1.9403870067 Rh,0,-0.4781622182,-0.4681784111,-0.0518820951 H,0,0.0085367392,-2.2315595506,-0.1643699851</p>	<p>S,0,1.6528808744,-0.8219185896,2.6783366914 H,0,-1.3523878571,1.3669215027,0.2097712634 C,0,-0.7347507599,-1.2483985715,-3.3316023828 H,0,-1.7659659238,-1.5212935489,-3.0780478621 C,0,-1.4129695621,1.6190824877,-3.094974269 H,0,-1.054440281,1.6639004719,-4.1290051112 C,0,-2.8872745632,1.2415499003,-3.082832773 H,0,-3.4830457439,2.0383351492,-3.5312930661 H,0,-3.2437952747,1.1001712849,-2.0594118227 H,0,-3.0930481043,0.3262596162,-3.6388835734 C,0,-1.1719384356,2.9608351904,-2.4288714943 H,0,-1.7048692754,3.7458246302,-2.9684354605 H,0,-0.1146848084,3.2254925269,-2.4089137677 H,0,-1.5331590038,2.9548393967,-1.3989163098 C,0,-0.624223944,-0.9785101578,-4.8213873752 H,0,-1.3632036769,-0.2607420636,-5.1777568395 H,0,-0.7738079895,-1.9030179184,-5.3823577288 H,0,0.36804867,-0.6019558662,-5.081744006 C,0,0.1858028955,-2.3735604695,-2.8903434978 H,0,-0.0612220695,-3.2931767141,-3.423250169 H,0,0.1029373313,-2.570270101,-1.8203927567 H,0,1.2289223428,-2.1354332978,-3.1085719142 C,0,-0.6920547161,1.1844270742,3.3417956639 H,0,-1.7347693131,1.43249802,3.1107542238 C,0,0.19137185,2.3318226491,2.8822846961 H,0,-0.0663333976,3.2448315471,3.4214568599 H,0,0.0808591731,2.5271811725,1.8145925568 H,0,1.2443766697,2.1188432105,3.077850818 C,0,-0.5431100684,0.9162153968,4.8285335914 H,0,-1.2567198417,0.1805346828,5.1997623545 H,0,-0.7029330642,1.8364319794,5.393720079 H,0,0.4633247083,0.5635836569,5.067120984 C,0,-1.3055690388,-1.6985141547,3.1163797791 H,0,-0.9239086678,-1.735237552,4.1424217416 C,0,-2.7885456335,-1.3570417724,3.1363244069 H,0,-3.3549398438,-2.1683122284,3.5967229926 H,0,-3.1703488488,-1.2239410733,2.1209450939 H,0,-3.0045430451,-0.4472856965,3.6975572644 C,0,-1.0462789499,-3.03357415,2.4437158793 H,0,-1.5484087363,-3.8316435767,2.9935383595 H,0,0.0164230067,-3.2724606409,2.4009988021 H,0,-1.4293638521,-3.0356646482,1.4216696548 Rh,0,-0.4856467536,-0.0280765836,0.001960475 H,0,-1.3255369134,-1.4419190144,-0.1874787081</p>
 <p>6a+py</p>	 <p>6a+py</p>
<p>HF=-2543.0008307 ZPE= 0.561355 NImag=0</p> <p>Htot= -2542.403092 Gtot= -2542.504854</p> <p>C,0,-1.8436314317,0.0929603299,-0.3969240182 C,0,-4.688260831,0.1336900099,-0.5363115986 C,0,-2.5962067836,-0.9939338471,-0.8775509957 C,0,-2.6092321611,1.2167487598,-0.0395586599 C,0,-4.0015076291,1.2550073355,-0.102664658 C,0,-3.9891326459,-0.9941997711,-0.9332056735 H,0,-4.540588579,2.1528101049,0.1742231958 H,0,-4.5239516998,-1.8659099977,-1.290201609 H,0,-5.770181642,0.1440221168,-0.5817500677 P,0,0.1548735451,-2.1687653249,-0.7489881277</p>	<p>HF=-2543.0252626 ZPE= 0.561220 NImag=0</p> <p>Htot= -2542.427689 Gtot= -2542.529312</p> <p>C,0,-1.8485997794,0.0966831784,-0.3995771665 C,0,-4.6957340222,0.131985033,-0.5311052059 C,0,-2.6019111195,-0.9941769216,-0.8725374658 C,0,-2.6157640203,1.2223484097,-0.0473591782 C,0,-4.0088419279,1.2566549379,-0.105948488 C,0,-3.995689651,-0.9968481435,-0.9238545932 H,0,-4.5499609575,2.1542313923,0.168521413 H,0,-4.5312413657,-1.8709919449,-1.274469601 H,0,-5.7780568773,0.1402238386,-0.5726878901 P,0,0.1557906966,-2.1720266958,-0.7466015658</p>

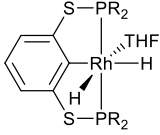
<p>P,0,0.1139520192,2.3321734848,-0.3206320339 S,0,-1.8065321853,-2.4763813874,-1.5292439545 S,0,-1.8150926291,2.7474085021,0.5057972047 C,0,1.2345366236,-2.8434551679,-2.1108800153 H,0,0.8415806089,-3.8391316799,-2.342946329 C,0,0.2695847592,-3.4794521655,0.5913758722 H,0,1.2292144216,-3.2685977672,1.0790904389 C,0,-0.8533538277,-3.292153583,1.6014338872 H,0,-0.6725624917,-3.9023292545,2.4883250574 H,0,-1.8058472354,-3.601931732,1.1694060866 H,0,-0.9633057083,-2.2572915522,1.9164049134 C,0,0.26740673,-4.903359279,0.058473107 H,0,0.2622262047,-5.6142008111,0.8872160779 H,0,1.1330847038,-5.1320548801,-0.5615946861 H,0,-0.6331862778,-5.0903529105,-0.5316184972 C,0,1.1653232161,-1.9847045093,-3.3612594148 H,0,0.1378599727,-1.8146079679,-3.6835774088 H,0,1.7025788833,-2.470297238,-4.1778824196 H,0,1.6285300335,-1.0130098126,-3.185326975 C,0,2.6651068109,-2.9596271794,-1.601650955 H,0,3.318517907,-3.3339963135,-2.3914634157 H,0,2.7586871111,-3.6358255015,-0.7509395552 H,0,3.0358284651,-1.9796778876,-1.2931820187 C,0,1.1973781085,3.5150320419,0.6382736717 H,0,2.08064167,3.5989963047,-0.0054303189 C,0,1.6283755887,2.9058905644,1.9608099394 H,0,2.3012756477,3.5826891919,2.4904910132 H,0,2.143749137,1.9585621482,1.808347287 H,0,0.767568034,2.7234429691,2.6085588923 C,0,0.5870074087,4.8956778177,0.8249170092 H,0,0.2561477663,5.3448525747,-0.1111870934 H,0,1.3162230181,5.572389202,1.274381264 H,0,-0.273350987,4.8545347707,1.4951676293 C,0,0.0788454079,3.1047623764,-2.0224165617 H,0,-0.0740610249,4.1769674993,-1.8583756145 C,0,1.4167781178,2.8796821995,-2.7133449295 H,0,1.4101385268,3.3397207901,-3.7029610742 H,0,1.6086122207,1.8125746192,-2.839394861 H,0,2.2570643015,3.3018210189,-2.1609859045 C,0,-1.0723397309,2.5656354223,-2.8536767975 H,0,-1.0733836328,3.0364111156,-3.8382759811 H,0,-2.0380165502,2.7564537697,-2.386663935 H,0,-0.9797056046,1.4870783399,-2.9967224112 Rh,0,0.2910275528,0.0573959041,-0.2705684542 H,0,0.3518554002,0.1729277621,-1.8181976342 H,0,1.9524554171,0.057292956,-0.2778603131 N,0,0.3223594041,-0.1292480867,2.016939947 C,0,0.4154709305,-0.3635528807,4.7863343796 C,0,1.4293315522,-0.5587682142,2.6365247926 C,0,-0.7398480787,0.1806277721,2.7703217404 C,0,-0.731330307,0.083479327,4.1520094679 C,0,1.5159468443,-0.6948182559,4.0103300595 H,0,2.2639660329,-0.7854335095,1.9822411106 H,0,-1.6198814332,0.507366903,2.2293469757 H,0,-1.6167144653,0.3515888604,4.7125670913 H,0,2.4340554343,-1.0501057905,4.4587676659 H,0,0.4522901356,-0.4536420067,5.8647775186</p>	<p>P,0,0.1114712892,2.3440743038,-0.3251786721 S,0,-1.8135378266,-2.4797863733,-1.5175069579 S,0,-1.825987144,2.7571395506,0.4888858035 C,0,1.2264942191,-2.850087976,-2.1142167924 H,0,0.8271244165,-3.8440685199,-2.3424577347 C,0,0.2774639718,-3.4766990671,0.5971934582 H,0,1.2386153431,-3.2578862817,1.0777054407 C,0,-0.8394285713,-3.2904793184,1.6132968033 H,0,-0.631459498,-3.8680193192,2.516317489 H,0,-1.7890266969,-3.6413676062,1.206406007 H,0,-0.976642913,-2.2509017305,1.9020495512 C,0,0.282700833,-4.9034817942,0.0738211088 H,0,0.2912956861,-5.6067050479,0.9095291654 H,0,1.1455433547,-5.1325245549,-0.5503048785 H,0,-0.620326697,-5.1085956966,-0.5067456749 C,0,1.1586055415,-1.9946537961,-3.3659821336 H,0,0.1325633676,-1.8157310242,-3.689269445 H,0,1.6868218215,-2.4889779943,-4.183774303 H,0,1.6329276686,-1.026266761,-3.2003610696 C,0,2.6587326316,-2.9773270778,-1.6143224632 H,0,3.298975955,-3.3747741158,-2.4041336113 H,0,2.7535247403,-3.6402189599,-0.7534480181 H,0,3.051646444,-1.9995139005,-1.3271399597 C,0,1.1950737737,3.5207582081,0.6401595155 H,0,2.0815145924,3.5962040398,-0.000018471 C,0,1.6185670017,2.9169087612,1.9667021719 H,0,2.2949194617,3.5949703932,2.4910533166 H,0,2.1337682094,1.9678027348,1.8244115406 H,0,0.7592790402,2.7434470033,2.6187832086 C,0,0.5950325292,4.9063179751,0.8177882397 H,0,0.2664400532,5.3543908373,-0.1199799572 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H,0,-1.6180694849,0.5200534445,2.2394495114 H,0,-1.6222649355,0.3347048297,4.7166930045 H,0,2.4191946225,-1.0936577965,4.4558609312 H,0,0.4384071969,-0.499497634,5.8648502191</p>
 <p>6-NMeH₂ (5)</p>	 <p>6-NMeH₂ (5)</p>
<p>HF=-2390.5475428 ZPE= 0.538098 NImag=0 Htot= -2389.974704</p>	<p>HF=-2390.5693803 ZPE=0.538240 NImag=0 Htot=-2389.996563</p>

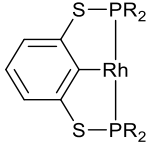
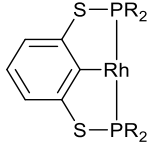
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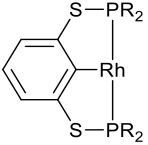
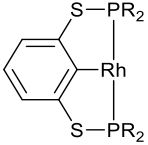
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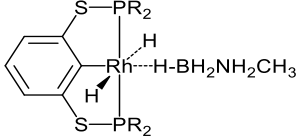
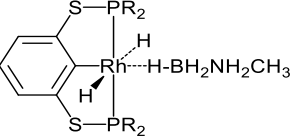
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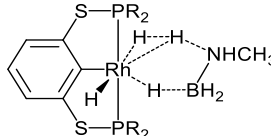
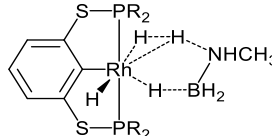
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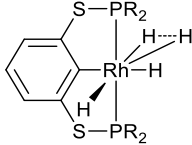
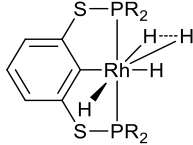
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H,0,2.9912608146,3.8042125075,1.2538049614 H,0,2.9238241202,2.8658704312,-0.2398444755 H,0,2.4259691624,2.1253347295,1.2592437343 C,0,0.3262630042,3.7491654548,1.8795200454 H,0,0.9596867502,4.38061098,2.5058605985 H,0,0.2062309162,2.7909522954,2.3885064857 H,0,-0.6563575155,4.2120005435,1.8149438619 C,0,1.2993569529,-2.8530990267,-2.0723586652 H,0,0.9571443882,-3.8824218496,-2.2248426961 C,0,0.5636832633,-3.3898751788,0.7120282857 H,0,1.5687234903,-3.1193066608,1.0574366183 C,0,1.0918497868,-2.0803840203,-3.3634661304 H,0,1.5764108225,-2.5994907893,-4.1922221972</p>	<p>HF=-2527.1766681 ZPE=0.589207 NImag=0</p> <p>H=-2526.550335 G=-2526.653479</p> <p>H,0,0.4702245913,0.0684192997,-1.8738376678 Rh,0,0.2289341127,0.0688232782,-0.3616931199 H,0,1.881777597,0.0961944522,-0.1749802808 C,0,-1.8830477615,0.0214933905,-0.6646096404 C,0,-4.7189190065,-0.0684578991,-0.9612163513 C,0,-2.5795728668,-1.1582078971,-0.9877029205 C,0,-2.7022892582,1.1583312058,-0.5399916274 C,0,-4.0891926135,1.1328693541,-0.682342031 C,0,-3.9674545462,-1.2200552952,-1.119758397 H,0,-4.6710550823,2.041202427,-0.5809266899 H,0,-4.4572264689,-2.1581191879,-1.3520978132 H,0,-5.7962618228,-0.1048097448,-1.0675331088 P,0,0.2439696897,-2.1917481619,-0.683775164 P,0,0.0430372798,2.3400882039,-0.5720337189 O,0,-0.0573887862,0.2335847495,1.999020945 C,0,-1.3219497841,0.4206994543,2.6690316594 H,0,-1.9477748019,-0.4637518373,2.499025461 H,0,-1.8161793729,1.2808736772,2.2144235925 C,0,0.9837833014,-0.0232626713,2.9592616167 H,0,1.6403737442,0.853952154,3.0072428129 H,0,1.5772499024,-0.8678069146,2.6029748151 C,0,-0.9712751249,0.6012548198,4.1297529738 H,0,-1.784241836,0.3067838381,4.7910813037 H,0,-0.731571813,1.6469174888,4.3375766483 C,0,0.2723173672,-0.2670382787,4.2732649982 H,0,-0.0088871057,-1.3184062005,4.3658563142 H,0,0.8872385647,-0.0074212751,5.1333739322 S,0,-1.7325214754,-2.7163135377,-1.3046492862 S,0,-2.0122603565,2.7854773619,-0.1703748807 C,0,0.2714494093,3.0524300167,-2.2879835212 H,0,-0.0493503075,4.0967775942,-2.1986425391 C,0,-0.6232605666,2.3487391277,-3.2931645361 H,0,-0.5530811871,2.8461137135,-4.2624494392 H,0,-1.6705630245,2.3526916879,-2.9911184354 H,0,-0.3222568995,1.3085218793,-3.4328642922 C,0,1.7289921098,3.0053758736,-2.7200735174 H,0,2.3646024883,3.6647669032,-2.1299920057 H,0,1.8177625699,3.3191321842,-3.7621127256 H,0,2.1301899519,1.9913100791,-2.6464759159 C,0,0.970672998,3.5493778868,0.5268302325 H,0,0.9729883186,4.5007850654,-0.0175120603 C,0,2.4049941505,3.0691852061,0.7135003619 H,0,2.9813094358,3.8250494094,1.2513232285 H,0,2.9192102822,2.8582590727,-0.2223047714 H,0,2.4246214047,2.1463862454,1.2952160387 C,0,0.310666981,3.743920761,1.8816198699 H,0,0.9440639291,4.3689889725,2.5148774151 H,0,0.1815431143,2.7854277795,2.3878309467 H,0,-0.6672475916,4.2174625579,1.8160231823 C,0,1.2826209131,-2.8652700768,-2.0809646379 H,0,0.9265844663,-3.8890761115,-2.2386537844 C,0,0.5702684806,-3.3963779856,0.7126913858 H,0,1.5784639628,-3.1218579795,1.045025413 C,0,1.0838331616,-2.0813935487,-3.3658918041 H,0,1.5489716395,-2.6091994269,-4.2007865329</p>

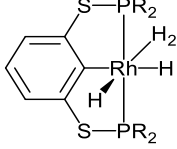
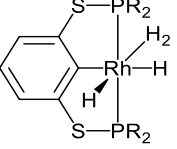
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 <p>3-singlet</p>	 <p>3-singlet</p>
<p>HF=-2293.454800 ZPE=0.454005 NImag=0</p> <p>Htot=-2292.969928 Gtot=-2293.062082</p> <p>C,0,1.5773179892,-0.0004505007,-0.0019315095 C,0,2.3507066057,-0.3086259599,1.1451200797 S,0,1.637139107,-0.7581938141,2.7267352069 P,0,-0.3624499037,-0.2562084167,2.2692834356 Rh,0,-0.417803166,-0.0001395521,0.0001985632 C,0,2.3483500381,0.307580411,-1.1506082176 S,0,1.6315326356,0.7573701392,-2.730692778 P,0,-0.3671791112,0.2557420818,-2.2690148026 C,0,4.4421231735,-0.0007138778,-0.0049425107 C,0,3.7434212486,-0.3004865456,1.1482236403 C,0,3.7410534223,0.2991846327,-1.1566386491 H,0,4.2733132932,-0.5317388854,2.0641727923 H,0,4.2690608391,0.5303530927,-2.073696342 H,0,5.5244066278,-0.0008064534,-0.0060778401 C,0,-0.7198502124,-1.2283024782,-3.3533538764 H,0,-1.776647834,-1.4456240783,-3.1556724684 C,0,-1.3145733147,1.6498749975,-3.0751068482 H,0,-0.9237991202,1.7584996504,-4.0926656937 C,0,-2.7943313191,1.2993133592,-3.1382883132 H,0,-3.3658953379,2.1311179268,-3.5530486497 H,0,-3.1945116882,1.100021545,-2.140676099 H,0,-2.9933203936,0.4243372875,-3.7576598407 C,0,-1.0743927393,2.9392310958,-2.3068383942 H,0,-1.595982308,3.771950616,-2.782067896 H,0,-0.0141303312,3.1849824354,-2.2561599878 H,0,-1.4387555594,2.8508919276,-1.2805467151 C,0,-0.5243710609,-0.9668548736,-4.8361944931 H,0,-1.1873589569,-0.1894149302,-5.2173410325 H,0,-0.7183175343,-1.8728549085,-5.4134359492 H,0,0.5046486966,-0.6641271993,-5.0424624889 C,0,0.1165286233,-2.3994717731,-2.8617228448 H,0,-0.1403039755,-3.3106860729,-3.4043046359 H,0,-0.0297727829,-2.5745808314,-1.7941795575 H,0,1.1795436562,-2.2059111472,-3.0186904963 C,0,-0.7126849497,1.2276231154,3.3546973443 H,0,-1.769893702,1.4450514604,3.159348359 C,0,0.1226984691,2.3988498849,2.8615101044 H,0,-0.1329518053,3.3099767766,3.4047957327 H,0,-0.0258497421,2.5741602888,1.7943114749 H,0,1.1860335434,2.2052178589,3.0161978388</p>	<p>HF=-2293.4778599 ZPE=0.454039 NImag=0</p> <p>Htot=-2292.993079 Gtot=-2293.084050</p> <p>C,0,1.5909153933,-0.0038790508,0.0017383575 C,0,2.3689747081,-0.2818215273,1.1569742109 S,0,1.655383008,-0.6877320296,2.7516547571 P,0,-0.354964349,-0.2378549901,2.2764641598 Rh,0,-0.4050673986,0.0000797032,-0.0002808031 C,0,2.3723654197,0.2709524103,-1.1519533509 S,0,1.663583643,0.6798362262,-2.7480169536 P,0,-0.3494901119,0.237831321,-2.2769825461 C,0,4.4650490721,-0.0096609878,0.0045750034 C,0,3.7620331484,-0.2770345413,1.1635414459 C,0,3.7654036211,0.2605473166,-1.1557735899 H,0,4.2911710837,-0.4860923126,2.0856210269 H,0,4.2971969299,0.467473692,-2.076805757 H,0,5.5475985819,-0.0118494194,0.005640843 C,0,-0.7536604185,-1.2379653703,-3.3537835793 H,0,-1.8176748701,-1.4130367132,-3.1531333066 C,0,-1.2672952084,1.657690224,-3.0737462873 H,0,-0.8779489573,1.7663976452,-4.0916329891 C,0,-2.7540771813,1.3404151418,-3.1351903972 H,0,-3.3075241145,2.1914172604,-3.5364078954 H,0,-3.1580326433,1.1356280805,-2.1398319764 H,0,-2.9762862267,0.4806491507,-3.7679380704 C,0,-0.9997068781,2.9354369838,-2.296499803 H,0,-1.4999519821,3.7835039625,-2.7683743189 H,0,0.0651962505,3.1615285171,-2.2398258484 H,0,-1.3698829005,2.8525542957,-1.2712497756 C,0,-0.5547937342,-0.9914498812,-4.8379753219 H,0,-1.1769916983,-0.180187907,-5.2177922993 H,0,-0.8034807035,-1.8873765115,-5.4107580227 H,0,0.4871170381,-0.7472134267,-5.0577942676 C,0,0.0352894026,-2.4397110297,-2.8606775901 H,0,-0.2584694609,-3.3411477056,-3.4017534083 H,0,-0.1185032723,-2.6115588458,-1.7931571526 H,0,1.1063548161,-2.2944318482,-3.0168480992 C,0,-0.7555534066,1.2395591565,3.352390623 H,0,-1.8184547898,1.4187981935,3.1495332456 C,0,0.0391212023,2.4381823173,2.8608863496 H,0,-0.2521890712,3.3407780694,3.4013533507 H,0,-0.111819612,2.6106136154,1.7930520356 H,0,1.109286657,2.2886924448,3.0192363494</p>

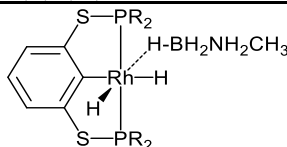
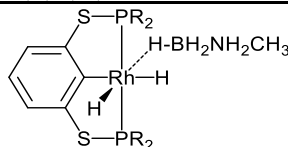
<p>C,0,-0.5140182607,0.9658413768,4.8370553407 H,0,-1.176216479,0.1883442128,5.219457626 H,0,-0.7066779277,1.8717221842,5.4149151642 H,0,0.5154313528,0.6630240666,5.0410379856 C,0,-1.3083663818,-1.6504014261,3.0769949441 H,0,-0.9156642267,-1.7591646559,4.0937967025 C,0,-2.7879897572,-1.2997932979,3.1430153094 H,0,-3.3587971125,-2.1316167318,3.5587798397 H,0,-3.1900538663,-1.1003937772,2.1461814001 H,0,-2.9857737956,-0.4248687577,3.7628467279 C,0,-1.0696688479,-2.939663176,2.3081061061 H,0,-1.5903655045,-3.7724366108,2.784220115 H,0,-0.0095062591,-3.1854225789,2.2553779522 H,0,-1.4359780536,-2.851176113,1.2825191446</p>	<p>C,0,-0.5607333353,0.9923247251,4.8370013134 H,0,-1.186891086,0.1835220921,5.2155523094 H,0,-0.8070961422,1.8892409144,5.4092393053 H,0,0.4797548622,0.7440183874,5.0589902299 C,0,-1.2800057743,-1.6540633719,3.071359935 H,0,-0.893209353,-1.7642564547,4.0900571725 C,0,-2.7656546137,-1.3309464612,3.1296942764 H,0,-3.3232858346,-2.1797685797,3.5297360541 H,0,-3.1667139009,-1.1245719526,2.1334921861 H,0,-2.9858109829,-0.4703165976,3.7619835126 C,0,-1.0158292459,-2.9328900299,2.2947238496 H,0,-1.5203346795,-3.7789714822,2.765625368 H,0,0.0482972193,-3.1631384687,2.2402223702 H,0,-1.3836003342,-2.8486133213,1.2687240723</p>
 <p>3-triplet</p>	 <p>3-triplet</p>
<p>HF=-2293.4107867 ZPE=0.453607 NImag=0</p> <p>Htot=-2292.926258 Gtot=-2293.018416</p> <p>C,0,1.6606015232,-0.0005398604,-0.0020149492 C,0,2.4162103582,-0.1673190179,1.1828385093 S,0,1.6666659066,-0.4081731658,2.7904544651 P,0,-0.4183192846,-0.2194882022,2.2884589789 Rh,0,-0.4258543749,-0.0005500784,0.0001500183 C,0,2.4137488862,0.1662580583,-1.1884315734 S,0,1.6608704799,0.4071890284,-2.7944772632 P,0,-0.4230791825,0.2186484297,-2.2881457102 C,0,4.4921151062,-0.000527844,-0.004952049 C,0,3.8085076899,-0.1678943034,1.1881983984 C,0,3.8060321803,0.1668413666,-1.1966804027 H,0,4.3565041496,-0.296683317,2.1132928855 H,0,4.3521071019,0.2956487101,-2.1229079238 H,0,5.57549474,-0.0005221439,-0.0060757942 C,0,-0.9493317308,-1.2049133444,-3.379104815 H,0,-2.035776117,-1.2368242273,-3.2339964589 C,0,-1.1116175119,1.7413419325,-3.1238086323 H,0,-0.6469330265,1.8102806081,-4.1130703411 C,0,-2.6198398046,1.6136782771,-3.2743563263 H,0,-3.0408370096,2.5357485578,-3.6787000474 H,0,-3.0939124716,1.4327354831,-2.3059627606 H,0,-2.9069615808,0.8016680794,-3.9429853077 C,0,-0.7294948758,2.9628612508,-2.3038942479 H,0,-1.079918244,3.8766625264,-2.7866527471 H,0,0.3503342205,3.0393178439,-2.1738456921 H,0,-1.1798508561,2.9127133978,-1.308954484 C,0,-0.6415004862,-1.0074575115,-4.8529079351 H,0,-1.1199225748,-0.1184396618,-5.2652801355 H,0,-0.9891688656,-1.8641395907,-5.4335384199 H,0,0.4342834515,-0.9181004977,-5.0168333827 C,0,-0.3493329211,-2.4911167492,-2.8335930126 H,0,-0.7075126174,-3.3534987919,-3.3980215977 H,0,-0.6033974331,-2.6381924752,-1.782173694 H,0,0.7397985166,-2.4711291244,-2.9089179693 C,0,-0.9421590358,1.2042414668,3.380359457 H,0,-2.0289055929,1.2362141241,3.2375447657 C,0,-0.3432224963,2.4903350113,2.8334226792 H,0,-0.7001460656,3.3528118073,3.3985018534 H,0,-0.599498731,2.6373012892,1.7825245404 H,0,0.7460642883,2.4702778677,2.9064467775</p>	<p>HF=-2293.4324386 ZPE=0.453315 NImag=0</p> <p>Htot=-2292.948128 Gtot=-2293.040520</p> <p>C,0,1.6747358541,-0.0004511913,-0.0020250788 C,0,2.4290467698,-0.1460284758,1.1829127159 S,0,1.6765630399,-0.3550768435,2.7983132762 P,0,-0.4155407485,-0.20071594,2.3026080331 Rh,0,-0.4271831662,-0.0003492072,0.0001690779 C,0,2.4265850181,0.1450537824,-1.1885354479 S,0,1.6707509772,0.354176155,-2.8023616648 P,0,-0.4203273235,0.2000089214,-2.3022887939 C,0,4.5067250424,-0.0005865096,-0.0049814408 C,0,3.8223759299,-0.1473851146,1.1904410651 C,0,3.8198956474,0.1462772015,-1.1989726023 H,0,4.3713432609,-0.2606575145,2.1174069201 H,0,4.3669373609,0.2594980183,-2.1270824413 H,0,5.5902820024,-0.0006375986,-0.0061124305 C,0,-0.9701185704,-1.2082900209,-3.4012990869 H,0,-2.0573194533,-1.2155872607,-3.258470537 C,0,-1.0856563992,1.7386708738,-3.1296456549 H,0,-0.6131004027,1.8139280096,-4.1143740354 C,0,-2.5930811031,1.6286167669,-3.2947405737 H,0,-3.000255675,2.5616495511,-3.6891457031 H,0,-3.0811256505,1.4395702951,-2.3342566984 H,0,-2.8837714888,0.8310053377,-3.9791244674 C,0,-0.701165216,2.9482486076,-2.2947612949 H,0,-1.0284297179,3.8707475313,-2.7781312994 H,0,0.3771103894,3.0127197383,-2.1424085346 H,0,-1.1712305974,2.9018392015,-1.3083657928 C,0,-0.6581211507,-1.0111504994,-4.8734486266 H,0,-1.1064474833,-0.1036724511,-5.2799481923 H,0,-1.0375896458,-1.8514237015,-5.4589312341 H,0,0.4193963704,-0.9594028069,-5.0438576415 C,0,-0.4038129064,-2.5111488638,-2.8623814921 H,0,-0.784755671,-3.3615955481,-3.430723462 H,0,-0.6631039932,-2.6602351621,-1.8120812726 H,0,0.6858017862,-2.5241925726,-2.9360553099 C,0,-0.9629066284,1.2076306271,3.4027675743 H,0,-2.0504041359,1.2150209733,3.2622194378 C,0,-0.3976190897,2.5104407722,2.862664707 H,0,-0.7773024493,3.3609202729,3.4317997125 H,0,-0.6590911054,2.6595471462,1.8129080192 H,0,0.6921482342,2.5233931888,2.9340621358</p>

<p>C,0,-0.631227706,1.0069442222,4.8535329153 H,0,-1.1088459109,0.1180154978,5.2670269067 H,0,-0.9776012567,1.8637255717,5.4347905142 H,0,0.4448934245,0.917524086,5.015194866 C,0,-1.1052601031,-1.7420251907,3.1257204391 H,0,-0.6384602219,-1.8109446213,4.1139868572 C,0,-2.6131372682,-1.6141420698,3.2795012813 H,0,-3.0333897158,-2.5361171348,3.684835717 H,0,-3.0892673477,-1.4332232874,2.3121131965 H,0,-2.8987080316,-0.8020295898,3.9486706888 C,0,-0.7250683524,-2.963664503,2.3050869261 H,0,-1.0745773767,-3.8773778557,2.7886739037 H,0,0.354467703,-3.0402798249,2.1727214057 H,0,-1.1775575451,-2.9135375096,1.3111147265</p>	<p>C,0,-0.647839471,1.0104625969,4.8742593225 H,0,-1.0953951021,0.1030253782,5.2816984307 H,0,-1.0260010091,1.8507705712,5.4605372659 H,0,0.4300284464,0.9586159625,5.0424067582 C,0,-1.0792800965,-1.7393183366,3.1313520438 H,0,-0.6047010378,-1.8145995449,4.1151054967 C,0,-2.5863532984,-1.629149721,3.2995507833 H,0,-2.99278328,-2.5621498132,3.694799904 H,0,-3.0763618177,-1.440073948,2.3400732539 H,0,-2.8755743483,-0.8315126245,3.9845267595 C,0,-0.6965987973,-2.9489318085,2.2956887445 H,0,-1.0229338561,-3.8714020352,2.7797412501 H,0,0.3813559351,-3.0134833072,2.141114988 H,0,-1.1686923931,-2.9024980304,1.3102634378</p>
 <p>6b+$\text{BH}_3\text{NH}_2\text{Me-Eq}$</p>	 <p>6b+$\text{BH}_3\text{NH}_2\text{Me-Eq}^*$</p>
<p>HF=-2417.2106675 ZPE= 0.570451 NImag=0</p> <p>Htot= -2416.603803 Gtot= -2416.705146</p> <p>C,0,-2.0039447508,0.1481932403,-0.0890161103 C,0,-4.8460913428,-0.0720770204,0.0092982407 C,0,-2.7681395238,-0.3176176009,-1.1775146942 C,0,-2.758521355,0.524517344,1.040637688 C,0,-4.1449909287,0.402619715,1.1015780769 C,0,-4.1573891923,-0.4216645173,-1.1362944159 H,0,-4.667047813,0.6820629072,2.0082352812 H,0,-4.6919634548,-0.7715920262,-2.0106858602 H,0,-5.9240470438,-0.1614163452,0.0481647372 P,0,-0.1727983636,0.1589372822,-2.4379678676 P,0,-0.0558826265,0.5023007845,2.1299468116 S,0,-2.0331110577,-0.8017005514,-2.7368760158 S,0,-2.0063543692,1.2155643775,2.5138042981 C,0,-0.2866830936,1.7809027324,-3.3570542313 H,0,-0.4641214427,1.5273207274,-4.4064038176 C,0,0.9566668878,-0.8760201672,-3.5098732419 H,0,1.9124480633,-0.3452685379,-3.4524966281 C,0,1.144137468,-2.2642307473,-2.9248439084 H,0,1.8807109726,-2.8210582502,-3.5072735386 H,0,0.2084070523,-2.825539507,-2.934944449 H,0,1.4776174654,-2.2154902475,-1.8900847618 C,0,0.5080927337,-0.9450335636,-4.9630894489 H,0,1.1936379927,-1.5759585582,-5.5316815772 H,0,0.4889334823,0.0297211381,-5.4479563511 H,0,-0.4861600956,-1.3873582623,-5.0549873186 C,0,-1.4499333508,2.6159181084,-2.8528232773 H,0,-2.4035636961,2.1055538623,-2.9874171479 H,0,-1.4929388499,3.5607630443,-3.3971708012 H,0,-1.3333936718,2.8406708324,-1.7914242821 C,0,1.0406836427,2.5131341454,-3.2145074251 H,0,0.9997803334,3.4757968289,-3.7266052899 H,0,1.879072295,1.9530232455,-3.6316195818 H,0,1.257729781,2.7046639995,-2.160907302 C,0,0.0687096068,-1.0215127848,3.2178183672 H,0,1.0711180054,-1.4185151504,3.0038817943 C,0,-0.960493607,-2.0488183847,2.7739584129 H,0,-0.8013979843,-2.9937835435,3.2957280357 H,0,-0.9098471416,-2.2295804679,1.6998045066 H,0,-1.9686248413,-1.7048515517,3.0115672944 C,0,-0.0508225508,-0.7179815661,4.7017805034</p>	<p>HF=-2417.2350763 ZPE= 0.570459 NImag= 0</p> <p>Htot= -2416.628182 Gtot= -2416.730818</p> <p>* Single-Point Energy using Gas Phase Geometry</p>

<p>H,0,0.7516568963,-0.0815726235,5.0747237183 H,0,-0.0315515437,-1.6429286334,5.2808121284 H,0,-1.0015373247,-0.2235071309,4.9137196403 C,0,1.0089795457,1.7632395818,2.9978990517 H,0,0.578474905,1.877105128,3.9991259482 C,0,2.4362022495,1.2445270724,3.1201804149 H,0,3.0524388109,1.9584038593,3.6688300155 H,0,2.8905740935,1.1295781847,2.1328804882 H,0,2.4981614025,0.2929917683,3.6524019281 C,0,0.9693992794,3.1018997997,2.2814823172 H,0,1.523080645,3.8486376833,2.8533985428 H,0,-0.050737655,3.4591959121,2.1465885386 H,0,1.4216684253,3.0234970972,1.2920544338 Rh,0,0.0353859622,0.285980635,-0.14800468 H,0,-0.1804449602,1.9076928072,-0.2116649316 H,0,1.9063165154,0.7432803777,-0.125107652 B,0,2.9131999775,0.0680464271,-0.4021566567 H,0,0.2360694352,-1.4260046518,-0.0792303813 H,0,3.8602765497,0.7066251361,-0.0196962174 N,0,2.8384492482,-1.2931046338,0.4625335695 H,0,2.9785057799,-0.2478523277,-1.5562694943 C,0,3.892996104,-2.2719944783,0.1530186845 H,0,2.8602753979,-1.0645329975,1.4544619668 H,0,1.8860285795,-1.6660684095,0.2937665824 H,0,3.8040945254,-3.1647588586,0.7696873644 H,0,3.8091989005,-2.5451985626,-0.8956487886 H,0,4.8656799204,-1.811795726,0.3107573636</p>	
 <p>7b+BH₃NH₂Me-Eq-TS</p>	 <p>7b+BH₃NH₂Me-Eq-TS*</p>
<p>HF=-2417.193640 ZPE= 0.565643 NImag=1 (-502)</p> <p>Htot= -2416.591908 Gtot= -2416.692428</p> <p>P,0,-0.1494046367,0.5531806086,-2.245890451 Rh,0,-0.0252971921,0.2935249873,0.0372083995 C,0,-2.079408612,0.1692773092,0.0170737567 P,0,-0.1766799289,0.2084276553,2.3484427083 H,0,-0.3398778598,1.826773421,0.1285527423 H,0,0.3213164571,-1.5706770075,-0.0782938218 H,0,1.7909585336,0.7241651292,-0.0305118064 B,0,2.8013382798,-0.0020535668,0.2459820647 N,0,2.6554022027,-1.3603490974,-0.5142072856 C,0,3.6635189982,-2.3555427378,-0.1762452244 C,0,-4.9177619198,-0.0467501754,-0.02964189 C,0,-2.8243839443,-0.2537722007,1.1335755949 C,0,-2.849105673,0.5288807564,-1.1068825148 C,0,-4.2363075044,0.4038637338,-1.1446721248 C,0,-4.2140866726,-0.3616801554,1.1170316326 H,0,-4.7751820757,0.6647198333,-2.0468394153 H,0,-4.7373482426,-0.6856726814,2.0079859362 H,0,-5.9959903273,-0.1391696232,-0.0503595221 S,0,-2.0657914865,-0.6792332698,2.7002646339 S,0,-2.1229544096,1.2211927067,-2.5946135514 C,0,-0.1798673828,1.8726546172,3.1917384751 H,0,-0.2508220753,1.6723476623,4.2650670605 C,0,0.9176179234,-0.8456997058,3.4323850214 H,0,1.8714726649,-0.3081472399,3.4244831293 C,0,1.1302126919,-2.216683222,2.8158364633 H,0,1.7791365603,-2.8163900888,3.4562405232 H,0,0.1841911855,-2.7496806567,2.703716901</p>	<p>HF=-2417.2146324 ZPE= 0.564523 NImag = 3 (-569; -80; -46)</p> <p>Htot= -2416.615383 Gtot= -2416.712123</p> <p>* Single-Point Energy using Gas Phase Geometry</p>

<p>H,0,1.5950345598,-2.1429258793,1.8361116614 C,0,0.4039481507,-0.9547364664,4.8614228195 H,0,1.1106660267,-1.5297307236,5.4619075745 H,0,0.2757249293,0.0111661749,5.3479829207 H,0,-0.5518603104,-1.4809460474,4.8994724978 C,0,-1.3727300545,2.7107284473,2.76903272 H,0,-2.3180747687,2.2245503206,3.0089270862 H,0,-1.3492864349,3.6756106679,3.2777325566 H,0,-1.3566139752,2.900645861,1.6943876349 C,0,1.1408553206,2.5678710479,2.884450464 H,0,1.1860008079,3.5320922088,3.3929532813 H,0,2.0095310097,1.9865292284,3.1956493936 H,0,1.2381959526,2.7496561737,1.8117699321 C,0,0.0134271748,-0.9516590398,-3.3452036275 H,0,1.0296000552,-1.3146332837,-3.1465252828 C,0,-0.9806086589,-2.0168171609,-2.9097846214 H,0,-0.8096506201,-2.9395701349,-3.4656545158 H,0,-0.9032834899,-2.2390311575,-1.8458705697 H,0,-2.0029392323,-1.6925116864,-3.1117945825 C,0,-0.1348523812,-0.6226905217,-4.8215514459 H,0,0.6326299307,0.0599556694,-5.1854175939 H,0,-0.0724205501,-1.5341745305,-5.4182346016 H,0,-1.1106232162,-0.1726814423,-5.0175825146 C,0,0.8934104238,1.8623988104,-3.0575124071 H,0,0.4499784933,2.0307056218,-4.0456199739 C,0,2.3231155002,1.3604971003,-3.2165079603 H,0,2.9347078632,2.12548329,-3.6968887846 H,0,2.7744456304,1.1513103711,-2.2439801641 H,0,2.3901328105,0.4609215588,-3.829807102 C,0,0.8443507472,3.1545598132,-2.2590064378 H,0,1.3770540206,3.9440900812,-2.7910184645 H,0,-0.1785361835,3.489367409,-2.0873771581 H,0,1.3220247242,3.0226896338,-1.2865818172 H,0,3.7170664224,0.6892904123,-0.1476348808 H,0,2.8629735888,-0.2047320965,1.4326812316 H,0,2.6776712771,-1.2096892241,-1.5201437895 H,0,1.2188678232,-1.5736894207,-0.2527312201 H,0,3.4968209867,-3.2932392441,-0.710283591 H,0,3.6145500671,-2.5615142487,0.8932357362 H,0,4.6824259249,-2.0137710851,-0.391552039</p>	
 <p>6a+H₂</p>	 <p>6a+H₂</p>
<p>HF=-2295.8302617 ZPE= 0.486852 NImag=0</p> <p>Htot= -2295.311552 Gtot= -2295.403129</p> <p>C,0,-1.9824991514,0.063907122,-0.0361697493 C,0,-4.8151428917,-0.1585344516,-0.0571907097 C,0,-2.7405112737,0.1937606956,-1.2098826813 C,0,-2.7328124134,-0.1559606921,1.1289127739 C,0,-4.122125621,-0.2607901391,1.137088636 C,0,-4.1295182123,0.0729703542,-1.2369114251 H,0,-4.656095925,-0.4168172012,2.0662202838 H,0,-4.6700512907,0.1632567032,-2.1710545831 H,0,-5.8942005117,-0.2477629022,-0.0669736122 P,0,0.0522234041,0.189345446,-2.2985147783 P,0,-0.1124853519,0.6728670917,2.2228745616 S,0,-1.9797738748,0.5764308437,-2.7969720656 S,0,-1.9374882693,-0.2944837488,2.7435727042 C,0,0.954149037,1.4979241706,-3.2691492525</p>	<p>HF=-2295.8500899 ZPE= 0.486224 NImag=0</p> <p>Htot= -2295.331871 Gtot= -2295.423705</p> <p>C,0,-2.0033070466,0.0567711844,-0.0329048421 C,0,-4.8377740453,-0.1669387622,-0.0533161205 C,0,-2.7605681815,0.1621183614,-1.2106770962 C,0,-2.7563209189,-0.1399139922,1.1361019537 C,0,-4.1461361194,-0.2462198274,1.1436874942 C,0,-4.1503849897,0.0412611301,-1.2364277785 H,0,-4.6827386895,-0.3858451125,2.0742058921 H,0,-4.691139307,0.1131142319,-2.1723328024 H,0,-5.9170406507,-0.2566831945,-0.0628252771 P,0,0.045188348,0.1723160262,-2.3075252597 P,0,-0.1149954941,0.6699491814,2.2233767632 S,0,-2.0014637492,0.5079470516,-2.8060635288 S,0,-1.9660348729,-0.2504888204,2.755621881 C,0,0.9065176841,1.5215715305,-3.2612349857</p>

<p>H,0,0.5471684691,1.4509119129,-4.285185606 C,0,0.4298671124,-1.4016366568,-3.2116248302 H,0,1.4704124108,-1.6146300735,-2.9389398275 C,0,-0.4584166301,-2.5227988747,-2.6959377686 H,0,-0.1731760123,-3.4708231777,-3.1539118648 H,0,-1.5026499781,-2.3311640524,-2.9486507779 H,0,-0.3981175109,-2.6407592649,-1.6154321912 C,0,0.3092454374,-1.2657259926,-4.7208811874 H,0,0.4943282291,-2.2280714111,-5.2012667532 H,0,1.0150512992,-0.550405965,-5.1415855768 H,0,-0.6995026224,-0.9528456309,-5.0001299541 C,0,0.6969005886,2.8815153694,-2.6982369031 H,0,0.-0.3683307026,3.0893859291,-2.5956102251 H,0,1.1302417142,3.6414466347,-3.3504527883 H,0,1.1571123388,2.9817693478,-1.7140875798 C,0,2.4420769846,1.1765224703,-3.2953528702 H,0,2.986766389,1.961434352,-3.8221694469 H,0,2.6624157103,0.2328971543,-3.7951012043 H,0,2.8378844705,1.1193634246,-2.2791422231 C,0,1.055222745,0.0178126032,3.5214015497 H,0,1.9135731824,0.694189524,3.4386441501 C,0,1.5144055026,-1.3870800153,3.1690815445 H,0,2.1987034733,-1.7633859941,3.9308368436 H,0,2.0311255245,-1.40907195,2.2107447842 H,0,0.6682608227,-2.0754440385,3.1162025376 C,0,0.4936411816,0.0901263317,4.9332452142 H,0,0.1732776385,1.0936164109,5.2116556984 H,0,1.2501160243,-0.2236435605,5.6545279577 H,0,-0.361764057,-0.5777761396,5.0493893521 C,0,-0.3492801537,2.4634526762,2.6895736408 H,0,-0.549355414,2.4654461612,3.7661452016 C,0,0.9276625613,3.2402005027,2.4016219804 H,0,0.7949435949,4.2912599087,2.6627610849 H,0,1.1798300024,3.1874595664,1.3404965118 H,0,1.7847744565,2.8683811975,2.9641762966 C,0,-1.5455123216,3.0623491345,1.9698532726 H,0,-1.6786696233,4.1024674864,2.2714200275 H,0,-2.4669788854,2.5249768316,2.1920663776 H,0,-1.402641219,3.0433326194,0.8876976304 Rh,0,0.1610478182,0.2382225791,-0.0138321933 H,0,-0.0232139199,1.7668751127,-0.2233682281 H,0,1.7721805112,0.5939574423,0.0016797957 H,0,0.8926299537,-1.4409228349,0.1887884971 H,0,0.0928977197,-1.6016123431,0.2804119488</p>	<p>H,0,0.4959703377,1.4739571598,-4.2756882962 C,0,0.4716097321,-1.3956071164,-3.236924488 H,0,1.5212972219,-1.5675844331,-2.9704165786 C,0,-0.3642238719,-2.5556338667,-2.7230088848 H,0,-0.0394278694,-3.4878501595,-3.1879123138 H,0,-1.4184406167,-2.4143721909,-2.9689957231 H,0,-0.2902502172,-2.6793892011,-1.6437744667 C,0,0.3399964502,-1.2570664922,-4.7443689015 H,0,0.5729958294,-2.2074253048,-5.2286252582 H,0,1.0080230527,-0.5067488878,-5.1662526182 H,0,-0.683110823,-0.9956033789,-5.0251199559 C,0,0.6130259456,2.8919863055,-2.6778857459 H,0,-0.4560366684,3.068715001,-2.5539157289 H,0,1.0064788582,3.668594773,-3.3363554045 H,0,1.0900866283,3.0099575182,-1.7035400888 C,0,2.4026436465,1.2474633879,-3.3027139543 H,0,2.9152705282,2.051367035,-3.8338375201 H,0,2.6505444545,0.3133661614,-3.8073391667 H,0,2.8154644149,1.2021296813,-2.2925954619 C,0,1.0517692506,-0.00615954,3.5104347949 H,0,1.947177333,0.6084597954,3.3640814848 C,0,1.4107901532,-1.4503083453,3.2070517597 H,0,2.1020191824,-1.8309105818,3.9608246862 H,0,1.8915420909,-1.5488486566,2.2346417592 H,0,0.5276988878,-2.0928954717,3.2171617406 C,0,0.5533608284,0.1668355864,4.9359366088 H,0,0.3333207729,1.2043001457,5.1865469148 H,0,1.3104937696,-0.1828357492,5.6403372399 H,0,-0.3486940065,-0.4212211794,5.1174439894 C,0,-0.3236266017,2.4659538469,2.681581833 H,0,-0.5769193898,2.4686709215,3.7465080274 C,0,0.9850904405,3.2095978872,2.4629453761 H,0,0.8601762854,4.2663397931,2.7059839199 H,0,1.301684113,3.1449534775,1.4193575429 H,0,1.7975084929,2.8266423039,3.0815852741 C,0,-1.4662739693,3.1029449556,1.9111333548 H,0,-1.6024001801,4.135524504,2.2377613008 H,0,-2.4098828226,2.5785634865,2.0632107291 H,0,-1.2630121627,3.1189487427,0.8383858463 Rh,0,0.1393170473,0.2069145066,-0.0134645165 H,0,-0.0048461222,1.7366857486,-0.2244127116 H,0,1.7666938085,0.5211132187,0.0015157012 H,0,0.790608139,-1.530993974,0.2068369797 H,0,-0.0094923413,-1.6398024022,0.3035666269</p>
 <p>6a+H₂-TS HF=-2295.8176407 ZPE= 0.481049 NImag=1 (-563) Htot= -2295.303156 Gtot= -2295.398420 C,0,-2.0232546338,0.033575236,-0.0381524116 C,0,-4.8739977618,-0.1348679757,-0.0687454035 C,0,-2.7770106797,0.0125398661,-1.2277991319 C,0,-2.8029106482,-0.036462549,1.1340377055 C,0,-4.194159018,-0.1124297322,1.1361627852 C,0,-4.1694049543,-0.0744255797,-1.2565207825 H,0,-4.7396712759,-0.1501425353,2.0708088772 H,0,-4.6970160153,-0.0935322447,-2.2020475052 H,0,-5.9550557024,-0.1959010269,-0.0814473802 P,0,0.0309193453,0.0795355043,-2.2925398217</p>	 <p>6a+H₂-TS* HF=-2295.8367011 ZPE= 0.480470 NImag=1 (-572; -253; -15) Htot= -2295.324256 Gtot= -2295.415280 * Single-Point Energy Using Gas Phase Geometry</p>

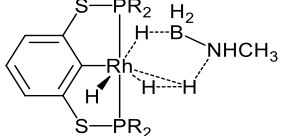
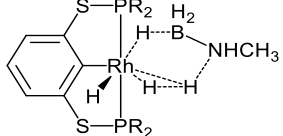
<p>P,0,-0.1294522943,0.6337828462,2.1947051085 S,0,-2.0197884097,0.0900370587,-2.8539097163 S,0,-2.0574671776,-0.0443581625,2.7742776859 C,0,0.6699313597,1.6135340651,-3.1466842276 H,0,0.2716346659,1.57023034,-4.1660513679 C,0,0.733369784,-1.3157605688,-3.3228269516 H,0,1.810305421,-1.2511826268,-3.1284194856 C,0,0.2251460764,-2.6471386789,-2.7973589395 H,0,0.6464612274,-3.4715087529,-3.374507304 H,0,-0.8624575007,-2.7069679429,-2.8759853035 H,0,0.4931208619,-2.7957884325,-1.7524939492 C,0,0.4765745949,-1.1602247064,-4.8124382635 H,0,0.9046080549,-2.0019234035,-5.3600205106 H,0,0.9132887274,-0.2496892206,-5.2225905152 H,0,-0.5946332891,-1.1470090896,-5.0247497544 C,0,0.1305933513,2.8603095655,-2.4667369001 H,0,-0.954737472,2.8287414156,-2.3639997229 H,0,0.3926095816,3.7500876335,-3.0417057241 H,0,0.5552270702,2.9692876191,-1.4667703734 C,0,2.1901749095,1.6087445629,-3.1929076011 H,0,2.5583151006,2.5370149116,-3.6328493476 H,0,2.5898931451,0.7853073178,-3.785241278 H,0,2.6119569249,1.5328429834,-2.1880852192 C,0,0.9571676905,-0.0679172386,3.5382659326 H,0,1.9249797221,0.4069231487,3.3385461426 C,0,1.1142089378,-1.5680201672,3.3508596102 H,0,1.7840258673,-1.9780280577,4.1081727412 H,0,1.5263663976,-1.8056581788,2.3701794365 H,0,0.1534578937,-2.0780142632,3.4439860192 C,0,0.503653462,0.2893014792,4.9446117304 H,0,0.448712708,1.3653937315,5.1077373189 H,0,1.1990564957,-0.1175757023,5.6809833774 H,0,-0.4795357969,-0.1330647006,5.1612900108 C,0,-0.1725815383,2.4678523884,2.5449141997 H,0,-0.5311056121,2.568100779,3.574594671 C,0,1.2194151052,3.0685353572,2.4252149754 H,0,1.1804184127,4.1464594218,2.5903775627 H,0,1.6296942068,2.9067400642,1.4255854339 H,0,1.922925152,2.6525379797,3.1472474286 C,0,-1.1612053477,3.1445879461,1.6096745431 H,0,-1.2111807427,4.2138605058,1.8222901572 H,0,-2.1647278959,2.7319626759,1.7117359031 H,0,-0.8588866653,3.0148245854,0.5684683096 Rh,0,0.1459594645,0.0622154196,-0.0058034474 H,0,1.182737813,1.2176120904,-0.126199538 H,0,1.7750311277,-0.0197341015,0.0497345572 H,0,0.1462302632,-2.1655766541,0.4704722331 H,0,-0.6129165901,-2.1719818052,0.4403860202</p>	
<p>H₂ HF=-1.1717115 ZPE= 0.009886 NImag=0 Htot= -1.158521 Gtot= -1.173317 H,0,0.,0.,0.3721688168 H,0,0.,0.,-0.3721688168</p>	<p>H₂ HF=-1.1712241 ZPE= 0.009871 NImag=0 Htot= -1.158048 Gtot= -1.172845 H,0,0.,0.,0.3723236728 H,0,0.,0.,-0.3723236728</p>
 <p>6a+BH₃NH₂Me-Ax (7)</p>	 <p>6a+BH₃NH₂Me-Ax* (7)</p>
<p>HF=-2417.2199715 ZPE=0.571611 NImag=0</p>	<p>HF=-2417.2432975 ZPE= NImag=0</p>

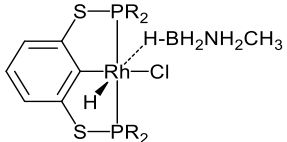
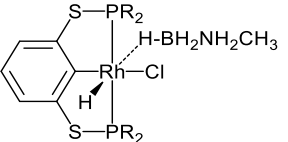
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Gtot= -2416.713300

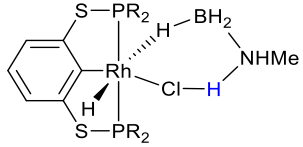
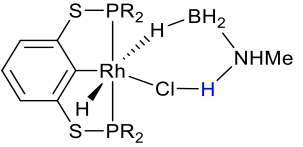
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C,0,-1.2216001603,1.6439752367,-1.4061917098
C,0,-1.3076362713,2.8735867855,-2.0575149998
C,0,0.9777106875,3.3000824828,-1.4631362765
H,0,-2.2375181783,3.195412195,-2.5101932277
H,0,1.8433564124,3.9510946755,-1.4720076197
H,0,-0.2330110035,4.6428032218,-2.6131734219
P,0,2.2992957513,-0.364309972,0.3685963979
P,0,-2.2213396552,-0.497812709,0.3787252465
S,0,2.5403764299,1.7461129083,0.1131381813
S,0,-2.755618958,0.6782083291,-1.3477035887
C,0,3.161248312,-0.6742896921,1.9888771665
H,0,4.1633808273,-0.2426981882,1.8930297035
C,0,3.4560778844,-1.061398221,-0.9326955286
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H,0,2.0827700702,-0.3195916793,-2.4457223687
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C,0,-3.4338733536,-1.9109747867,0.2713148978
H,0,-3.2828727175,-2.4129180843,1.2342189972
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H,0,-3.6871373783,-3.7475403262,-0.825920045
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H,0,-5.2177912084,-0.860804148,0.9840054418
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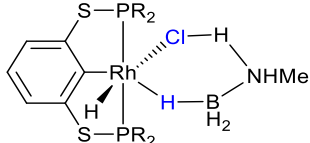
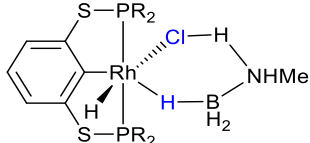
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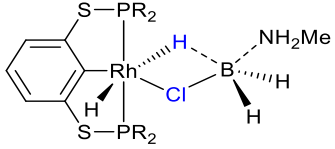
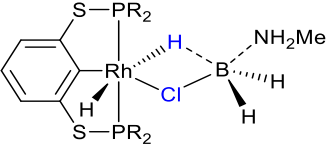
* Single-Point Energy using Gas Phase Geometry

<p>H,0,-0.7328221481,-0.074984087,-5.1055874814 H,0,0.7026106004,-1.1138996497,-4.9380854935 H,0,-0.9021456378,-1.8438853696,-4.992906028</p>	
 <p>6a+BH₃NH₂Me-Ax-TS</p>	 <p>6a+BH₃NH₂Me-Ax-TS</p>
<p>HF=-2417.1839851 ZPE= 0.563442 NImag=1 (-275.)</p> <p>Htot= -2416.584171 Gtot= -2416.684278</p>	<p>HF=-2417.2059613 ZPE= 0.562615 NImag= 1 (-298)</p> <p>Htot= -2416.606651 Gtot= -2416.707509</p>
<p>C,0,-1.9208072515,0.0333394972,-0.0618086525 C,0,-4.7568951554,0.15590053,-0.145671975 C,0,-2.619854864,0.5172580034,-1.1838187185 C,0,-2.7219583733,-0.3397539098,1.0324374868 C,0,-4.1137208737,-0.2810754334,0.996955514 C,0,-4.0112363159,0.5607746899,-1.2374227033 H,0,-4.6842969462,-0.5669785911,1.8714963743 H,0,-4.5020632581,0.9078003335,-2.1378229022 H,0,-5.8380845279,0.1919985386,-0.181543589 P,0,-0.0081020174,0.0066258831,-2.3297647241 P,0,-0.1518400807,0.0737702475,2.2757491948 S,0,-1.7761609859,1.1286691254,-2.6435474904 S,0,-2.017680434,-0.8664317914,2.5969880339 C,0,1.2933612083,0.9782759672,-3.2355974457 H,0,0.8981642776,1.1477410926,-4.2431748328 C,0,-0.2678110139,-1.5317884981,-3.3457083185 H,0,0.608605936,-2.1450924347,-3.107192034 C,0,-1.508518859,-2.260879177,-2.8526299131 H,0,-1.5604746519,-3.2510659182,-3.3064433082 H,0,-2.4127481786,-1.7150471576,-3.1280927928 H,0,-1.4992786955,-2.3915700308,-1.7709603278 C,0,-0.335316607,-1.2555621481,-4.8382609928 H,0,-0.5485674572,-2.180176142,-5.3770112751 H,0,0.5931306304,-0.8513739002,-5.2418194883 H,0,-1.1407849198,-0.5539343103,-5.0684137784 C,0,1.5493168063,2.3192957563,-2.5695145826 H,0,0.633569418,2.8975992466,-2.4503921652 H,0,2.2502063129,2.9059499818,-3.165450709 H,0,1.9826570227,2.1850696559,-1.577200537 C,0,2.5634127232,0.1408600563,-3.3252190454 H,0,3.3525282567,0.7056895317,-3.8233060569 H,0,2.4180502835,-0.7847895528,-3.8825706011 H,0,2.9283338051,-0.1275385071,-2.3308993742 C,0,0.9862842798,-0.7638768405,3.4965744706 H,0,1.9770586664,-0.4248289048,3.1684433968 C,0,0.9188520525,-2.2744342287,3.3445495263 H,0,1.74734641,-2.7387777977,3.8818350489 H,0,0.9657575455,-2.5933280412,2.3050833312 H,0,-0.0096120712,-2.6652580507,3.7628807735 C,0,0.76730003,-0.3391587506,4.9416732354 H,0,0.9828729273,0.7139422978,5.1170849399 H,0,1.4229371609,-0.9182594709,5.5939176072 H,0,-0.2582701412,-0.53296549,5.2627145282 C,0,-0.3327072547,1.8102190322,2.9349537897 H,0,-0.5738325097,1.6936476227,3.9958116407 C,0,1.0007926863,2.5295149751,2.7839367823 H,0,0.9363958865,3.5387736403,3.19318684 H,0,1.2691254747,2.6180436993,1.7285619647 H,0,1.8171063154,2.0183943112,3.297736492 C,0,-1.4626306223,2.5688590786,2.2623095519 H,0,-1.5258866505,3.5767368598,2.6760803055</p>	<p>C,0,-1.9234093456,0.0228770657,-0.039924046 C,0,-4.7580471177,0.126786177,-0.1375882144 C,0,-2.6184659333,0.5086882839,-1.1639640996 C,0,-2.726281535,-0.3546925681,1.0518517021 C,0,-4.1183226951,-0.3080231962,1.0082175449 C,0,-4.0101541256,0.5430155258,-1.2239682317 H,0,-4.6935156019,-0.6001979266,1.8778563795 H,0,-4.5009510634,0.8906296529,-2.1243863554 H,0,-5.8394795739,0.1531254752,-0.1797138096 P,0,0.0009748878,0.0014548245,-2.3119271799 P,0,-0.1611533499,0.0966969728,2.2999093768 S,0,-1.7663400848,1.1358779745,-2.6131198695 S,0,-2.020774432,-0.866719889,2.622953216 C,0,1.3161723963,0.976233695,-3.1920803515 H,0,0.9343500143,1.1554697662,-4.2029214837 C,0,-0.2640756868,-1.5257558418,-3.3446347379 H,0,0.5999281457,-2.1519668451,-3.0940343111 C,0,-1.5259274708,-2.2402447076,-2.8862173914 H,0,-1.5680289179,-3.2368684981,-3.3278233002 H,0,-2.4174498728,-1.6959805806,-3.2037938946 H,0,-1.563146396,-2.357834304,-1.8032439062 C,0,-0.2937520297,-1.2429939221,-4.8364567704 H,0,-0.5034656048,-2.1646834477,-5.3824860695 H,0,0.6477170413,-0.848097614,-5.2182139544 H,0,-1.0865476755,-0.5336617074,-5.0868243045 C,0,1.5744546316,2.3093927001,-2.5128064286 H,0,0.6645391516,2.8984930646,-2.3980265268 H,0,2.2832927463,2.8955227239,-3.1003060095 H,0,2.0038702076,2.167837188,-1.5192747762 C,0,2.5830809932,0.1342724855,-3.2720640716 H,0,3.3722714062,0.6930812488,-3.7774191578 H,0,2.4392527541,-0.7979511571,-3.8189890734 H,0,2.9497841168,-0.1211415267,-2.2747125297 C,0,0.9939571043,-0.7028068606,3.5266153939 H,0,1.9693132952,-0.3081297426,3.215550164 C,0,1.0068860205,-2.2110467159,3.3521981463 H,0,1.8519439207,-2.6412155548,3.8925800233 H,0,1.083685378,-2.5108633283,2.3087709994 H,0,0.0964617848,-2.6606597256,3.7516614602 C,0,0.7365283076,-0.3047961235,4.9718194007 H,0,0.8896165658,0.7577606619,5.15718498 H,0,1.4211224738,-0.8488062779,5.6251798157 H,0,-0.2774749728,-0.5609215705,5.2862077364 C,0,-0.3640301991,1.8413100204,2.927142853 H,0,-0.6230900137,1.7376043962,3.9852321508 C,0,0.9676152013,2.5658026235,2.7926180051 H,0,0.8842999567,3.5823804954,3.1805635739 H,0,1.2648499894,2.63991904,1.7433913043 H,0,1.7746436265,2.0733191814,3.3379460842 C,0,-1.4837008365,2.5877672396,2.2263066802 H,0,-1.5619879941,3.596950406,2.635211689</p>

<p>H,0,-2.4262655546,2.0836911488,2.4140239179 H,0,-1.2951118883,2.6571113023,1.1875340737 Rh,0,0.1297983591,-0.0944492041,-0.0168768285 H,0,0.0622786652,1.5075657157,-0.0806148337 H,0,1.9646722123,0.2095486004,0.1668378051 H,0,0.2340811704,-1.9037764102,0.0031028301 B,0,1.0473698988,-3.0497365274,-0.3265073807 H,0,0.5428232503,-3.3963281701,-1.3572743619 N,0,2.4762827798,-2.7152045086,-0.4397486142 H,0,0.7356908875,-3.6882849413,0.6482066519 C,0,3.3699196968,-2.6826705122,0.6844092579 H,0,2.932251217,-2.7901088194,-1.3315174838 H,0,1.958237207,-0.556551925,-0.106015866 H,0,4.4140639464,-2.6591203122,0.3690456996 H,0,3.214001929,-1.790107117,1.3152452812 H,0,3.2419347237,-3.5490898963,1.3456046568</p>	<p>H,0,-2.4499869951,2.1016830396,2.3597933925 H,0,-1.2957578471,2.6774933811,1.1546305371 Rh,0,0.121000613,-0.1232464189,0.0066613488 H,0,0.083138792,1.4664097759,-0.0578459191 H,0,1.9867208497,0.0926589616,0.2831361233 H,0,0.2072170013,-1.9722713109,0.0218446039 B,0,0.9670397027,-3.0834634159,-0.3122840241 H,0,0.4064525141,-3.4741245689,-1.3033322517 N,0,2.3998065243,-2.7830300124,-0.5293611158 H,0,0.7378854917,-3.7388689802,0.6810126161 C,0,3.3735529403,-2.7370229302,0.52216196 H,0,2.788584338,-2.821771936,-1.4549299549 H,0,1.9755641606,-0.583070077,-0.1533820964 H,0,4.3913136297,-2.7955881446,0.1314656754 H,0,3.3232851744,-1.8074731262,1.1190960301 H,0,3.2491974216,-3.5612304942,1.2364425503</p>
 <p>3a+BH₃NH₂Me-Ax</p>	 <p>3a+BH₃NH₂Me-Ax</p>
<p>HF=-2876.8959509 ZPE= 0.566485 NImag=0</p> <p>Htot= -2876.291333 Gtot= -2876.396174</p> <p>C,0,-0.0444417981,1.1472972718,-0.7264484772 C,0,-0.1016489112,3.6030525964,-2.1636504526 C,0,1.0525108323,2.0372677519,-0.7467321339 C,0,-1.1979683674,1.6094551862,-1.396594702 C,0,-1.2330636338,2.8077422465,-2.1083653431 C,0,1.0385226031,3.2250455344,-1.4755022974 H,0,-2.1475883971,3.1204485409,-2.5968410133 H,0,1.9185056277,3.8558592675,-1.4919457046 H,0,-0.1159550988,4.5293711625,-2.7235095583 P,0,2.3110044264,-0.3787629706,0.3896930531 P,0,-2.2739543277,-0.4305509767,0.4079901875 S,0,2.5325508464,1.7362195886,0.2177697661 S,0,-2.7555086535,0.6932754804,-1.3513063517 C,0,3.1464369615,-0.7578178149,2.0053690538 H,0,4.1142247098,-0.2434046903,1.9729363143 C,0,3.4724447937,-1.009732107,-0.9352430491 H,0,3.2421247177,-2.0795514,-0.9924301568 C,0,3.1314522545,-0.3553274211,-2.2664413588 H,0,3.5921507191,-0.9028671313,-3.0895353567 H,0,3.4928024655,0.6734781774,-2.2915062119 H,0,2.0575451089,-0.3379722209,-2.4420425099 C,0,4.9407884114,-0.7946973645,-0.6049792553 H,0,5.5618668313,-1.1280032147,-1.4384113814 H,0,5.2668429204,-1.3349528302,0.2818476454 H,0,5.1486492556,0.2673770486,-0.4528989591 C,0,2.3269897959,-0.225646066,3.170054661 H,0,2.1108529108,0.838584421,3.068059334 H,0,2.8720014738,-0.3713053562,4.104003733 H,0,1.3818997984,-0.7675659719,3.2430282259 C,0,3.3584178037,-2.2635085856,2.1233070321 H,0,3.8695537808,-2.4882289762,3.0607295103 H,0,3.96353635,-2.6729040766,1.3145112935 H,0,2.3987105884,-2.782506342,2.1279458443 C,0,-3.4015211341,-1.9027829793,0.3393211764 H,0,-3.1970872565,-2.3778801396,1.3058896284 C,0,-2.9644489163,-2.8657084099,-0.7485561939 H,0,-3.6071622234,-3.7471215907,-0.7421277352 H,0,-1.9373100748,-3.1910576389,-0.5966149495</p>	<p>HF=-2876.9225379 ZPE= 0.566367 NImag=0</p> <p>Htot= -2876.317975 Gtot= -2876.423270</p> <p>C,0,-0.0479836388,1.1447782413,-0.7010450766 C,0,-0.1024001867,3.5972430416,-2.1458078881 C,0,1.0442906689,2.0402635571,-0.7131554037 C,0,-1.1957463155,1.5981902902,-1.3862233999 C,0,-1.2283953951,2.794136092,-2.1028005073 C,0,1.0316206192,3.2274570764,-1.4432120529 H,0,-2.1382305414,3.1002474187,-2.6043808535 H,0,1.9076427549,3.864216685,-1.4511388936 H,0,-0.1158455563,4.5225596603,-2.707671083 P,0,2.3180271612,-0.3768971255,0.4000505337 P,0,-2.2827613514,-0.4329559735,0.4208124994 S,0,2.5197454524,1.7434099087,0.2587605053 S,0,-2.7496854822,0.680827368,-1.3472597717 C,0,3.1697791458,-0.7572931005,2.0085093157 H,0,4.1274830393,-0.2249605167,1.9701424962 C,0,3.479164124,-0.9842517727,-0.9348025694 H,0,3.2608781757,-2.0566425,-0.9916650268 C,0,3.1219305204,-0.3305643452,-2.2618564451 H,0,3.563232584,-0.8856900256,-3.0910179927 H,0,3.4981424513,0.6928926723,-2.3010139079 H,0,2.0457222262,-0.2947847368,-2.4240066069 C,0,4.9475390115,-0.7576472105,-0.6159995346 H,0,5.5623422962,-1.0852959395,-1.4568482265 H,0,5.289114475,-1.2983040806,0.2649324385 H,0,5.153226467,0.3049420306,-0.4637940734 C,0,2.3558825279,-0.2485884801,3.1860588583 H,0,2.1223933457,0.8137108123,3.1016204413 H,0,2.9128895237,-0.3951905716,4.1132407528 H,0,1.4185809976,-0.8025230767,3.2678094233 C,0,3.4166794259,-2.2570020103,2.1175726289 H,0,3.9519647549,-2.4730688567,3.0439778831 H,0,4.0131089547,-2.6541303192,1.2963237035 H,0,2.4701672408,-2.7987362744,2.1405579492 C,0,-3.4327113469,-1.8906145033,0.3450420359 H,0,-3.243552843,-2.3755172667,1.3093560331 C,0,-3.0163093387,-2.8537912701,-0.7502517691 H,0,-3.671132888,-3.7267162418,-0.742325806 H,0,-1.9934171418,-3.1973396078,-0.6097244491</p>

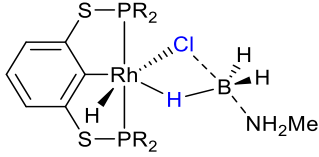
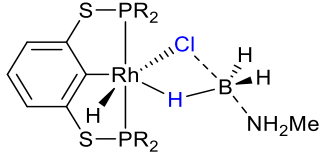
<p>H,0,-3.0397500547,-2.4137931285,-1.7406951546 C,0,-4.8729348671,-1.532317323,0.2374027854 H,0,-5.2170833832,-0.9178998681,1.0686115085 H,0,-5.4805646466,-2.438483128,0.2306807415 H,0,-5.0870925617,-0.9951776594,-0.6893684671 C,0,-2.9123280445,0.5936613901,1.8274766467 H,0,-3.9905751079,0.6892793033,1.6645653087 C,0,-2.6469328586,-0.1578889004,3.1261800735 H,0,-2.9768111209,0.4418837072,3.9757801568 H,0,-1.5814306464,-0.3649877411,3.2482273683 H,0,-3.1662083665,-1.114993647,3.1726043304 C,0,-2.3007216589,1.9839500082,1.8431428317 H,0,-2.7112522594,2.5560673253,2.6764631747 H,0,-2.5058149392,2.5354803583,0.9257672346 H,0,-1.217682018,1.9411873231,1.972874904 Rh,0,0.0038562247,-0.6320087779,0.280160895 H,0,0.0410968747,0.2400512183,1.5473401142 Cl,0,-0.1996905863,-2.69641348,1.7065576617 H,0,-0.0102072619,-1.9231502116,-1.2590552202 B,0,0.0779540784,-2.2004308771,-2.4565177133 H,0,1.2138042148,-2.4172019336,-2.7764883478 H,0,-0.685629367,-3.0871659004,-2.7225624775 N,0,-0.4240302107,-0.8919749798,-3.2615370278 C,0,-0.3114087841,-1.0053969144,-4.7249929656 H,0,-1.39073698,-0.6954311791,-2.9919678209 H,0,0.0849924277,-0.068675913,-2.9372809707 H,0,-0.6912375183,-0.1158154816,-5.2251560628 H,0,0.7351042891,-1.1524713215,-4.9808525384 H,0,-0.8699404617,-1.8790507673,-5.0506350764</p>	<p>H,0,-3.0942828519,-2.3975408398,-1.740300919 C,0,-4.8988822824,-1.5006777745,0.2463188445 H,0,-5.2355151021,-0.8838619596,1.0788857941 H,0,-5.5164883811,-2.4005589203,0.2415781759 H,0,-5.112226476,-0.9622765621,-0.6800987074 C,0,-2.9207334204,0.6055691606,1.8310480346 H,0,-3.9947449932,0.7172558155,1.6530866683 C,0,-2.6889336947,-0.1424113297,3.1365435604 H,0,-3.052031349,0.454689654,3.974835687 H,0,-1.6251713772,-0.3313149415,3.2976688772 H,0,-3.2005040592,-1.104560572,3.1712600304 C,0,-2.288077499,1.9852045848,1.8558631714 H,0,-2.7063212798,2.5644823689,2.680920992 H,0,-2.4690761054,2.5425086875,0.9366059634 H,0,-1.2081849973,1.9287966311,2.008232095 Rh,0,0.0055598455,-0.6444210194,0.2866405617 H,0,0.048591742,0.2049806156,1.5690416472 Cl,0,-0.1405302624,-2.774952828,1.6681318349 H,0,-0.1101312995,-1.9098488939,-1.2774692892 B,0,0.0503020106,-2.2035321524,-2.4616352413 H,0,1.2036384578,-2.4151888192,-2.719185221 H,0,-0.6825041552,-3.1162029563,-2.7378580257 N,0,-0.4324567792,-0.9288109173,-3.317513416 C,0,-0.253848511,-1.0664297155,-4.7734230213 H,0,-1.4133949798,-0.7420481788,-3.1016306691 H,0,0.0525425423,-0.0909567654,-2.9940998632 H,0,-0.6242475196,-0.1886068455,-5.3001011584 H,0,0.8046486781,-1.1998094108,-4.9838077893 H,0,-0.7889002192,-1.9503956646,-5.1108055775</p>
 <p>3a+BH₃NH₂Me-Ax-cyclic</p>	 <p>3a+BH₃NH₂Me-Ax-cyclic*</p>
<p>HF=-2876.9039952 ZPE= 0.566773 NImag=0</p> <p>Htot=-2876.299300 Gtot=-2876.403618</p> <p>C,0,-0.0076413925,1.6071620154,-0.4450001278 C,0,0.0059853119,4.269309242,-1.4508151769 C,0,1.1069846465,2.459781039,-0.3141881303 C,0,-1.1399645634,2.198553843,-1.0387682971 C,0,-1.1389898987,3.4996035944,-1.5369839261 C,0,1.1288244831,3.7539882962,-0.8301568766 H,0,-2.0403349199,3.9065380997,-1.9778187954 H,0,2.0262028173,4.3526393121,-0.7370712648 H,0,0.0167226663,5.2760600244,-1.8482931939 P,0,2.3112426433,-0.125662436,0.3794533007 P,0,-2.2990655686,-0.0755750648,0.3515911577 S,0,2.5847226116,1.9709643858,0.5717942974 S,0,-2.7186139536,1.3478340273,-1.1575889562 C,0,3.1846316814,-0.7839951988,1.8829565042 H,0,4.1435212489,-0.2543052297,1.92877706 C,0,3.4165856907,-0.5546225379,-1.0627206343 H,0,3.2884958069,-1.6355893253,-1.1760435647 C,0,2.9012961288,0.1331820409,-2.3172981913 H,0,3.4407960862,-0.2306340409,-3.1927341007 H,0,3.0531532212,1.2124016702,-2.2561899411 H,0,1.8391769604,-0.0495528116,-2.479369742 C,0,4.8780221125,-0.229348752,-0.8029400371 H,0,5.4726164914,-0.4604822188,-1.688567938 H,0,5.2975257202,-0.7954358872,0.0285862534 H,0,5.0093063158,0.8342131812,-0.5919882745</p>	<p>HF=-2876.9281878 ZPE= 0.565348 NImag=0</p> <p>Htot=-2876.325239 Gtot=-2876.429277</p> <p>* Single-Point Energy using Gas Phase Geometry</p>

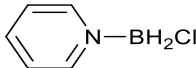
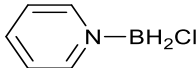
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 <p>3a-BH₃NH₂Me-Eq-cyclic</p> <p>HF=-2876.9273702 ZPE= 0.567022 NImag=0</p> <p>Htot= -2876.322578 Gtot= -2876.426282</p> <p>C,0,-2.010890825,0.0845745551,-0.1134075957 C,0,-4.8490270803,-0.0352295496,-0.0869795878 C,0,-2.7505671129,-0.4385691461,-1.1900900302 C,0,-2.7771453216,0.6081855065,0.9467060279 C,0,-4.1681088517,0.5305935593,0.975359878 C,0,-4.1428526328,-0.504321884,-1.1787103872 H,0,-4.7099214923,0.9131897572,1.8313011934 H,0,-4.6674226134,-0.910082659,-2.0348969557 H,0,-5.9297920394,-0.0962059766,-0.0705255963 P,0,-0.1570808764,0.0515639548,-2.4229963895 P,0,-0.1469335772,0.4784267037,2.1816037293 S,0,-1.9751381458,-0.9987737518,-2.7073130664</p>	<p>C,0,-2.010890825,0.0845745551,-0.1134075957 C,0,-4.8490270803,-0.0352295496,-0.0869795878 C,0,-2.7505671129,-0.4385691461,-1.1900900302 C,0,-2.7771453216,0.6081855065,0.9467060279 C,0,-4.1681088517,0.5305935593,0.975359878 C,0,-4.1428526328,-0.504321884,-1.1787103872 H,0,-4.7099214923,0.9131897572,1.8313011934 H,0,-4.6674226134,-0.910082659,-2.0348969557 H,0,-5.9297920394,-0.0962059766,-0.0705255963 P,0,-0.1570808764,0.0515639548,-2.4229963895 P,0,-0.1469335772,0.4784267037,2.1816037293 S,0,-1.9751381458,-0.9987737518,-2.7073130664</p>

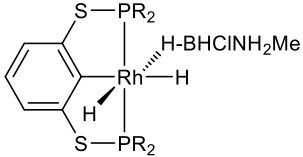
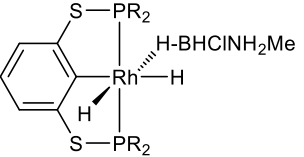
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 <p>3a+BH₃NH₂Me-Ax-S_N2-TS</p>	 <p>3a+BH₃NH₂Me-Ax-S_N2-TS</p>
<p>HF=-2876.8536889 ZPE= 0.562831 NImag=1 (-263)</p> <p>Htot= -2876.252198 Gtot= -2876.359080</p>	<p>HF=-2876.8746884 ZPE= 0.562432 NImag=1 (-285)</p> <p>Htot= -2876.273446 Gtot= -2876.380357</p>

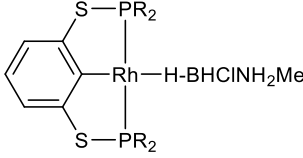
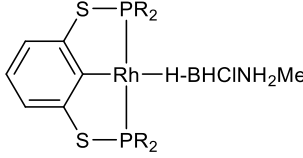
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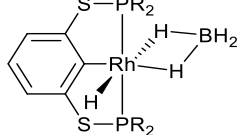
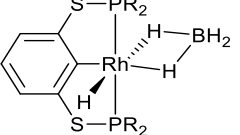
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H,0,2.952614,-3.3214422,1.459414
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H,0,-2.7510622,-2.6348085,-0.4163517
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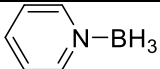
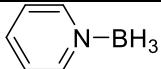
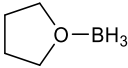
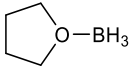
	
<p>3a+BH₃NH₂Me-Eq-Sn₂-TS</p> <p>HF=-2876.8529186 ZPE= 0.563245 NImag=1 (-308)</p> <p>Htot=-2876.251307 Gtot=-2876.356720</p> <p>Rh,0,-0.2359801633,-0.4540269449,-0.0893952005 C,0,-2.174790642,0.1931328377,-0.0810502497 Cl,0,-0.3415839997,-3.0000314898,0.1998684127 B,0,1.9089984233,-2.0667318874,-0.1255152037 N,0,4.0023680617,-1.0669620275,-0.4483711882 H,0,1.5836974015,-0.8714460045,-0.0800542623 H,0,0.0855043394,1.0641379184,-0.184313161 P,0,-0.2524563393,-0.0980552736,2.1943008438 P,0,-0.4349697809,-0.413410806,-2.401255168 C,0,-4.9034436684,0.9859132495,-0.0283765203 C,0,-3.0397747944,-0.0123479377,-1.1726076788 C,0,-2.7433024811,0.8682938119,1.0169716909 C,0,-4.0856939175,-1.2383581337,1.0574096171 C,0,-4.3783455039,0.3746011389,-1.1512008945 H,0,-4.4821989383,1.7220643864,1.9411431402 H,0,-4.9995206114,0.2016817019,-2.0210499568 H,0,-5.9459651617,1.2759743958,-0.003941684 S,0,-2.4960295886,-0.754398888,-2.7148766801 S,0,-1.7837892529,1.3384515085,2.4585414026 C,0,-0.0614112482,1.2501762703,-3.1631117316 H,0,-0.3071791788,1.1534010854,-4.224390351 C,0,0.39853965,-1.6293501029,-3.549698828 H,0,1.4445104627,-1.5793467292,-3.222241523 C,0,-0.1038746627,-3.0460779078,-3.3191796152 H,0,0.5248410894,-3.747829409,-3.8698487787 H,0,-1.1257104392,-3.1593642018,-3.6842924075 C,0,-0.0944474134,-3.3215729141,-2.2663141667 C,0,0.3121459765,-1.243370062,-5.020147412 H,0,0.7631385852,-2.0299732035,-5.6274675818 H,0,0.8325161922,-0.3153564568,-5.2541664898 H,0,-0.7247674024,-1.1410703371,-5.3472067587 C,0,-0.9141075429,2.3594257953,-2.5741961033 H,0,-1.9785166063,2.1639496201,-2.7024921382 H,0,-0.6842348781,3.3049656635,-3.0684165479 H,0,-0.7253979055,2.4858564325,-1.5070098354 C,0,1.4279684113,1.5283279136,-3.0034202712 H,0,1.6880615201,2.4919205077,-3.444458159 H,0,2.0487359638,0.7685621921,-3.4829349659 H,0,1.7001534093,1.5642171993,-1.9447159614 C,0,-0.7055019039,-1.4900225371,3.3463905263 H,0,0.0172706369,-2.273153498,3.0867675636 C,0,-2.1033128068,-1.9914333437,3.0124506464 H,0,-2.3065722974,-2.9081113455,3.5672864228 H,0,-2.2128824488,-2.2124091782,1.9520663904 H,0,-2.8550468947,-1.2531433807,3.2976082331 C,0,-0.5939805162,-1.1089195351,4.8134656305 H,0,0.4195108155,-0.8487330604,5.1176655751 H,0,-0.9174455597,-1.9430441572,5.4383069136 H,0,-1.2458725468,-0.2625683388,5.0441262639 C,0,1.2257154926,0.738650107,2.9593898598 H,0,0.8994056347,1.0750324354,3.950023724 C,0,2.3685138846,-0.2569092801,3.1111128851 H,0,3.2242292966,0.2266901522,3.5855685833 H,0,2.688019123,-0.6302019509,2.1368192821</p>	<p>3a+BH₃NH₂Me-Eq-Sn₂-TS</p> <p>HF=-2876.8770809 ZPE= 0.563093 NImag=1 (-320)</p> <p>Htot=-2876.275559 Gtot=-2876.381084</p> <p>Rh,0,-0.2606140541,-0.481159287,-0.086795302 C,0,-2.1953044081,0.1784326476,-0.0873848635 Cl,0,-0.3630734991,-3.0533569676,0.1999837561 B,0,1.8391244912,-2.1326666851,-0.1100762153 N,0,3.994277924,-1.0986760121,-0.4574409462 H,0,1.5496336122,-0.9283198418,-0.0683727252 H,0,0.0603612613,1.0311060705,-0.1818838409 P,0,-0.2625434898,-0.1002390074,2.1986294879 P,0,-0.4340955567,-0.4101250818,-2.4039973607 C,0,-4.922714229,0.9766608261,-0.0463041039 C,0,-3.0543840935,-0.0183077909,-1.1856161024 C,0,-2.7676095588,0.8526328656,1.0097839587 C,0,-4.1097902821,1.225546502,1.0442474366 C,0,-4.3932281239,0.3690437272,-1.1693109259 H,0,-4.5114104873,1.7098763311,1.9255616355 H,0,-5.0119609118,0.2015269322,-2.0421898047 H,0,-5.9651653818,1.2680691808,-0.0257716639 S,0,-2.4986349414,-0.7482717469,-2.7303324247 S,0,-1.8117588305,1.3240621899,2.4534502461 C,0,-0.0506167044,1.2610518732,-3.1411512228 H,0,-0.2979848118,1.1778643889,-4.203151773 C,0,0.4070377033,-1.6131910305,-3.5598675569 H,0,1.449565475,-1.565693708,-3.2214925178 C,0,-0.097895056,-3.0312560346,-3.3516577649 H,0,0.5508068844,-3.7309958223,-3.8816974052 H,0,-1.1063146691,-3.1503233916,-3.7516596063 H,0,-0.1217554481,-3.3135693765,-2.3006533704 C,0,0.3392938148,-1.211869857,-5.0262039408 H,0,0.8050360601,-1.9902729363,-5.6336903202 H,0,0.8598327899,-0.2798888693,-5.2436545124 H,0,-0.6920295176,-1.1122081368,-5.3716065879 C,0,-0.8902373403,2.3728576405,-2.5408921021 H,0,-1.9585959279,2.189501451,-2.657445168 H,0,-0.6602688086,3.3169640813,-3.0385234834 H,0,-0.6878014469,2.5036871454,-1.476220387 C,0,1.4407199397,1.5243882751,-2.9815621374 H,0,1.7065923694,2.4882293079,-3.4192270143 H,0,2.0566258569,0.7638501997,-3.4658866003 H,0,1.7188304186,1.5555827017,-1.9241841407 C,0,-0.6929071372,-1.4803375386,3.3741404094 H,0,0.036956246,-2.2577976937,3.1181745406 C,0,-2.0879974806,-2.000965727,3.0633854652 H,0,-2.267124278,-2.9260750779,3.6133507131 H,0,-2.2204112311,-2.2147787165,2.0036255052 H,0,-2.8483514985,-1.2799600366,3.3697134644 C,0,-0.5647783858,-1.0880811784,4.8361336564 H,0,0.4500048506,-0.8136864464,5.1232481435 H,0,-0.8660587504,-1.9242604721,5.4700025363 H,0,-1.2239355782,-0.2501608193,5.0770698722 C,0,1.2167877951,0.7585770058,2.9351250812 H,0,0.8994877988,1.1006878922,3.9264760686 C,0,2.3694014313,-0.2255305015,3.0819641574 H,0,3.2187046431,0.2666904625,3.5594571368 H,0,2.6982785255,-0.5869349748,2.106142332</p>



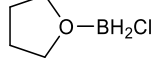
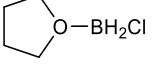
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BH₂Cl-NH₂Me HF=-582.204028 ZPE= 0.092579 NImag=0 Htot= -582.104811 Gtot= -582.140485 H,0,-0.0430486387,-0.0975205793,0.1454215727 B,0,1.1448206036,-0.042005455,0.0128880924 Cl,0,1.8017268638,1.6863774263,0.2447234059 H,0,1.5835310569,-0.5662322444,-0.9691505019 N,0,1.7762201635,-0.8587597427,1.2778076057 H,0,1.4897931118,-0.3867214531,2.1320443457 H,0,2.7880200742,-0.7608157092,1.2424675714 C,0,1.3959381197,-2.283799219,1.3221058398 H,0,1.8362890506,-2.790929809,2.1780073362 H,0,1.7271354528,-2.7571411886,0.4022668919 H,0,0.3128450202,-2.3496023354,1.3713731864	BH₂Cl-NH₂Me HF=-582.2167677 ZPE= 0.092859 NImag=0 Htot= -582.117329 Gtot= -582.152874 H,0,-0.0384053952,-0.0924608969,0.145172405 B,0,1.1521919466,-0.0507889453,0.0273393797 Cl,0,1.7883595563,1.7058631583,0.2170211321 H,0,1.5838511487,-0.559926812,-0.9664373406 N,0,1.7771486434,-0.8567016111,1.2782970996 H,0,1.4926639091,-0.4019732654,2.1432590075 H,0,2.7914304079,-0.7762229932,1.2533125296 C,0,1.3927278875,-2.2819715008,1.3166522927 H,0,1.8359194003,-2.7830650931,2.1741605237 H,0,1.7274807898,-2.7591943062,0.3999095817 H,0,0.3099025832,-2.3507080553,1.3712687391
H₂B-NHMe HF=-121.362449 ZPE= 0.076349 NImag=0 Htot= -121.281394 Gtot= -121.310843 B,0,0.1007608775,0.0303447865,1.1205281451 H,0,0.0204718444,1.1019248219,1.6292715438 H,0,0.3391926353,-0.9553592964,1.7442427758 N,0,-0.0904258688,-0.0744979088,-0.2495517279 H,0,-0.2926970503,0.751949854,-0.7881624321 C,0,-0.0309194576,-1.293903938,-1.0398044398 H,0,0.9496776026,-1.7655935304,-0.96831633 H,0,-0.220536577,-1.0800713637,-2.0897950517 H,0,-0.7755244357,-2.0183324522,-0.7082339791	H₂B-NHMe HF=-121.3641148 ZPE= 0.076245 NImag=0 Htot= -121.283166 Gtot= -121.312607 B,0,0.1005243991,0.0298870043,1.1185146582 H,0,0.020462524,1.101896371,1.6291820718 H,0,0.3394481922,-0.9531693389,1.7480660836 N,0,-0.0900893311,-0.0759964777,-0.2487756321 H,0,-0.292578846,0.7508395174,-0.7884573348 C,0,-0.0308718672,-1.2945584105,-1.0401247524 H,0,0.9500252977,-1.7661498402,-0.969625453 H,0,-0.2208561842,-1.0772690166,-2.0891918764 H,0,-0.776064613,-2.0190188337,-0.7094092511
 Py+BH₂Cl HF=-734.6506784 ZPE=0.115062 NImag=0 Htot=-734.528338 Gtot= -734.566937 B,0,-0.0005771488,0.035648503,-0.0592518535 Cl,0,1.8643141814,-0.0366596172,0.0609323332 H,0,-0.3990181398,1.1588285562,0.0431269341 H,0,-0.3990182439,-0.5809623385,-1.0036065723 N,0,-0.5204712878,-0.7519592678,1.2498424614 C,0,-1.3056858584,-2.1133404618,3.5126139048 C,0,-0.7087017926,-2.0784818509,1.2067076364	 Py+BH₂Cl HF=-734.6664267 ZPE=0.115318 NImag=0 Htot=-734.542983 Gtot= -734.584158 B,0,-0.0074029276,0.0287241904,-0.0477428526 Cl,0,1.8758905235,-0.0110745451,0.0184070137 H,0,-0.3999968129,1.1546146083,0.0450971987 H,0,-0.3999969168,-0.5807289914,-0.9989606226 N,0,-0.5074675981,-0.7547020878,1.2544013408 C,0,-1.3122040685,-2.1127544633,3.511639909 C,0,-0.7019730405,-2.0822215974,1.2097768541

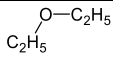
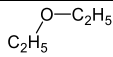
<p>C,0,-0.7087016737,-0.0924325783,2.4016008419 C,0,-1.1028540447,-0.742961998,3.5520221245 C,0,-1.1028541672,-2.7901193019,2.3203636824 H,0,-0.5260783847,-2.5353556465,0.243598608 H,0,-0.5260781748,0.9724868109,2.3540684619 H,0,-1.2476975082,-0.1778727952,4.4617298284 H,0,-1.2476977285,-3.8585535011,2.2472730031 H,0,-1.6179415346,-2.6475723232,4.4005684366</p>	<p>C,0,-0.7019729215,-0.0933922849,2.4063426519 C,0,-1.1050977125,-0.7432474111,3.5526673688 C,0,-1.105097835,-2.7905556631,2.3209181099 H,0,-0.5209249731,-2.5449852724,0.2494122972 H,0,-0.5209247626,0.9718615501,2.365299567 H,0,-1.2546605789,-0.1769987995,4.4607319874 H,0,-1.2546607992,-3.8580813498,2.2460333951 H,0,-1.6325710826,-2.6457656933,4.3975656125</p>
 <p>7+BH₂CINH₂Me-Ax</p>	 <p>7+BH₂CINH₂Me-Ax*</p>
<p>HF=-2876.8763045 ZPE=0.564430 NImag= 0</p> <p>Htot=-2876.274069 Gtot= -2876.378708</p> <p>C,0,-0.0884555351,1.1319486789,-0.7955743111 C,0,-0.2331233629,3.6629869685,-2.0922809129 C,0,0.9799514295,2.0510364003,-0.7871084216 C,0,-1.254183329,1.6011057354,-1.4292506764 C,0,-1.3439544797,2.8352251857,-2.0721157965 C,0,0.9284109095,3.282259453,-1.4391357484 H,0,-2.2712642459,3.1517804302,-2.5334545135 H,0,1.7857008829,3.9441499126,-1.4286040215 H,0,-0.2802540133,4.6197592651,-2.5971375751 P,0,2.2724435737,-0.3947334002,0.340669945 P,0,-2.2528324474,-0.4921818801,0.3978342739 S,0,2.4819506273,1.7274747822,0.1490534978 S,0,-2.7775829343,0.6210752168,-1.3729983437 C,0,3.1418138048,-0.7410822699,1.9495233882 H,0,4.1398542992,-0.29852339,1.8632979476 C,0,3.4423752521,-1.0234376892,-0.9853572681 H,0,3.1757759814,-2.0812750532,-1.0848774844 C,0,3.1474561785,-0.313068113,-2.3009582719 H,0,3.5370289668,-0.8883432481,-3.1420167907 H,0,3.6095487665,0.6743505062,-2.3132820375 H,0,2.0793619935,-0.1681964839,-2.4590961121 C,0,4.9141330615,-0.8804766545,-0.6341451633 H,0,5.5297356288,-1.1978797246,-1.4779773735 H,0,5.2118332237,-1.4760679959,0.2272983296 H,0,5.1633824507,0.1637700767,-0.4297413763 C,0,2.4151253866,-0.1102390187,3.1247554217 H,0,2.2573024115,0.9593526286,2.985483974 H,0,2.9922267994,-0.2524938567,4.0398921078 H,0,1.4409487428,-0.580695614,3.2678489157 C,0,3.2569586225,-2.2502410588,2.1243848481 H,0,3.7754589616,-2.4821423041,3.0559161279 H,0,3.8035884914,-2.7329288363,1.3138984415 H,0,2.2636263285,-2.7008137193,2.168386916 C,0,-3.4815764122,-1.8914827881,0.3560040099 H,0,-3.3446775166,-2.3453780129,1.3445157169 C,0,-3.0777285109,-2.9099604767,-0.693074515 H,0,-3.7494053031,-3.7691253712,-0.6706989905 H,0,-2.0626819293,-3.2711752775,-0.5385554483 H,0,-3.1278753868,-2.4892622046,-1.6997271325 C,0,-4.9277528433,-1.4477640165,0.202965656 H,0,-5.2516260774,-0.7716051936,0.9934628132 H,0,-5.5875695102,-2.3166536429,0.2268373832 H,0,-5.0899378743,-0.9466517101,-0.7533602448 C,0,-2.8577267664,0.5852310574,1.7988172852 H,0,-3.9255458463,0.7364619827,1.6126115847 C,0,-2.6660671506,-0.1541776613,3.1163382843</p>	<p>HF=-2876.9017785 ZPE=0.564035 NImag=0</p> <p>Htot=-2876.299836 Gtto= -2876.404737</p> <p>* Single-Point Energy using Gas Phase Geometry</p>

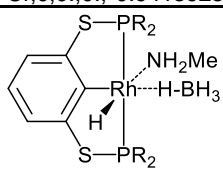
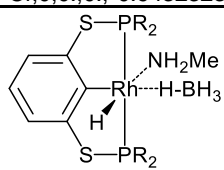
<p>H,0,-2.9913093711,0.4729362176,3.947840248 H,0,-1.6135742466,-0.3985889005,3.2755159518 H,0,-3.2342928093,-1.083469972,3.1651311009 C,0,-2.174115494,1.9417907472,1.8145896994 H,0,-2.5560847992,2.5360095523,2.6464593116 H,0,-2.3482780563,2.5008823198,0.8959809535 H,0,-1.0943160367,1.8421906249,1.9425895301 Rh,0,0.0100530917,-0.7511681149,0.2542769118 H,0,0.0542785538,0.0273546756,1.5812752388 H,0,0.0626321521,-2.0816320876,1.2109850181 H,0,-0.1090209958,-2.110613312,-1.2154206941 B,0,0.1719688517,-2.2629989703,-2.4035704464 H,0,1.3418089933,-2.3469659693,-2.6120708887 Cl,0,-0.724230869,-3.7508007618,-3.0585871895 N,0,-0.4046419851,-0.9868570245,-3.180201322 C,0,-0.1193683722,-0.9288554053,-4.626212406 H,0,-1.4127731901,-0.9250115697,-3.0128170738 H,0,-0.0392666112,-0.154142664,-2.7065244683 H,0,-0.5423754988,-0.028915618,-5.0680090774 H,0,0.9588608715,-0.9360877518,-4.7660916148 H,0,-0.5401644782,-1.8123151302,-5.0985236219</p>	
 <p>3+BH₂CINH₂Me-Eq</p>	 <p>3+BH₂CINH₂Me-Eq</p>
<p>HF=-2875.7002151 ZPE=0.547991 NImag=0</p> <p>Htot=-2875.114859 Gtot=-2875.219606</p> <p>C,0,-1.9704459342,-0.032963506,-0.1334594956 C,0,-4.833235274,-0.2828621471,-0.1364442012 C,0,-2.7338391334,-0.2610805272,-1.3077771315 C,0,-2.7656267651,0.082117598,1.0353195348 C,0,-4.1532121001,-0.0458241948,1.0422071281 C,0,-4.1217378059,-0.3806791181,-1.3166407652 H,0,-4.6958974754,0.0445187811,1.9751624582 H,0,-4.6396734574,-0.546467091,-2.2532007643 H,0,-5.911366489,-0.3799041711,-0.136774137 P,0,-0.0633287237,0.2323801687,-2.3962854416 P,0,-0.043976272,0.4471212258,2.12684074 S,0,-2.0004490336,-0.4152539351,-2.9400852655 S,0,-2.086819752,0.4259607646,2.6619415001 C,0,0.0524273229,1.9899703074,-3.0203415762 H,0,-0.1648007545,1.9679534898,-4.0930007604 C,0,1.0182332702,-0.738833161,-3.5703392925 H,0,2.0280199205,-0.3935828266,-3.3217665415 C,0,0.9274340999,-2.2207080937,-3.2466878467 H,0,1.6885476245,-2.7840615156,-3.7895594502 H,0,-0.0500597731,-2.6224466483,-3.5166604925 H,0,1.064497884,-2.4028355445,-2.1795203592 C,0,0.7390736191,-0.4691182558,-5.040153773 H,0,1.3810764268,-1.0899744517,-5.6680355083 H,0,0.9211361577,0.5686844746,-5.3165996558 H,0,-0.294774934,-0.7096072867,-5.2978084802 C,0,-0.9871108299,2.8498732824,-2.3208817417 H,0,-1.9995390521,2.4920859627,-2.507617866 H,0,-0.9221914193,3.8827790039,-2.6673989455 H,0,-0.8309463038,2.8402509393,-1.2397025401 C,0,1.4649221363,2.5084082078,-2.7858201221 H,0,1.554750576,3.5413012191,-3.1266219435 H,0,2.2228441961,1.923356253,-3.3090106089 H,0,1.709572215,2.4884264283,-1.7201854748</p>	<p>HF=-2875.7269588 ZPE=0.548123 NImag=0</p> <p>Htot=-2875.141427 Gtot=-2875.246631</p> <p>C,0,-1.9925148825,-0.0177884237,-0.1156921086 C,0,-4.8628123394,-0.2499221036,-0.1326623615 C,0,-2.7558548401,-0.2373497512,-1.2936786281 C,0,-2.7966057659,0.0994556806,1.0491795563 C,0,-4.1855669311,-0.019855124,1.049189219 C,0,-4.1451360586,-0.349039057,-1.3091583905 H,0,-4.7327870295,0.0721400563,1.9796848026 H,0,-4.6605605359,-0.5097776208,-2.2483301472 H,0,-5.9417672535,-0.3403048374,-0.1382549465 P,0,-0.0628448403,0.2116587996,-2.3825868917 P,0,-0.0751984053,0.4643874092,2.152083723 S,0,-2.0196239682,-0.3940956579,-2.9232637579 S,0,-2.1244911572,0.433295913,2.6793568126 C,0,0.0950326387,1.9580307772,-3.0314975542 H,0,-0.1363572089,1.9298197328,-4.1008831831 C,0,0.984030988,-0.8028194812,-3.5526752996 H,0,2.0030287471,-0.4808590066,-3.3127451809 C,0,0.8558012848,-2.2790034624,-3.2174240895 H,0,1.6236302379,-2.8606154037,-3.7314008972 H,0,-0.1171417222,-2.668925092,-3.5207050512 H,0,0.9507475818,-2.4611285255,-2.1451207574 C,0,0.7117569456,-0.5382451062,-5.023920751 H,0,1.3387235797,-1.1823819834,-5.6442497892 H,0,0.9227069344,0.4910483863,-5.3122299625 H,0,-0.3266794014,-0.7549876156,-5.285293245 C,0,-0.9050515541,2.8614715578,-2.3313036563 H,0,-1.9330678282,2.535034678,-2.4915043484 H,0,-0.8169670306,3.8849372832,-2.7015843088 H,0,-0.7293029767,2.873433494,-1.2527651135 C,0,1.5249781114,2.4373692671,-2.8244963272 H,0,1.6390315991,3.4618231466,-3.1844132717 H,0,2.2591597234,1.8237000683,-3.3488507178 H,0,1.7875296125,2.4305725485,-1.7626654921</p>

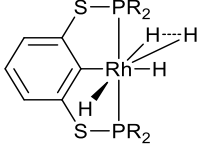
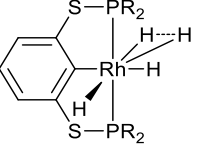
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 <p>4+BH_3 (6+BH_3)</p>	 <p>4+BH_3 (6+BH_3)</p>
<p>HF=-2321.3327509 ZPE=0.503907 NImag=0</p> <p>Htot=-2320.796044 Gtot=-2320.889085</p> <p>C,0,-0.0077809921,1.8391168964,-0.3675273255 C,0,-0.0995110478,4.31681214,-1.7677761459 C,0,1.155213155,2.5242118446,-0.774926036 C,0,-1.2136057264,2.5260698803,-0.6164581278 C,0,-1.2667425007,3.7267800591,-1.3220376454 C,0,1.1157686256,3.7249113903,-1.4814218519 H,0,-2.2235206043,4.1970868534,-1.5107775391 H,0,2.0396145094,4.193744062,-1.7959698229 H,0,-0.1358344102,5.2460072274,-2.3216392349 P,0,2.3457910935,0.0349077221,0.3050432257 P,0,-2.2536182196,0.0384917315,0.6126691961 S,0,2.8125178259,1.9840181561,-0.3534515184 S,0,-2.8008444387,1.9884167921,0.0220650279 C,0,3.3890155227,-0.1835634837,1.8285756874 H,0,4.398108896,0.1463726252,1.5569681626 C,0,3.096493527,-1.0737066151,-0.9891956968 H,0,2.815138344,-2.0771985807,-0.65122062 C,0,2.4401181339,-0.8078343145,-2.334882252 H,0,2.7982628026,-1.5253777766,-3.0739432761 H,0,2.6836866055,0.193451712,-2.6949321514 H,0,1.3547013591,-0.8929701916,-2.2831901723 C,0,4.6086299215,-0.9444454677,-1.0687463699</p>	<p>HF=-2321.3529514 ZPE=0.503620 NImag=0</p> <p>Htot=-2320.816361 Gtot=-2320.909935</p> <p>C,0,-0.0089055543,1.8372139681,-0.3836446826 C,0,-0.0982165101,4.3362603756,-1.7475869208 C,0,1.1552164002,2.5282493583,-0.7797198581 C,0,-1.2143445503,2.5300832508,-0.6212006158 C,0,-1.266064061,3.7412440649,-1.309780928 C,0,1.1166221613,3.7393991538,-1.46917948 H,0,-2.2217929357,4.2167857314,-1.4920073074 H,0,2.0402937322,4.213485636,-1.7771353353 H,0,-0.1337091028,5.2730587714,-2.2889721065 P,0,2.3531538988,0.0263155328,0.2893840331 P,0,-2.2630643426,0.0298753278,0.5981678573 S,0,2.812471036,1.9815396959,-0.36763389 S,0,-2.8027826262,1.9858825637,0.0080123689 C,0,3.3572339167,-0.1749835841,1.841983911 H,0,4.3705844501,0.1567503551,1.5902857959 C,0,3.15454562,-1.0745973597,-0.9813332097 H,0,2.88412196,-2.0811925154,-0.6443448028 C,0,2.5289730176,-0.8327938305,-2.3448989463 H,0,2.9105164729,-1.5587216677,-3.0643849215 H,0,2.7731062919,0.1637485552,-2.7181029176 H,0,1.4429529489,-0.9273796126,-2.3221343787 C,0,4.6658591226,-0.926215128,-1.0232195832</p>

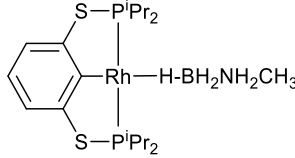
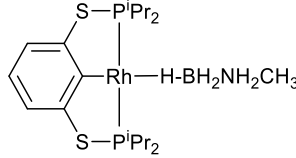
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 <p>BH₃-Pyridine HF=-274.994381 ZPE=0.121311 NImag=0 Htot=-274.865670 Gtot=-274.903736</p> <p>H,0,0.1202192692,0.0000000158,-0.205985255 B,0,-0.0027663059,0.000000174,0.9972753115 H,0,-0.5114771864,-1.0136616544,1.4034477431 H,0,-0.5114771966,1.0136616855,1.4034477395 N,0,1.5057327857,0.000000026,1.5660709593 C,0,4.1326236196,0.000000408,2.4424154507 C,0,2.1527614965,-1.1550661247,1.7849801529 C,0,2.1527614848,1.155066184,1.7849801488 C,0,3.4616410009,1.1916778735,2.2188971397 C,0,3.4616410129,-1.1916777994,2.2188971439 H,0,1.5692399514,-2.0459131421,1.5969655095 H,0,1.5692399308,2.0459131948,1.5969655022 H,0,3.9403262427,2.1469579215,2.3828026626 H,0,3.9403262644,-2.146957842,2.3828026703 H,0,5.1580857334,0.000000466,2.788084532</p>	 <p>BH₃-Pyridine HF=-275.0068089 ZPE=0.121596 NImag=0 Htot=-274.877882 Gtot=-274.915580</p> <p>H,0,0.1069529764,0.0000000158,-0.2072784161 B,0,0.0045368069,0.000000174,0.9987048766 H,0,-0.5172074791,-1.0085958131,1.4042250712 H,0,-0.5172074893,1.0085958441,1.4042250676 N,0,1.5084154044,0.000000026,1.5651245418 C,0,4.1310299726,0.000000408,2.444063874 C,0,2.1543506928,-1.1564311619,1.7832900995 C,0,2.1543506811,1.1564312212,1.7832900954 C,0,3.4617291282,1.1920669796,2.2197487196 C,0,3.4617291402,-1.1920669055,2.2197487239 H,0,1.5766724331,-2.0506291881,1.5943053228 H,0,1.5766724124,2.0506292409,1.5943053155 H,0,3.9403126249,2.1472348549,2.383618601 H,0,3.9403126466,-2.1472347754,2.3836186086 H,0,5.1562281522,0.000000466,2.7909808309</p>
 <p>BH₃-THF</p>	 <p>BH₃-THF</p>

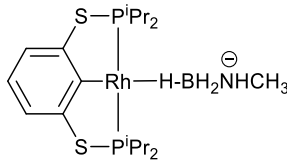
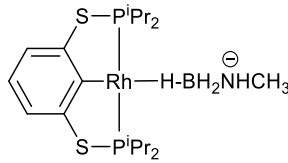
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 <p>THF</p>	 <p>THF</p>
<p>HF=-232.4896731 ZPE= 0.116872 NImag=0</p> <p>Htot= -232.366918 Gtot= -232.400584</p> <p>H,0,0.0019218513,-0.0233791083,0.0420362714 C,0,-0.025652044,0.0087195796,1.1301710376 C,0,1.0378184651,0.9137357156,1.7240645557 O,0,0.539428123,1.3423546255,2.9904877351 C,0,-0.8456808139,1.0148257378,3.0911497096 C,0,-1.2962822637,0.6287195447,1.6945060249 H,0,0.0925698065,-1.0128970689,1.4981320975 H,0,1.2108167065,1.7902612329,1.0850169107 H,0,1.9997017401,0.4187223562,1.8758394103 H,0,-1.3796788798,1.8747174931,3.5019118085 H,0,-0.9722016227,0.1779337733,3.7913008301 H,0,-1.5703123067,1.5174710179,1.1217052928 H,0,-2.1517080209,-0.0451310571,1.6942711665</p>	<p>HF=-232.4954183 ZPE=0.116842 NImag=0</p> <p>Htot=-232.372719 Gtot= -232.406185</p> <p>H,0,0.0031780932,-0.0236465763,0.0431260903 C,0,-0.0255436802,0.0084993852,1.131279997 C,0,1.0377425407,0.9129112566,1.7220410514 O,0,0.5406814162,1.3434233692,2.9921354288 C,0,-0.8475954387,1.0139527592,3.0905562561 C,0,-1.2955927716,0.6296201095,1.6944459997 H,0,0.0930159149,-1.0125605379,1.5010854804 H,0,1.2098493257,1.7900508306,1.0834769147 H,0,2.0004895557,0.4183286741,1.8724453104 H,0,-1.3827876225,1.8731320084,3.5022546057 H,0,-0.9730697707,0.1765789315,3.7904276722 H,0,-1.5680868785,1.5194126352,1.1222641558 H,0,-2.1515399432,-0.0436490029,1.6950538882</p>
 <p>BH₂Cl-THF</p>	 <p>BH₂Cl-THF</p>
<p>HF=-718.7984314 ZPE= 0.143392 NImag=0</p> <p>Htot= -718.646385 Gtot= -718.688387</p> <p>H,0,-0.4219523358,-0.7172464136,0.1234463467 B,0,-0.3318007314,-0.3701127486,1.2618496487 H,0,-0.4686703055,-1.2231160429,2.0963330173 Cl,0,-1.2951474663,1.1484599157,1.6451750371 O,0,1.2170058416,0.0774852387,1.3938206882 C,0,2.1590205178,-0.8954781405,0.8456496337 H,0,2.2100381723,-0.7111751937,-0.2246172414 H,0,1.7493541644,-1.8935854121,1.0236047266 C,0,1.666428532,0.5073139974,2.7292661773</p>	<p>HF=-718.8112539 ZPE= 0.143531 NImag=0</p> <p>Htot= -718.659118 Gtot= -718.700770</p> <p>H,0,-0.4113650261,-0.7170776615,0.118188779 B,0,-0.3201528757,-0.3468322988,1.2501452444 H,0,-0.5483755309,-1.1683552667,2.0956494132 Cl,0,-1.271409289,1.2182702713,1.5554929491 O,0,1.204697866,0.0476876318,1.415985805 C,0,2.157717613,-0.9194559364,0.8574126842 H,0,2.1859473195,-0.7418119486,-0.2147736581 H,0,1.7719731794,-1.9232531575,1.0534219201 C,0,1.6582011553,0.4730698928,2.7581910739</p>

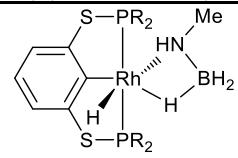
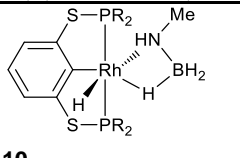
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F_3B-OEt_2 BF₃ diethyl ether adduct HF=-558.3666815 ZPE= 0.151743 NImag=0 Htot=-558.203130 Gtot= -558.251940 B,0,-0.1659396099,-0.4639057696,1.024133947 O,0,1.2300644215,-0.2165648299,1.9166635318 F,0,0.3248757566,-0.7651223185,-0.2043061072 F,0,-0.7921692086,0.7325718713,1.1454715958 F,0,-0.796465588,-1.492492192,1.6592828353 C,0,2.3948362297,-1.0357303745,1.6188962396 H,0,3.2015951415,-0.6568025959,2.2491089674 H,0,2.6353644364,-0.8068033752,0.5832212184 C,0,1.0175509465,0.0717628043,3.3272797605 H,0,-0.0600306692,0.172018433,3.4397490225 H,0,1.3333927275,-0.8002800906,3.9046216366 C,0,2.1428289809,-2.5035178903,1.8265940673 H,0,3.0599112922,-3.0580722693,1.6307429391 H,0,1.3706673955,-2.8657913432,1.1517124556 H,0,1.8330466426,-2.7233676993,2.8481368335 C,0,1.7449733252,1.3268550912,3.7145554671 H,0,1.3898674481,2.1697197479,3.1243136517 H,0,2.8213857889,1.2336968558,3.5702225857 H,0,1.5708492427,1.5473447449,4.7670180521	F_3B-OEt_2 BF₃ diethyl ether adduct HF=-558.3764891 ZPE=0.151735 NImag=0 Htot=-558.213055 Gtot= -558.261308 B,0,-0.1336793084,-0.4522737721,1.050179393 O,0,1.2171086316,-0.228385565,1.9171292676 F,0,0.3248453669,-0.7418994049,-0.2016257326 F,0,-0.7832590451,0.743697975,1.1627259386 F,0,-0.8045932626,-1.4868561369,1.649738968 C,0,2.3925102825,-1.0484175779,1.6201472929 H,0,3.1856928898,-0.6686994517,2.265184146 H,0,2.6475691626,-0.8077807071,0.5906825166 C,0,1.0166470128,0.0726860645,3.3363877847 H,0,-0.0599358583,0.1637116083,3.4642121634 H,0,1.3502417415,-0.7941908304,3.9100991598 C,0,2.1404328252,-2.5140086435,1.8186879832 H,0,3.0675378302,-3.0598609282,1.6446273428 H,0,1.3918352039,-2.8875219656,1.1227643466 H,0,1.8092871443,-2.7372145002,2.8329954372 C,0,1.7380470425,1.334134506,3.7006537943 H,0,1.3652061185,2.1746623541,3.1170524709 H,0,2.812904181,1.2498338759,3.5398524303 H,0,1.5782067411,1.5539018998,4.7559239968
 Diethyl ether HF=-233.7031866 ZPE= 0.136680 NImag=0 Htot= -233.558732 Gtot= -233.595973 O,0,0.0267423821,0.0463195029,0.9189594691 C,0,-0.0174847433,-0.0302840421,-0.4905753719 H,0,1.0055142118,-0.0220689242,-0.8991497921 H,0,-0.5218697886,0.8597665864,-0.8991497371 C,0,0.6960486199,1.2055919545,1.3692140113 H,0,1.7241804467,1.2226974667,0.9740181671 H,0,0.1967964463,2.1045329773,0.9740182221 C,0,0.698138275,1.2092112498,2.8726569063 H,0,1.2066357707,0.327799644,3.2611850743 H,0,-0.3194352937,1.2088771307,3.2611851292 H,0,1.2080603102,2.092422152,3.2553205067 C,0,-0.7430510633,-1.2870018239,-0.8837317488 H,0,-0.2335395016,-2.1666570158,-0.4925604678 H,0,-0.7958859184,-1.3785144152,-1.9678661198 H,0,-1.759610566,-1.2855795292,-0.4925604129	 Diethyl ether HF=-233.7080048 ZPE=0.136515 NImag=0 Htot= -233.563728 Gtot= -233.600940 O,0,0.0246405032,0.0426789415,0.9221851264 C,0,-0.0190214435,-0.032945685,-0.4897048123 H,0,1.0040413892,-0.0246690218,-0.8974433728 H,0,-0.5233851277,0.8571910357,-0.8974433178 C,0,0.6952304448,1.2041748334,1.3719573709 H,0,1.7229908713,1.2205879676,0.9764628562 H,0,0.1955643545,2.1024480251,0.9764629112 C,0,0.6997768859,1.2120494071,2.8739568998 H,0,1.2109182151,0.3335303399,3.2676374901 H,0,-0.3166135876,1.2154511842,3.267637545 H,0,1.2109861552,2.0974898648,3.2511000532 C,0,-0.7432548085,-1.2873547207,-0.887233765 H,0,-0.2350060657,-2.1708838943,-0.501092558 H,0,-0.7930903318,-1.3736723166,-1.9724260855 H,0,-1.7625378683,-1.2889630501,-0.501092503
H-Cl HF=-460.8061245 ZPE= 0.006842 NImag=0	H-Cl HF=-460.8099664 ZPE=0.006757 NImag=0

<p>Htot= -460.795978 Gtot= -460.817166</p> <p>H,0,0.,0.,0.3413925711 Cl,0,0.,0.,-0.9413925711</p>  <p>LRh-H-H-BH₃-Eq-NH₂Me-Ax</p> <p>HF=-2417.2224136 ZPE= 0.571248 NImag=0</p> <p>Htot= -2416.614281 Gtot= -2416.714948</p> <p>C,0,-2.0190944466,0.0561936273,-0.2095166222 C,0,-4.8584821827,-0.1396356496,-0.1691691595 C,0,-2.7677911399,-0.3472057742,-1.3328320186 C,0,-2.7886875324,0.4292953781,0.9113448037 C,0,-4.1770665661,0.3108502586,0.9468392839 C,0,-4.1576418003,-0.4492856913,-1.3203648001 H,0,-4.7185405444,0.5792936873,1.8452678404 H,0,-4.6843757157,-0.7588579284,-2.2144038853 H,0,-5.9369930451,-0.2298337228,-0.1482035021 P,0,-0.1344787086,0.1965454723,-2.4927411747 P,0,-0.0668114589,0.5028661948,2.0667411746 S,0,-2.0040029412,-0.7158507682,-2.9228006959 S,0,-2.0593372304,1.1565056314,2.3818208746 C,0,-0.2779862154,1.9298464201,-3.1694843924 H,0,-0.494478448,1.8079428181,-4.234946735 C,0,1.0460010717,-0.6444341062,-3.6722282836 H,0,2.0176718489,-0.2530303913,-3.3481777268 C,0,1.0582696522,-2.1501045525,-3.4696894786 H,0,1.7964017768,-2.6057370207,-4.1308781794 H,0,0.0875545021,-2.5939586797,-3.6969827793 H,0,1.3352565186,-2.4154771548,-2.4523148627 C,0,0.8098947651,-0.2888295789,-5.1333199693 H,0,1.49939429,-0.8525708011,-5.7638430907 H,0,0.9713868648,0.7669318467,-5.3441867224 H,0,-0.2026376949,-0.5459802517,-5.4522883001 C,0,-1.4252640071,2.6967577001,-2.5360864841 H,0,-2.378577554,2.1841083322,-2.6644418983 H,0,-1.508228467,3.6815823235,-2.9985759127 H,0,-1.266483413,2.8431306858,-1.4664697872 C,0,1.0554387425,2.6426587485,-2.9896803167 H,0,0.9975606655,3.6580343777,-3.3846090694 H,0,1.8767715397,2.1368270372,-3.4992999606 H,0,1.317943022,2.7117624354,-1.9317868116 C,0,0.1324381293,-0.8961015614,3.2921005387 H,0,1.0921313698,-1.3448914915,3.0036081199 C,0,-0.99167622,-1.9070540306,3.0944357983 H,0,-0.7342159997,-2.8651741036,3.548394515 H,0,-1.2323546341,-2.0745790725,2.0447440819 H,0,-1.907714046,-1.5488863862,3.5650684929 C,0,0.1887550902,-0.4458242508,4.7428806451 H,0,1.0470645259,0.1867227945,4.9623332024 H,0,0.2450105504,-1.3140697351,5.4019981403 H,0,-0.7177264886,0.1029004695,5.0101116287 C,0,0.9476304608,1.90071713,2.7578596505 H,0,0.5453690164,2.0787547551,3.7621155328 C,0,2.4101448458,1.4848886631,2.853136179 H,0,2.990853948,2.2862590649,3.3127407009 H,0,2.8271031581,1.2889492801,1.8648987455 H,0,2.5609631452,0.5847848659,3.4490057587</p>	<p>Htot=-460.799905 Gtot= -460.821097</p> <p>H,0,0.,0.,0.3432323259 Cl,0,0.,0.,-0.9432323259</p>  <p>LRh-H-H-BH₃-Eq-NH₂Me-Ax</p> <p>HF=-2417.2454588 ZPE=0.570552 NImag=0</p> <p>Htot=-2416.637753 Gtot=-2416.739049</p> <p>C,0,-2.0296931163,0.0524922867,-0.2076712704 C,0,-4.870740929,-0.1425479923,-0.1699024813 C,0,-2.778603632,-0.3410109649,-1.3355137871 C,0,-2.8005733651,0.4196956761,0.9150477238 C,0,-4.1894451631,0.3011855786,0.9487465624 C,0,-4.1689190728,-0.4441570108,-1.3224576811 H,0,-4.7321827366,0.5648660008,1.8480974057 H,0,-4.696371094,-0.7480766376,-2.2182619518 H,0,-5.9494236684,-0.2330669988,-0.1499503748 P,0,-0.1396533426,0.1966421943,-2.4978659166 P,0,-0.0774274825,0.4935168952,2.0812357255 S,0,-2.0192041415,-0.6979058542,-2.9282751278 S,0,-2.0755875786,1.1382629064,2.3907028099 C,0,-0.2633820833,1.9342944088,-3.1673402023 H,0,-0.4868385095,1.8179183485,-4.2319163681 C,0,1.0351338074,-0.6537778086,-3.6759598814 H,0,2.0085523809,-0.2733041849,-3.3447964515 C,0,1.0300013978,-2.1603444134,-3.4869611994 H,0,1.7926300268,-2.6127736209,-4.1226890609 H,0,0.0688072397,-2.5991681361,-3.7603168722 H,0,1.2607060717,-2.4453469869,-2.4631053918 C,0,0.8163292386,-0.2839344938,-5.1353436554 H,0,1.5088714726,-0.8495491239,-5.7614622425 H,0,0.9922421544,0.7714303441,-5.3369807052 H,0,-0.1936777822,-0.5294484655,-5.4714736255 C,0,-1.3930087276,2.7204515998,-2.5281399365 H,0,-2.3564370495,2.2215303176,-2.6377506701 H,0,-1.4713221814,3.7000900819,-3.0032509172 H,0,-1.219533556,2.8835884272,-1.4628389769 C,0,1.0810591982,2.6262589809,-2.995263871 H,0,1.0364731425,3.6407356386,-3.3951939008 H,0,1.8928683579,2.1067859166,-3.5066633181 H,0,1.350645606,2.6993427686,-1.939039575 C,0,0.1327129362,-0.8921317745,3.3196721351 H,0,1.098488726,-1.3324440551,3.0405159534 C,0,-0.9723642312,-1.9230445917,3.1261831038 H,0,-0.6961518662,-2.8729289422,3.5868380816 H,0,-1.2072191661,-2.1071735238,2.0778677853 H,0,-1.8968458925,-1.5839187573,3.5951240086 C,0,0.1801575199,-0.4295189842,4.766139363 H,0,1.0306862451,0.2143221685,4.984408054 H,0,0.2481548135,-1.2938635564,5.4298808296 H,0,-0.7327356015,0.1084205233,5.0338840718 C,0,0.926168831,1.9069734402,2.7598557115 H,0,0.5233989504,2.0878655979,3.7629386627 C,0,2.3911149145,1.5048084196,2.8626802057 H,0,2.9605774386,2.308202404,3.3333934083 H,0,2.8192494422,1.3276783296,1.8755019321 H,0,2.5495893481,0.6019728708,3.4526765313</p>
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<p>C,0,0.787576469,3.1654030122,1.9312911167 H,0,1.2855544595,3.9988353466,2.4289698009 H,0,-0.2589419447,3.4335051118,1.7847503887 H,0,1.2470195302,3.0427274318,0.9493093924 Rh,0,0.0397859256,0.0868235821,-0.1977291845 H,0,-0.0671998047,1.6351300805,-0.2673480606 H,0,1.8405205878,0.413467235,-0.2725904043 B,0,2.7162168276,-0.5124565733,-0.0833990801 N,0,0.2725800124,-2.2300886934,-0.0101253089 H,0,3.7019693025,0.1853035148,-0.0303127043 H,0,2.5198819829,-1.099149025,0.9615960208 H,0,2.7220345621,-1.2498450255,-1.047864357 H,0,1.1381380111,-2.3825858185,-0.52144183 H,0,0.5301106905,-2.4095705341,0.9546482065 C,0,-0.7868005285,-3.1429769167,-0.4379366335 H,0,-0.5363551884,-4.1964603174,-0.2864469717 H,0,-1.7047906087,-2.9203984082,0.1060635585 H,0,-0.9966576858,-2.9781256974,-1.4931396383</p>	<p>C,0,0.7610274798,3.1664432083,1.9281630727 H,0,1.2496607568,4.0051812433,2.4271764503 H,0,-0.2857487389,3.431319555,1.7755487634 H,0,1.2269946269,3.0489324445,0.9483885287 Rh,0,0.0241423972,0.0743026268,-0.1925904785 H,0,-0.0882640261,1.6223703062,-0.2623022379 H,0,1.8486800056,0.3865919368,-0.2595000545 B,0,2.7614635443,-0.4967393901,-0.1382138388 N,0,0.2680653018,-2.2413530419,-0.0114550306 H,0,3.740685137,0.2170501041,-0.1194539714 H,0,2.6334541876,-1.1072764385,0.9026663521 H,0,2.7471930654,-1.225109404,-1.1086927418 H,0,1.122939834,-2.4089133009,-0.5350470294 H,0,0.5307861116,-2.4421318885,0.9480588262 C,0,-0.796198228,-3.1502457168,-0.4368023954 H,0,-0.5369908554,-4.2042506275,-0.3039913819 H,0,-1.7061997492,-2.9438641664,0.1266212933 H,0,-1.0219625406,-2.9749270975,-1.487198863</p>
 <p>6a+H₂</p>	 <p>6a+H₂</p>
<p>HF=-2295.8302617 ZPE= 0.486852 NImag=0</p> <p>Htot= -2295.311552 Gtot= -2295.403129</p> <p>C,0,-1.9824991514,0.063907122,-0.0361697493 C,0,-4.8151428917,-0.1585344516,-0.0571907097 C,0,-2.7405112737,0.1937606956,-1.2098826813 C,0,-2.7328124134,-0.1559606921,1.1289127739 C,0,-4.122125621,-0.2607901391,1.137088636 C,0,-4.1295182123,0.0729703542,-1.2369114251 H,0,-4.656095925,-0.4168172012,2.0662202838 H,0,-4.6700512907,0.1632567032,-2.1710545831 H,0,-5.8942005117,-0.2477629022,-0.0669736122 P,0,0.0522234041,0.189345446,-2.2985147783 P,0,-0.1124853519,0.6728670917,2.228745616 S,0,-1.9797738748,0.5764308437,-2.7969720656 S,0,-1.9374882693,-0.2944837488,2.7435727042 C,0,0.954149037,1.4979241706,-3.2691492525 H,0,0.5471684691,1.4509119129,-4.285185606 C,0,0.4298671124,-1.4016366568,-3.2116248302 H,0,1.4704124108,-1.6146300735,-2.9389398275 C,0,-0.4584166301,-2.5227988747,-2.6959377686 H,0,-0.1731760123,-3.4708231777,-3.1539118648 H,0,-1.5026499781,-2.3311640524,-2.9486507779 H,0,-0.3981175109,-2.6407592649,-1.6154321912 C,0,0.3092454374,-1.2657259926,-4.7208811874 H,0,0.4943282291,-2.2280714111,-5.2012667532 H,0,1.0150512992,-0.550405965,-5.1415855768 H,0,-0.6995026224,-0.9528456309,-5.0001299541 C,0,0.6969005886,2.8815153694,-2.6982369031 H,0,-0.3683307026,3.0893859291,-2.5956102251 H,0,1.1302417142,3.6414466347,-3.3504527883 C,0,1.1571123388,2.9817693478,-1.7140875798 H,0,2.4420769846,1.1765224703,-3.2953528702 H,0,2.986766389,1.961434352,-3.8221694469 H,0,2.6624157103,0.2328971543,-3.7951012043 H,0,2.8378844705,1.1193634246,-2.2791422231 C,0,1.0552222745,0.0178126032,3.5214015497 H,0,1.9135731824,0.694189524,3.4386441501 C,0,1.5144055026,-1.3870800153,3.1690815445</p>	<p>HF=-2295.8500899 ZPE= 0.486224 NImag=0</p> <p>Htot= -2295.331871 Gtot= -2295.423705</p> <p>C,0,-2.0033070466,0.0567711844,-0.0329048421 C,0,-4.8377740453,-0.1669387622,-0.0533161205 C,0,-2.7605681815,0.1621183614,-1.2106770962 C,0,-2.7563209189,-0.1399139922,1.1361019537 C,0,-4.1461361194,-0.2462198274,1.1436874942 C,0,-4.1503849897,0.0412611301,-1.2364277785 H,0,-4.6827386895,-0.3858451125,2.0742058921 H,0,-4.691139307,0.1131142319,-2.1723328024 H,0,-5.9170406507,-0.2566831945,-0.0628252771 P,0,0.045188348,0.1723160262,-2.3075252597 P,0,-0.1149954941,0.6699491814,2.2233767632 S,0,-2.0014637492,0.5079470516,-2.8060635288 S,0,-1.9660348729,-0.2504888204,2.755621881 C,0,0.9065176841,1.5215715305,-3.2612349857 H,0,0.4959703377,1.4739571598,-4.2756882962 C,0,0.4716097321,-1.3956071164,-3.236924488 H,0,1.5212972219,-1.5675844331,-2.9704165786 C,0,-0.3642238719,-2.5556338667,-2.7230088848 H,0,-0.0394278694,-3.4878501595,-3.1879123138 H,0,-1.4184406167,-2.4143721909,-2.9689957231 H,0,-0.2902502172,-2.6793892011,-1.6437744667 C,0,0.3399964502,-1.2570664922,-4.7443689015 H,0,0.5729958294,-2.2074253048,-5.2286252582 H,0,1.0080230527,-0.5067488878,-5.1662526182 H,0,-0.683110823,-0.9956033789,-5.0251199559 C,0,0.6130259456,2.8919863055,-2.6778857459 H,0,-0.4560366684,3.068715001,-2.5539157289 H,0,1.0064788582,3.668594773,-3.3363554045 H,0,1.0900866283,3.0099575182,-1.7035400888 C,0,2.4026436465,1.2474633879,-3.3027139543 H,0,2.9152705282,2.051367035,-3.8338375201 H,0,2.6505444545,0.3133661614,-3.8073391667 H,0,2.8154644149,1.2021296813,-2.2925954619 C,0,1.0517692506,-0.00615954,3.5104347949 H,0,1.947177333,0.6084597954,3.3640814848 C,0,1.4107901532,-1.4503083453,3.2070517597</p>

<p>H,0,2.1987034733,-1.7633859941,3.9308368436 H,0,2.0311255245,-1.40907195,2.2107447842 H,0,0.6682608227,-2.0754440385,3.1162025376 C,0,0.4936411816,0.0901263317,4.9332452142 H,0,0.1732776385,1.0936164109,5.2116556984 H,0,1.2501160243,-0.2236435605,5.6545279577 H,0,-0.361764057,-0.5777761396,5.0493893521 C,0,-0.3492801537,2.4634526762,2.6895736408 H,0,-0.549355414,2.4654461612,3.7661452016 C,0,0.9276625613,3.2402005027,2.4016219804 H,0,0.7949435949,4.2912599087,2.6627610849 H,0,1.1798300024,3.1874595664,1.3404965118 H,0,1.7847744565,2.8683811975,2.9641762966 C,0,-1.5455123216,3.0623491345,1.9698532726 H,0,-1.6786696233,4.1024674864,2.2714200275 H,0,-2.4669788854,2.5249768316,2.1920663776 H,0,-1.402641219,3.0433326194,0.8876976304 Rh,0,0.1610478182,0.2382225791,-0.0138321933 H,0,-0.0232139199,1.7668751127,-0.2233682281 H,0,1.7721805112,0.5939574423,0.0016797957 H,0,0.8926299537,-1.4409228349,0.1887884971 H,0,0.0928977197,-1.6016123431,0.2804119488</p>	<p>H,0,2.1020191824,-1.8309105818,3.9608246862 H,0,1.8915420909,-1.5488486566,2.2346417592 H,0,0.5276988878,-2.0928954717,3.2171617406 C,0,0.5533608284,0.1668355864,4.9359366088 H,0,0.3333207729,1.2043001457,5.1865469148 H,0,1.3104937696,-0.1828357492,5.6403372399 H,0,-0.3486940065,-0.4212211794,5.1174439894 C,0,-0.3236266017,2.4659538469,2.681581833 H,0,-0.5769193898,2.4686709215,3.7465080274 C,0,0.9850904405,3.2095978872,2.4629453761 H,0,0.8601762854,4.2663397931,2.7059839199 H,0,1.301684113,3.1449534775,1.4193575429 H,0,1.7975084929,2.8266423039,3.0815852741 C,0,-1.4662739693,3.1029449556,1.9111333548 H,0,-1.6024001801,4.135524504,2.2377613008 H,0,-2.4098828226,2.5785634865,2.0632107291 H,0,-1.2630121627,3.1189487427,0.8383858463 Rh,0,0.1393170473,0.2069145066,-0.0134645165 H,0,-0.0048461222,1.7366857486,-0.2244127116 H,0,1.7666938085,0.5211132187,0.0015157012 H,0,0.790608139,-1.530993974,0.2068369797 H,0,-0.0094923413,-1.6398024022,0.3035666269</p>
LRh-H-H2-Ax-TS-M06L.out	LRh-H-H2-Ax-TS-M06L-SCRF-SP.out
 <p>8</p>	 <p>8</p>
<p>HF=-1.1717115 ZPE= 0.009886 NImag=0</p> <p>Htot=-1.158521 Gtot=-1.173317</p> <p>C,0,-1.9796056834,-0.0048582354,-0.1281693639 C,0,-4.8418032878,-0.2948718476,-0.099461064 C,0,-2.7492756569,-0.2960025947,-1.28418469 C,0,-2.7730130694,0.1648750464,1.0346358763 C,0,-4.1577523952,0.0131999951,1.0605951259 C,0,-4.1355826894,-0.4358347153,-1.2784046697 H,0,-4.6950228769,0.1419009599,1.9922132537 H,0,-4.6564222771,-0.6507779541,-2.2033640711 H,0,-5.9179901139,-0.41124047,-0.0871620811 P,0,-0.0968612373,0.2207510968,-2.4092379499 P,0,-0.0434335016,0.4694332721,2.119769013 S,0,-2.0229333958,-0.4951143994,-2.913611662 S,0,-2.0878380242,0.6378526305,2.6250046339 C,0,-0.0364348223,1.9575445907,-3.0966748262 H,0,-0.3216368257,1.8993418319,-4.1520529772 C,0,0.9853669337,-0.7643276999,-3.5696362521 H,0,1.987464108,-0.3690929032,-3.3731967311 C,0,0.9649164348,-2.2293496446,-3.1680562992 H,0,1.7139598992,-2.7952951977,-3.7250897671 H,0,-0.0116215393,-2.6763117662,-3.3598724536 H,0,1.1708938409,-2.3470678474,-2.1030512213 C,0,0.6455674247,-0.5789156525,-5.0395806069 H,0,1.3012136283,-1.1929017078,-5.6603086099 H,0,0.7612533914,0.4533999546,-5.3680059521 H,0,-0.380770558,-0.8861168383,-5.2522456201 C,0,-1.039716379,2.8273961729,-2.3569117661 H,0,-2.055417439,2.4426317265,-2.4503694242 H,0,-1.0247512913,3.8455039581,-2.7503267377 H,0,-0.8017556579,2.8666954793,-1.2909554052 C,0,1.3807253148,2.4992433291,-2.9688061293 H,0,1.4278833068,3.5314388341,-3.3205334118</p>	<p>HF=-2416.0670239 ZPE=0.555540 NImag=0</p> <p>Htot=-2415.475323 Gtot=-2415.576691</p> <p>C,0,-1.9981739542,0.0243374025,-0.1159648141 C,0,-4.8627261204,-0.2825356941,-0.0707939242 C,0,-2.773292221,-0.2919251962,-1.263535838 C,0,-2.7910692638,0.2132912489,1.0462561003 C,0,-4.1751489687,0.0519382162,1.0804067439 C,0,-4.1592217227,-0.4407420672,-1.2496149248 H,0,-4.7106162395,0.1943468478,2.0114016146 H,0,-4.683328079,-0.6763694863,-2.1680477224 H,0,-5.9382210864,-0.4065860447,-0.0519110868 P,0,-0.1202732067,0.2216075277,-2.4112608517 P,0,-0.0529079467,0.4787582289,2.1373764397 S,0,-2.0508598238,-0.5144922518,-2.8909081588 S,0,-2.1008732263,0.7272056963,2.6202131224 C,0,-0.0699408599,1.933820782,-3.1605722228 H,0,-0.3827271044,1.8393183901,-4.2053449878 C,0,0.9576726689,-0.7973573277,-3.5469391695 H,0,1.9598218425,-0.4011923877,-3.3540627811 C,0,0.9310587216,-2.2547754906,-3.1198550005 H,0,1.7130807188,-2.8212597007,-3.6295781125 H,0,-0.0275713343,-2.718905861,-3.3574911006 H,0,1.0801392601,-2.3611650041,-2.0437095496 C,0,0.6323778424,-0.639048363,-5.0225555617 H,0,1.2881282379,-1.2740236702,-5.6224789621 H,0,0.7640762615,0.3836171163,-5.3750512525 H,0,-0.3942529851,-0.9409388666,-5.2432615381 C,0,-1.046915252,2.8381610538,-2.4291527927 H,0,-2.0675041455,2.4554040852,-2.4702064871 H,0,-1.0457379966,3.8369121234,-2.8708512036 H,0,-0.7748762997,2.931498686,-1.3745252259 C,0,1.3520506427,2.4717738162,-3.0929289539 H,0,1.3925791031,3.4901020839,-3.484996231</p>

<p>H,0,2.10683935,1.9229909643,-3.5438247983 H,0,1.7038107819,2.4896006028,-1.9245045613 C,0,0.5671152607,-0.8012652834,3.3621994841 H,0,1.65038024,-0.8525418102,3.176377574 C,0,-0.0687055922,-2.1492867547,3.0558214093 H,0,0.3839344716,-2.9430490767,3.6532679366 H,0,0.0099746708,-2.4149931455,1.9988293213 H,0,-1.1345804406,-2.1237554617,3.2871507446 C,0,0.3469292321,-0.4036495058,4.8120145495 H,0,0.8675987726,0.5156076232,5.0788684094 H,0,0.6990275137,-1.1882050594,5.4847410157 H,0,-0.7172921738,-0.2592084278,5.009928459 C,0,0.6666011506,2.0755297904,2.7590359353 H,0,0.2289315476,2.2450441553,3.7490432096 C,0,2.1810858723,1.9822327678,2.8767306153 H,0,2.5959202477,2.9449423556,3.1802099359 H,0,2.6355354159,1.7180060155,1.9196012773 H,0,2.5025615152,1.2451908824,3.6137857943 C,0,0.2483075787,3.2016570451,1.8269761482 H,0,0.5811121298,4.166027428,2.2150933319 H,0,-0.8341842715,3.2395806425,1.699958966 H,0,0.692321062,3.060193061,0.8381107544 Rh,0,0.0542173601,0.1545562435,-0.134549726 H,0,1.9582178253,0.4509721686,-0.0722591307 B,0,2.8148476826,-0.4351722951,-0.2528662836 H,0,3.7903857795,-0.1085609853,0.3728939635 N,0,2.2774528743,-1.8257135019,0.3807143044 H,0,3.0300634221,-0.641910208,-1.415495802 C,0,3.1158201478,-3.0012870223,0.0822443516 H,0,2.1754017762,-1.7227325709,1.3878222516 H,0,1.3096505665,-1.9433731492,0.0410914902 H,0,2.71786669,-3.9019402427,0.5469119975 H,0,3.1558550645,-3.1309873771,-0.9959414984 H,0,4.1240919148,-2.8133432723,0.4431954099</p>	<p>H,0,2.0593854514,1.8722467691,-3.6677501077 H,0,1.7089247371,2.502863516,-2.0599419825 C,0,0.4875887751,-0.8395578857,3.3620673365 H,0,1.5722172397,-0.9169252173,3.2007015502 C,0,-0.1676471342,-2.1626432529,3.0009789771 H,0,0.2325756558,-2.9753695244,3.6106383552 H,0,-0.0300149407,-2.4195263788,1.9475873736 H,0,-1.2443893629,-2.1190293344,3.1753820811 C,0,0.2411761138,-0.4732174986,4.8148760408 H,0,0.7733667643,0.4276558978,5.1203112051 H,0,0.5656586842,-1.2823070969,5.4729006494 H,0,-0.8236072139,-0.3151420581,4.9998502399 C,0,0.7029677496,2.0472024194,2.8195790294 H,0,0.2444300099,2.2219931593,3.7989853326 C,0,2.2069947564,1.8899794312,2.9835401948 H,0,2.6497984857,2.8314006848,3.3145572657 H,0,2.6837497224,1.624719583,2.0370193459 H,0,2.475478811,1.1318413404,3.720336141 C,0,0.3642642385,3.2044934635,1.8947617165 H,0,0.7159926911,4.1484584659,2.316227721 H,0,-0.7098735034,3.290288717,1.7247405222 H,0,0.8432019415,3.0701680309,0.92136129 Rh,0,0.0331062382,0.1993050207,-0.1324514086 H,0,1.95727053,0.5116081727,-0.0831564998 B,0,2.8502275951,-0.3334604294,-0.2814908273 H,0,3.8334433345,0.0517899936,0.2996509264 N,0,2.3981676732,-1.7317011136,0.3831721663 H,0,3.0356013768,-0.5357250656,-1.4505634127 C,0,3.2522115681,-2.8861480196,0.0493317677 H,0,2.3557728641,-1.6273349639,1.3944580052 H,0,1.4209643412,-1.8940175064,0.1021884913 H,0,2.8915948129,-3.7927377768,0.532063866 H,0,3.2523237582,-3.0202065063,-1.0290895435 H,0,4.2690297726,-2.6774549299,0.3732456243</p>
 <p>9</p>	 <p>9*</p>
<p>HF=-2415.4953898 ZPE=0.538147 NImag=0</p> <p>Htot=-2414.920870 Gtot= -2415.023563</p> <p>C,0,-2.0324959659,0.0979710532,-0.0648069092 C,0,-4.9128131234,0.2673607425,-0.1584864619 C,0,-2.8018943526,-0.1572791587,-1.2324092229 C,0,-2.8395681169,0.4634000864,1.0474496854 C,0,-4.2309251831,0.5369256642,1.0148711095 C,0,-4.1920823276,-0.0737307172,-1.2891364357 H,0,-4.7758995931,0.8078555195,1.9118769518 H,0,-4.7058243945,-0.2761241003,-2.2219499964 H,0,-5.9943098116,0.3266738103,-0.1925548732 P,0,-0.0156071625,-0.3076029636,-2.2307776451 P,0,-0.1354891944,0.2696914884,2.245811016 S,0,-2.0481247628,-0.6142238308,-2.7987871047 S,0,-2.1346506902,0.9024126844,2.6419582478 C,0,0.5186076854,1.1061203196,-3.338250934 H,0,0.1966343214,0.8746089198,-4.3601464046 C,0,0.8253076873,-1.794612877,-2.9852431838 H,0,1.8865358077,-1.5441060483,-2.8887681552 C,0,0.5573105688,-3.0088491807,-2.1122874291 H,0,1.0840148797,-3.8859010203,-2.4967543658 H,0,-0.5100918984,-3.2405241994,-2.0778501138</p>	<p>HF=-2415.5465161 ZPE= 0.538321 NImag=0</p> <p>Htot= -2414.973653 Gtot= -2415.070763</p> <p>* Single-Point Energy using Gas Phase Geometry</p>

<p>H,0,0.8951989746,-2.8241609968,-1.0904949198 C,0,0.4785624583,-2.0358848522,-4.4439249062 H,0,1.0338947876,-2.8933712157,-4.8329531754 H,0,0.7170185302,-1.1789395847,-5.0761787862 H,0,-0.5850467767,-2.2551871453,-4.5650785802 C,0,-0.1784380036,2.3730164644,-2.8688170889 H,0,-1.2636581343,2.2645472931,-2.8860497313 H,0,0.0927494047,3.2222336821,-3.5013783626 H,0,0.1085148696,2.6020675024,-1.8390086034 C,0,2.0329980829,1.252865437,-3.2889245401 H,0,2.3470986704,2.1472934658,-3.8330594971 H,0,2.5507170226,0.3990719302,-3.7272575753 H,0,2.3814757732,1.345433736,-2.257531539 C,0,0.0651559399,-1.2124683514,3.3670668577 H,0,1.1215904507,-1.4653499342,3.216671006 C,0,-0.7886541514,-2.3499137813,2.829977953 H,0,-0.6073777469,-3.2692628415,3.3924100539 H,0,-0.5779172795,-2.5384859379,1.7746483431 H,0,-1.8524250003,-2.1105873016,2.9082115629 C,0,-0.2231102365,-0.9298313779,4.8300369334 H,0,0.4355987754,-0.1655573711,5.2454580987 H,0,-0.0902413526,-1.8347972466,5.4290085737 H,0,-1.2550399218,-0.5956494633,4.9673800589 C,0,0.8558485499,1.6074371348,3.0943487314 H,0,0.3775633074,1.8104185458,4.0604096163 C,0,2.2867379611,1.1339239073,3.3110024628 H,0,2.8961287212,1.9517539036,3.7044506324 H,0,2.7351592154,0.7928005449,2.3752017985 H,0,2.3480083983,0.3043038675,4.0160261709 C,0,0.8095174255,2.8638282374,2.2388320596 H,0,1.3438357941,3.6830688137,2.7269034716 H,0,-0.2158637985,3.1847145718,2.0505389887 H,0,1.2799177361,2.6768541388,1.2704160809 Rh,0,0.0082536858,0.0168462247,-0.0015785942 H,0,1.8332695679,0.294939042,0.0885545596 B,0,2.7349127421,-0.615916042,0.0772769246 H,0,3.7167701891,0.0538075981,0.3709660158 N,0,2.4622395811,-1.6882854391,1.1435515533 H,0,2.8700227783,-1.0452408043,-1.0654403076 C,0,3.4871854367,-2.7031204717,1.1985523786 H,0,1.5707435642,-2.1407792791,0.9556778396 H,0,3.2721719034,-3.4648903803,1.9586645151 H,0,3.6659444081,-3.2349067432,0.2430015102 H,0,4.4405033232,-2.2376186721,1.4685766812</p>	
<p>[NMeH₃]⁺ HF=-96.2312945 ZPE=0.079420 NImag=0 Htot=-96.147478 Gtot=-96.174004 H,0,-1.8239327615,0.4745176337,0.8218886607 H,0,-1.8239327615,0.4745176337,-0.8218886607 H,0,-1.8239327467,-0.9490352848,0. N,0,-1.4478058695,-0.000000019,0. C,0,0.0557568029,0.0000000137,0. H,0,0.3997449184,-0.514318698,0.8908261462 H,0,0.3997449184,-0.514318698,-0.8908261462 H,0,0.3997449024,1.0286374478,0.</p>	<p>[NMeH₃]⁺ HF=-96.3031897 ZPE=0.080102 NImag=0 Htot=-96.218763 Gtot=-96.245143 H,0,-1.8196877164,0.473768768,0.8205915871 H,0,-1.8196877164,0.473768768,-0.8205915871 H,0,-1.8196877017,-0.9475375532,0. N,0,-1.4413354685,-0.000000018,0. C,0,0.0483231007,0.0000000136,0. H,0,0.3956784639,-0.5136436749,0.8896569717 H,0,0.3956784639,-0.5136436749,-0.8896569717 H,0,0.395678448,1.0272874014,0.</p>
 <p>10</p>	 <p>10</p>
<p>HF=-2416.0411419</p>	<p>HF=-2416.0610866</p>

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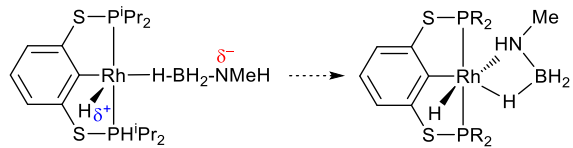
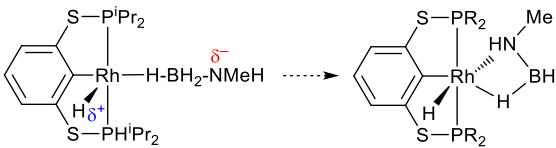
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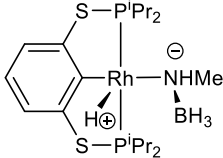
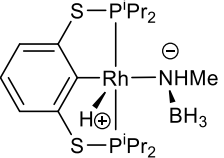
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P,0,0.2377996986,-0.4613525784,-2.2319260716
P,0,0.3936079366,0.4255712179,2.2296527073
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S,0,-1.5249118007,1.3365385307,2.3056041252
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C,0,1.8292232219,-2.63657957,-3.0555788185
H,0,2.4866490162,-3.0639961292,-3.8141991874
H,0,0.9672570353,-3.301336537,-2.9646358182
H,0,2.381971392,-2.6327628241,-2.117339247
C,0,0.8797215104,-1.2147080836,-4.8981368709
H,0,1.5886230758,-1.7154720213,-5.5596612819
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N,0,1.1999736691,-2.4633169328,0.2635275475
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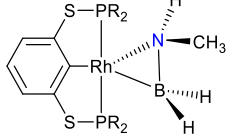
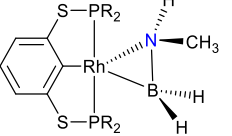
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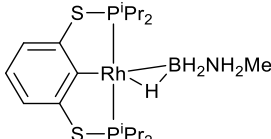
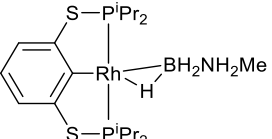
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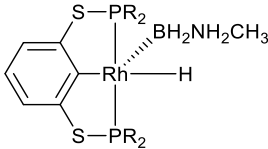
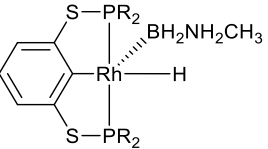
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C,0,-2.3182081588,0.2804028809,1.0470150071
C,0,-3.7059582763,0.1671270848,1.0998602811
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H,0,-4.1796186597,-1.6723779252,-1.6937518268
H,0,-5.4527794777,-0.6496253353,0.1645879541
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S,0,-1.4615378465,-1.7245645299,-2.383064348
S,0,-1.5708789057,1.3252408802,2.3009945336
C,0,-0.2008984251,1.1256509528,-3.0887735733
H,0,-0.517518883,0.8291258046,-4.0926584762
C,0,1.4521356372,-1.2635609897,-3.4418964257
H,0,2.3539900635,-0.6532602899,-3.3162829437
C,0,1.7993979393,-2.6936359732,-3.0590447507
H,0,2.4624660336,-3.1215387788,-3.812866994
H,0,0.9134843903,-3.3305331664,-3.0124370485
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C,0,0.9911437491,-1.1789093616,-4.89007814
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H,0,3.3710782634,-1.9932183866,-0.3984209129
C,0,0.8082019612,-3.4292814629,1.2878445684
H,0,1.0538155404,-2.878900959,-0.629072993

<p>H,0,-0.2832516823,-3.6465183122,1.1911384499 H,0,1.3314696723,-4.3735253716,1.1690394297 H,0,0.9917763317,-3.0379338448,2.25861062</p>	<p>H,0,-0.2543928306,-3.6731917322,1.212782029 H,0,1.3755531887,-4.3625868407,1.1948685971 H,0,1.0033912311,-3.0315083254,2.2809676498</p>
	
<p>HF=-2416.0411419 ZPE=0.552443 NImag=0 Htot=-2415.453784 Gtot=-2415.550779</p>	<p>HF=-2416.061086 ZPE=0.551757 NImag=0 Htot=-2415.474143 Gtot=-2415.571867</p>
<p>C,0,-1.5221260184,-0.3521828308,0.0728495022 C,0,-4.353050105,-0.5658067157,0.1800787266 C,0,-2.2645309715,-1.0425660304,-0.9006060317 C,0,-2.2885228851,0.2838772817,1.0675634814 C,0,-3.6747062154,0.1669565724,1.1389554862 C,0,-3.6520493596,-1.157141779,-0.8560240497 H,0,-4.2169133428,0.6481744355,1.943330846 H,0,-4.1772750901,-1.6902761563,-1.6385402271 H,0,-5.4303252119,-0.6598881762,0.2302581628 P,0,0.2377996986,-0.4613525784,-2.2319260716 P,0,0.3936079366,0.4255712179,2.2296527073 S,0,-1.4660103721,-1.7344650855,-2.3616881061 S,0,-1.5249118007,1.3365385307,2.3056041252 C,0,-0.2549704513,1.1354584143,-3.0696631266 H,0,-0.579903921,0.8430000978,-4.0721977056 C,0,1.4097465493,-1.2346645196,-3.4707403333 H,0,2.2909334465,-0.5861249996,-3.4049493958 C,0,1.8292232219,-2.63657957,-3.0555788185 H,0,2.4866490162,-3.0639961292,-3.8141991874 H,0,0.9672570353,-3.301336537,-2.9646358182 H,0,2.381971392,-2.6327628241,-2.117339247 C,0,0.8797215104,-1.2147080836,-4.8981368709 H,0,1.5886230758,-1.7154720213,-5.5596612819 H,0,0.7348912169,-0.2070818724,-5.2839794992 H,0,-0.0707812729,-1.7458392005,-4.9797464386 C,0,-1.4125250959,1.8332125795,-2.3779029745 H,0,-2.3091385536,1.2154579947,-2.3519807358 H,0,-1.6534223969,2.7526067399,-2.9146770463 H,0,-1.1600663439,2.1002968558,-1.3502312913 C,0,0.9657343267,2.040945568,-3.1659571077 H,0,0.6947236017,2.9853920374,-3.6401923777 H,0,1.7749358238,1.6014811642,-3.7505012114 H,0,1.3551866694,2.2709453766,-2.1715538111 C,0,0.3644640815,-0.7366090951,3.6964209909 H,0,1.2696474678,-1.3409531293,3.5571836643 C,0,-0.8672625673,-1.6294994946,3.6012501934 H,0,-0.758907218,-2.499985813,4.2500175875 H,0,-1.0519655022,-1.9828950709,2.5873516143 H,0,-1.7552009576,-1.0812463387,3.9180854185 C,0,0.41395942,-0.0352538985,5.0437190619 H,0,1.3441745664,0.5056111375,5.2122817848 H,0,0.3112600286,-0.7662989658,5.8477876425 H,0,-0.4151033968,0.6699077596,5.1427317551 C,0,1.5341492198,1.8026957352,2.7455137065 H,0,1.1410378617,2.1662520025,3.7013974676 C,0,2.9348712081,1.2387427007,2.9498434283 H,0,3.608774691,2.0261381658,3.290762363 H,0,3.3300448409,0.8391112251,2.0150104126 H,0,2.9666658985,0.4344138616,3.6851541085 C,0,1.5393235762,2.9479327476,1.7480055351 H,0,2.1233595044,3.7808407352,2.1430653614 H,0,0.534126181,3.3096379455,1.5313026405</p>	<p>C,0,-1.539778608,-0.351714088,0.0578782556 C,0,-4.3745257214,-0.557980954,0.1283178929 C,0,-2.2730730108,-1.0327308666,-0.9301657251 C,0,-2.3182081588,0.2804028809,1.0470150071 C,0,-3.7059582763,0.1671270848,1.0998602811 C,0,-3.661770789,-1.1446871496,-0.9023312675 H,0,-4.2582230308,0.6452944278,1.8995020542 H,0,-4.1796186597,-1.6723779252,-1.6937518288 H,0,-5.4527794777,-0.6496253353,0.1645879541 P,0,0.259317151,-0.4712735087,-2.2340562178 P,0,0.3571329131,0.4268372585,2.2451424393 S,0,-1.4615378465,-1.7245645299,-2.383064348 S,0,-1.5708789057,1.3252408802,2.3009945336 C,0,-0.2008984251,1.1256509598,-3.0887735733 H,0,-0.517518883,0.8291258046,-4.0926584762 C,0,1.4521356372,-1.2635609897,-3.4418964257 H,0,2.3539900635,-0.6532602899,-3.3162829437 C,0,1.7993979393,-2.6936359732,-3.0590447507 H,0,2.4624660336,-3.1215387788,-3.812866994 H,0,0.9134843903,-3.3305331664,-3.0124370485 H,0,2.328396302,-2.7458949129,-2.109087575 C,0,0.9911437491,-1.1789093616,-4.89007814 H,0,1.7154610888,-1.6841263368,-5.5316870425 H,0,0.9026597301,-0.1554360299,-5.2508205176 H,0,0.0290889016,-1.6738887298,-5.0397143171 C,0,-1.3555224643,1.8481295866,-2.420230889 H,0,-2.2617744493,1.2439956316,-2.3903901841 H,0,-1.5828694688,2.7585270519,-2.978519535 H,0,-1.1104964649,2.1385665324,-1.3968460284 C,0,1.034078655,2.0108324528,-3.1792157568 H,0,0.783351949,2.9523820602,-3.670880244 H,0,1.8453985672,1.5525060158,-3.7463277889 H,0,1.4151316567,2.2519595492,-2.1839185914 C,0,0.3247360093,-0.7336864194,3.713061359 H,0,1.2374874212,-1.3282971352,3.5832944507 C,0,-0.8933558803,-1.6427283685,3.6095939921 H,0,-0.7738734313,-2.5143832487,4.2553793282 H,0,-1.0710252995,-1.9979914126,2.5947367447 H,0,-1.7918890422,-1.1128567744,3.9288369404 C,0,0.3593779028,-0.033151562,5.0605204147 H,0,1.283463088,0.5162711259,5.2362960299 H,0,0.2619400972,-0.7682645091,5.8620725522 H,0,-0.4768115321,0.6632794768,5.1625187239 C,0,1.4821653462,1.8154910159,2.7663557033 H,0,1.0785340018,2.1746145668,3.7193156788 C,0,2.8868654998,1.2684646903,2.9835148659 H,0,3.5412442346,2.0599198718,3.3530773812 H,0,3.3088088955,0.8993155975,2.0475071807 H,0,2.9225909205,0.4503685418,3.7033781451 C,0,1.4881090511,2.9617684628,1.7712991781 H,0,2.0586947193,3.7995659798,2.1766392998 H,0,0.4840937336,3.3197266801,1.5419603686</p>

<p>H,0,1.9929356404,2.637795687,0.8058940128 Rh,0,0.5466287455,-0.3208606859,0.0547407004 H,0,0.4655014259,1.2335788095,-0.1750861798 H,0,2.3560089621,-0.4270497827,0.0640024351 B,0,2.5270529675,-1.7111711792,0.4158280525 H,0,2.8886542578,-1.696074873,1.5652506829 N,0,1.1999736691,-2.4633169328,0.2635275475 H,0,3.3862658458,-2.0068435177,-0.3793369793 C,0,0.7851129263,-3.4286484723,1.2652629732 H,0,1.054612221,-2.8735697235,-0.6493957546 H,0,-0.2832516823,-3.6465183122,1.1911384499 H,0,1.3314696723,-4.3735253716,1.1690394297 H,0,0.9917763317,-3.0379338448,2.25861062</p>	<p>H,0,1.9591457683,2.6627332414,0.8338600844 Rh,0,0.5261333404,-0.3211705234,0.0647821655 H,0,0.4337663711,1.2309771161,-0.1678598307 H,0,2.347005866,-0.4185557616,0.0950929519 B,0,2.5239204457,-1.7009803816,0.413901051 H,0,2.9134593916,-1.6999153868,1.5556968717 N,0,1.2004986395,-2.4606054277,0.2799922196 H,0,3.3710782634,-1.9932183866,-0.3984209129 C,0,0.8082019612,-3.4292814629,1.2878445684 H,0,1.0538155404,-2.878900959,-0.629072993 H,0,-0.2543928306,-3.6731917322,1.212782029 H,0,1.3755531887,-4.3625868407,1.1948685971 H,0,1.0033912311,-3.0315083254,2.2809676498</p>
	
<p>HF=-2416.011758 ZPE= 0.550951 NImag=0</p> <p>Htot=-2415.424954 Gtot=-2415.523790</p> <p>C,0,-1.6179930474,-0.1624310424,0.0903024179 C,0,-2.3783443274,-0.7361323903,-0.9497726792 C,0,-3.7636650707,-0.8670037526,-0.8978302242 C,0,-4.4521510331,-0.4313490732,0.2196518943 C,0,-3.7587341241,0.1378731197,1.2713549103 C,0,-2.3738868434,0.2761348644,1.1937522835 Rh,0,0.4486803513,-0.1892632169,0.0593101901 H,0,0.4134005868,1.3119958655,-0.1757835252 P,0,0.3932681134,0.4701509668,2.2994869833 S,0,-1.620584305,1.0686106184,2.6092766075 P,0,0.2056755896,-0.311301376,-2.2277595373 S,0,-1.6247367518,-1.3541677243,-2.4642598925 N,0,2.6177426483,-0.6589358485,-0.0456760302 B,0,3.489559,0.5880187968,-0.5453158472 H,0,4.6687871696,0.3053492211,-0.4238823236 H,0,-4.2863041233,0.4743916176,2.1550091149 H,0,-4.2963026464,-1.3039201638,-1.7332471208 H,0,-5.5285728792,-0.5341856153,0.2697731776 C,0,-0.0622375562,1.2943462355,-3.1385890916 H,0,-0.3511675443,0.9824750017,-4.1484451968 C,0,1.4031142725,-1.3002282319,-3.2496892534 H,0,2.3587912156,-0.816532157,-3.0087504692 C,0,1.4365010509,-2.7449096257,-2.7684707813 H,0,2.2996763297,-3.2632774052,-3.1873184287 H,0,0.5394941368,-3.283164472,-3.0764063154 H,0,1.4956260033,-2.8226945661,-1.6807123761 C,0,1.1570514715,-1.2142354747,-4.747770902 H,0,1.8818853493,-1.8326787657,-5.2795011862 H,0,1.2561906629,-0.198969721,-5.1290315677 H,0,0.1623241623,-1.5800904936,-5.0117083744 C,0,-1.2100166615,2.0852020265,-2.5328039322 H,0,-2.1413903908,1.5204863448,-2.5149478957 H,0,-1.3766649524,2.9905112723,-3.1182900756 H,0,-0.9860681397,2.3915016261,-1.5087656092 C,0,1.2149313163,2.1169663022,-3.1946782685 H,0,1.0365610347,3.0283889763,-3.7680667203 H,0,2.0456291901,1.5842127657,-3.6568553969 H,0,1.5453221261,2.4033048296,-2.1947419405 C,0,0.6794364029,-0.7929502723,3.6475430819 H,0,1.7483336365,-1.0190408932,3.5709175394 C,0,-0.1142019126,-2.046044377,3.3104856109 H,0,0.0800380093,-2.8327266625,4.0405710241</p>	<p>HF=-2416.0404668 ZPE= 0.550970 NImag=0</p> <p>Htot= -2415.453738 Gtot= -2415.552157</p> <p>C,0,-1.610083312,-0.1795977716,0.0960891172 C,0,-2.3735233177,-0.7758953669,-0.9291917062 C,0,-3.7589833379,-0.9082595848,-0.8732824048 C,0,-4.4467459052,-0.447091969,0.2345481817 C,0,-3.7525508778,0.1505530771,1.2701032034 C,0,-2.3673777307,0.2878686694,1.1874427226 Rh,0,0.4606763612,-0.1834446215,0.0515906561 H,0,0.4508199936,1.3176242343,-0.1975770994 P,0,0.4005701214,0.4915489097,2.2943862033 S,0,-1.611254788,1.1226561897,2.5763423297 P,0,0.1903443541,-0.3165040201,-2.2306267723 S,0,-1.6177955453,-1.4117703324,-2.4351690522 N,0,2.6498827599,-0.5984113478,-0.07940251 B,0,3.5828443362,0.6078288818,-0.5232968788 H,0,4.747626878,0.233075099,-0.4970292244 H,0,-4.2812909025,0.5104196316,2.1440777605 H,0,-4.2936457816,-1.3631372647,-1.6980048549 H,0,-5.5232383047,-0.5498320872,0.2885854376 C,0,-0.1170612422,1.2746982888,-3.1514466284 H,0,-0.4140381487,0.9527569557,-4.1554188373 C,0,1.4056565351,-1.2852664071,-3.2512436068 H,0,2.351625627,-0.7756935495,-3.0258969616 C,0,1.4849971716,-2.7221944536,-2.7544074755 H,0,2.3701785532,-3.213584886,-3.1603123205 H,0,0.6126027726,-3.2970583673,-3.0678963106 H,0,1.5380222674,-2.7923130704,-1.6651975804 C,0,1.1535471242,-1.2222406173,-4.7485641997 H,0,1.8978677914,-1.8231864514,-5.274155798 H,0,1.2213177997,-0.2088080732,-5.1419623225 H,0,0.1715762294,-1.6229598139,-5.0096999859 C,0,-1.2611822542,2.0605774397,-2.5352729652 H,0,-2.1912644394,1.493397123,-2.5063878667 H,0,-1.4408930282,2.9624549555,-3.1230165363 H,0,-1.0276242448,2.3739424997,-1.5150928063 C,0,1.1512636972,2.10809608,-3.2318500627 H,0,0.9617882641,3.0046060663,-3.8252826675 H,0,1.9844396866,1.5755093619,-3.6907612654 H,0,1.4792214949,2.427407291,-2.2407757382 C,0,0.647147463,-0.783955316,3.6386373008 H,0,1.7141974448,-1.0236485321,3.5723059724 C,0,-0.1577299913,-2.025603769,3.288615507 H,0,0.0297159341,-2.82035007,4.0122580883</p>

<p>H,0,0.139002553,-2.4374840419,2.3228554796 H,0,-1.1867256581,-1.8414997085,3.3180655865 C,0,0.3713109823,-0.2765945697,5.0417174588 H,0,0.9884085714,0.5790408182,5.3157743457 H,0,0.5509742584,-1.0589486866,5.7811661493 H,0,-0.6761570632,0.0190290583,5.1251810305 C,0,1.2581451822,2.021777973,2.8741674751 H,0,0.7175109629,2.2976051405,3.7881211863 C,0,2.7230482897,1.7868151892,3.2096245804 H,0,3.1442135894,2.6905518927,3.6527586057 H,0,3.2974240682,1.5702251802,2.3080899661 H,0,2.8712592932,0.976379568,3.9249403821 C,0,1.0914883609,3.1306943556,1.846791997 H,0,1.4704674534,4.0713192445,2.2488946091 H,0,0.0457710559,3.279602842,1.5746372748 H,0,1.6634428999,2.9013942156,0.9452142093 H,0,3.2008683602,0.7670668883,-1.7124369454 H,0,3.2020775287,1.5617301502,0.1245752513 C,0,3.1744820129,-1.2994499549,1.1436402636 H,0,2.6831792724,-1.3505151196,-0.7873863022 H,0,2.561896979,-2.1353615013,1.5009021907 H,0,4.1894368225,-1.6671957949,0.9591994337 H,0,3.2495475043,-0.5636877687,1.9440859984</p>	<p>H,0,0.0898128372,-2.4154509684,2.29866936 H,0,-1.2294989933,-1.8157028625,3.3001559663 C,0,0.329501142,-0.2755962429,5.0328936519 H,0,0.9452562879,0.5763784511,5.3215234292 H,0,0.5013832261,-1.0647300406,5.7675476805 H,0,-0.7180410447,0.0212751466,5.1135290045 C,0,1.273991936,2.0295436052,2.8927476994 H,0,0.7091521603,2.3214142701,3.7865405703 C,0,2.7193077787,1.7685767198,3.2850523087 H,0,3.1406660387,2.6685011957,3.7366303142 H,0,3.3271329512,1.5330986697,2.4111134783 H,0,2.8265086167,0.9626398186,4.0122265383 C,0,1.1659162841,3.1366758731,1.8570873399 H,0,1.5597577193,4.0689348535,2.2654535146 H,0,0.133424377,3.3169687012,1.5541359405 H,0,1.7521575739,2.8922211257,0.9688485706 H,0,3.2611877469,0.9187527313,-1.6538891637 H,0,3.4228428601,1.540223373,0.2404337849 C,0,3.1551926422,-1.3063524976,1.0946361732 H,0,2.6920851709,-1.2691425378,-0.8420037339 H,0,2.5014741515,-2.1314987722,1.3998740498 H,0,4.1572222095,-1.7143407117,0.9190401254 H,0,3.2379896193,-0.6104204124,1.9299374547</p>
	
<p>HF=-2414.8523814 ZPE= 0.534398 NImag=0</p> <p>Htot=-2414.282912 Gtot=-2414.380466</p> <p>C,0,-1.6386266318,-0.2220790438,0.0196022056 C,0,-4.505856749,-0.1530107462,0.0938907122 C,0,-2.4568156563,-0.7059603533,-1.0303170488 C,0,-2.3740202258,0.3136778814,1.1003764314 C,0,-3.7673395059,0.3422477807,1.1510596991 C,0,-3.8496087061,-0.6731511047,-1.0051531242 H,0,-4.2657187429,0.7483230662,2.0224175311 H,0,-4.4118096202,-1.0471131236,-1.8516526267 H,0,-5.5879269834,-0.130324208,0.1245110624 P,0,0.1594780165,-0.5549695645,-2.2180273434 P,0,0.3592043341,0.2016255502,2.2578439561 S,0,-1.771014741,-1.3753009205,-2.5485381214 S,0,-1.5810728048,1.0310392752,2.5275710832 C,0,0.0560240432,1.0735076891,-3.1427012004 H,0,-0.3586692703,0.8019687976,-4.1198097999 C,0,1.2201496019,-1.6457812903,-3.3034607971 H,0,2.234670843,-1.2739970087,-3.1092017005 C,0,1.1236213,-3.0912081035,-2.8310274645 H,0,1.9213449171,-3.6959454724,-3.2653582951 H,0,0.1711084867,-3.5319202489,-3.1266735865 H,0,1.1742956637,-3.1787081711,-1.7428620247 C,0,0.9293368356,-1.5307071477,-4.7915967187 H,0,1.5607602492,-2.2194308279,-5.3563308538 H,0,1.1131299829,-0.5289600832,-5.1774925941 H,0,-0.1089644785,-1.7889863637,-5.0109141785 C,0,-0.9130727117,2.0125136314,-2.4426173046 H,0,-1.9156665506,1.5923776416,-2.3733044542 H,0,-0.9789024411,2.9545885746,-2.9901637147 H,0,-0.5748420239,2.2298047403,-1.4263047455 C,0,1.4128428622,1.733081744,-3.3326087358 H,0,1.312042193,2.5945975071,-3.9956558342 H,0,2.1586105803,1.0669489848,-3.7693370022</p>	<p>HF=-2414.8723784 ZPE= 0.534167 NImag=0</p> <p>Htot=-2414.303044 Gtot=-2414.400974</p> <p>C,0,-1.635984696,-0.1922422017,0.0361643858 C,0,-4.5040385076,-0.1267425887,0.130225846 C,0,-2.4615219401,-0.7002384961,-0.9970779243 C,0,-2.365192776,0.3596414259,1.1139417373 C,0,-3.7586546347,0.3885259336,1.1735425655 C,0,-3.8547279012,-0.6694300707,-0.9626509822 H,0,-4.2534937811,0.8096479618,2.0401148349 H,0,-4.4243724355,-1.0619714412,-1.796030903 H,0,-5.5861534541,-0.1037850134,0.1675243128 P,0,0.1490356502,-0.5523885488,-2.2216712682 P,0,0.3775981348,0.2328863075,2.2608276761 S,0,-1.7805247635,-1.4086796466,-2.5008768476 S,0,-1.5571346851,1.091271682,2.5263150165 C,0,0.0163652112,1.0384112773,-3.2060794931 H,0,-0.4026447371,0.7247976717,-4.1685303321 C,0,1.2231472674,-1.6676247011,-3.2658959791 H,0,2.2314929671,-1.2762277327,-3.0740137294 C,0,1.1420017285,-3.0980115203,-2.7481823224 H,0,1.9674902334,-3.6975044524,-3.1362233552 H,0,0.2122518979,-3.5732193276,-3.0634893166 H,0,1.1603777234,-3.1525892366,-1.6562873073 C,0,0.9498316065,-1.6039059533,-4.7595632548 H,0,1.6058777723,-2.295075894,-5.2930965021 H,0,1.1166693847,-0.6114444428,-5.1766063682 H,0,-0.0778109431,-1.8951335996,-4.988444177 C,0,-0.9548223709,1.9954802391,-2.5360358797 H,0,-1.9538551118,1.5713628127,-2.4377530727 H,0,-1.0385098679,2.9122739544,-3.123454655 H,0,-0.6089659859,2.2654378351,-1.534766627 C,0,1.3639007885,1.7037187831,-3.4356869717 H,0,1.249524098,2.5243277998,-4.1472952662 H,0,2.1183506382,1.0257649199,-3.8381128437</p>

<p>H,0,1.8084097279,2.092438526,-2.3826329965 C,0,0.4362250614,-1.0518635013,3.6557426783 H,0,1.4740101171,-1.4055357645,3.6360397161 C,0,-0.4807561395,-2.2131858554,3.30193669 H,0,-0.3917383427,-3.0162756878,4.0355662822 H,0,-0.2566971387,-2.6196359863,2.3133168217 H,0,-1.523347157,-1.8887012787,3.2881051702 C,0,0.1291157994,-0.4881481125,5.031545234 H,0,0.8296948508,0.2904091325,5.33415497 H,0,0.1738213198,-1.2775104788,5.7846040437 H,0,-0.8772923868,-0.0662689591,5.0597546697 C,0,1.3331284315,1.6614196305,2.9228203157 H,0,0.7674534007,1.9783137945,3.807331995 C,0,2.7414297461,1.2918265112,3.3627485193 H,0,3.2147044089,2.1463671082,3.8499718192 H,0,3.3678703249,1.022841587,2.51263222 H,0,2.7582936578,0.4650638907,4.0746179116 C,0,1.3236331706,2.7979036238,1.9123019789 H,0,1.8296203798,3.6742856319,2.3215220897 H,0,0.3057386067,3.0861971433,1.6504712753 H,0,1.8354972886,2.5096981343,0.9933081266 Rh,0,0.4205056994,-0.5014717808,0.039874252 B,0,2.748058494,0.0600417868,-0.3636295936 H,0,3.1461803873,0.8061554173,0.4682864004 N,0,2.5483907661,-1.3190702784,0.0035003949 H,0,2.8447253813,0.3059816055,-1.5208099624 C,0,2.969555329,-1.9311496293,1.2517659845 H,0,2.5039028009,-1.9954344762,-0.746873203 H,0,2.2359083293,-2.6580514183,1.6064463359 H,0,3.9326455651,-2.4361625452,1.1403177597 H,0,3.081313054,-1.1536118535,2.0049576898</p>	<p>H,0,1.7561993321,2.1253115071,-2.5102187923 C,0,0.4179101066,-1.068096689,3.6147249835 H,0,1.4506104351,-1.4357796844,3.5858055607 C,0,-0.5118376672,-2.2036629769,3.2166040331 H,0,-0.4281740613,-3.0369658964,3.9170489369 H,0,-0.2942896812,-2.5756356193,2.2126282651 H,0,-1.5531528929,-1.8736235918,3.219977793 C,0,0.1125698994,-0.5522708637,5.0086866651 H,0,0.8217400626,0.20389419,5.3465244835 H,0,0.1444340986,-1.3712571128,5.7307680748 H,0,-0.8887338835,-0.1191512574,5.0545117045 C,0,1.3610013443,1.6552450269,2.9915861312 H,0,0.7879011036,1.9421155995,3.8815709147 C,0,2.757309856,1.249633186,3.4367411535 H,0,3.2308725742,2.0786080126,3.9669286829 H,0,3.3967340854,1.0076548251,2.5878270449 H,0,2.7551718595,0.3951315831,4.1150534692 C,0,1.3838551325,2.8361370704,2.0349896334 H,0,1.8785591111,3.6906291701,2.5013739106 H,0,0.3769086856,3.1452986936,1.7536409877 H,0,1.9245374562,2.5951161724,1.1190706587 Rh,0,0.4269322581,-0.4524766695,0.0342623964 B,0,2.7386366763,0.1688630053,-0.3400299907 H,0,3.1277605277,0.8775889591,0.5282500692 N,0,2.5657513935,-1.2286295522,-0.0447133647 H,0,2.8206379314,0.4778477869,-1.4839312871 C,0,2.9906198807,-1.8991919265,1.1714392113 H,0,2.5425853035,-1.8674231767,-0.8288990444 H,0,2.273351323,-2.6651112004,1.4738877796 H,0,3.9657340272,-2.3750498263,1.0375704464 H,0,3.0790502114,-1.1664674812,1.9713474932</p>
	
<p>HF=-2416.0376055 ZPE= 0.555265 NImag=0</p> <p>Htot= -2415.445913 Gtot= -2415.548499</p> <p>C,0,-0.045589,1.6547339,-0.718832 C,0,-0.2647339,4.4249245,-1.5023073 Rh,0,0.1189062,-0.3397102,-0.2448825 C,0,1.0665182,2.5291302,-0.8507962 C,0,-1.2762409,2.3063175,-0.9931662 C,0,-1.3952036,3.6421642,-1.3688451 C,0,0.9695948,3.8644527,-1.2381615 H,0,-2.3758918,4.0640006,-1.5520296 H,0,1.8682919,4.462454,-1.3281072 H,0,-0.345597,5.4628578,-1.7989952 B,0,0.5588336,-2.853771,-0.3963732 P,0,2.3716752,-0.0098659,-0.1152629 P,0,-2.1256656,-0.2835121,0.0518296 S,0,2.7546148,2.0264162,-0.5148829 S,0,-2.8598573,1.4679111,-0.8726997 C,0,3.1942073,-0.2456295,1.5490389 H,0,4.1667871,0.2548381,1.4827313 C,0,3.4972316,-0.9012804,-1.3116452 H,0,3.3467689,-1.9575895,-1.0565309 C,0,2.9942845,-0.6695008,-2.7276332 H,0,3.567297,-1.2642493,-3.4413957 H,0,3.0986478,0.3808933,-3.0062639 H,0,1.9403041,-0.9334367,-2.824145 C,0,4.9652385,-0.5395499,-1.164658</p>	<p>HF=-2416.0643144 ZPE= 0.555596 NImag=0</p> <p>Htot= -2415.472441 Gtot= -2415.573939</p> <p>C,0,-0.0449085219,1.6659208389,-0.7159278897 C,0,-0.2526478441,4.4416067245,-1.4929248923 Rh,0,0.1095924296,-0.3262523793,-0.2446994541 C,0,1.0707645228,2.5389631933,-0.8416960665 C,0,-1.2738914978,2.3225285232,-0.9960456281 C,0,-1.3861500855,3.660607191,-1.3682432139 C,0,0.9794321329,3.8763690273,-1.2251708581 H,0,-2.3641466484,4.0872738288,-1.556465352 H,0,1.879545401,4.473585282,-1.3100316911 H,0,-0.3293018172,5.4809901125,-1.7867192712 B,0,0.5399857399,-2.8523303389,-0.4019364243 P,0,2.3661848828,-0.0191984676,-0.113875392 P,0,-2.1397992404,-0.2704667344,0.0543221481 S,0,2.755542319,2.0249332345,-0.5039086662 S,0,-2.8586789107,1.483821978,-0.8921461986 C,0,3.1996283828,-0.2633243538,1.5450845716 H,0,4.1762398415,0.2279482762,1.4715579883 C,0,3.488020757,-0.9019578163,-1.3212202276 H,0,3.3302589116,-1.9592389045,-1.0754664543 C,0,2.9879715579,-0.6573173419,-2.7351454506 H,0,3.5446675171,-1.2658767103,-3.450724297 H,0,3.1166078613,0.38948195,-3.0184433995 H,0,1.9276596672,-0.8965065743,-2.8335151696 C,0,4.9591761359,-0.5571627924,-1.1731330948</p>

<p>H,0,5.5689463,-1.0844362,-1.8934114 H,0,5.3600034,-0.7718895,-0.1751382 H,0,5.1217344,0.5260713,-1.3475605 C,0,2.3552568,0.4326674,2.6194729 H,0,2.1632875,1.4791982,2.3801461 H,0,2.8567934,0.3888839,3.5883266 H,0,1.3869033,-0.065996,2.7111439 C,0,3.3999524,-1.7203387,1.8566277 H,0,3.8533933,-1.8406698,2.8424256 H,0,4.0475169,-2.2175463,1.1337352 H,0,2.4467095,-2.2522234,1.8644033 C,0,-3.3187181,-1.551865,-0.6650626 H,0,-3.1640636,-2.4435143,-0.0387434 C,0,-2.9155629,-1.8597946,-2.1003769 H,0,-3.4742754,-2.7104424,-2.4982232 H,0,-1.8439811,-2.0593367,-2.1928933 H,0,-3.1198414,-0.9996552,-2.7393988 C,0,-4.7884567,-1.1783963,-0.5614561 H,0,-5.1042658,-1.0098673,0.4677782 H,0,-5.4176304,-1.9702869,-0.9733783 H,0,-4.99668,-0.2705287,-1.1299692 C,0,-2.6878647,-0.1520607,1.8343716 H,0,-3.7709786,0.0083099,1.8277471 C,0,-2.3611662,-1.4454257,2.5677643 H,0,-2.6300955,-1.3710315,3.6230476 H,0,-1.2875777,-1.6507742,2.5150748 H,0,-2.8952771,-2.3076846,2.1609455 C,0,-2.0087017,1.0414306,2.4853632 H,0,-2.3171181,1.1364719,3.5282235 H,0,-2.2534549,1.9710471,1.9718646 H,0,-0.9226611,0.9269251,2.4520958 H,0,0.3633222,-2.068208,0.5528358 N,0,-0.7069625,-3.8731411,-0.3192091 C,0,-0.672375,-4.9443491,-1.3343688 H,0,-0.7663503,-4.2813324,0.6098105 H,0,-1.5564875,-3.3235699,-0.4362381 H,0,-1.5364464,-5.6020994,-1.2544685 H,0,-0.6512683,-4.4800579,-2.3164892 H,0,0.2424367,-5.5157012,-1.2040544 H,0,0.5371716,-2.378564,-1.5045838 H,0,1.5424739,-3.5059643,-0.1652096</p>	<p>H,0,5.5552919464,-1.1048049316,-1.9066916224 H,0,5.3544495547,-0.8021045121,-0.1867744013 H,0,5.1327021565,0.5072409888,-1.3495452403 C,0,2.3797370772,0.4153668376,2.6287489713 H,0,2.1859640754,1.4643218249,2.4000732702 H,0,2.8977090402,0.368508559,3.5892181249 H,0,1.4117833638,-0.0799250182,2.7399932792 C,0,3.3974661664,-1.7394479968,1.8487062666 H,0,3.8809644805,-1.8616376766,2.8203519311 H,0,4.0173025858,-2.2476287441,1.1091244357 H,0,2.4394688006,-2.2614941478,1.8915490869 C,0,-3.3220702002,-1.5473394975,-0.6542999123 H,0,-3.139348899,-2.4346175063,-0.0319295705 C,0,-2.9383506725,-1.8548791166,-2.0937639453 H,0,-3.4799772063,-2.726284707,-2.4697779638 H,0,-1.8650909685,-2.0310812361,-2.2075047415 H,0,-3.181414386,-1.0123918775,-2.7431651847 C,0,-4.7946831801,-1.1958099356,-0.5281205087 H,0,-5.1024190586,-1.0393982951,0.5057053166 H,0,-5.4156377866,-1.9967960743,-0.9356796288 H,0,-5.0318832942,-0.2902941261,-1.0900620565 C,0,-2.7130117087,-0.1136439772,1.8315195724 H,0,-3.7949185349,0.0519853904,1.8107963519 C,0,-2.4052831655,-1.4005901872,2.5826834044 H,0,-2.6979602641,-1.3132740442,3.6310200046 H,0,-1.3323933631,-1.6137435861,2.5594607647 H,0,-2.9319526414,-2.2661673521,2.1744349384 C,0,-2.0385552197,1.0815807274,2.4816943105 H,0,-2.3665871465,1.1884016247,3.5178655171 H,0,-2.2684768643,2.0108701033,1.9597313879 H,0,-0.9521972559,0.9638226387,2.4750627244 H,0,0.3142824861,-2.0712094633,0.5453445572 N,0,-0.6842880507,-3.9068014288,-0.3598922341 C,0,-0.5755311906,-4.9954447109,-1.3510217637 H,0,-0.7679074308,-4.3060566872,0.5718672644 H,0,-1.5540075019,-3.4018395884,-0.5189153587 H,0,-1.4262667777,-5.6715741145,-1.2886248221 H,0,-0.5263144593,-4.5563590347,-2.3439545706 H,0,0.3441145259,-5.5444455963,-1.1678559989 H,0,0.5360268748,-2.354183698,-1.501537853 H,0,1.5455616857,-3.4679746738,-0.1604029193</p>
	
<p>HF=-2416.0082412 ZPE=0.553602 NImag=0</p> <p>Htot=-2415.419079 Gtot=-2415.517947</p> <p>C,0,-0.0671000015,1.2383565367,-0.8409810585 C,0,-0.1849932226,3.813183802,-2.0679900614 Rh,0,0.0563252214,-0.6721644054,0.0836497236 C,0,0.9977679887,2.1606705345,-0.7953336713 C,0,-1.2279116789,1.7393094712,-1.4609758056 C,0,-1.2983225239,2.9916756345,-2.070150167 C,0,0.9656503275,3.4092379875,-1.4111751087 H,0,-2.220249439,3.325840319,-2.529855319 H,0,1.82876525,4.062267305,-1.3700622143 H,0,-0.2221315163,4.7799678561,-2.5544719114 B,0,0.1142783684,-1.8084492063,-1.7549967806 P,0,2.3154746998,-0.307502408,0.1573657854 P,0,-2.2269415737,-0.5203275795,0.1377207198 S,0,2.4827663959,1.8194587024,0.1689787447</p>	<p>HF=-2416.0337455 ZPE=0.553709 NImag=0</p> <p>Htot=-2415.444588 Gtot=-2415.542578</p> <p>C,0,-0.0611051806,1.2401772208,-0.8288934963 C,0,-0.1701629618,3.8116251486,-2.068799349 Rh,0,0.0543427253,-0.6653484659,0.1120746067 C,0,1.0042209198,2.1632004692,-0.7811757353 C,0,-1.2178849362,1.7393298731,-1.4594139187 C,0,-1.283201349,2.9891774422,-2.0760782853 C,0,0.9762859576,3.4098654056,-1.4025162408 H,0,-2.2009595421,3.3222410138,-2.5455983081 H,0,1.8386954733,4.064199994,-1.3592407072 H,0,-0.2039099416,4.7765462854,-2.5598260831 B,0,0.1079160879,-1.8068661364,-1.7288088282 P,0,2.3220372234,-0.3140216213,0.1706976866 P,0,-2.2365993825,-0.5179906274,0.1516755129 S,0,2.4850736222,1.8202913844,0.1894060499</p>

<p>S,0,-2.7816691196,0.829695056,-1.4137212836 C,0,3.1399835233,-0.7502239206,1.7718105044 H,0,4.1133485174,-0.2490205045,1.7933888057 C,0,3.5444655887,-0.788336156,-1.1779952989 H,0,3.3397369019,-1.8501874718,-1.3596355567 C,0,3.2577632937,-0.004084323,-2.453265635 H,0,3.7891375855,-0.4522686925,-3.2945397649 H,0,3.6033782578,1.0246051476,-2.3464339873 H,0,2.1979444123,0.0274091237,-2.6981866593 C,0,4.9933304525,-0.6001228047,-0.7588984918 H,0,5.6564213931,-0.8282091528,-1.5957950974 H,0,5.2899343139,-1.2342680436,0.0757296887 H,0,5.1782589188,0.4396449585,-0.4779607995 C,0,2.285132792,-0.2584396025,2.9295678149 H,0,2.146777942,0.8219591302,2.9029870408 H,0,2.7452904742,-0.5207887336,3.8839192289 H,0,1.2982431352,-0.7292699686,2.8925213888 C,0,3.332863271,-2.2582250392,1.8476581542 H,0,3.8484584101,-2.5314549589,2.7699947458 H,0,3.917330756,-2.6561437294,1.0158816971 H,0,2.3598182694,-2.7553324665,1.8494276865 C,0,-3.5556992875,-1.8319478251,-0.0502766022 H,0,-3.2867367499,-2.563188008,0.7215799331 C,0,-3.4991671111,-2.5136374847,-1.4078973138 H,0,-4.224566144,-3.3282526946,-1.4500365394 H,0,-2.5156306337,-2.9207920475,-1.6286724914 H,0,-3.733120155,-1.8126889095,-2.2099064706 C,0,-4.9592023675,-1.3101496008,0.2254437172 H,0,-5.0822471349,-0.9461964451,1.2441886248 H,0,-5.6908215816,-2.1061266095,0.0728780035 H,0,-5.2186288474,-0.4961013225,-0.4543347203 C,0,-2.7110239522,0.3225949631,1.7398503738 H,0,-3.7322222581,0.6936439691,1.6120943236 C,0,-2.6610703384,-0.6858024298,2.8804288961 H,0,-2.8783307892,-0.1932700512,3.8300905046 H,0,-1.6680003548,-1.1352744913,2.9571385342 H,0,-3.3828876649,-1.4948367523,2.7604383749 C,0,-1.7901486482,1.5035937091,2.0058103305 H,0,-2.0770956701,2.0032011115,2.9333030812 H,0,-1.8190258483,2.236710155,1.2004170801 H,0,-0.7503358996,1.1783128484,2.1112486177 H,0,0.148265955,-2.1197672335,0.9636491268 N,0,0.0024578885,-3.3795621273,-1.2911445511 C,0,1.2966255514,-4.0352835516,-1.0355011183 H,0,-0.5154855359,-3.3383276062,-0.4090879492 H,0,-0.5385039138,-3.9180485978,-1.9650556235 H,0,1.1688557381,-5.0604218437,-0.6907383713 H,0,1.8872764649,-4.0183823885,-1.9476602667 H,0,1.8017645425,-3.4524078843,-0.2672426193 H,0,-0.8674344038,-1.5336740734,-2.3837421285 H,0,1.1656309687,-1.7072278754,-2.3144888138</p>	<p>S,0,-2.7707966861,0.8281565962,-1.4203633219 C,0,3.1768294196,-0.7604118676,1.768746623 H,0,4.1491317157,-0.2568934502,1.7708914216 C,0,3.5350661023,-0.782093423,-1.1842955316 H,0,3.3237325429,-1.8415420603,-1.3705086579 C,0,3.2398346402,0.012095572,-2.4508143642 H,0,3.7435416291,-0.4457793099,-3.3043452599 H,0,3.6122956317,1.0326762427,-2.3528848193 H,0,2.1770910677,0.0700596845,-2.6789678316 C,0,4.9904907133,-0.6064759145,-0.7848062214 H,0,5.6378263494,-0.8355821355,-1.6342849542 H,0,5.2977353462,-1.2489787962,0.0394595425 H,0,5.193537742,0.4292377845,-0.5009586278 C,0,2.352140124,-0.2787711843,2.9509034381 H,0,2.2028086374,0.8007790179,2.937296005 H,0,2.8447714961,-0.5385719227,3.890051157 H,0,1.3689474877,-0.7579032359,2.9490416973 C,0,3.3793170638,-2.2673059309,1.8342290519 H,0,3.9263140067,-2.5368987511,2.7398698773 H,0,3.9402384465,-2.6631323813,0.9858205816 H,0,2.4127846653,-2.7754730089,1.8679494238 C,0,-3.5612878077,-1.8321950894,-0.0435717238 H,0,-3.307020419,-2.5463952853,0.7487180791 C,0,-3.4813647164,-2.5468240987,-1.3818346731 H,0,-4.2254281995,-3.3449776579,-1.4218070255 H,0,-2.506081597,-2.9913597567,-1.562806408 H,0,-3.6804233807,-1.8661372444,-2.2107880473 C,0,-4.9694772175,-1.3064864816,0.1945584518 H,0,-5.1120441371,-0.9070535433,1.1974840387 H,0,-5.6937939567,-2.1128475115,0.0609666424 H,0,-5.2286015206,-0.52074916,-0.5183388936 C,0,-2.7516312539,0.3432032631,1.7353191519 H,0,-3.766586368,0.7197004082,1.5783141545 C,0,-2.7429754743,-0.6523098648,2.8870858768 H,0,-2.9863955654,-0.1460644507,3.8235113684 H,0,-1.75685838,-1.1081994478,3.0052108421 H,0,-3.4667441671,-1.4578622286,2.7566008997 C,0,-1.8318503307,1.5199445962,2.0172986611 H,0,-2.1426045237,2.028919634,2.93239726 H,0,-1.8354025558,2.2510252761,1.2090207177 H,0,-0.7970616684,1.1921243452,2.1574961133 H,0,0.1378517094,-2.1147849921,0.9879406969 N,0,0.0141577221,-3.379672803,-1.314331635 C,0,1.3058815053,-4.0336509874,-1.0413743033 H,0,-0.5480440549,-3.410902052,-0.4625934837 H,0,-0.4861431308,-3.9007000764,-2.0331098727 H,0,1.1679635795,-5.0651467304,-0.7210238135 H,0,1.9126916693,-4.0052339921,-1.9427944746 H,0,1.8007092434,-3.4710091927,-0.2521343925 H,0,-0.8780673925,-1.5232936399,-2.3507439097 H,0,1.1510647318,-1.6755288477,-2.2992514318</p>
<p>HF=-2511.8687787 ZPE=0.617626 NImag=1 (-560.5730)</p> <p>Htot=-2511.211432 Gtot=-2511.320869</p> <p>Rh,0,0.2475364513,-0.2267768668,-0.687939515 C,0,-0.5394987088,-0.176979558,-2.6391283665 C,0,-1.6142047562,-0.0930254755,-5.3059264181 C,0,-0.9672076752,-1.3240656619,-3.3488376246</p>	<p>HF=-2511.9003438 ZPE=0.619028 NImag=1 (-615.9213)</p> <p>Htot=-2511.241920 Gtot=-2511.349910</p> <p>Rh,0,0.2044103277,-0.2095414248,-0.7412546301 C,0,-0.5200786351,-0.1785673226,-2.7115722108 C,0,-1.512693598,-0.1208185315,-5.4158523383 C,0,-0.8774759379,-1.338337274,-3.4438227071</p>

C,0,-0.657199925,1.011349315,-3.3996311409	C,0,-0.6664598228,1.0100795542,-3.470904433
C,0,-1.1884917931,1.0683043996,-4.6872209342	C,0,-1.155837188,1.0526488233,-4.7763632302
C,0,-1.4889707329,-1.2990638094,-4.641083071	C,0,-1.3606097361,-1.3249794668,-4.752100276
H,0,-1.2624268164,2.0177527562,-5.2037068999	H,0,-1.2524256244,2.0011853599,-5.2914785718
H,0,-1.792636526,-2.2202382721,-5.1236221139	H,0,-1.6136399786,-2.2539694615,-5.2494576166
H,0,-2.0271696397,-0.060015988,-6.3065462761	H,0,-1.8940141695,-0.0982669986,-6.429535574
P,0,0.2275676437,-2.4759618104,-0.8882953515	P,0,0.2171559859,-2.4676966768,-0.9088605704
P,0,0.3697007628,2.0247531273,-0.7940785693	P,0,0.3104848212,2.0430859467,-0.8423564581
S,0,-0.0720765034,2.6021018823,-2.795840596	S,0,-0.1869278849,2.6232658391,-2.8363347095
S,0,-0.854645972,-2.9790455675,-2.6511477595	S,0,-0.7239335938,-2.9917087582,-2.7525986883
C,0,1.9254466991,-3.21380316,-1.1843247107	C,0,1.9318337938,-3.2080032524,-1.0669151973
H,0,2.4486553209,-3.0227077998,-0.239695939	H,0,2.3763651484,-3.0011370611,-0.0859693886
C,0,1.929337683,-4.7015432403,-1.4845191638	C,0,1.962915962,-4.7003694747,-1.3373647812
H,0,2.9425098589,-5.0445730391,-1.7043810889	H,0,2.9930432722,-5.0461511552,-1.4508151716
H,0,1.3139962821,-4.9207594334,-2.3603024395	H,0,1.4378978403,-4.9427372592,-2.2646266794
H,0,1.5589380625,-5.3021567229,-0.6525747659	H,0,1.5142964151,-5.2860458684,-0.5338372568
C,0,2.6051694969,-2.4106535182,-2.2833238881	C,0,2.7019765888,-2.4244677139,-2.1173312586
H,0,3.6365226595,-2.7406772138,-2.4215303922	H,0,3.7444004586,-2.7479154677,-2.1545598671
H,0,2.6057778636,-1.3435906478,-2.0510221879	H,0,2.6771761861,-1.3522599108,-1.9094089458
H,0,2.0817194002,-2.537506855,-3.233355758	H,0,2.271146886,-2.5744829778,-3.1099740782
C,0,2.0366109412,2.8328883516,-0.5468661952	C,0,1.9718664397,2.8758502996,-0.6300132032
H,0,1.9644393765,3.8544975171,-0.9362598993	H,0,1.8740046332,3.8935242392,-1.0238189817
C,0,2.3969330485,2.8652368376,0.930413869	C,0,2.3610755948,2.9290368698,0.8387234333
H,0,1.6785710505,3.4294913592,1.5291854467	H,0,1.6428139559,3.4789451148,1.4500026024
H,0,3.3770331062,3.325009047,1.073272907	H,0,3.3310537414,3.4177309472,0.9555238578
H,0,2.4387003809,1.8499643438,1.3297910177	H,0,2.4447502024,1.921006456,1.2497962341
C,0,3.075550497,2.0607830408,-1.3445243727	C,0,3.0110970504,2.1205492667,-1.4411302664
H,0,4.057041488,2.5313047033,-1.2580386301	H,0,3.9810805419,2.6198827801,-1.3870325788
H,0,2.8137842134,2.0069069813,-2.4014368226	H,0,2.7302312051,2.0412019469,-2.4920875273
H,0,3.1527285751,1.0381020989,-0.9669713529	H,0,3.1302806685,1.1061481476,-1.0524072011
C,0,-0.8143818242,3.1187102444,0.1713392944	C,0,-0.8627003354,3.113347782,0.157959167
H,0,-0.6212752656,2.8485352679,1.2189415478	H,0,-0.6212042405,2.8478869826,1.1962736147
C,0,-2.2397992406,2.7304395324,-0.1952901134	C,0,-2.2926572009,2.6924656899,-0.1438874846
H,0,-2.9625696913,3.1923811357,0.4821438007	H,0,-2.9949684996,3.1535439218,0.5549474633
H,0,-2.3802484064,1.6467012157,-0.1819180123	H,0,-2.4156711375,1.6073196016,-0.0998894318
H,0,-2.4719283011,3.062164105,-1.2082356611	H,0,-2.578143479,3.001252392,-1.1509685493
C,0,-0.5848366093,4.6083832786,-0.0153059774	C,0,-0.6739747987,4.6072988692,-0.0355279206
H,0,-1.3339220039,5.1866001552,0.5307764255	H,0,-1.407184391,5.1665746408,0.5508435688
H,0,-0.6729742831,4.8798153654,-1.069858135	H,0,-0.8209213036,4.8864314347,-1.0817498117
H,0,0.3961822575,4.9302747824,0.3341141427	H,0,0.3149075735,4.9519795041,0.2675526568
C,0,-0.549816405,-3.68342516,0.3179412957	C,0,-0.6514316867,-3.6666232316,0.2411318348
H,0,-0.462370474,-4.6823916539,-0.1209594655	H,0,-0.5793432616,-4.6593640309,-0.2152233132
C,0,0.2239420412,-3.6499353926,1.6279193508	C,0,0.0629427574,-3.6860785036,1.5836905684
H,0,0.3359493673,-2.6275091495,2.001305841	H,0,0.2003866413,-2.6758174752,1.9800852696
H,0,1.2349172082,-4.0431766939,1.5164253699	H,0,1.0577013219,-4.1279120921,1.5150829879
H,0,-0.2761462017,-4.2467756995,2.394203099	H,0,-0.5010324463,-4.2676988202,2.3167815704
C,0,-2.0286550341,-3.3778021272,0.4989879716	C,0,-2.122774151,-3.3117859139,0.3681095563
H,0,-2.2011544809,-2.316421728,0.6976396684	H,0,-2.2656623936,-2.2745539964,0.6818557239
H,0,-2.4507914456,-3.9582754132,1.3228639521	H,0,-2.6170295451,-3.9589412317,1.0965215421
H,0,-2.5938673008,-3.6033512057,-0.4034454747	H,0,-2.6434530498,-3.4168835921,-0.5829597252
H,0,0.9543988896,-0.2419750496,0.9014953457	H,0,0.8524513955,-0.1952853434,0.8811842093
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B,0,0.1807799567,0.1879769548,2.6560279056	B,0,0.2164494185,0.1624704347,2.5923282651
H,0,0.4545675272,1.3217455766,2.4773028774	H,0,0.5031606309,1.3021829725,2.4720317069
N,0,-0.4086974711,0.6323301495,4.6234874598	N,0,-0.2698209688,0.520098374,4.6431994863
H,0,0.4935816548,0.4268291234,5.0375109705	H,0,0.6391635045,0.2542636318,5.0058507486
H,0,-1.0651300472,0.0163114358,5.0943694039	H,0,-0.9301899742,-0.099854978,5.1038482051
N,0,-1.204850816,-0.2802696166,2.0823226531	N,0,-1.2324429881,-0.2404321943,2.1172318537
H,0,-1.3396231812,-1.2754540938,2.2494045096	H,0,-1.4023074738,-1.225522151,2.3125941025
H,0,-1.015280379,-0.2282790749,1.0203709361	H,0,-1.1387237112,-0.1986301568,1.0653494487
C,0,-2.4339428834,0.4551617774,2.4212147325	C,0,-2.3937488372,0.5531015511,2.5610253707
H,0,-2.2495469349,1.5192727101,2.2984907899	H,0,-2.1582465995,1.609167351,2.4612560986
H,0,-2.7383724331,0.2584766727,3.4472223607	H,0,-2.6310982379,0.3349373483,3.5986596662
H,0,-3.2387344521,0.160047634,1.7498310578	H,0,-3.2586675018,0.3192719108,1.9431386191
C,0,-0.7519350304,2.0348340556,4.880188445	C,0,-0.542864332,1.9097646388,5.0134372344
H,0,-1.7637563945,2.2348080258,4.5338842226	H,0,-1.5624129997,2.1739869471,4.7390757476
H,0,-0.0755801177,2.6678903466,4.3072264927	H,0,0.1305125809,2.5621623135,4.4576016217
H,0,-0.6888645558,2.3144713888,5.9337122391	H,0,-0.415795225,2.1091166677,6.0801256341

<p>HF=-2511.8916872 ZPE= 0.618783 NImag=0</p> <p>Htot= -2511.233285 Gtot= -2511.343783</p> <p>Rh,0,0.2521766283,-0.2489408003,-0.6616215962 C,0,-0.6406578718,-0.1908066626,-2.5663444166 C,0,-1.8920719711,-0.0895358507,-5.1539531539 C,0,-1.2598116769,-1.3045336432,-3.1824629522 C,0,-0.6616707291,0.9669443308,-3.3818516446 C,0,-1.2797489762,1.0350243088,-4.6292805133 C,0,-1.8675747694,-1.2720615032,-4.4360235305 H,0,-1.2757466018,1.9626818136,-5.1889748182 H,0,-2.3140838379,-2.1687308646,-4.8487813305 H,0,-2.3717942029,-0.0483978043,-6.1241497675 P,0,0.1783183874,-2.4829846691,-0.9016119761 P,0,0.4971325719,1.9834954498,-0.8486559833 S,0,0.1722577277,2.4869347171,-2.8952524735 S,0,-1.280359913,-2.92610831,-2.3951536904 C,0,1.7556004612,-3.244841318,-1.5747035859 H,0,2.4796136563,-3.0713446162,-0.7692139029 C,0,1.6603112684,-4.7307205273,-1.8700806812 H,0,2.5907931955,-5.0933807507,-2.3121105901 H,0,0.8589011018,-4.9303684074,-2.5852847184 H,0,1.4720687821,-5.3284589501,-0.9770484278 C,0,2.1948767383,-2.4514640325,-2.7963306741 H,0,3.1620752441,-2.8071210221,-3.1572490476 H,0,2.2701514047,-1.3858942392,-2.5713310989 H,0,1.4730871891,-2.5617005613,-3.6086653305 C,0,2.2003748074,2.6925755967,-0.5516522387 H,0,2.2199035391,3.6999929868,-0.9822287318 C,0,2.4750343452,2.7659352346,0.9434819562 H,0,1.785627347,3.4294705787,1.4684913162 H,0,3.4873431416,3.1315128227,1.1280191855 H,0,2.3915136132,1.7735491089,1.3933065511 C,0,3.2265133917,1.8198730137,-1.256657686 H,0,4.2334123731,2.22017608,-1.1196888161 H,0,3.0273880737,1.7510345847,-2.3263146649 H,0,3.1991342053,0.8061691583,-0.8486421446 C,0,-0.642919944,3.1992870596,0.0226664237 H,0,-0.5121997202,2.9543201244,1.0861073546 C,0,-2.0786515698,2.906251085,-0.389022545 H,0,-2.7879113593,3.4318279611,0.2554904737 H,0,-2.3009573075,1.8380601092,-0.363503054 H,0,-2.2509100703,3.2379184184,-1.414054519 C,0,-0.2973400344,4.6603491534,-0.2060928323 H,0,-1.027605153,5.312131818,0.2797649007 H,0,-0.3169166004,4.8921818626,-1.273709896 H,0,0.6871450927,4.9270327164,0.1783944126 C,0,-0.3329605451,-3.7063838315,0.4246466911 H,0,-0.4377943763,-4.6860267204,-0.0531125972 C,0,0.7486570869,-3.7757113889,1.4922006951 H,0,0.9867938634,-2.7744833406,1.866281914 H,0,1.6787482865,-4.2018217633,1.115622354 H,0,0.4247460576,-4.3896125851,2.3360025551 C,0,-1.6727596108,-3.3056226844,1.0148812332 H,0,-1.6078178053,-2.3073979888,1.4547384574 H,0,-1.9843309658,-4.0039334584,1.795380826 H,0,-2.453504498,-3.2629238938,0.2560820207 H,0,1.0997125158,-0.3019419201,0.8389746022</p>	<p>HF=-2511.9314477 ZPE=0.621805 NImag=0</p> <p>Htot=-2511.270281 Gtot= -2511.379142</p> <p>Rh,0,0.29857385,-0.2653855201,-0.7028828868 C,0,-0.6046318116,-0.1942380309,-2.6080379422 C,0,-1.8373351146,-0.0840379774,-5.2073901597 C,0,-1.2295636715,-1.3036478772,-3.2289530254 C,0,-0.6111056821,0.9636625965,-3.4254840235 C,0,-1.220311581,1.0366746165,-4.6778726907 C,0,-1.8281483364,-1.2667174484,-4.4879041161 H,0,-1.2060793328,1.9636152477,-5.239288545 H,0,-2.2804999704,-2.1588876256,-4.9050164317 H,0,-2.3098741046,-0.0395069746,-6.1813246643 P,0,0.1890422893,-2.5032095937,-0.9217348267 P,0,0.5167780946,1.972903411,-0.8620010187 S,0,0.2310506712,2.4748100486,-2.9255751648 S,0,-1.2730719475,-2.9204911969,-2.434309482 C,0,1.7506074614,-3.3057778678,-1.586827511 H,0,2.4696074683,-3.1507236612,-0.7733794076 C,0,1.6263763571,-4.7885021972,-1.8833735095 H,0,2.559849324,-5.173977047,-2.3003665593 H,0,0.8412564082,-4.9746869915,-2.6203015892 H,0,1.4016542168,-5.3818312759,-0.9958886921 C,0,2.2264081311,-2.5247492223,-2.8012441923 H,0,3.1908722869,-2.9028131828,-3.1478932243 H,0,2.3284621036,-1.4608105819,-2.5761789914 H,0,1.5180172653,-2.616769573,-3.6280193548 C,0,2.1917904621,2.7361719156,-0.5325041761 H,0,2.1895789059,3.7408363472,-0.9696893316 C,0,2.427075312,2.8322341566,0.9675296047 H,0,1.7055279201,3.4780500817,1.4706206278 H,0,3.4223188494,3.233956326,1.1713205435 H,0,2.3685852627,1.8435286645,1.4294581967 C,0,3.265702228,1.8954084305,-1.2020071586 H,0,4.2534061287,2.3365560988,-1.0483802067 H,0,3.0993202206,1.8037195413,-2.276030841 H,0,3.2729742295,0.8861542474,-0.7821820478 C,0,-0.6742483853,3.1577699632,-0.08185976298 H,0,-0.5570597457,2.9133644406,1.045887575 C,0,-2.0947075557,2.8289934105,-0.4515936305 H,0,-2.8247427326,3.3450161322,0.1773020282 H,0,-2.297511282,1.7573303014,-0.4148596073 H,0,-2.2632283111,3.1489944735,-1.4815353175 C,0,-0.3647960128,4.6279317147,-0.2365146672 H,0,-1.1192962402,5.2552972833,0.2451162648 H,0,-0.3779817619,4.8713543106,-1.3018772924 H,0,0.6057023444,4.9229390747,0.1628773925 C,0,-0.3641958768,-3.719408288,0.3941586397 H,0,-0.5057705081,-4.6876870463,-0.0974968447 C,0,0.7151349319,-3.8476904388,1.4579295862 H,0,0.9774672777,-2.867417235,1.8681478236 H,0,1.6344512952,-4.2893483723,1.0724592081 H,0,0.3718144631,-4.4784033754,2.2815708143 C,0,-1.6849622939,-3.2797811757,0.9980749873 H,0,-1.5779185826,-2.3055371385,1.480662902 H,0,-2.0277092326,-3.9944194743,1.7503837876 H,0,-2.4667845811,-3.1774550716,0.2454907503 H,0,1.1419978405,-0.3314475651,0.7872573481</p>

H,0,1.1588913842,0.3995122236,3.9800920306	H,0,1.1989997266,0.6000966508,3.8245221712
B,0,0.09033104,0.848455137,3.6770461339	B,0,0.0768104073,0.9833693195,3.6526462685
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H,0,-2.4570057915,1.6667023261,6.0986411172	H,0,-2.2745427622,1.5476490856,6.2987208129s

References for Supporting Information

- 1 A. L. Colebatch, B. W. Hawkey Gilder, G. R. Whittell, N. L. Oldroyd, I. Manners and A. S. Weller, *Chem. Eur. J.*, 2018, **24**, 5450-5455.
- 2 R. C. Todd, M. M. Hossain, K. V. Josyula, P. Gao, J. Kuo and C. T. Tan, *Tetrahedron Lett.*, 2007, **48**, 2335-2337.
- 3 M. Potyten, K. V. B. Josyula, M. Schuck, S. Lu, P. Gao and C. Hewitt, *Org. Process Res. Dev.*, 2007, **11**, 210-214.
- 4 H. Brown, *Quantitative Analysis of Active Metals and Metal Hydrides via Gas Buret, Vol. 1*, Inc.: Milwaukee, 1997.
- 5 H.-J. Drexler, A. Preetz, T. Schmidt and D. Heller, in *The Handbook of Homogeneous Hydrogenation*, 2006, pp. 257-293.
- 6 C. A. Jaska, K. Temple, A. J. Lough and I. Manners, *J. Am. Chem. Soc.*, 2003, **125**, 9424-9434.
- 7 G. Sheldrick, *Acta Crystallogr., Sect. A*, 2008, **64**, 112-122.
- 8 G. Sheldrick, *Acta Crystallogr., Sect. C*, 2015, **71**, 3-8.
- 9 K. Nakamoto, in *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, **2008**, pp. 149-354.
- 10 a) J. Burés, *Angew. Chem. Int. Ed.*, 2016, **55**, 2028-2031; b) J. Burés, *Angew. Chem. Int. Ed.*, 2016, **55**, 16084-16087.
- 11 Y. Zhao and D. G. Truhlar, *J. Chem. Phys.*, 2006, **125**, 194101: 1-18.
- 12 A. Schaefer, C. Huber and R. Ahlrichs, *J. Chem. Phys.*, 1994, **100**, 5829-5835.
- 13 P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299-310.
- 14 J. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396
- 15 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.