I. GENERAL METHODS

All experiments were performed under Ar atmosphere using standard Schlenk and vacuum-line techniques or in an MBraun glove box. Glassware was flame dried on a Schlenk line or kept at 120 °C overnight prior to use. Solvents were dried and stored over 4 Å molecular sieves under Ar. Deuterated solvents were purchased from Eurisotop, degassed and distilled from the proper drying agent, and stored over 4 Å molecular sieves under Ar. The argon was provided by PANGAS and further purified with an MBraun >99 HP gas purification system. Air sensitive compounds were handled in a glovebox (MBraun lab master 130 or 150B-G). Chemicals were received from ABCR, Acros, Aldrich, Fluka, Lancaster or STREM. The following compounds were prepared by previously reported methods: diammoniate of diborane,[S1] **4**, **5** and **6**[S2]. IR spectra were recorded on a Perkin-Elmer-Spectrum 2000 FT-IR-Raman spectrometer with KBr beam splitter (range 500 - 4000 cm^{-1}). For solid compounds the ATR technique was used. The absorption bands are described as follows: very strong (vs), strong (s), middle (m), weak (w), or broad (br). Samples were prepared in open glass capillaries. Solution NMR measurements were carried out on Bruker Avance 200, 300, 400, 500 MHz and 500 MHz cryoprobe spectrometers at room temperature (unless indicated otherwise). Solid state NMR measurements were carried out on Bruker Avance 700 MHz spectrometers equipped with a 2.5 mm two channel probe at room temperature. The sample spun at 20 kHz. For ^{11}B solid state MAS NMR, a Hahn echo pulse-sequence was used with an echo delay of 1.6 ms. Chemical shifts δ are given as dimensionless numbers and the absolute values of the coupling constants are given in Hertz (Hz), the first atom mentioned in the subscript always refers to the atom that was used to observe the coupling. Multiplicities are abbreviated as singlet (s), doublet (d), triplet (t), quartet (q), virtual triplet (vt), virtual doublet of doublets (vdd) and broad (br). NMR spectra were referenced to TMS (^{1}H, ^{13}C and ^{29}Si), $BF_3{\cdot}OEt_2$ (^{11}B), $CFCl_3$ (^{19}F), H_3PO_4 (^{31}P) and $Rh(acac)_3$ (^{103}Rh). Quaternary carbons are indicated as C_{quat}, aromatic carbon and hydrogens as C_{ar} and CH_{ar}, benzylic carbons and hydrogens as and CH_{benz}, olefinic carbons and hydrogens as CH_{olefin}. Single crystals suitable for X-ray diffraction analysis were coated with polyisobutylene oil in a glovebox, transferred to a nylon loop and then transferred to the goniometer of a Bruker X8 APEX2 or D8-Venture diffractometer equipped with a molybdenum X-ray tube (λ = 0.71073 Å) and a copper X-ray tube (λ = 1.5406 Å). Preliminary data were collected to determine the crystal system. The space group was identified, and the data were processed using the Bruker SAINT+ program and corrected for absorption using SADABS. The structures were solved using direct methods (SHELXT) on OLEX2 completed by Fourier transformation and refined by full-matrix least-squares procedures. Thermo gravimetric analysis was carried out in a NETZSCH STA 449 F5

JUPITER instrument coupled to a NETZSCH QMS 403 D AËOLOS mass spectrometer. Sample and reference crucibles made of Al_2O_3 were used. The gas flow was set to 50 + 20 mL Ar min^{-1}. The sample was heated from 40 to 1500 °C at a heating rate of 10 K min^{-1}. Scanning electron microscopy (SEM) of the as-obtained particles were performed with secondary electrons (SE) on a 1530 Gemini (Zeiss; field emission gun (FEG)) using a low voltage electron beam (V_{acc} = 1 KV) to minimize charging. The DLS measurements were performed with a Zetasizer Nano ZS (Malvern Instruments Ltd., Malvern, UK) equipped with a max 4 mW He–Ne laser (emitting at 633 nm). Each measurement was performed at the non-invasive backscatter angle (NIBS) of 173° at a temperature of 25 °C and was preceded by a 30 s equilibration time.

II. SYNTHESIS AND CHARACTERIZATION DATA

Ammonia borane: To a solution of sodium borohydride (1.00 g, 26.4 mmol, 1.0 equiv) in THF (50 ml) ammonium sulfate (6.99 g, 52.9 mmol, 2.0 equiv) was added. The reaction mixture was placed in an ultrasonic bath at 40°C overnight. The precipitate was filtered off and the solvent was removed under reduced pressure giving a white solid. The product was recrystallized from diethyl ether.

^{11}B-NMR (96 MHz, THF-d_8, 298K): δ (ppm) −24.1 (q, J = 95.4 Hz).

^{15}N ammonia borane: ^{15}N labelled AB was synthesized following the previous protocol using $(^{15}NH_4)_2SO_4$.

***N*-propargylamine-borane:** The synthesis is adapted from a previously reported procedure. [S3]

A mixture of sodium borohydride (700 mg, 18.5 mmol, 1.0 equiv) and propargylamine hydrochloride (6.772 g, 74.05 mmol, 4 equiv) in THF (50 mL) was placed in an ultrasonic bath overnight. The resulting suspension was filtered and the solvent evaporated, leading to a white powder (1.034 g, 63 % yield).

^{1}H NMR (300 MHz, THF-d_8) δ (ppm) 1.38 (m br, 3 H, BH_3), 2.75 (t, $^4J_{HH}$ = 2.6 Hz, 1 H, C≡C*H*), 3.25 (m, 2 H, CH_2), 2.58 (dt, $^2J_{HH}$ = 11.2 Hz, $^3J_{HRh}$ = 2.1 Hz, 1 H, TMS-CH_2), 5.14 (s br, 2 H, NH_3). ^{13}C NMR (75.5 MHz, THF-d_8) 37.8 (s, 1 C, *C*H_2), 74.3 (s, 1 C, C≡*C*H), 80.4 (s, 1 C, *C*≡CH). δ (ppm ^{11}B NMR (96 MHz, THF-d_8): δ (ppm) −18.25 (q, J = 96.5 Hz). ^{15}N NMR (30.4 MHz, THF-d_8). δ (ppm) 29.0 (s). IR (ATR, cm^{-1}): 3252.9 (s, ν_{NH}), 3227.3 (m, $\nu_{C\equiv C-H}$), 2393.8 (m, ν_{B-H}), 2324.0 (s, ν_{B-H}), 2284.8 (m, ν_{B-H}), 2126.2 (w, $\nu_{C\equiv C}$), 1580.8 (s), 1359.9 (s), 1273.8 (s), 1166.2 (vs), 1040.7 (vs), 696.1 (vs), 493.8 (vs). Anal. Calcd for C_3H_8BN: C, 52.29; H, 11.70; N, 20.33. Found: C, 52.29; H, 11.56; N, 20.23.

III. CATALYTIC DEHYDROGENATION OF AB AND SUBSTITUTED AMINE BORANES BY Rh COMPLEXES

A) DEHYDROGENATION OF AB. CATALYST SCREENING IN NMR SCALE REACTIONS

Ammonia borane (17.0 mg, 551 µmol), catalyst **4**, **5** or **6** (1.9 µmol, 0.35 mol%) and sodium tetraphenylborate as internal NMR standard (4.5 mg, 13 µmol, 2.4 mol%) were dissolved in 0.5 mL dimethoxyethane. The solution was placed in a J. Young NMR tube and heated at 80°C inside a 400 MHz spectrometer. The conversion to borazine was followed by ^{11}B NMR applying 30° pulses, with a cycle delay of 2 s to avoid saturation of the sodium tetraphenylborate.

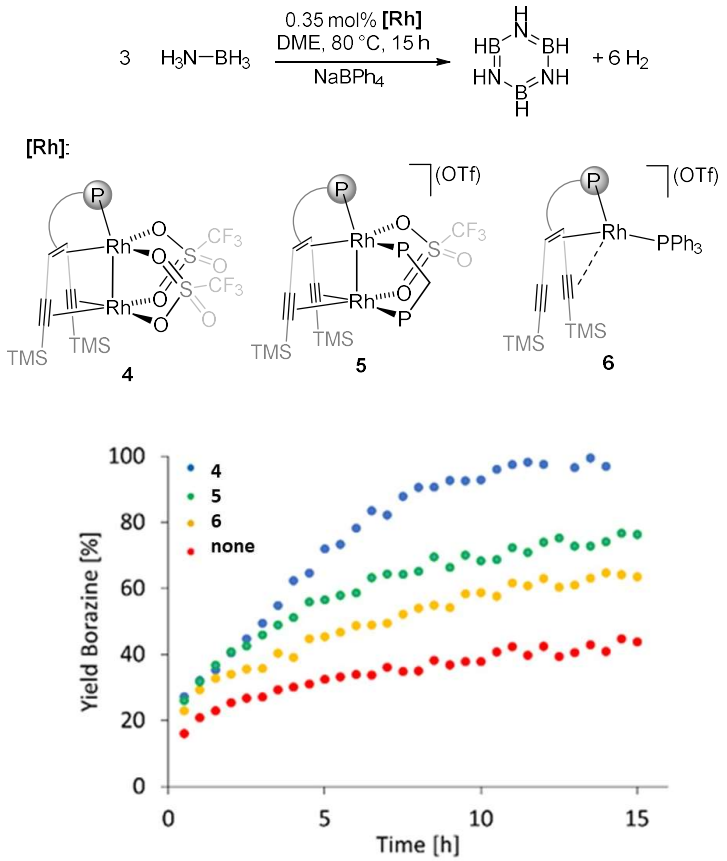


Figure S1. NMR yield quantification of borazine by ^{11}B NMR formed in the non-catalyzed decomposition of AB and in catalytic experiments with complexes **4** -**6**.

B) SCALE UP AND ISOLATION OF BORAZINE

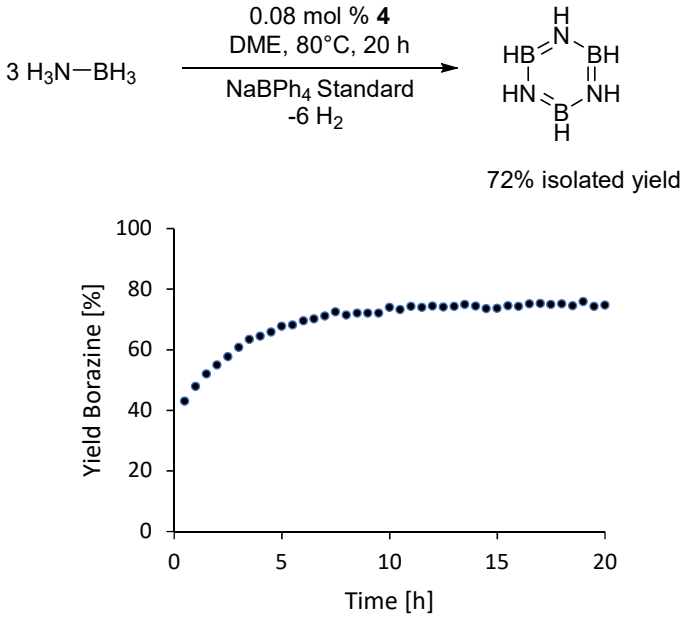
Ammonia borane (572.4 mg, 18.54 mmol), catalyst **4** (16 mg, 15 µmol, 0.08 mol%) and sodium tetraphenylborate (501 mg, 1.46 mmol, 7.9 mol%) were dissolved in 10 mL dimethoxyethane and heated in a stainless steel 50 mL autoclave to 80°C. The evolution of the reaction was monitored by ^{11}B NMR analysis of aliquots taken regularly. After 20 h the reaction was stopped and analysis of the mixture indicated formation of borazine in 75% NMR yield (TON = 938). The separation of borazine

from the catalyst and residual side products was performed by distillation under vacuum (0.01 mbar). The reaction mixture was frozen, and a vacuum was applied. Upon gradual warming of the solution to room temperature, the product and partial 1,2-dimethoxyethane (DME) were condensed in a secondary bulb cooled with liquid nitrogen. The borazine was isolated in 72% NMR yield ($NaBPh_4$ was used as internal standard)

Stock solutions of borazine (0.5 M) in dimethoxyethane (DME) were used for the reactions with borazine described in the following sections.

$^{11}B\{^1H\}$ NMR (128 Hz, DME, 278 K) δ (ppm) = 31.3 ($^1J_{BH}$ = 137 Hz).

a)



b)

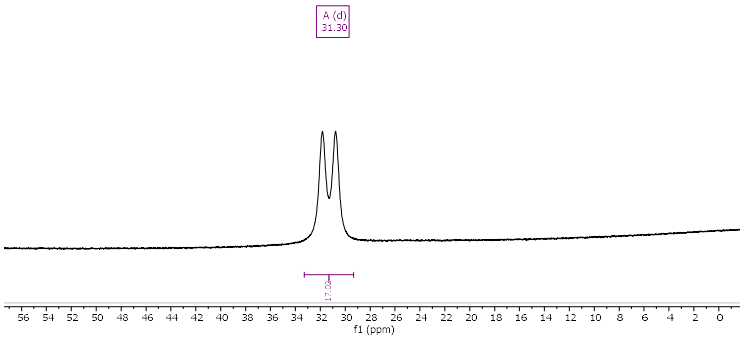


Figure S2. a) Catalytic test with complex **4** (0.08 mol%) achieving TON_{max} = 938. b) $^{11}B\{^1H\}$ NMR of isolated borazine in DME.

C) CATALYTIC FORMATION OF BORAZINE: MERCURY AND TRIPHENYLPHOSPHINE AS ADDITIVES

Test A. To a solution of ammonia borane (34.8 mg, 1.13 mmol), catalyst **4** (4.5 mg, 4.2 µmol, 0.37 mol%) and sodium tetraphenylborate (9.8 mg, 29 µmol, 2.6 mol%) in dimethoxyethane (1 mL) were added three drops of mercury. The reaction mixture was stirred at 80°C for 10 h, after which the solution was cooled down to room temperature and analyzed by ^{11}B NMR spectroscopy. The same experiment was repeated without mercury using an identical setup (Figure S3). No change in reaction time or conversion could be observed.

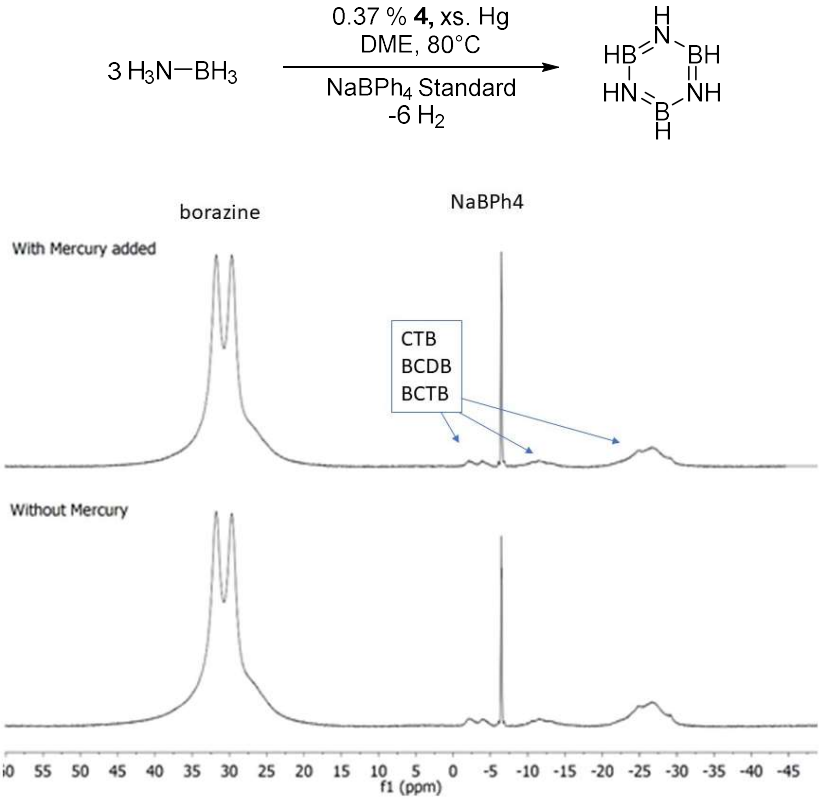


Figure S3. ^{11}B NMR spectra (64.2 MHz) of the catalysis with (top) and without (bottom) mercury.

Test B1. To a 25 mL Schlenk flask (with a glass ground joint and an additional side arm with a needle valve gas inlet) containing a solution of ammonia borane (34.9 mg, 1.13 mmol), catalyst **4** (4.6 mg, 4.2 µmol, 0.38 mol%) and sodium tetraphenylborate (10.1 mg, 29.5 µmol, 2.6 %) in dimethoxyethane (1 mL) was added triphenylphosphine (33.6 mg, 128 µmol, 11.3 mol%) The reaction mixture was heated at 80°C for 10 h. A substantial amount of a white precipitate was formed, identified as polyaminoborane. ^{11}B NMR analysis of the filtrate indicate no conversion of the ammonia borane to borazine.

Test B2. To a 25 mL Schlenk flask (with a glass ground joint and an additional side arm with a needle valve gas inlet) containing a solution of ammonia borane (34.9 mg, 1.13 mmol), catalyst **4** (4.6 mg, 4.2 µmol, 0.38 mol%) and sodium tetraphenylborate (10.1 mg, 29.5 µmol, 2.6 %) in dimethoxyethane (1 mL) was added triphenylphosphine (0.5 mg, 2.1 µmol, 0.19 mol%) The reaction mixture was heated at 80°C for 10 h. ^{11}B NMR analysis of the filtrate showed the formation of product but not complete conversion, having a proportional loss of catalytic activity (change in conversion is proportional to using half of the amount of catalyst then usually), which is an indication for the existence of a homogenous catalyst.

D) CATALYTIC FORMATION OF BORAZINE: SOLVENT EFFECT

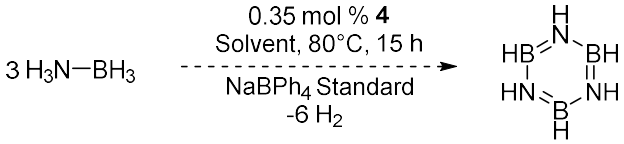


Table S1. Influence of solvent in the Rh(I)-catalyzed dehydrogenation of ammonia borane to borazine.

Entry	Solvent	Yield [%][a]
1	**DME**	95
2	**diglyme**	75
3	**ACN**	<5[b]
4	**THF**	nd

[a] Yield borazine determined by ^{11}B NMR with $NaBPh_4$ as internal standard. [b] Polyaminoborane formed as only dehydrogenation product.

Diglyme: Ammonia borane (17.0 mg, 551 µmol), catalyst **4** (2.1 mg, 1.9 µmol, 0.35 mol%) and sodium tetraphenylborate as internal standard (4.9 mg, 14 µmol, 2.6 %) were dissolved in diethylene glycol dimethyl ether (0.5 mL). The solution was placed in a J. Young NMR tube and heated inside a 400 MHz NMR magnet to 80°C. The reaction was followed during 16 h by ^{11}B NMR spectroscopy, applying 30° pulses with a cycle delay of 2 sec to avoid saturation of the sodium tetraphenylborate.

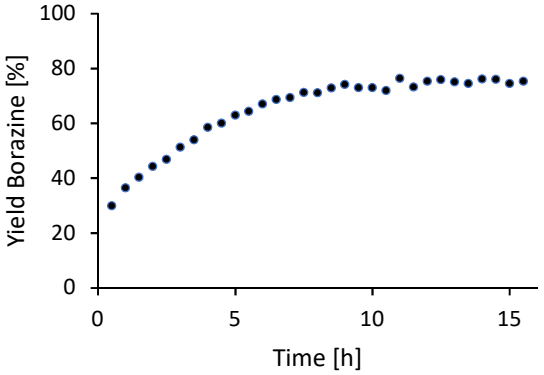


Figure S4. Monitoring the formation of borazine in the dehydrogenation of AB catalyzed by **4** in diglyme. Yield after 15h: 75 %, TOF: 8, TON: 212.

Acetonitrile: Ammonia borane (17.2 mg, 557 µmol), **4** (2.1 mg, 1.9 µmol, 0.34 mol%) and sodium tetraphenylborate as internal standard (7.0 mg, 20 µmol, 3.6 %) were dissolved in 0.5 mL acetonitrile. The solution was placed in a J. Young NMR tube. The reaction was followed at room temperature by ^{11}B NMR spectroscopy, applying 30° pulses with a cycle delay of 2 s to avoid saturation of the sodium

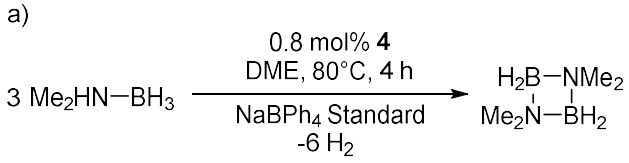
tetraphenylborate. Only traces of borazine were observed and most of the product precipitated from the reaction mixture as polyaminoborane.

Tetrahydrofuran is not a suitable solvent for the reaction since its polymerizes during the reaction. Identification of the reaction products was not possible.

E) CATALYTIC DEHYDROGENATION OF N-SUBSTITUTED AMINE BORANES

Catalytic dehydrogenation of Me_2HN-BH_3

a)



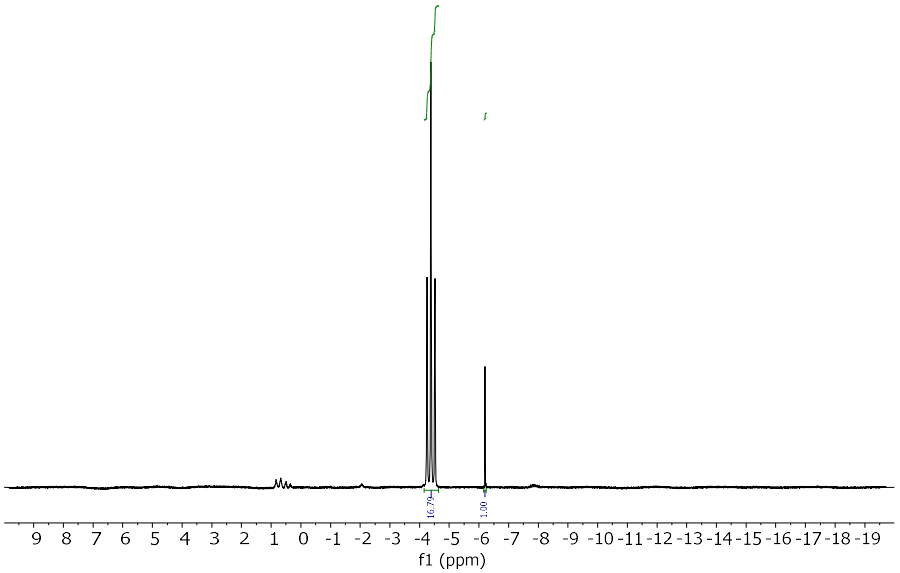
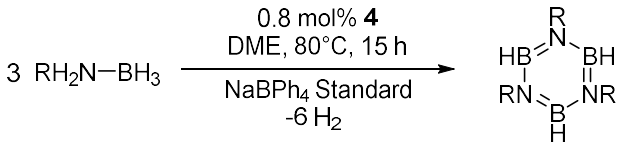


Figure S5. a) Rh-catalyzed dehydrogenation of Me_2NH-BH3. b) $^{11}B\{^1H\}$ NMR of the reaction in DME after 4h.

N-dimethylamine-borane (21.8 mg, 0.370 mmol, 1.0 equiv), catalyst **4** (3.2 mg, 3.0 µmol, 0.8 mol%) and sodium tetraphenylborate internal standard (9.8 mg, 29 µmol, 7.7 mol%) were dissolved in 0.5 mL of dimethoxyethane. The solution was placed in a J. Young NMR tube and heated at 80°C inside of a 400 MHz NMR spectrometer. ^{11}B NMR spectra were recorded periodically. Nearly complete conversion of the amine borane to the dimer $[Me_2NBH_2]_2$ was observed after 4 h.

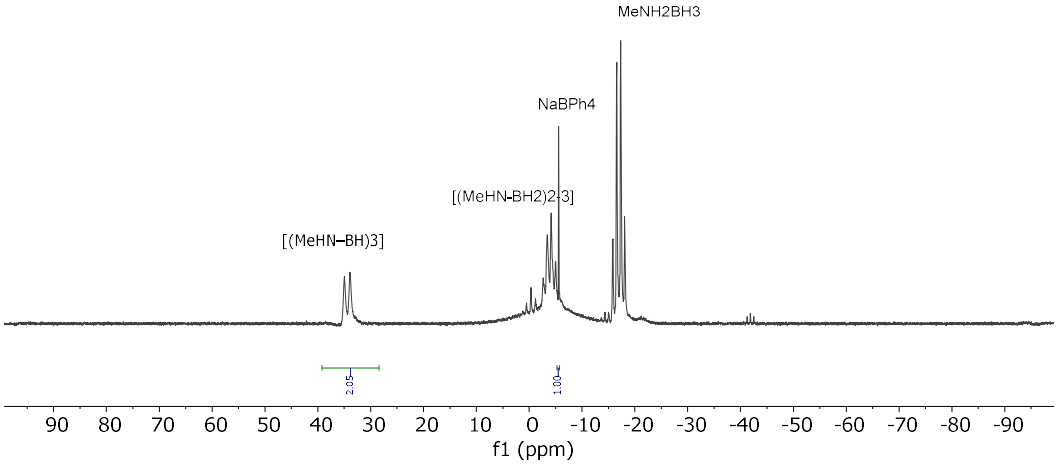
Catalytic dehydrogenation of RH_2N-BH_3 (R = Me, tBu)

a)



R = Me, 65% NMR yield
R = ^{t}Bu, 45% NMR yield (85% after 35h)

b)



c)

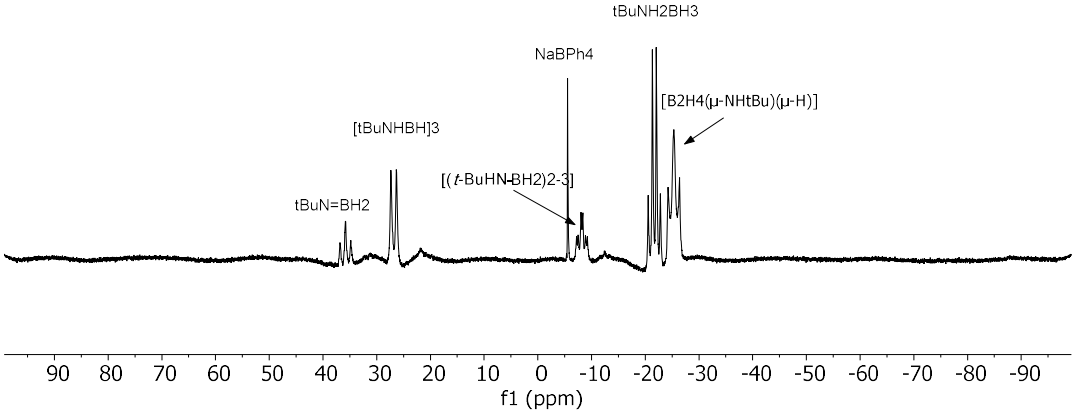


Figure S6. a) Rh-catalyzed dehydrogenation of N-substituted amine boranes to borazines. b) $^{11}B\{^1H\}$ NMR recorded during the reaction of $MeNH_2BH_3$ in DME. c) $^{11}B\{^1H\}$ NMR recorded during the reaction of tBuNH$_2$BH$_3$ in DME.

The mono substituted amine borane (0.370 mmol, 1 equiv), **4** (3.2 mg, 3.0 µmol, 0.8 mol%) and sodium tetraphenylborate internal standard (4.7 mg, 13 µmol, 3.6 mol%) were dissolved in 0.5 mL of dimethoxyethane. The solution was placed in a J. Young NMR tube and heated at 80°C inside of a 400 MHz NMR spectrometer. Conversion of the amino borane to the corresponding substituted borazine was monitored by ^{11}B NMR spectroscopic analysis.

Catalytic dehydrogenation of N-propargylamineborane

Complex **4** (24.3 mg, 22.5 µmol, 0.8 mol%) was dissolved in 15 mL of dimethoxyethane and heated at 80°C. *N*-propargylamine-borane **7** (250.0 mg, 2.81 mmol, 1 equiv) was dissolved in 5 mL dimethoxyethane and added drop wise to the catalyst solution at 80 °C. The reaction mixture was stirred at 80°C overnight. The resulting solution was cooled to 60°C and filtered, leading to a pale solid. The solid was washed with dimethoxyethane (20 mL) and hexane (2 x 10 mL). Drying under high vacuum led to an off-white solid (135 mg) characterized by solid state NMR and TGA analysis.

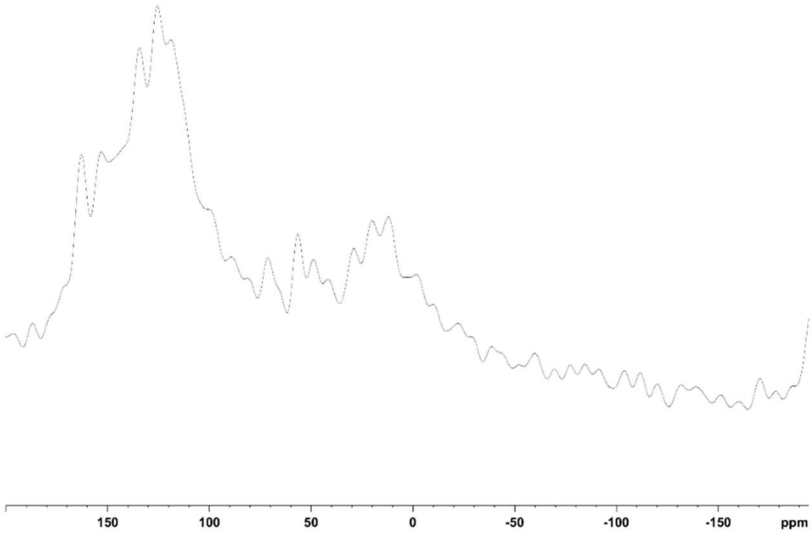


Figure S7. ^{13}C MAS NMR spectra of ***BCNHr^{cat}***. The main signal is observed in the carbon double bond region indicating the formation of a cross-linked polymer, in which the triple bonds were hydroborated.

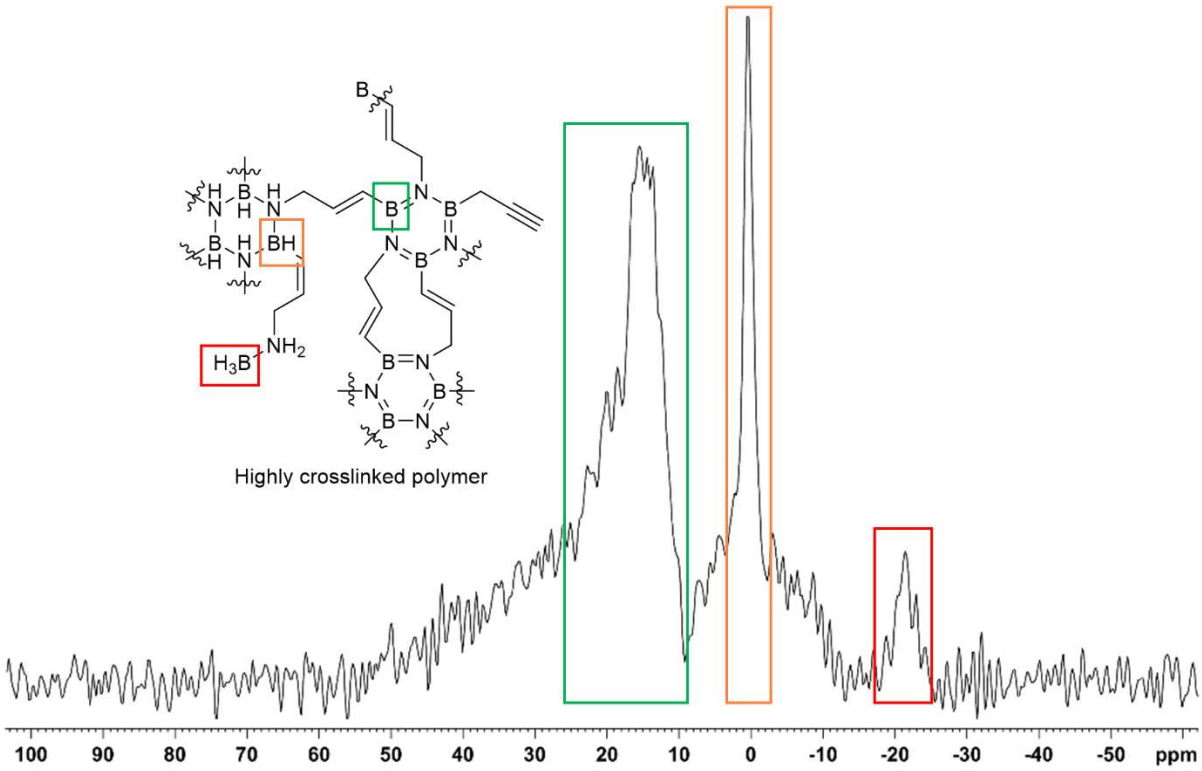


Figure S8. ^{11}B Hahn-Echo MAS NMR spectrum of ***BCNH^{cat}***. The signal at 17 ppm is assigned to *B*=N in borazine rings. The signal at 0 ppm corresponds likely to BH_2-NR_2 in cyclic units, and the signal at -21 ppm to residual BH_3 groups.

The dehydrogenation of the *N*-propargylamine-borane **7** was additionally performed without the catalyst under otherwise identical conditions. The resulting ^{11}B Hahn-Echo MAS NMR spectrum is presented in Figure S9.

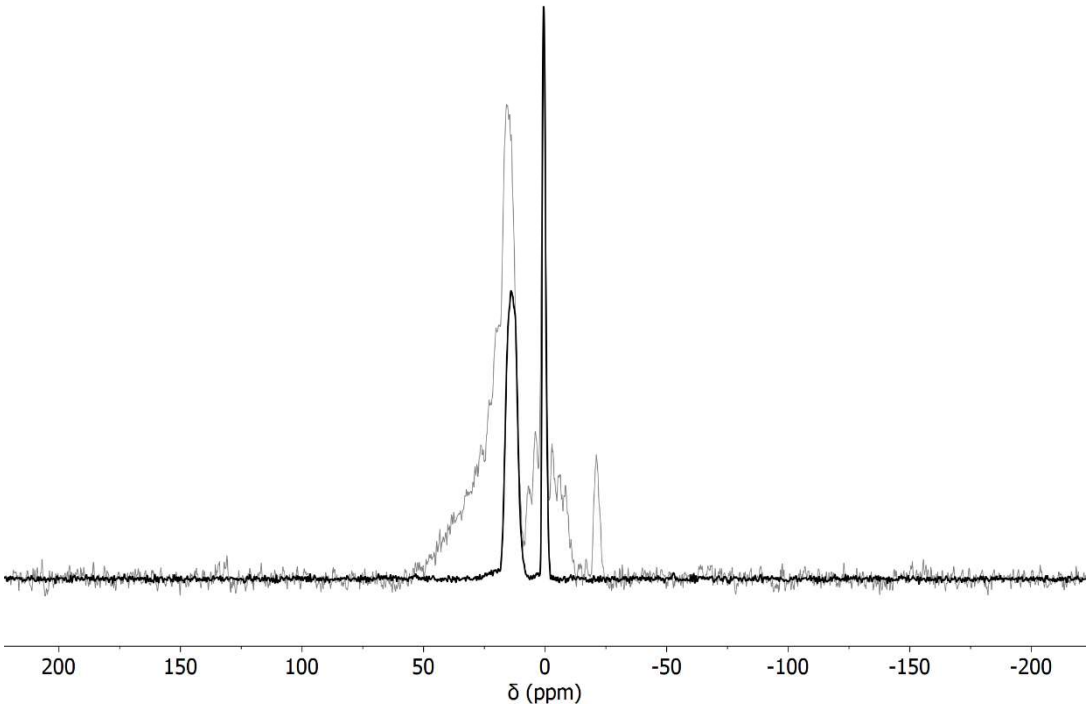


Figure S9. ^{11}B Hahn-Echo MAS NMR spectrum of the thermal dehydrogenation of *N*-propargylamine-borane **7** (black spectrum), compared to the catalytic dehydrogenated material (***BCNHr^{cat}***) (grey spectrum). In the catalytic dehydrogenation, significantly more borazine rings are formed, as indicated by the larger area of the signals between 0 and 50 ppm.

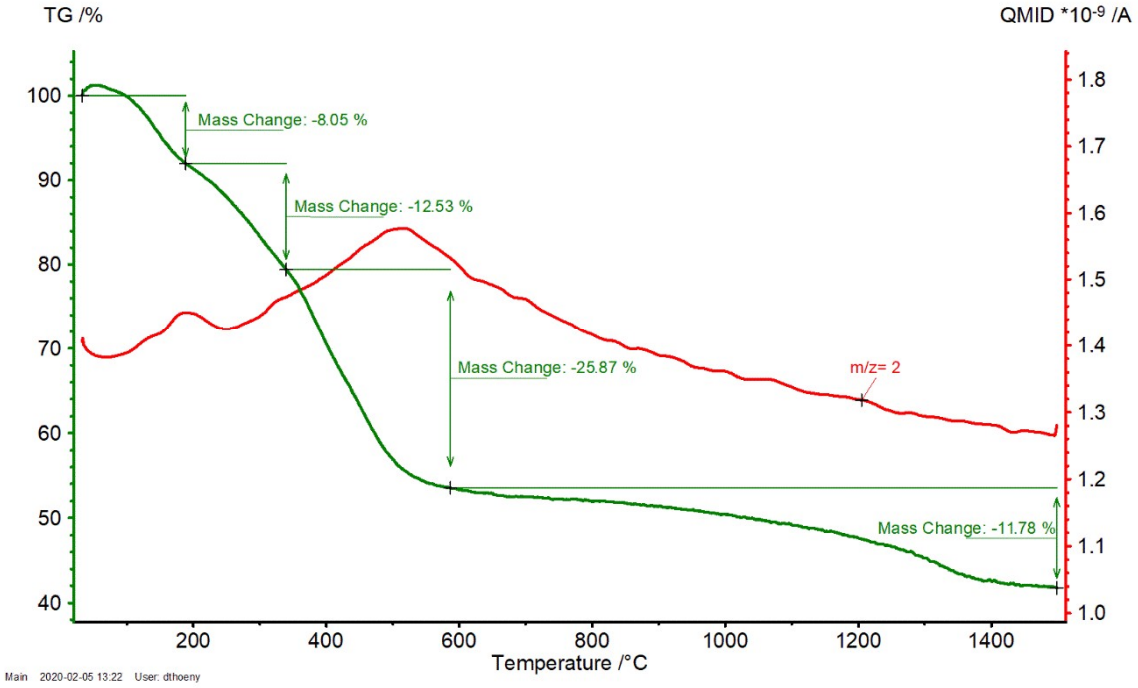


Figure S10. TGA of ***BCNHr^{cat}***. The m/z = 2 corresponds to dihydrogen.

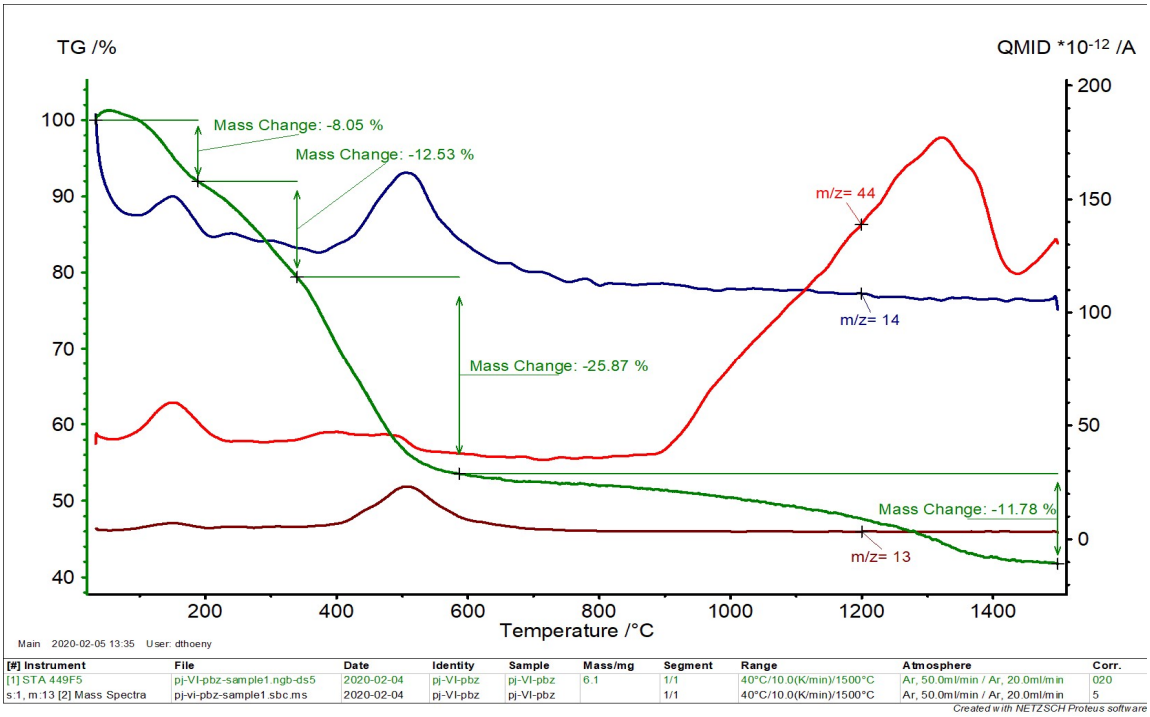


Figure S11. TGA of ***BCNHr^{cat}***. The m/z = 13 and 14 corresponds to $^{10}BH_3$ and $^{11}BH_3$, respectively. The presence of this fragment is in line with the incomplete dehydrogenation observed in NMR (see Figure S7). m/z = 44 corresponds to $H_3C\text{-}CH{=}NH_2^+$.

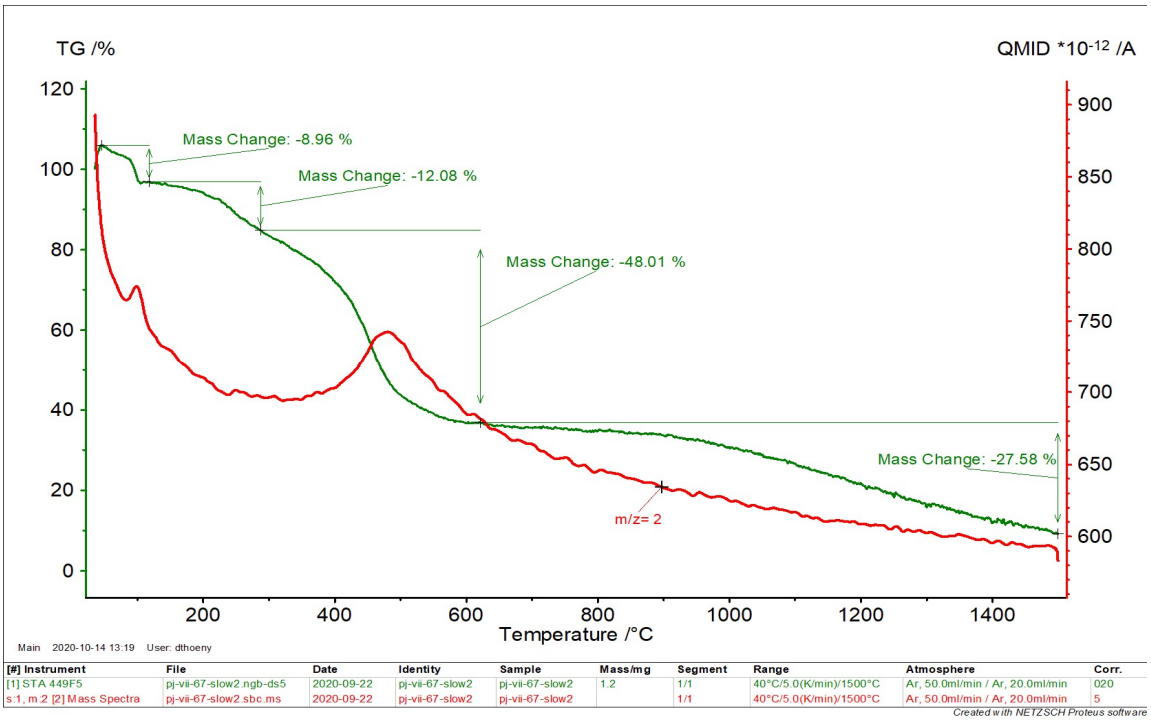


Figure S12. TGA of *N*-propargylamine-borane **7**. The m/z = 2 corresponds to dihydrogen.

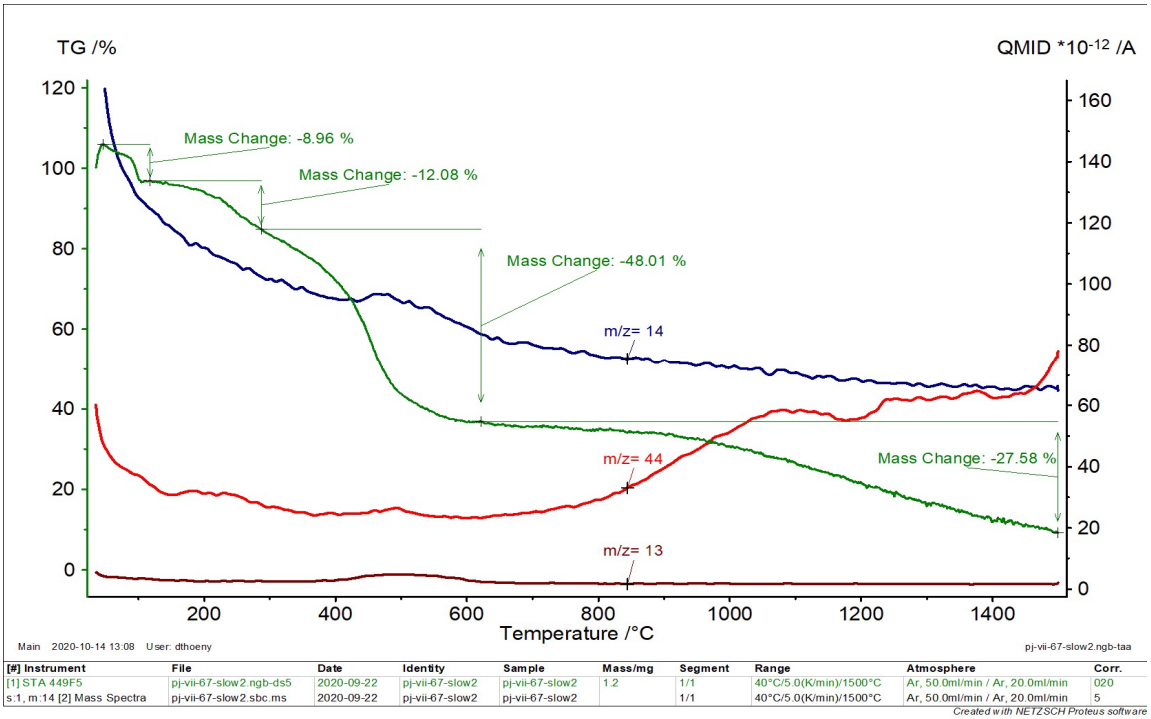


Figure S13. TGA of *N*-propargylamine-borane **7**. The m/z = 13 and 14 corresponds to $^{10}BH_3$ and $^{11}BH_3$, respectively. The presence of this fragment is in line with the incomplete dehydrogenation observed by NMR (see Figure S7). m/z = 44 corresponds to $H_3C\text{-}CH{=}NH_2^+$.

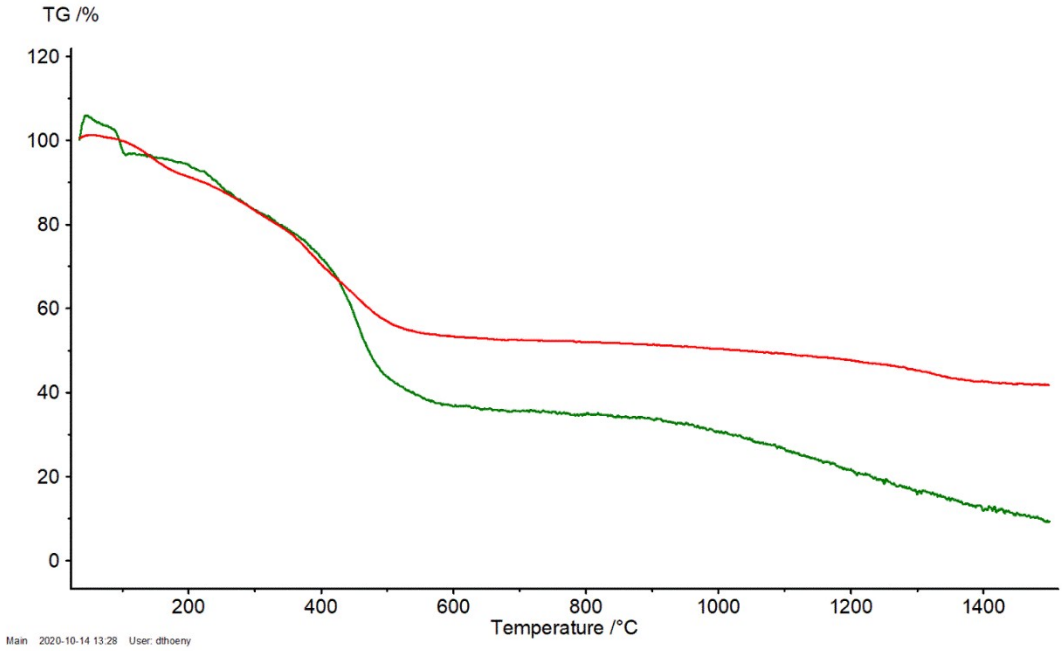


Figure S14. Comparison of the TGA of *N*-propargylamine-borane **7** (green) and of ***BCNHr^{cat}*** (red). Note that only the polymeric material shows a loss of hydrogen at 200°C.

A sample of the polymer (16.1 mg) was heated under an Argon flow to 200°C for 4-12 h, resulting in the formation of the material ***BCNHp^{cat}***. IR, NMR and TGA analysis of this material after thermal treatment is presented in Figures S14-S16.

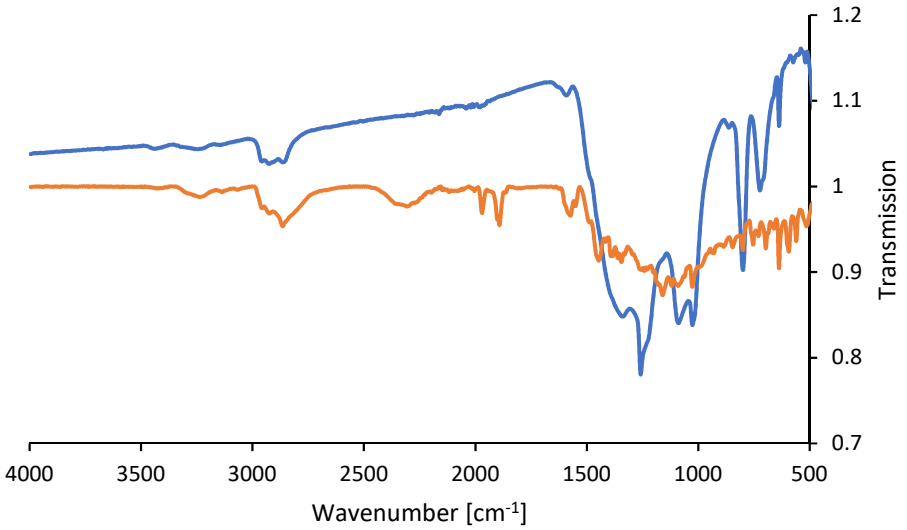


Figure S15. IR spectra of ***BCNHr^{cat}*** (orange) and ***BCNHp^{cat}*** (blue) of heating the sample to 200°C. Note the clear change, leading to a more polymeric character. Additionally, all signals from B-H groups (2306 cm^{-1}) as well as signals from C≡C bonds (1970 and 1892 cm^{-1}) vanished.

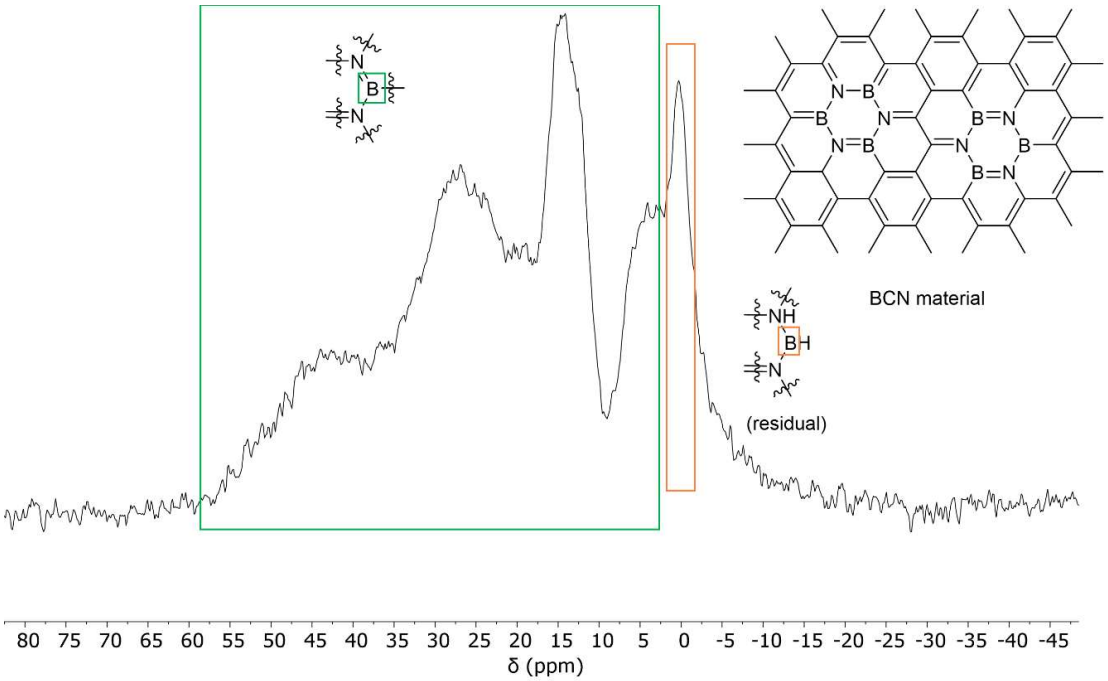
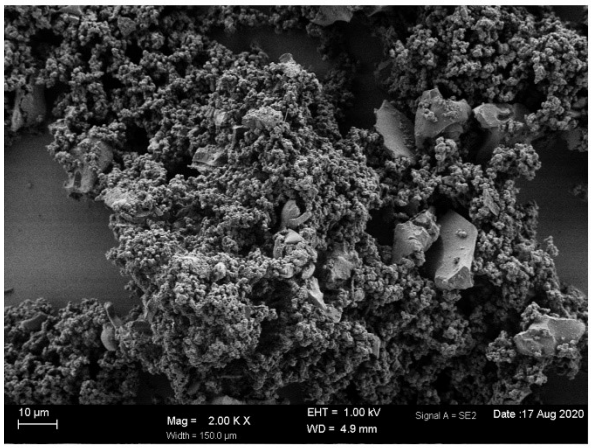


Figure S16. ^{11}B Hahn-Echo MAS NMR spectrum of ***BCNHp^{cat}***.

After Catalytic Dehydrogenation:



After 12h treatment at 200°C:

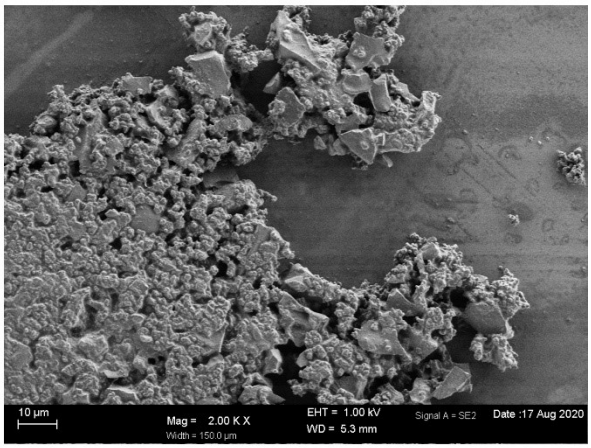
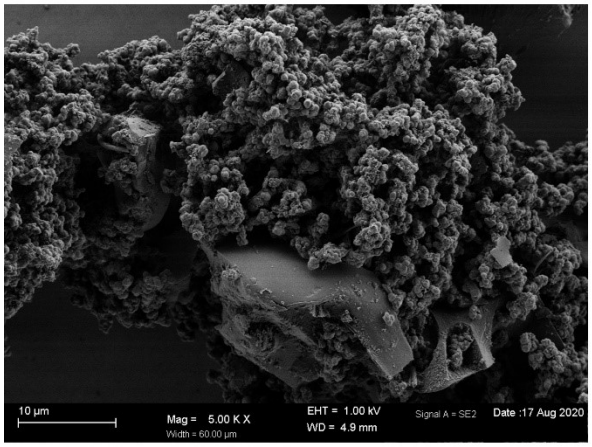


Figure S17. SEM images of ***BCNHr^{cat}*** (left) and ***BCNHp^{cat}*** (right) at a magnification of 2.00 K.

After Catalytic Dehydrogenation:



After 12h treatment at 200°C:

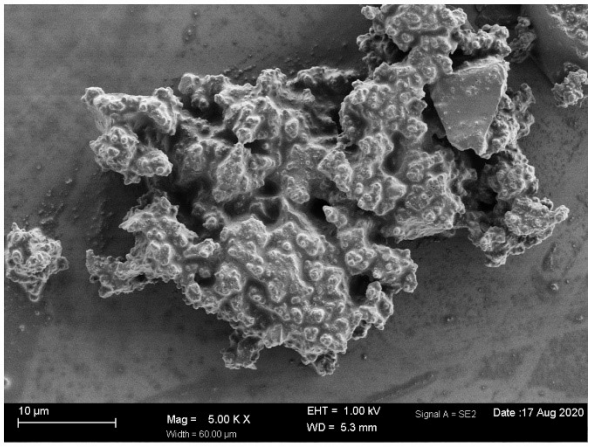
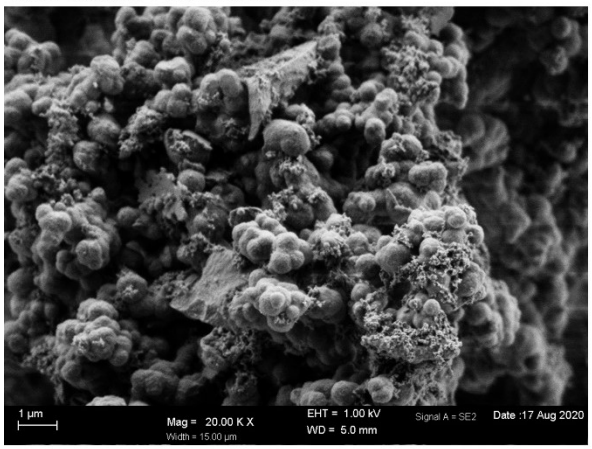


Figure S18. SEM images of ***BCNHr^{cat}*** (left) and ***BCNHp^{cat}*** (right) at a magnification of 5.00 K.

After Catalytic Dehydrogenation:



After 12h treatment at 200°C:

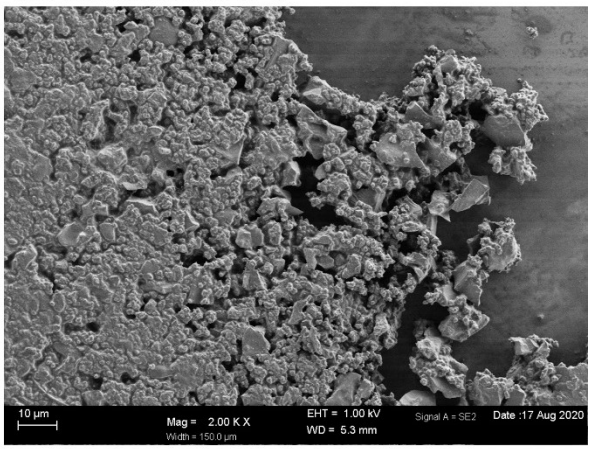
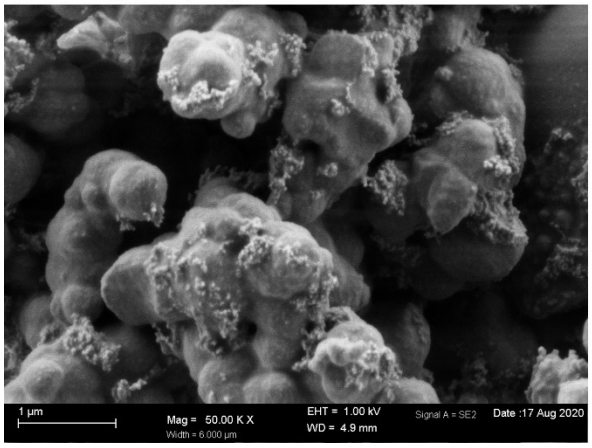


Figure S19. SEM images of ***BCNHr^{cat}*** (left) and ***BCNHp^{cat}*** (right) at a magnification 2.00 K.

After Catalytic Dehydrogenation:



After 12h treatment at 200°C:

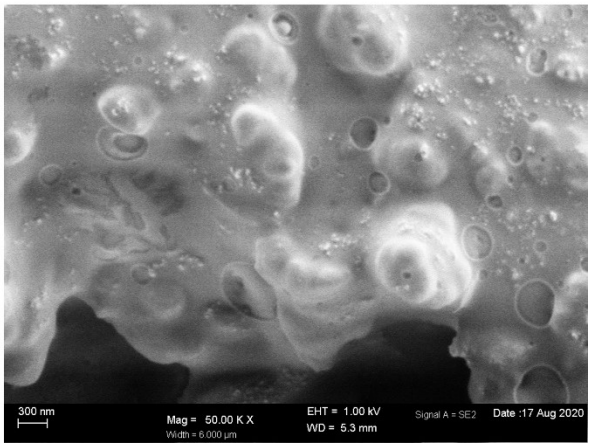


Figure S20. SEM images of ***BCNHr^{cat}*** (left) and ***BCNHp^{cat}*** (right) at a magnification of 50.00 K.

F) ^{11}B NMR MONITORING OF AB DEHYDROGENATION CATALYZED BY COMPLEX 4.

Ammonia borane (17.0 mg, 551 µmol), catalyst **4** (1.9 µmol, 0.35 mol%) and sodium tetraphenylborate (4.5 mg, 13 µmol, 2.4 mol%) were dissolved in 0.5 mL dimethoxyethane. The solution was placed in a J. Young NMR tube and heated at 80°C inside a 400 MHz spectrometer. ^{11}B{^{1}H} NMR analysis after 30 min indicates the formation of borazine and several intermediates, which are assigned based on comparison of the observed chemical shifts with previously reported in the literature.[S4]

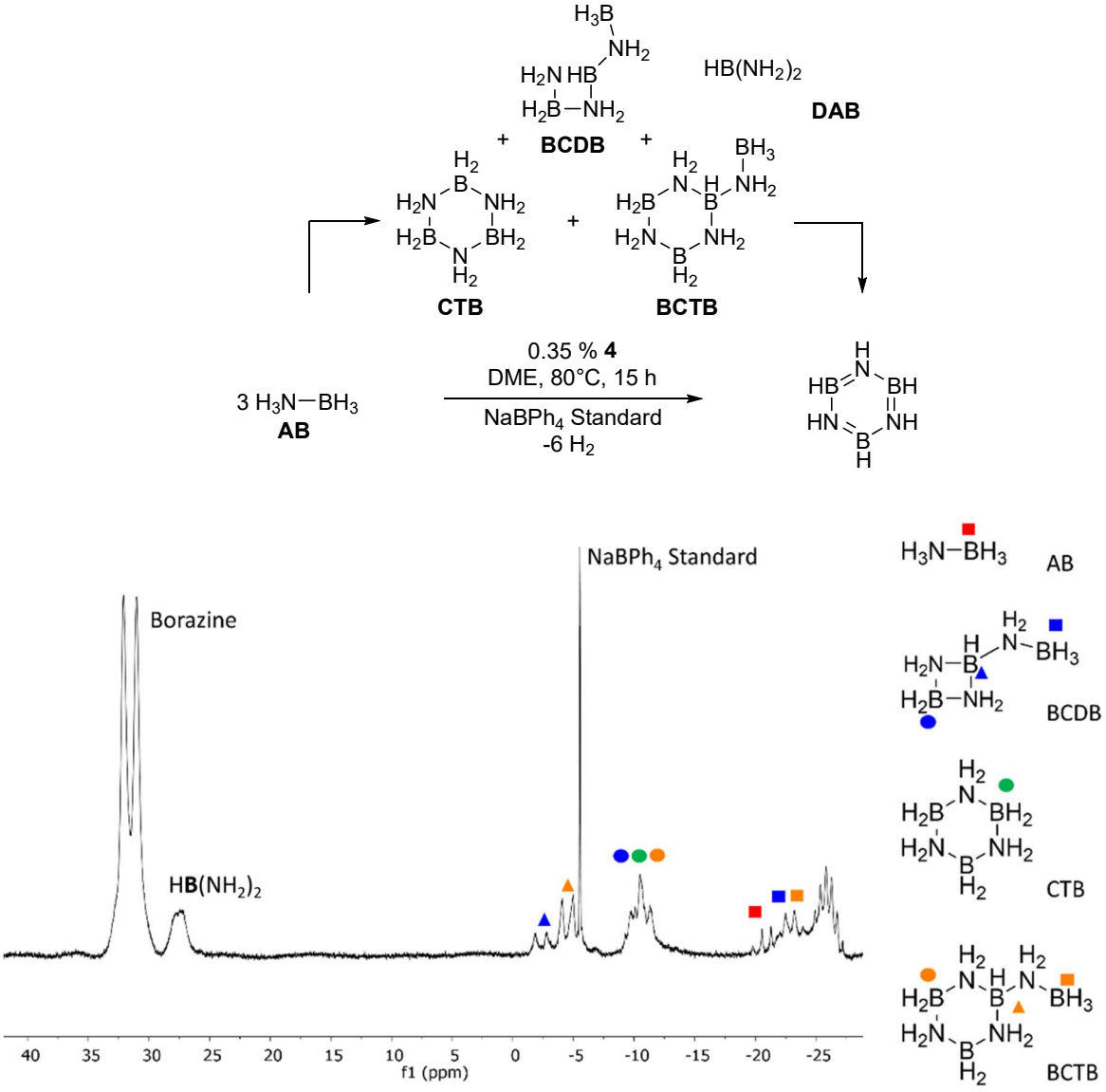
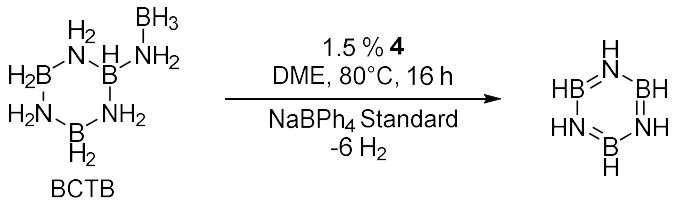


Figure S21. ^{11}B NMR (128.4 MHz) of the dehydrogenation of ammonia borane with 0.35 % **4** after 30 min at 80°C. The observed intermediates are depicted on the right. **AB**, ammonia borane; **BCDB**, *B*-(cyclodiborazanyl)amine-borane; **CTB**, cyclotriborazane; **BCTB**, *B*-(cyclotriborazanyl)amine-borane; **DAB**, diaminoborane.

G) DEHYDROGENATION OF B-(CYCLOTRIBORAZANYL)AMINE-BORANE (BCTB) CATALYZED BY 4.

B-(cyclotriborazanyl)amine-borane (**BCTB**, 15.3 mg, 0.132 mmol, 1 equiv) and **4** (2.1 mg, 1.9 µmol, 1.5 mol%) were dissolved in 0.5 mL of dimethoxyethane. The solution was placed in a J. Young NMR tube and heated at 80°C inside of a 400 MHz NMR magnet. After 16 h, borazine is formed in 63% NMR yield (Figure S41). Without catalyst, the conversion of BCTB is very low, leading to a mixture of products.



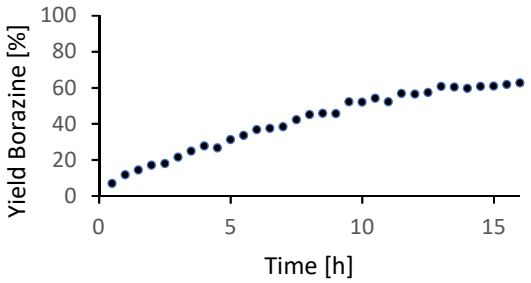
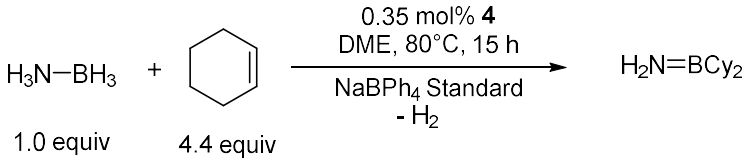


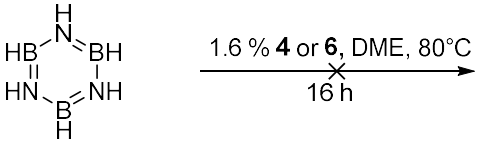
Figure S22. Yield of borazine determined by ^{11}B NMR. TOF = 4.8 h^{-1}, TON = 57.

H) TRAPPING EXPERIMENTS: HYDROBORATION OF CYCLOHEXENE BY $H_2N{=}BH_2$



Ammonia borane (17.1 mg, 0.554 mmol, 1.0 equiv), **4** (2.1 mg, 1.9 µmol, 0.35 mol%) and sodium triphenylborate (5.6 mg, 16.4 µmol, 3.0 mol%) were added to a solution of cyclohexene (250 µL, 203 mg, 2.47 mmol, 4.4 equiv) in 0.5 mL of dimethoxyethane. The solution was placed in a J. Young NMR tube and heated at 80°C inside of a 400 MHz NMR magnet. After 30 min, ^{11}B NMR showed quantitative formation of dicyclohexyl aminoborane $H_2N{=}BCy_2$ (^{11}B δ = 48.7 ppm).[S5]

I) DEHYDROGENATION OF BORAZINE WITH COMPLEX 4 OR 6



Complex **4** or **6** (1.3 µmol, 1.6 mol%) was added to a solution of borazine in dimethoxyethane (0.5 mL, 0.16 M, 80 µmol) and stirred at 80°C. After 15 h, analysis of the solution by ^{11}B NMR showed no conversion of borazine.

J) DEHYDROGENATION OF DIAMMONIATE OF DIBORANE (DADB) WITH 4

Diammoniate of diborane (DADB, 11.9 mg, 193 µmol, 1 equiv), **4** (1.4 mg, 1.3 µmol, 0.67 mol%) and sodium tetraphenylborate (5.0 mg, 15 µmol, 7.6 mol%) were dissolved in dimethoxyethane (0.5 mL). The solution was placed in a J. Young NMR tube and heated at 80°C inside a 400 MHz NMR magnet. The reaction was followed by ^{11}B NMR applying 30° pulses, with a cycle delay of 2 sec. Analysis of the solution by ^{11}B NMR indicated the formation of borazine in 50% NMR yield. Polyaminoborane, formed as insoluble solid was isolated from the reaction mixture in 32 % yield.

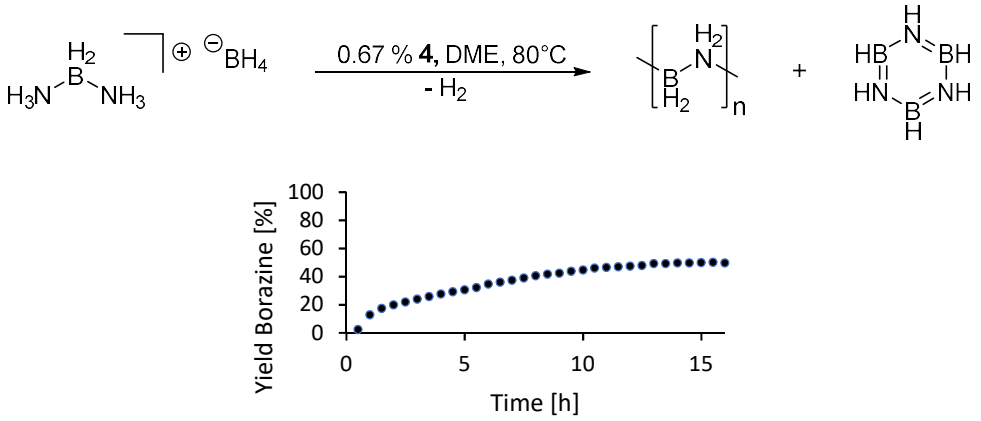


Figure S23. Formation of borazine by dehydrogenation of DADB catalyzed by **4**.

K) SYNTHESIS AND CHARACTERIZATION OF COMPLEX 11 AND H/D EXCHANGE EXPERIMENTS

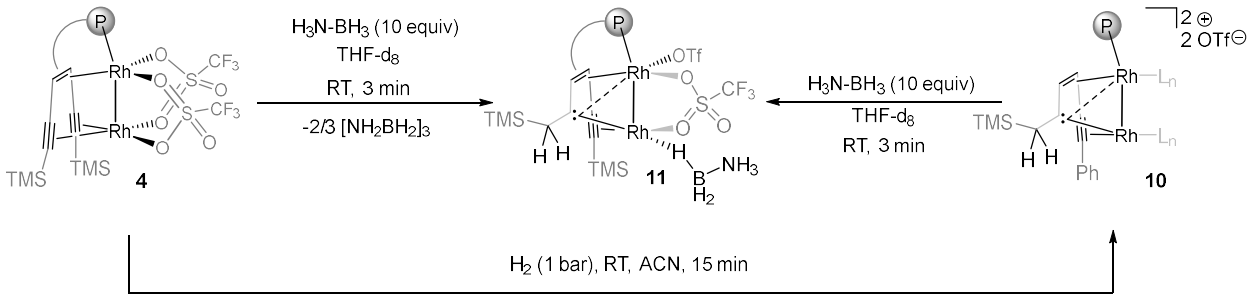


Figure S24. Formation of intermediate **11** by reaction of **4** with ammonia borane.

Method A. Complex **4** (10.1 mg, 9.4 μmol) and ammonia borane (3 mg, 94 μmol, 10 equiv) were dissolved in THF-d_8 (0.5 mL). Formation of complex **11** was observed within minutes by NMR analysis of the reaction mixture.

Method B. Following a previously reported procedure, complex **4** (15.2 mg, 14.1 μmol) was dissolved in acetonitrile and placed in a J. Young NMR tube. The tube was freed from argon by three freeze pump thaw cycles and pressurized with hydrogen (1 bar). The tube was shaken for 15 min and freed from hydrogen by three freeze pump thaw cycles. The acetonitrile was removed under vacuum affording complex **10**.[S2] To a solution of complex **10** (14 μmol) in THF-d_8 (0.5 mL) was added ammonia borane (3.7 mg, 0.12 mmol, 8.5 equiv) and the mixture analyzed immediately by NMR spectroscopy. Formation of complex **11** was observed within minutes.

^{1}H NMR (400 MHz, THF-d_8) δ (ppm) = -11.37 (dd br, $^1J_{HRh}$ = 25.3 Hz, $^3J_{HP}$ = 5.0 Hz, 1 H, Rh-H), 0.32 (s, 9 H, CH_3SiCH$_2$), 0.37 (s, 9 H, CH_3Si-C≡C), 2.58 (dt, $^2J_{HH}$ = 11.2 Hz, $^3J_{HRh}$ = 2.1 Hz, 1 H, TMS-CH$_2$), 2.60 (br, 2 H, BH$_2$), 3.14 (d, $^2J_{HH}$ = 11.1 Hz, 1 H, TMS-CH$_2$), 5.24 (d, $^2J_{HP}$ = 14.7 Hz, 1 H, CH$_{benz}$), 5.70 (s br, 3 H, NH$_3$), 6.93-7.45 (m, 12 H, CH$_{ar}$), 7.71 (m, 4 H, CH$_{ar}$), 8.22 (d, J = 7.7 Hz, 2 H, CH$_{ar}$). An accurate integration of all the signals from the complex was not possible due to overlapping with those corresponding to AB.

^{13}C NMR (125.8 MHz, THF-d_8) δ (ppm) = 0.7 (s, 1 C, CH$_3$Si-C≡C), 1.0 (s, 1 C, CH$_3$Si-CH$_2$), 45.7 (s, 1 C, CH$_2$) 51.3 (d, $^1J_{CP}$ = 19.8 Hz, 1 C, CH$_{benz}$), 79.0 (m, 1 C, C=C-C$_{Carbene}$), 80.7 (s, 1 C, TMS-C≡C), 98.9 (s, 1 C, C=C-C$_{Carbene}$), 107.6 (s, 1 C, TMS-C≡C), 118.1-142.9 (CH$_{ar}$ and C$_{ar}$), 184.0 (1 C, C$_{Carbene}$).

^{11}B NMR (160.5 MHz, THF-d_8) δ (ppm) = −0.24 (t br, $^1J_{BH}$ = 118 Hz).

^{15}N NMR (50.7 MHz, THF-d_8). δ (ppm) = 40.9 (q, $^1J_{NH}$ = 70.1 Hz).

^{19}F{^{1}H} NMR (188.3 MHz, THF-d_8) δ (ppm) −79.4 (s).

^{29}Si NMR (99.4 MHz, THF-d_8) δ (ppm) = −12.2 (s, 1 Si, CH$_3$Si-C≡C), 0.3 (s, 1 Si, CH$_3$SiCH$_2$).

^{13}P{^{1}H} NMR (202.5 MHz, THF-d_8) δ (ppm) 53.7 (dd, $^1J_{PRh}$ = 144.3 Hz, $^2J_{PRh}$ = 18.7 Hz).

^{103}Rh NMR (15.8 MHz, THF-d_8) δ (ppm) = −7752 (d, $^2J_{RhP}$ = 17 Hz, 1 Rh, P-Rh), −7500 (d, $^1J_{RhP}$ = 143 Hz, 1 Rh, P-Rh).

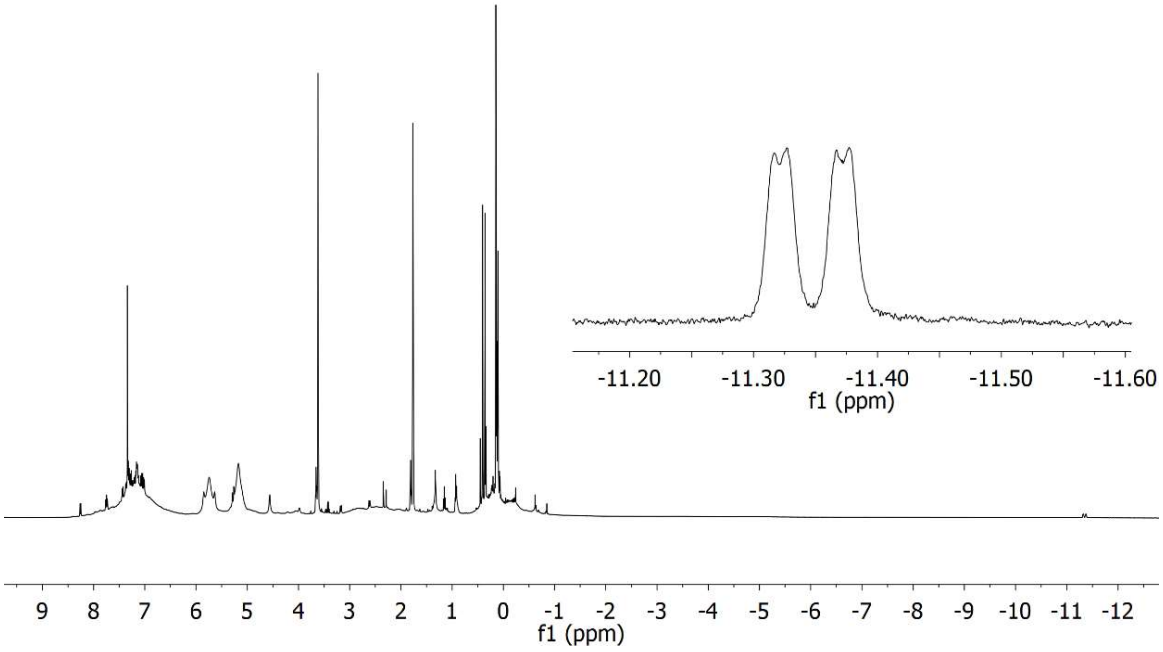


Figure S25. ^{1}H NMR (400 MHz, THF-d_8) spectrum of **11**.

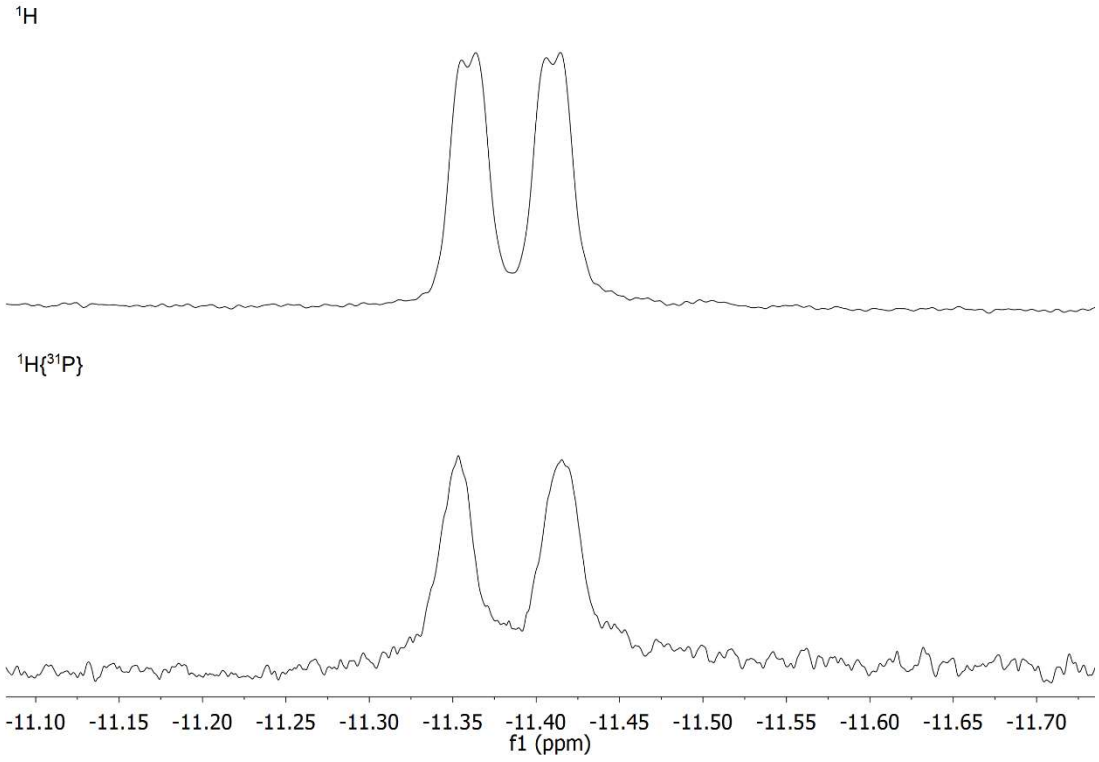


Figure S26. Comparison of ^{1}H (top) and ^{1}H{^{31}P} (bottom) spectra indicates that the coupling of J = 5.0 Hz is a ^{1}H-^{31}P coupling.

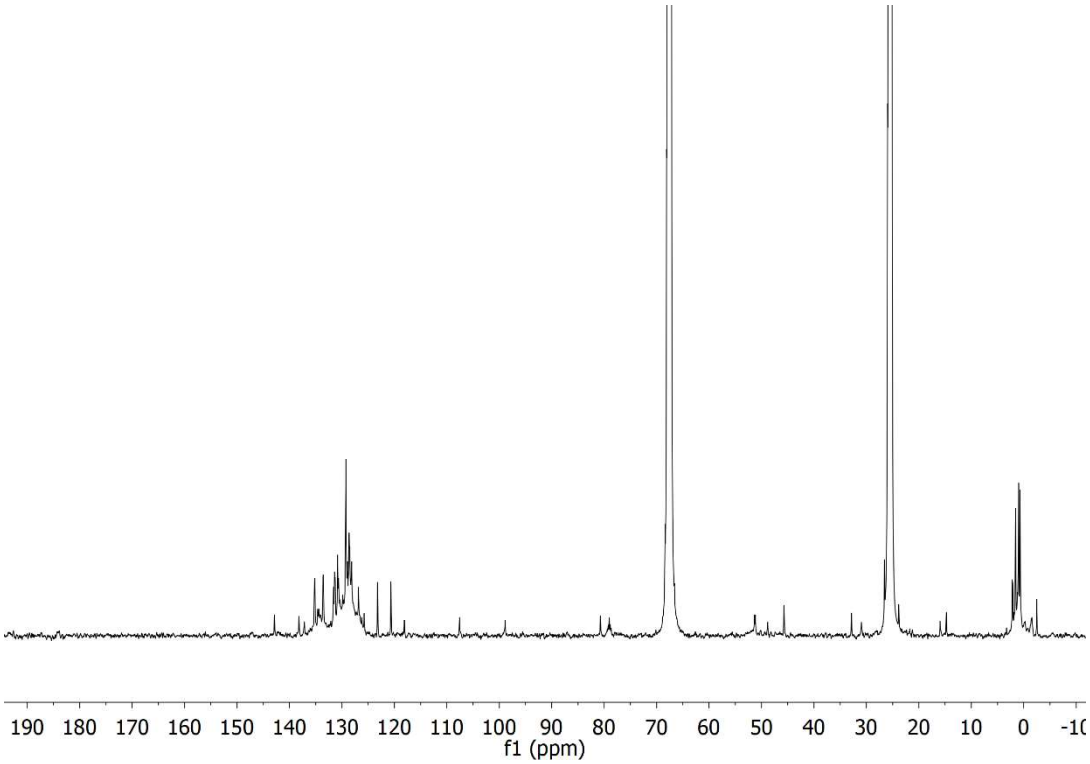


Figure S27. $^{13}C\{^{1}H\}$ NMR (125.8 MHz, THF-d_8) spectrum of **11**.

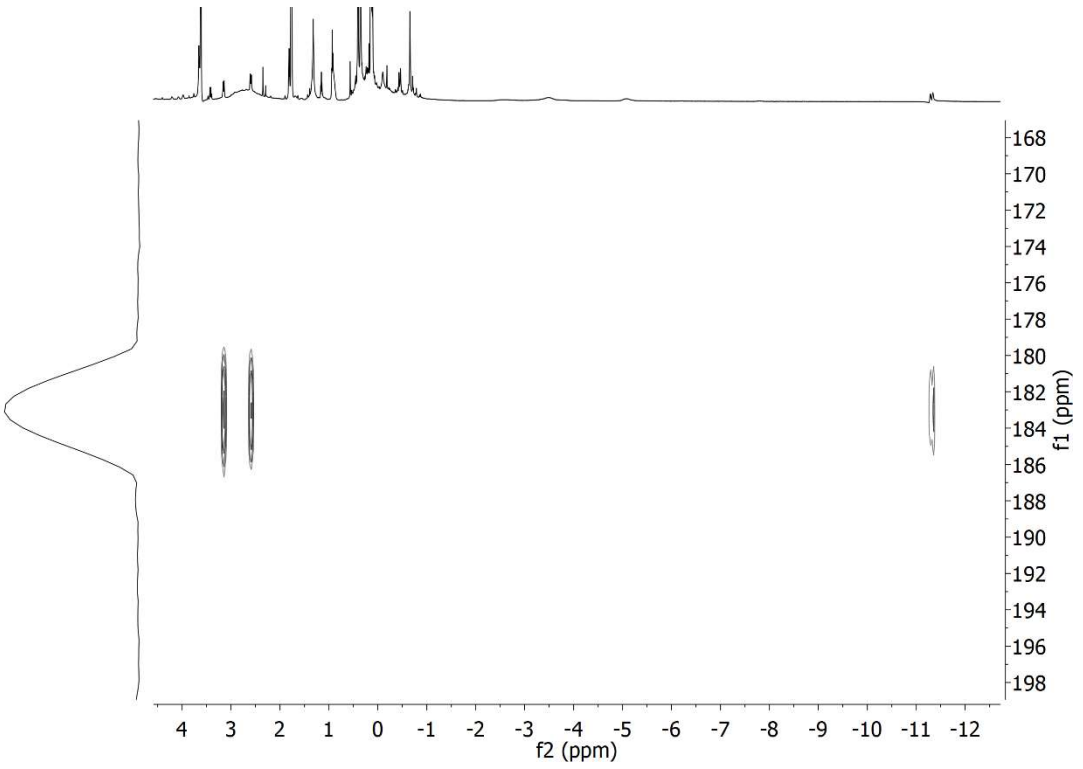


Figure S28. $^{1}H^{13}C$ HMBC spectrum of complex **11**. Selected region showing the ^{13}C carbene resonance.

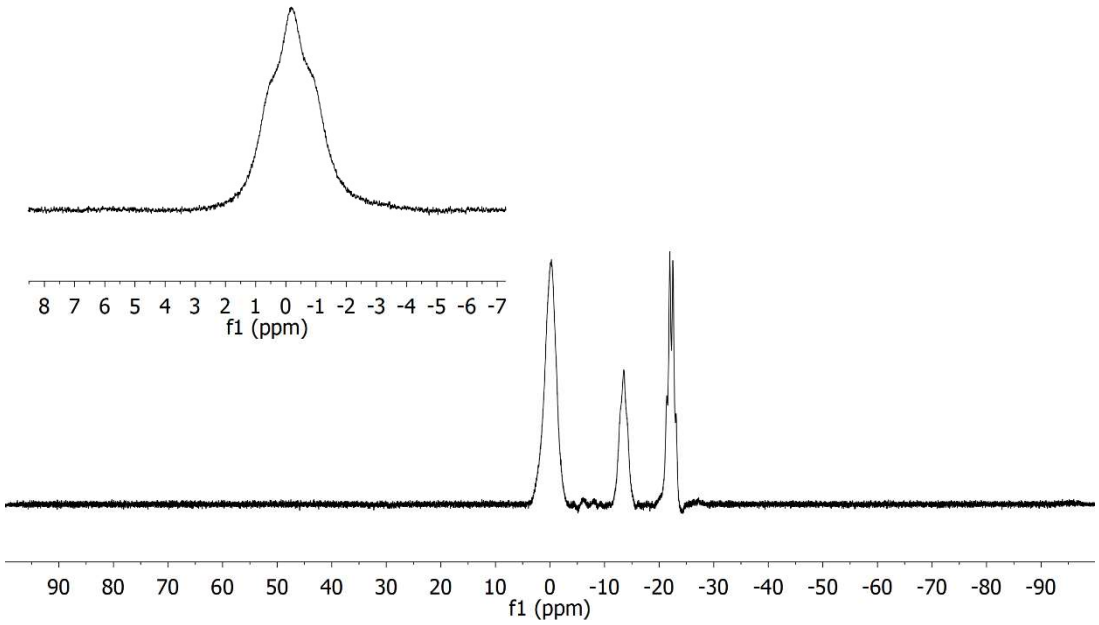


Figure S29. ^{11}B NMR (160.5 MHz, THF-d_8) spectrum of the reaction mixture of complex **4** and **AB**. Top: Amplified area of signal assigned to borane ligand in **11**. Other signals: **CTB** (−13.4 ppm), ammonia borane (−22.2 ppm).

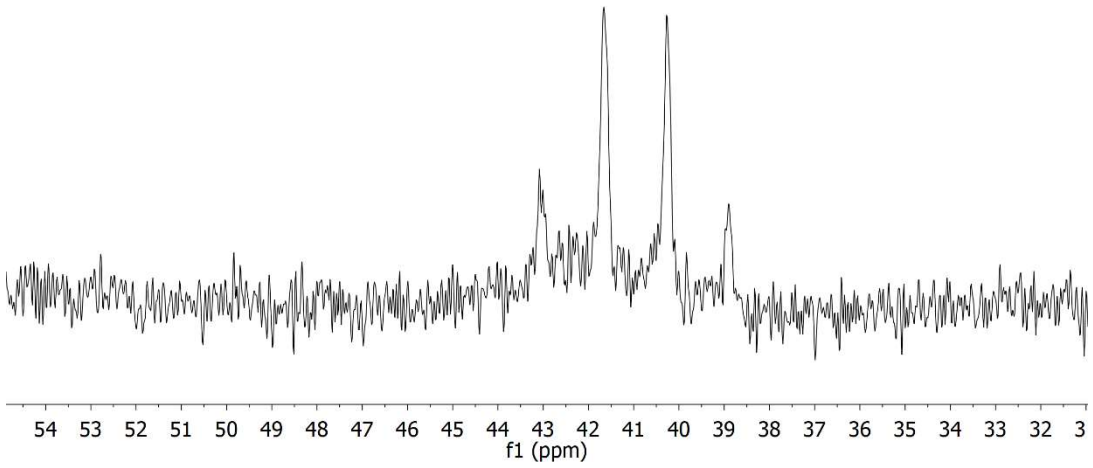


Figure S30. ^{15}N NMR (50.7 MHz, THF-d_8) spectrum of **11**.

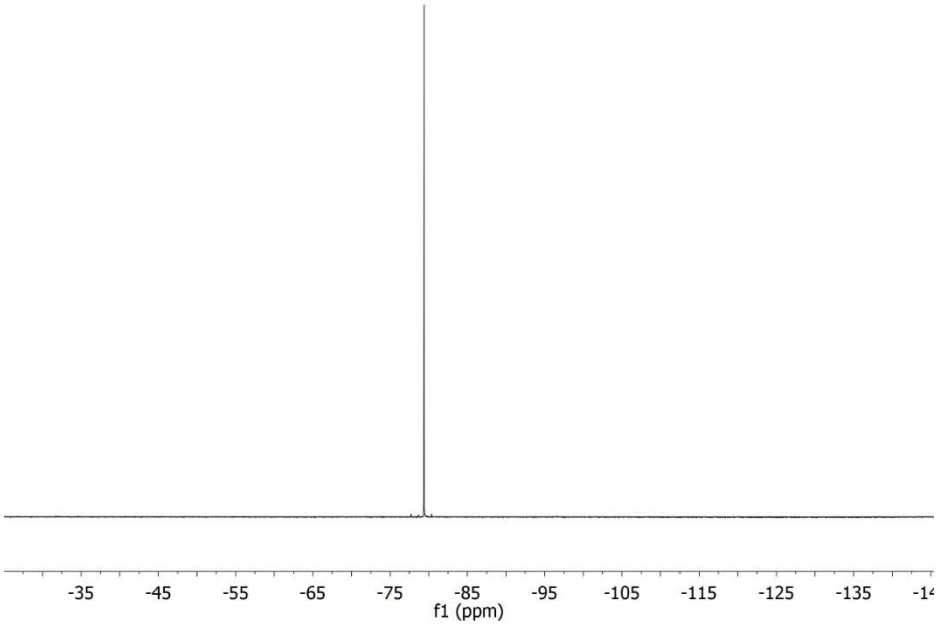


Figure S31. $^{19}F\{^{1}H\}$ NMR (188.3 MHz, THF-d_8) of **11**.

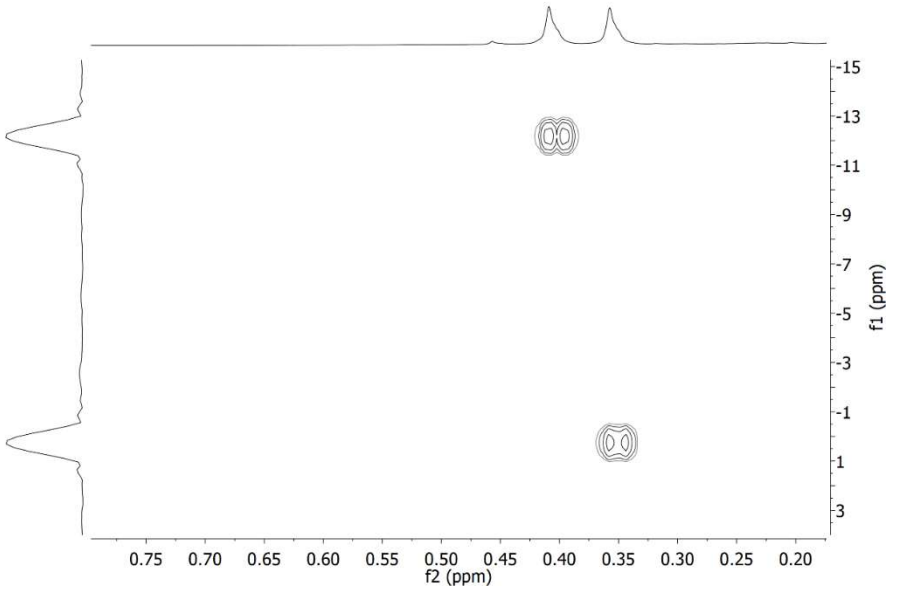


Figure S32. $^{1}H^{29}Si$ HMQC (400 MHz, 99.4 MHz, THF-d_8) spectrum of **11**.

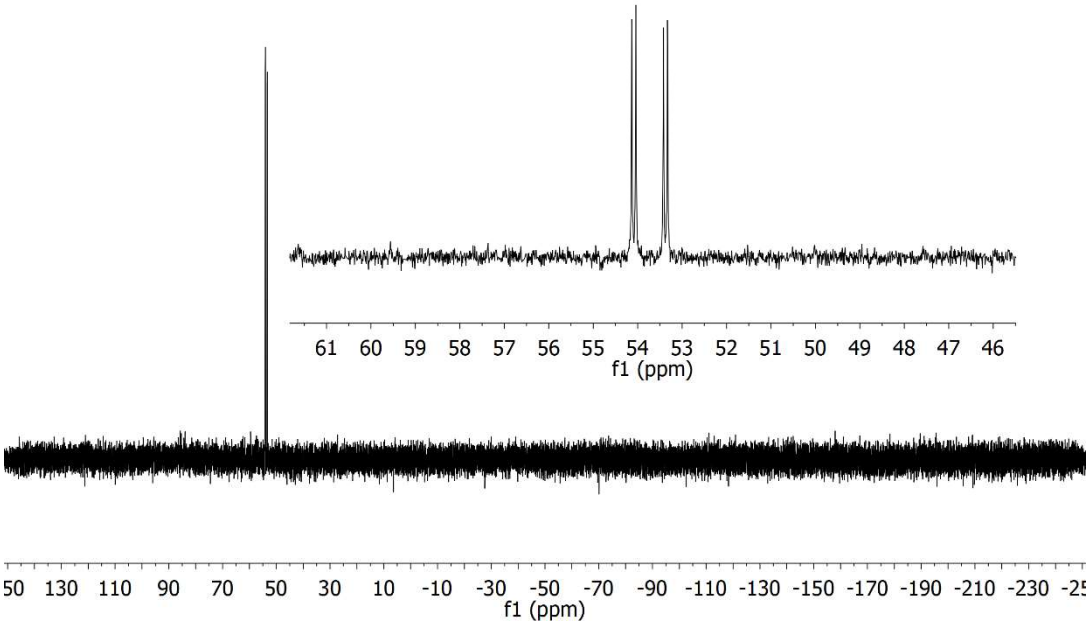


Figure S33. $^{31}P\{^{1}H\}$ NMR (202.5 MHz, THF-d_8) spectrum of **11**.

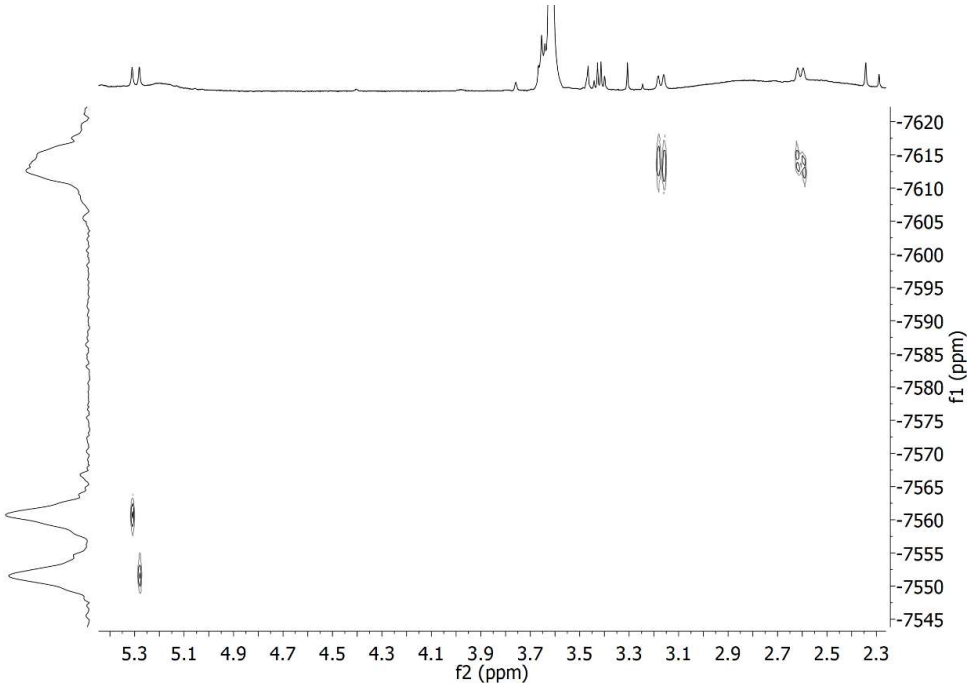


Figure S34. ^{1}H-^{103}Rh (400MHz, 15.8 MHz, THF-d_8) HMQC spectrum of **11**.

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L) CATALYTIC DEHYDROGENATION OF AMMONIA BORANE BY COMPLEX 11

Complex **11** was prepared in situ and used in the catalytic test. Complex **4** (10.1 mg, 9.4 µmol) and ammonia borane (0.9 mg, 30 µmol) were dissolved in THF (1 mL). After 3 min at room temperature 198 µL from the resulting solution were taken and the solvent was evaporated. The obtained solid was dissolved in dimethoxyethane (0.5 mL). Ammonia borane (17.2 mg, 557 µmol) and sodium tetraphenylborate (6.9 mg, 20 µmol) were added to the solution of complex **11**. The reaction mixture was placed in a J. Young NMR tube and heated at 80°C inside a 400 MHz NMR magnet. The reaction was monitored by ^{11}B NMR applying 30° pulses, with a cycle delay of 2 sec. The same experiment was accomplished using catalyst **4** for comparison. The obtained yield of borazine vs. time for both experiments is depicted in Figure S35.

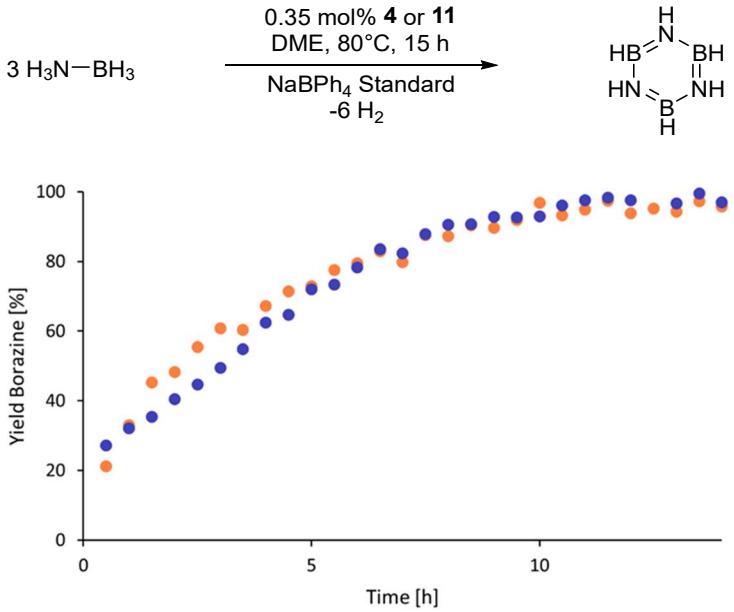
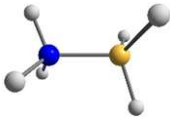


Figure S35. Comparison of borazine obtained in the catalyzed dehydrogenation of AB by complex **4** (blue) or complex **11** (orange)

IV. COMPUTATIONAL DETAILS

Density functional calculations were performed using Gaussian09[S6], revision D.01. Geometry optimizations were performed using the PBE0-D3[S7] functional in combination with the def2-SVP basis set.[S8] Solvent effects were taken into account implicitly using the SMD[S9] method with THF as solvent. The nature of each stationary point was confirmed by frequency calculations (no imaginary frequencies for minima and one for transition states). Intrinsic reaction coordinate (IRC) calculations were performed to obtain additional proof for the position of the transition state geometries. Cartesian coordinates are given in angstroms and energies in Hartree.

H_3NBH_3



E(RPBE1PBE) = -83.0629971307

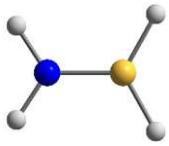
- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.069787 (Hartree/Particle)
Thermal correction to Energy= 0.073494
Thermal correction to Enthalpy= 0.074438
Thermal correction to Gibbs Free Energy= 0.046415
Sum of electronic and zero-point Energies= -82.993210
Sum of electronic and thermal Energies= -82.989504
Sum of electronic and thermal Enthalpies= -82.988559
Sum of electronic and thermal Free Energies= -83.016582

N	8.092500000	3.739075000	4.016606000
H	8.092500000	2.739675000	4.233850000
H	7.272068000	4.140007000	4.477256000
B	8.092500000	4.015799000	2.439262000
H	7.076621000	3.501594000	1.974317000
H	8.912932000	4.140007000	4.477256000
H	9.108379000	3.501594000	1.974317000
H	8.092500000	5.235149000	2.279492000

H_2NBH_2



E(RPBE1PBE) = -81.8730944296

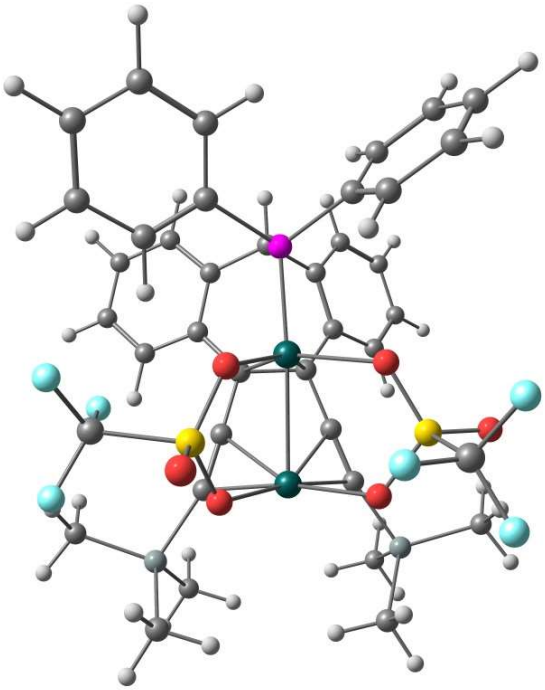
- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.047603 (Hartree/Particle)
Thermal correction to Energy= 0.050834
Thermal correction to Enthalpy= 0.051778
Thermal correction to Gibbs Free Energy= 0.025196
Sum of electronic and zero-point Energies= -81.825492
Sum of electronic and thermal Energies= -81.822260
Sum of electronic and thermal Enthalpies= -81.821316
Sum of electronic and thermal Free Energies= -81.847898

N	8.091343000	4.222953000	3.598251000
H	7.274921000	4.077105000	4.182047000
B	8.019771000	4.504534000	2.246620000
H	6.934964000	4.586254000	1.711482000
H	8.965554000	4.140532000	4.105806000
H	9.042439000	4.665676000	1.615906000

4



E(RPBE1PBE) = -4490.97466646

- Thermochemistry -

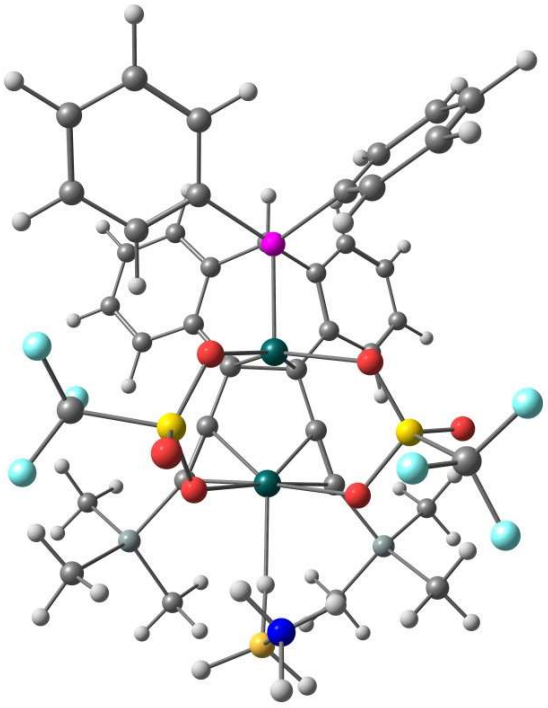
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.684778 (Hartree/Particle)
Thermal correction to Energy= 0.745663
Thermal correction to Enthalpy= 0.746607
Thermal correction to Gibbs Free Energy= 0.586536
Sum of electronic and zero-point Energies= -4490.289889
Sum of electronic and thermal Energies= -4490.229004
Sum of electronic and thermal Enthalpies= -4490.228060
Sum of electronic and thermal Free Energies= -4490.388130

Rh	2.509711000	3.111204000	5.394019000
Rh	4.379559000	3.872411000	3.704087000
S	1.583486000	2.880945000	2.273096000
S	2.464299000	6.279050000	4.794597000
P	6.213017000	4.243130000	2.505181000
Si	2.500133000	4.247818000	8.730351000
Si	1.717630000	-0.339138000	5.888752000
F	2.983307000	0.641054000	2.198775000
O	1.709145000	5.082327000	5.310843000
O	2.868596000	3.588926000	2.041528000
O	1.288795000	2.620742000	3.723930000
F	0.159177000	7.507104000	4.750735000
O	3.418052000	5.942421000	3.707630000
F	0.608019000	6.398957000	2.956386000
F	2.106721000	1.223169000	0.320103000
F	0.869199000	0.389068000	1.878251000
O	2.947699000	7.191029000	5.818370000
O	0.443664000	3.353339000	1.511773000
F	1.606990000	8.269589000	3.345995000
C	2.920501000	1.017755000	5.434335000
C	5.185109000	2.208401000	4.574385000
C	5.442790000	3.444011000	5.386518000
C	3.948964000	1.604713000	5.009243000
C	4.356954000	3.637207000	6.319946000
C	6.220906000	1.351641000	3.956597000
C	3.458901000	3.787158000	7.188652000
C	7.833495000	3.940187000	4.779349000
C	6.016962000	-0.033824000	3.875174000
H	5.116286000	-0.468166000	4.315449000
C	7.380437000	1.906303000	3.373743000
C	6.785342000	3.962696000	5.723154000
C	1.115619000	7.173000000	3.899610000
C	7.027910000	4.496026000	6.997536000
H	6.216551000	4.520294000	7.729192000
C	8.293903000	1.064481000	2.733560000
H	9.183590000	1.503456000	2.273790000
C	6.220949000	3.488113000	0.844324000
C	1.908905000	1.171508000	1.627529000
C	7.631073000	3.393930000	3.387700000
H	8.532904000	3.591451000	2.790900000
C	9.092676000	4.424060000	5.148500000
H	9.906171000	4.393600000	4.418039000
C	6.934338000	-0.859478000	3.233053000
H	6.750218000	-1.935341000	3.179338000
C	5.511147000	2.294757000	0.653622000
H	4.950515000	1.861946000	1.483372000
C	5.682981000	6.850068000	1.797691000
H	4.662878000	6.484238000	1.661792000
C	6.690491000	5.977805000	2.237341000
C	8.282029000	4.987152000	7.345020000
H	8.445793000	5.398956000	8.343900000
C	8.079657000	-0.309716000	2.658989000
H	8.803346000	-0.947815000	2.145964000
C	2.896370000	6.035021000	9.113906000
H	3.966919000	6.163164000	9.341922000
H	2.316174000	6.381817000	9.985137000
H	2.656361000	6.672510000	8.248535000
C	9.323308000	4.945545000	6.418851000
H	10.314273000	5.323482000	6.682093000
C	-0.016450000	0.260554000	5.526112000
H	-0.259642000	1.171143000	6.096970000
H	-0.745783000	-0.517576000	5.805984000
H	-0.140858000	0.488810000	4.457449000

C	5.515182000	1.668567000	-0.590037000
H	4.951607000	0.742728000	-0.729426000
C	5.976846000	8.187710000	1.547124000
H	5.184956000	8.859899000	1.207282000
C	0.685045000	4.003848000	8.338633000
H	0.375636000	4.654767000	7.506402000
H	0.067036000	4.248196000	9.218607000
H	0.469742000	2.959346000	8.059343000
C	3.065530000	3.088507000	10.091708000
H	2.863171000	2.037811000	9.828201000
H	2.533528000	3.312401000	11.031606000
H	4.146435000	3.191344000	10.279246000
C	6.224321000	2.231451000	-1.652016000
H	6.222505000	1.743959000	-2.630492000
C	2.177824000	-1.818560000	4.832882000
H	2.143482000	-1.561350000	3.762540000
H	1.474903000	-2.649942000	5.008322000
H	3.191730000	-2.178651000	5.070693000
C	6.929296000	4.052293000	-0.224303000
H	7.477103000	4.988681000	-0.090560000
C	1.949474000	-0.684985000	7.716353000
H	2.988718000	-0.976961000	7.936888000
H	1.286615000	-1.502747000	8.044701000
H	1.711966000	0.206868000	8.318844000
C	6.929579000	3.421535000	-1.467884000
H	7.480363000	3.867462000	-2.300084000
C	7.991165000	6.462783000	2.423081000
H	8.793741000	5.804499000	2.758327000
C	7.272975000	8.668394000	1.739753000
H	7.500538000	9.720528000	1.549593000
C	8.277198000	7.805498000	2.176859000
H	9.293967000	8.176765000	2.328357000

4(AB)



E(RPBE1PBE) = -4574.06488198

- Thermochemistry -

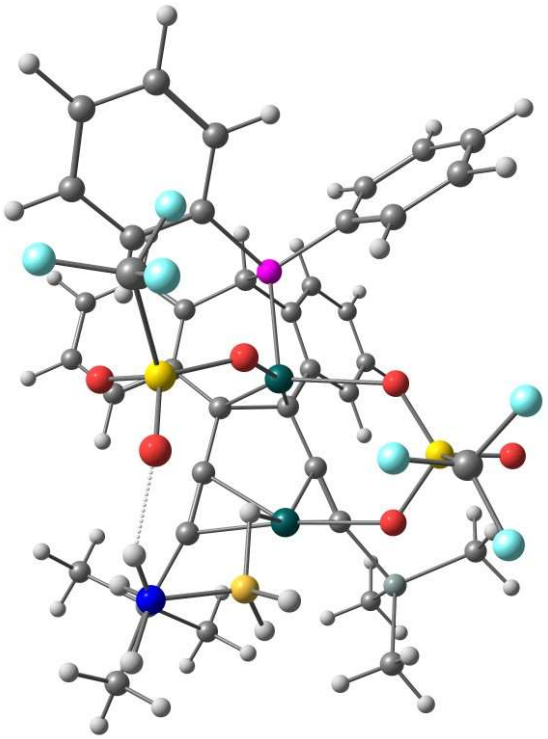
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.756778 (Hartree/Particle)
Thermal correction to Energy= 0.822075
Thermal correction to Enthalpy= 0.823019
Thermal correction to Gibbs Free Energy= 0.655437
Sum of electronic and zero-point Energies= -4573.308104
Sum of electronic and thermal Energies= -4573.242807
Sum of electronic and thermal Enthalpies= -4573.241863
Sum of electronic and thermal Free Energies= -4573.409445

Rh	7.342004000	-2.972918000	0.745995000
Rh	7.544788000	-2.626399000	-1.897125000
S	4.536164000	-3.530292000	-0.965070000
S	6.907612000	0.061656000	-0.303643000
P	8.044661000	-2.606353000	-4.065355000
Si	9.751668000	-1.239581000	2.834839000
Si	7.409930000	-6.384858000	2.037356000
F	5.417684000	-5.962325000	-1.437561000
O	6.621432000	-0.932995000	0.793597000
O	5.339041000	-3.030250000	-2.107100000
O	5.306108000	-3.615485000	0.324128000
F	5.478451000	1.707185000	1.131653000
O	6.695702000	-0.507383000	-1.657161000

F	4.332466000	0.522548000	-0.255619000
F	3.667954000	-5.404182000	-2.565021000
F	3.491977000	-5.879202000	-0.469703000
O	8.096441000	0.877948000	-0.116861000
O	3.209160000	-2.959550000	-0.807311000
F	5.522807000	2.171544000	-0.975600000
C	7.802147000	-5.058302000	0.779667000
C	8.841401000	-4.161316000	-1.545562000
C	9.485255000	-2.827136000	-1.325951000
C	8.232765000	-4.593263000	-0.312043000
C	9.277367000	-2.434750000	0.047621000
C	9.277180000	-5.162987000	-2.542174000
C	9.219087000	-2.109486000	1.267083000
C	10.790340000	-2.537820000	-3.458953000
C	9.209565000	-6.528304000	-2.229176000
H	8.875548000	-6.831648000	-1.234759000
C	9.710330000	-4.777631000	-3.829390000
C	10.649070000	-2.309568000	-2.073880000
C	5.460913000	1.194246000	-0.090376000
C	11.627809000	-1.561032000	-1.404151000
H	11.517229000	-1.376938000	-0.333533000
C	10.057216000	-5.763960000	-4.756780000
H	10.378667000	-5.459076000	-5.756451000
C	7.032547000	-3.703278000	-5.117454000
C	4.261285000	-5.314553000	-1.385626000
C	9.766000000	-3.325026000	-4.238839000
H	10.018845000	-3.283465000	-5.308275000
C	11.915599000	-2.034528000	-4.119819000
H	12.028455000	-2.225887000	-5.190720000
C	9.557136000	-7.499051000	-3.163182000
H	9.493737000	-8.556656000	-2.895103000
C	6.463706000	-4.846935000	-4.541385000
H	6.596505000	-5.037463000	-3.475253000
C	6.839719000	-0.238400000	-4.752606000
H	6.023549000	-0.617529000	-4.132700000
C	8.011452000	-0.995266000	-4.907602000
C	12.733550000	-1.053778000	-2.078448000
H	13.481052000	-0.471834000	-1.533593000
C	9.983018000	-7.116976000	-4.434475000
H	10.252174000	-7.870562000	-5.178646000
C	11.423164000	-0.480275000	2.440990000
H	12.159210000	-1.246995000	2.151269000
H	11.815180000	0.046758000	3.327195000
H	11.340504000	0.253159000	1.622999000
C	12.883148000	-1.295931000	-3.443244000
H	13.749720000	-0.907030000	-3.983578000
C	8.089924000	-5.859394000	3.698444000
H	9.164359000	-5.627193000	3.633866000
H	7.958707000	-6.671807000	4.432411000
H	7.562041000	-4.970937000	4.075658000
C	5.728955000	-5.734136000	-5.324043000
H	5.284835000	-6.619669000	-4.862770000
C	6.719209000	0.999352000	-5.377615000
H	5.803207000	1.581894000	-5.251013000
C	8.504915000	0.089557000	3.257935000
H	8.351677000	0.767841000	2.405778000
H	8.866835000	0.674956000	4.119641000
H	7.535234000	-0.354822000	3.526618000
C	9.886792000	-2.508872000	4.204697000
H	8.910221000	-2.976897000	4.401804000
H	10.225158000	-2.024386000	5.135755000
H	10.608684000	-3.300804000	3.949747000
C	5.554094000	-5.483749000	-6.685551000
H	4.973220000	-6.177341000	-7.299301000
C	5.555500000	-6.639496000	2.084060000
H	5.026903000	-5.686741000	2.232260000
H	5.290235000	-7.315865000	2.913720000
H	5.199203000	-7.093858000	1.147384000
C	6.851843000	-3.452959000	-6.483816000
H	7.282950000	-2.558593000	-6.941727000
C	8.265942000	-7.937246000	1.417195000
H	7.867273000	-8.246898000	0.437855000
H	8.098291000	-8.767851000	2.123594000
H	9.353403000	-7.790157000	1.321142000
C	6.114721000	-4.343624000	-7.263182000
H	5.974247000	-4.142303000	-8.328364000
C	9.060312000	-0.493711000	-5.687142000
H	9.982179000	-1.061361000	-5.820679000
C	7.768353000	1.497222000	-6.152658000
H	7.675323000	2.472410000	-6.637776000
C	8.936299000	0.751260000	-6.304651000
H	9.760919000	1.138138000	-6.908751000
N	4.671649000	-1.954965000	2.602257000
H	5.057705000	-1.077782000	2.241865000
B	5.760866000	-2.779126000	3.397668000
H	6.166527000	-2.115169000	4.341935000
H	4.355751000	-2.483726000	1.782182000
H	6.740574000	-2.986743000	2.630284000
H	5.286272000	-3.855734000	3.728666000
H	3.854075000	-1.732719000	3.173208000

4(AB)'



E(RPBE1PBE) = -4574.06393199

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.759264 (Hartree/Particle)
Thermal correction to Energy= 0.823562
Thermal correction to Enthalpy= 0.824507
Thermal correction to Gibbs Free Energy= 0.659019
Sum of electronic and zero-point Energies= -4573.304668
Sum of electronic and thermal Energies= -4573.240370
Sum of electronic and thermal Enthalpies= -4573.239425
Sum of electronic and thermal Free Energies= -4573.404913

Rh	7.379920000	-2.717186000	0.598497000
Rh	7.614695000	-2.509624000	-2.136180000
S	4.447896000	-3.609148000	-2.488525000
S	6.979888000	0.357740000	-0.457158000
P	8.241589000	-2.576328000	-4.263555000
Si	9.856338000	-1.173786000	2.652527000
Si	7.790068000	-6.016524000	2.173411000
F	4.130112000	-2.911870000	-5.029116000
O	7.004728000	-0.616107000	0.688857000
O	5.419186000	-2.481148000	-2.609458000
O	5.023730000	-4.951318000	-2.576451000
F	4.854601000	1.353790000	0.703692000
O	7.178452000	-0.262785000	-1.786550000
F	4.413917000	-0.109827000	-0.814452000
F	2.424013000	-2.530511000	-3.783896000
F	2.887443000	-4.548332000	-4.382973000
O	7.730849000	1.576971000	-0.199163000
O	3.453146000	-3.432980000	-1.411929000
F	5.062289000	1.863424000	-1.382325000
C	7.656873000	-4.852573000	0.714010000
C	8.710252000	-4.161103000	-1.672429000
C	9.511059000	-2.904621000	-1.479710000
C	8.058454000	-4.484588000	-0.424917000
C	9.386374000	-2.448884000	-0.117031000
C	9.055363000	-5.245711000	-2.618737000
C	9.412661000	-2.090009000	1.085970000
C	10.936344000	-2.885961000	-3.562036000
C	8.798921000	-6.579961000	-2.271993000
H	8.383044000	-6.803695000	-1.287592000
C	9.581728000	-4.964587000	-3.898708000
C	10.768189000	-2.583792000	-2.196022000
C	5.206344000	0.894156000	-0.489158000
C	11.819799000	-1.954309000	-1.511282000
H	11.696953000	-1.709311000	-0.454192000
C	9.835081000	-6.018391000	-4.780790000
H	10.227700000	-5.789988000	-5.775324000
C	7.181562000	-3.441809000	-5.473401000
C	3.410347000	-3.382626000	-4.024227000
C	9.839337000	-3.548327000	-4.352567000
H	10.126259000	-3.578096000	-5.413415000
C	12.148330000	-2.581299000	-4.189985000
H	12.273837000	-2.833625000	-5.246672000
C	9.052924000	-7.619115000	-3.162043000
H	8.838235000	-8.649477000	-2.867653000
C	6.657276000	-4.697645000	-5.138126000
H	6.825410000	-5.116901000	-4.146366000
C	7.571763000	0.042015000	-4.789793000
H	6.705630000	-0.176384000	-4.161294000
C	8.543296000	-0.945122000	-5.012094000
C	13.014857000	-1.642873000	-2.151123000
H	13.816145000	-1.151912000	-1.593314000
C	9.575354000	-7.339374000	-4.423637000
H	9.771694000	-8.145932000	-5.134271000
C	10.267505000	0.578732000	2.135804000
H	11.174208000	0.604658000	1.509702000
H	10.446977000	1.211459000	3.021156000
H	9.440299000	1.014494000	1.553414000
C	13.185354000	-1.962907000	-3.497350000
H	14.121262000	-1.727812000	-4.010198000
C	9.174321000	-5.347363000	3.243238000
H	10.098228000	-5.225325000	2.656786000
H	9.382201000	-6.034141000	4.080427000

H	8.899000000	-4.369040000	3.665416000
C	5.880533000	-5.398731000	-6.057085000
H	5.467567000	-6.371369000	-5.778605000
C	7.715611000	1.304832000	-5.358926000
H	6.954801000	2.068324000	-5.178227000
C	8.375556000	-1.214487000	3.799429000
H	7.513071000	-0.718455000	3.328100000
H	8.609312000	-0.682788000	4.736725000
H	8.085220000	-2.244475000	4.059777000
C	11.345559000	-2.022615000	3.418023000
H	11.113133000	-3.060285000	3.704646000
H	11.670505000	-1.482115000	4.322962000
H	12.192402000	-2.044348000	2.713239000
C	5.613453000	-4.852016000	-7.312241000
H	4.996003000	-5.399864000	-8.029120000
C	6.198262000	-6.103829000	3.161050000
H	5.866804000	-5.109881000	3.500898000
H	6.381277000	-6.715837000	4.060364000
H	5.378666000	-6.587714000	2.605727000
C	6.907977000	-2.893400000	-6.733544000
H	7.300057000	-1.910767000	-7.005611000
C	8.212444000	-7.704287000	1.472479000
H	7.423629000	-8.067663000	0.794468000
H	8.312655000	-8.434816000	2.292890000
H	9.164899000	-7.683529000	0.919951000
C	6.125456000	-3.598441000	-7.647022000
H	5.912061000	-3.160350000	-8.625510000
C	9.655063000	-0.653317000	-5.811705000
H	10.416305000	-1.408805000	-6.010074000
C	8.831293000	1.595608000	-6.145233000
H	8.947621000	2.590199000	-6.583741000
C	9.798452000	0.616264000	-6.370609000
H	10.672907000	0.839025000	-6.987299000
N	4.354439000	-4.277275000	1.066509000
H	4.944702000	-5.104592000	0.957161000
B	5.166496000	-2.947459000	1.215125000
H	5.746272000	-2.863311000	0.055600000
H	3.717927000	-4.449160000	1.847933000
H	5.934197000	-2.956264000	2.190484000
H	4.416763000	-1.993797000	1.227824000
H	3.796797000	-4.180111000	0.196108000

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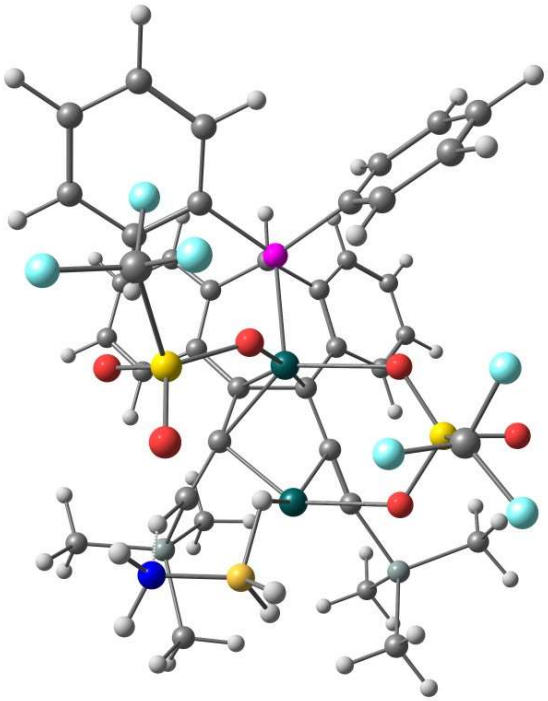

E(RPBE1PBE) = -4574.02416474

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.752352 (Hartree/Particle)
Thermal correction to Energy= 0.816189
Thermal correction to Enthalpy= 0.817133
Thermal correction to Gibbs Free Energy= 0.652328
Sum of electronic and zero-point Energies= -4573.271813
Sum of electronic and thermal Energies= -4573.207976
Sum of electronic and thermal Enthalpies= -4573.207031
Sum of electronic and thermal Free Energies= -4573.371836

Rh	7.269342000	-2.631260000	0.592983000
Rh	7.576574000	-2.533785000	-2.047361000
S	4.374860000	-3.310844000	-2.503307000
S	7.193104000	0.419032000	-0.530830000
P	8.214376000	-2.664687000	-4.199998000
Si	9.707146000	-1.372778000	2.913515000
Si	7.766986000	-5.973798000	1.672124000
F	4.173691000	-3.136241000	-5.139966000
O	7.072383000	-0.490192000	0.662504000
O	5.476682000	-2.298292000	-2.671229000
O	4.817334000	-4.704142000	-2.557457000
F	5.139782000	1.810312000	0.295370000
O	7.452781000	-0.282811000	-1.814861000

F	4.608085000	0.049058000	-0.825354000
F	2.893523000	-1.797727000	-4.048087000
F	2.424937000	-3.900979000	-4.144175000
O	8.006044000	1.597350000	-0.283272000
O	3.406492000	-2.974015000	-1.457649000
F	5.396815000	1.773415000	-1.847623000
C	7.029351000	-4.800833000	0.366056000
C	8.792222000	-4.136136000	-1.563507000
C	9.506387000	-2.863754000	-1.340284000
C	7.741437000	-4.249343000	-0.615239000
C	9.363836000	-2.452921000	0.036629000
C	9.198893000	-5.215641000	-2.483951000
C	9.350515000	-2.142259000	1.246505000
C	10.917088000	-2.720329000	-3.428994000
C	8.995140000	-6.553512000	-2.125313000
H	8.554898000	-6.784409000	-1.155590000
C	9.738713000	-4.916232000	-3.753130000
C	10.722906000	-2.429490000	-2.063652000
C	5.462693000	1.049172000	-0.739369000
C	11.704607000	-1.694267000	-1.381364000
H	11.557289000	-1.456110000	-0.325913000
C	10.077694000	-5.964931000	-4.612110000
H	10.482200000	-5.728874000	-5.599935000
C	7.241405000	-3.685505000	-5.349314000
C	3.413594000	-3.018761000	-4.061499000
C	9.895368000	-3.490511000	-4.224650000
H	10.205464000	-3.513954000	-5.279262000
C	12.091680000	-2.296138000	-4.057886000
H	12.242595000	-2.537529000	-5.113597000
C	9.336330000	-7.587485000	-2.991333000
H	9.167551000	-8.624446000	-2.691208000
C	6.737213000	-4.916356000	-4.910463000
H	6.857934000	-5.219776000	-3.870443000
C	7.253307000	-0.172457000	-4.806938000
H	6.400811000	-0.490569000	-4.201324000
C	8.345348000	-1.035296000	-4.987029000
C	12.861563000	-1.266774000	-2.023006000
H	13.609552000	-0.695391000	-1.468118000
C	9.884412000	-7.292735000	-4.238782000
H	10.149229000	-8.096652000	-4.929826000
C	10.471895000	0.292107000	2.525638000
H	11.437355000	0.179243000	2.006676000
H	10.646124000	0.866001000	3.450947000
H	9.799785000	0.875762000	1.876120000
C	13.061392000	-1.574171000	-3.367774000
H	13.968546000	-1.248335000	-3.882415000
C	9.641587000	-5.909642000	1.625745000
H	10.044648000	-6.268905000	0.665728000
H	10.066207000	-6.539492000	2.425160000
H	10.001712000	-4.879202000	1.776465000
C	6.045709000	-5.739093000	-5.795678000
H	5.648708000	-6.694093000	-5.443045000
C	7.264564000	1.093005000	-5.386390000
H	6.414392000	1.762718000	-5.235123000
C	8.098516000	-1.186639000	3.850664000
H	7.378739000	-0.583394000	3.276661000
H	8.286403000	-0.678893000	4.811435000
H	7.637766000	-2.162141000	4.071190000
C	10.890356000	-2.514256000	3.815517000
H	10.420772000	-3.488017000	4.028713000
H	11.190304000	-2.066978000	4.778024000
H	11.802347000	-2.694731000	3.224520000
C	5.844252000	-5.336563000	-7.115753000
H	5.293367000	-5.980647000	-7.806323000
C	7.133314000	-5.431893000	3.350966000
H	7.493634000	-4.425866000	3.615187000
H	7.491415000	-6.133281000	4.123134000
H	6.032706000	-5.423385000	3.390027000
C	7.034999000	-3.280094000	-6.674748000
H	7.414176000	-2.316316000	-7.023068000
C	7.107485000	-7.686629000	1.273936000
H	6.005347000	-7.690458000	1.289003000
H	7.460084000	-8.413047000	2.025304000
H	7.428888000	-8.046007000	0.283691000
C	6.336192000	-4.106104000	-7.552919000
H	6.172495000	-3.783265000	-8.584294000
C	9.443303000	-0.620655000	-5.750093000
H	10.298739000	-1.279603000	-5.906473000
C	8.363499000	1.507627000	-6.140523000
H	8.374816000	2.505358000	-6.586979000
C	9.449362000	0.651197000	-6.322160000
H	10.310746000	0.973113000	-6.912843000
N	4.516733000	-4.272562000	1.004548000
H	5.750689000	-4.772515000	0.502410000
B	5.033469000	-2.873443000	1.248452000
H	5.672759000	-2.569419000	0.099126000
H	4.292198000	-4.823689000	1.830788000
H	5.823043000	-2.791815000	2.211347000
H	4.247957000	-1.944176000	1.189124000
H	3.739527000	-4.299336000	0.344272000

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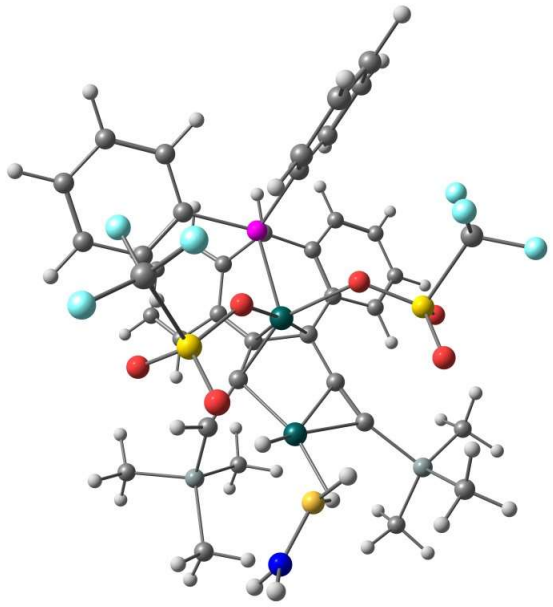


E(RPBE1PBE) = -4574.06157668

- Thermochemistry -

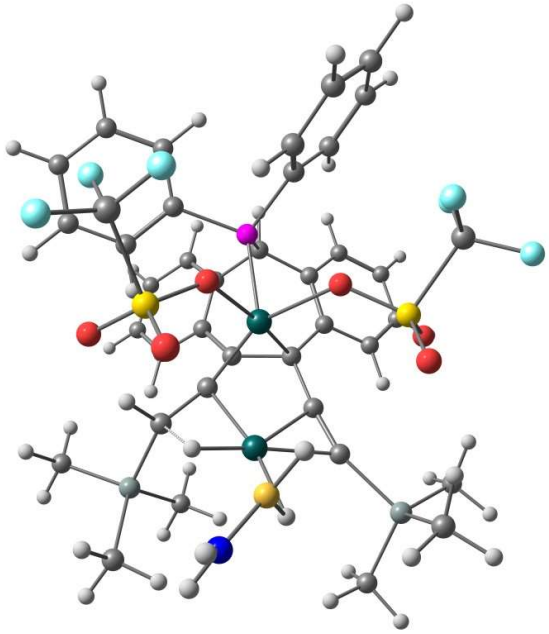
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.755039 (Hartree/Particle)
Thermal correction to Energy= 0.819762
Thermal correction to Enthalpy= 0.820706
Thermal correction to Gibbs Free Energy= 0.655124
Sum of electronic and zero-point Energies= -4573.306538
Sum of electronic and thermal Energies= -4573.241815
Sum of electronic and thermal Enthalpies= -4573.240871
Sum of electronic and thermal Free Energies= -4573.406452

Rh	7.290195000	-3.076824000	0.634606000
Rh	7.609508000	-2.556849000	-2.042400000
S	4.320888000	-3.170057000	-2.213722000
S	7.903211000	0.614045000	-1.271204000
P	8.195232000	-2.653384000	-4.209810000
Si	9.510064000	-1.065901000	2.769642000
Si	7.487068000	-6.304834000	1.143762000
F	3.816375000	-3.442466000	-4.786237000
O	6.922462000	0.898463000	-0.224957000
O	5.536841000	-2.393072000	-2.644569000
O	4.523254000	-4.621065000	-2.150731000
F	8.150825000	3.177916000	-1.703476000
O	7.458272000	-0.438303000	-2.259247000
F	6.623055000	2.244469000	-2.902067000
F	3.082448000	-1.609890000	-3.927390000
F	2.073239000	-3.471344000	-3.519937000
O	9.306947000	0.520942000	-0.875227000
O	3.578444000	-2.555870000	-1.117386000
F	8.702919000	1.952810000	-3.387753000
C	6.897638000	-5.032551000	-0.147407000
C	8.976555000	-4.134113000	-1.653875000
C	9.572239000	-2.835866000	-1.336368000
C	7.768115000	-4.281252000	-0.939170000
C	9.298448000	-2.459534000	0.028962000
C	9.480756000	-5.115481000	-2.633176000
C	9.198734000	-2.030293000	1.202329000
C	10.916972000	-2.431338000	-3.433030000
C	9.414495000	-6.480371000	-2.329979000
H	9.015988000	-6.793573000	-1.365814000
C	9.970925000	-4.709021000	-3.889096000
C	10.732898000	-2.252625000	-2.045526000
C	7.836536000	2.086431000	-2.392257000
C	11.666166000	-1.492966000	-1.327467000
H	11.512456000	-1.337116000	-0.259078000
C	10.393124000	-5.677313000	-4.803714000
H	10.755705000	-5.359306000	-5.784672000
C	7.272206000	-3.891756000	-5.165666000
C	3.258700000	-2.906857000	-3.708741000
C	9.966624000	-3.251607000	-4.273584000
H	10.262842000	-3.174078000	-5.330082000
C	12.040083000	-1.867809000	-4.048234000
H	12.189856000	-2.021827000	-5.120639000
C	9.844720000	-7.434944000	-3.244958000
H	9.788337000	-8.495818000	-2.989774000
C	6.672716000	-4.974442000	-4.511921000
H	6.683239000	-5.034209000	-3.422688000
C	6.775149000	-0.518396000	-5.170949000
H	5.942994000	-0.984831000	-4.637479000
C	8.050076000	-1.104448000	-5.132155000
C	12.772306000	-0.931932000	-1.954146000
H	13.484628000	-0.343011000	-1.371348000
C	10.337187000	-7.031758000	-4.486167000
H	10.668760000	-7.774859000	-5.215475000
C	11.115436000	-0.139713000	2.482132000
H	11.958627000	-0.828990000	2.315653000
H	11.359739000	0.493812000	3.351070000
H	11.015605000	0.512478000	1.599818000
C	12.963530000	-1.121280000	-3.321905000
H	13.829626000	-0.685777000	-3.826171000
C	9.305120000	-6.032784000	1.527273000
H	9.943769000	-6.084765000	0.631363000
H	9.660068000	-6.801885000	2.233250000
H	9.462625000	-5.047850000	1.995836000
C	6.027552000	-5.960138000	-5.254616000
H	5.548889000	-6.795331000	-4.738004000

C	6.581489000	0.668567000	-5.869035000
H	5.589526000	1.126123000	-5.890327000
C	8.088017000	0.124941000	3.015818000
H	7.844881000	0.635681000	2.069875000
H	8.358324000	0.883868000	3.768837000
H	7.180857000	-0.392797000	3.364425000
C	9.641332000	-2.301650000	4.173783000
H	8.720454000	-2.902783000	4.251438000
H	9.786126000	-1.782947000	5.135972000
H	10.489343000	-2.989904000	4.027679000
C	5.977242000	-5.869242000	-6.645324000
H	5.465169000	-6.641611000	-7.225220000
C	6.454464000	-6.064259000	2.693834000
H	6.702608000	-5.115452000	3.196035000
H	6.641517000	-6.883716000	3.407741000
H	5.378438000	-6.067165000	2.454596000
C	7.216235000	-3.796108000	-6.563098000
H	7.671796000	-2.945869000	-7.077801000
C	7.163749000	-8.033282000	0.476263000
H	6.091635000	-8.168364000	0.257906000
H	7.449870000	-8.784533000	1.231504000
H	7.723431000	-8.255876000	-0.445538000
C	6.569233000	-4.786700000	-7.298376000
H	6.523061000	-4.709342000	-8.387589000
C	9.124702000	-0.489114000	-5.782830000
H	10.125463000	-0.921371000	-5.750325000
C	7.653208000	1.280382000	-6.523006000
H	7.499153000	2.217266000	-7.064710000
C	8.920673000	0.702678000	-6.478497000
H	9.762550000	1.182520000	-6.983646000
N	4.500851000	-3.006909000	2.479273000
H	5.865523000	-5.147252000	-0.504499000
B	5.434355000	-2.315392000	1.700222000
H	5.754762000	-3.148105000	0.330220000
H	4.695530000	-3.882481000	2.949665000
H	6.671732000	-2.458114000	2.152021000
H	5.121826000	-1.252591000	1.216989000
H	3.534307000	-2.711389000	2.551635000

[TS2]



E(RPBE1PBE) = -4574.05614685

- Thermochemistry -

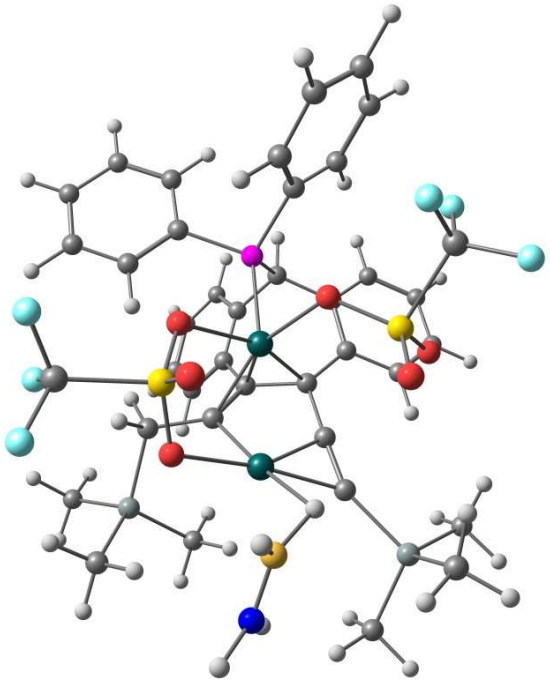
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.753604 (Hartree/Particle)
Thermal correction to Energy= 0.818408
Thermal correction to Enthalpy= 0.819353
Thermal correction to Gibbs Free Energy= 0.652295
Sum of electronic and zero-point Energies= -4573.302542
Sum of electronic and thermal Energies= -4573.237738
Sum of electronic and thermal Enthalpies= -4573.236794
Sum of electronic and thermal Free Energies= -4573.403852

Rh	7.444488000	-3.372960000	0.857616000
Rh	7.609529000	-2.650679000	-1.791285000
S	4.254563000	-3.351146000	-1.973615000
S	7.747148000	0.519886000	-0.963976000
P	8.113745000	-2.645535000	-3.981162000
Si	9.541389000	-1.193618000	2.958134000
Si	7.355442000	-6.682757000	1.027604000
F	3.788045000	-3.654474000	-4.556075000
O	6.840898000	0.823059000	0.142140000
O	5.510425000	-2.646216000	-2.397035000
O	4.393762000	-4.810166000	-1.870347000
F	7.944974000	3.083683000	-1.417343000
O	7.228967000	-0.547949000	-1.897231000
F	6.371159000	2.131319000	-2.538188000
F	3.082583000	-1.793736000	-3.734756000

F	2.026623000	-3.626695000	-3.316377000
O	9.175281000	0.429160000	-0.666908000
O	3.505359000	-2.681306000	-0.915812000
F	8.428803000	1.859428000	-3.122336000
C	6.937914000	-5.236068000	-0.149938000
C	9.063335000	-4.186187000	-1.534666000
C	9.600130000	-2.865798000	-1.179112000
C	7.901943000	-4.421540000	-0.773579000
C	9.338797000	-2.539635000	0.201097000
C	9.589350000	-5.095380000	-2.569542000
C	9.223641000	-2.148520000	1.388183000
C	10.846785000	-2.310209000	-3.303629000
C	9.631511000	-6.470584000	-2.311050000
H	9.306691000	-6.839898000	-1.338511000
C	10.006905000	-4.613246000	-3.824751000
C	10.705269000	-2.199340000	-1.903900000
C	7.609357000	1.986114000	-2.086929000
C	11.626495000	-1.425461000	-1.185953000
H	11.504492000	-1.324686000	-0.106753000
C	10.452914000	-5.519383000	-4.790103000
H	10.758854000	-5.145293000	-5.770529000
C	7.211361000	-3.904717000	-4.934281000
C	3.227963000	-3.091819000	-3.494366000
C	9.908525000	-3.144095000	-4.145432000
H	10.158555000	-3.005278000	-5.207350000
C	11.915533000	-1.662126000	-3.932404000
H	12.031952000	-1.760670000	-5.015431000
C	10.084633000	-7.362635000	-3.276869000
H	10.112380000	-8.432667000	-3.057783000
C	6.677877000	-5.027287000	-4.290165000
H	6.732612000	-5.117029000	-3.204754000
C	6.541578000	-0.567018000	-4.828528000
H	5.761800000	-1.083185000	-4.263680000
C	7.845475000	-1.085742000	-4.857616000
C	12.678953000	-0.781593000	-1.825337000
H	13.382735000	-0.182675000	-1.242300000
C	10.495146000	-6.885079000	-4.521495000
H	10.843342000	-7.579218000	-5.290226000
C	11.130592000	-0.238745000	2.671298000
H	11.980929000	-0.913226000	2.481813000
H	11.377004000	0.379938000	3.550315000
H	11.013764000	0.430406000	1.803906000
C	12.827086000	-0.900746000	-3.206334000
H	13.650070000	-0.399062000	-3.721197000
C	9.116352000	-6.517890000	1.654565000
H	9.857518000	-6.507115000	0.839757000
H	9.364663000	-7.362064000	2.319127000
H	9.238039000	-5.586149000	2.231016000
C	6.043734000	-6.018403000	-5.034524000
H	5.616658000	-6.884344000	-4.523247000
C	6.252864000	0.614594000	-5.502553000
H	5.237670000	1.017453000	-5.472809000
C	8.104788000	-0.030928000	3.247275000
H	7.844040000	0.504659000	2.320311000
H	8.371249000	0.706560000	4.022679000
H	7.208113000	-0.572293000	3.587644000
C	9.710171000	-2.444506000	4.346754000
H	8.791140000	-3.046717000	4.438594000
H	9.882314000	-1.941128000	5.312499000
H	10.551651000	-3.132678000	4.164938000
C	5.935883000	-5.893495000	-6.419395000
H	5.431004000	-6.669588000	-7.000583000
C	6.128370000	-6.564420000	2.444214000
H	6.348521000	-5.692317000	3.080614000
H	6.170652000	-7.465831000	3.077666000
H	5.098397000	-6.466500000	2.063875000
C	7.097339000	-3.776426000	-6.325122000
H	7.498735000	-2.895572000	-6.833323000
C	7.087034000	-8.283139000	0.081832000
H	6.048434000	-8.346871000	-0.282199000
H	7.267909000	-9.149538000	0.739849000
H	7.754322000	-8.376668000	-0.789106000
C	6.460759000	-4.771993000	-7.063310000
H	6.369314000	-4.667132000	-8.147367000
C	8.854133000	-0.405865000	-5.548219000
H	9.875771000	-0.786942000	-5.568909000
C	7.258374000	1.289110000	-6.198503000
H	7.029388000	2.220731000	-6.722568000
C	8.555670000	0.780336000	-6.218578000
H	9.346640000	1.309321000	-6.755937000
N	4.582303000	-3.108504000	2.536496000
H	5.972923000	-5.344004000	-0.672201000
B	5.610638000	-2.478411000	1.841968000
H	6.039506000	-4.072059000	0.626604000
H	4.707829000	-3.943551000	3.096757000
H	6.790421000	-2.720018000	2.360652000
H	5.409713000	-1.460279000	1.228775000
H	3.617390000	-2.805865000	2.465483000

9



E(RPBE1PBE) = -4574.09576552

- Thermochemistry -

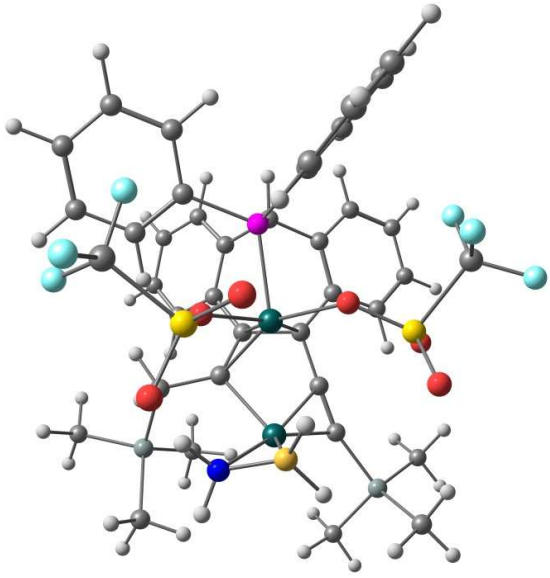
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.759051 (Hartree/Particle)
Thermal correction to Energy= 0.823657
Thermal correction to Enthalpy= 0.824601
Thermal correction to Gibbs Free Energy= 0.657996
Sum of electronic and zero-point Energies= -4573.336714
Sum of electronic and thermal Energies= -4573.272109
Sum of electronic and thermal Enthalpies= -4573.271164
Sum of electronic and thermal Free Energies= -4573.437770

Rh	7.153790000	-3.136862000	0.892143000
Rh	7.366363000	-2.639277000	-1.651363000
S	4.359429000	-3.096166000	-0.595982000
S	7.232400000	0.466493000	-0.832522000
P	7.863289000	-2.616890000	-3.850950000
Si	9.538219000	-1.471460000	3.194142000
Si	7.238993000	-6.838147000	0.881288000
F	3.696996000	-5.524670000	-1.376511000
O	6.348889000	0.697510000	0.308538000
O	5.140884000	-3.030391000	-1.862079000
O	5.131257000	-3.756497000	0.521899000
F	7.268897000	3.053750000	-1.199047000
O	6.740255000	-0.594439000	-1.791604000
F	5.758389000	2.040875000	-2.354476000
F	2.284526000	-3.986063000	-1.902045000
F	2.414437000	-4.681306000	0.135093000
O	8.671150000	0.425974000	-0.577176000
O	3.591388000	-1.921761000	-0.231049000
F	7.828440000	1.921536000	-2.943323000
C	7.009163000	-5.722072000	-0.665037000
C	8.863096000	-4.100672000	-1.354980000
C	9.343487000	-2.754834000	-1.027323000
C	7.713262000	-4.424232000	-0.564949000
C	9.083310000	-2.504291000	0.364358000
C	9.510103000	-4.968878000	-2.365243000
C	9.013860000	-2.301680000	1.604931000
C	10.565998000	-2.139902000	-3.148710000
C	9.801814000	-6.302822000	-2.044977000
H	9.570479000	-6.675869000	-1.047070000
C	9.876636000	-4.480245000	-3.636149000
C	10.422035000	-2.043762000	-1.747240000
C	7.003726000	1.959155000	-1.904764000
C	11.309208000	-1.233902000	-1.027062000
H	11.188304000	-1.150637000	0.053123000
C	10.458838000	-5.347424000	-4.565352000
H	10.720667000	-4.964741000	-5.555422000
C	7.059229000	-3.906170000	-4.857787000
C	3.106290000	-4.412159000	-0.959306000
C	9.677633000	-3.027548000	-3.992801000
H	9.943677000	-2.893443000	-5.051537000
C	11.599905000	-1.434265000	-3.773790000
H	11.719611000	-1.519479000	-4.857665000
C	10.397745000	-7.152406000	-2.971440000
H	10.614277000	-8.187715000	-2.697018000
C	6.313244000	-4.912197000	-4.235002000
H	6.169282000	-4.890201000	-3.154054000
C	6.213370000	-0.625208000	-4.750273000
H	5.447741000	-1.187665000	-4.209084000
C	7.542603000	-1.074963000	-4.751172000
C	12.327256000	-0.533381000	-1.663071000
H	13.003811000	0.093030000	-1.076497000
C	10.712354000	-6.677881000	-4.244081000
H	11.166183000	-7.340742000	-4.984941000
C	11.226953000	-0.729812000	2.849190000
H	11.951048000	-1.491178000	2.518801000
H	11.621893000	-0.261797000	3.766629000
H	11.160438000	0.052023000	2.075890000
C	12.474947000	-0.632682000	-3.045537000
H	13.269872000	-0.086816000	-3.559675000
C	8.815649000	-6.408769000	1.816889000
H	9.718139000	-6.477396000	1.188539000
H	8.951398000	-7.097596000	2.667479000
H	8.771303000	-5.381790000	2.216718000

C	5.739355000	-5.927797000	-4.999224000
H	5.151710000	-6.706922000	-4.506995000
C	5.874427000	0.545732000	-5.419756000
H	4.838727000	0.893846000	-5.410004000
C	8.313556000	-0.115488000	3.610253000
H	8.046769000	0.460471000	2.709613000
H	8.767647000	0.576214000	4.339473000
H	7.386410000	-0.508264000	4.054934000
C	9.648726000	-2.753226000	4.559696000
H	8.666004000	-3.190613000	4.796727000
H	10.029487000	-2.286766000	5.483758000
H	10.333812000	-3.572332000	4.287508000
C	5.910112000	-5.942602000	-6.382895000
H	5.459283000	-6.738766000	-6.981177000
C	5.760531000	-6.624690000	2.019475000
H	5.677639000	-5.585936000	2.374553000
H	5.849097000	-7.286211000	2.897499000
H	4.821061000	-6.873764000	1.499555000
C	7.220509000	-3.915895000	-6.250127000
H	7.787562000	-3.122476000	-6.745428000
C	7.313452000	-8.610735000	0.255790000
H	6.407976000	-8.861796000	-0.321525000
H	7.385539000	-9.324783000	1.093075000
H	8.184401000	-8.771262000	-0.400799000
C	6.649371000	-4.935426000	-7.007733000
H	6.777287000	-4.941569000	-8.093219000
C	8.526989000	-0.334141000	-5.412556000
H	9.567954000	-0.659520000	-5.410900000
C	6.857960000	1.281127000	-6.085072000
H	6.591514000	2.205226000	-6.604687000
C	8.180419000	0.841897000	-6.079123000
H	8.953924000	1.418398000	-6.592750000
N	5.893525000	-3.238207000	3.716744000
H	7.304615000	-6.291568000	-1.560187000
B	5.627737000	-2.328528000	2.710600000
H	5.924312000	-5.568762000	-0.709719000
H	6.803122000	-3.651203000	3.889373000
H	6.557264000	-1.822467000	2.041319000
H	4.538940000	-1.845464000	2.552377000
H	5.170043000	-3.589708000	4.335343000

9’



E(RPBE1PBE) = -4574.09579399

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.758532 (Hartree/Particle)
Thermal correction to Energy= 0.822909
Thermal correction to Enthalpy= 0.823853
Thermal correction to Gibbs Free Energy= 0.657865
Sum of electronic and zero-point Energies= -4573.337262
Sum of electronic and thermal Energies= -4573.272885
Sum of electronic and thermal Enthalpies= -4573.271941
Sum of electronic and thermal Free Energies= -4573.437929

Rh	7.417099000	-2.957755000	0.979204000
Rh	7.482761000	-2.526536000	-1.660832000
S	3.968626000	-2.600689000	-2.158734000
S	7.526016000	0.643447000	-0.974620000
P	7.931097000	-2.582383000	-3.871922000
Si	9.838187000	-1.555754000	3.233669000
Si	7.385045000	-6.639157000	1.039315000
F	3.432177000	-4.856274000	-3.406956000
O	6.575714000	1.189374000	-0.009906000
O	5.396149000	-3.047850000	-2.193082000
O	3.236098000	-3.150478000	-1.008766000
F	8.160532000	3.084289000	-1.643023000
O	6.957975000	-0.464039000	-1.832462000
F	6.536687000	2.272605000	-2.801533000
F	3.875578000	-3.206068000	-4.724089000
F	1.978271000	-3.295769000	-3.708954000

O	8.896106000	0.410566000	-0.519205000
O	3.732139000	-1.202922000	-2.505888000
F	8.561415000	1.634214000	-3.183361000
C	7.019286000	-5.530490000	-0.496151000
C	8.926896000	-4.026962000	-1.356537000
C	9.478418000	-2.691593000	-1.088765000
C	7.790947000	-4.267671000	-0.511063000
C	9.340207000	-2.414630000	0.314214000
C	9.498232000	-4.955670000	-2.360595000
C	9.362567000	-2.209989000	1.550675000
C	10.662583000	-2.185742000	-3.261678000
C	9.709648000	-6.300805000	-2.026240000
H	9.477133000	-6.644957000	-1.019988000
C	9.865694000	-4.515639000	-3.649544000
C	10.559961000	-2.041290000	-1.861899000
C	7.701350000	1.986698000	-2.236646000
C	11.488152000	-1.230171000	-1.194497000
H	11.399744000	-1.102333000	-0.114474000
C	10.372894000	-5.433225000	-4.573715000
H	10.633030000	-5.084881000	-5.576714000
C	7.057428000	-3.859179000	-4.834955000
C	3.276158000	-3.550046000	-3.591158000
C	9.721479000	-3.068143000	-4.046117000
H	9.956342000	-2.980599000	-5.116869000
C	11.694467000	-1.530693000	-3.941510000
H	11.777701000	-1.656847000	-5.024798000
C	10.227980000	-7.203305000	-2.949322000
H	10.380011000	-8.246090000	-2.660377000
C	6.606997000	-5.022737000	-4.202506000
H	6.713164000	-5.126252000	-3.123449000
C	6.345902000	-0.512589000	-4.721614000
H	5.587653000	-0.971446000	-4.083169000
C	7.640273000	-1.049780000	-4.793481000
C	12.505240000	-0.580309000	-1.883899000
H	13.214193000	0.048093000	-1.339307000
C	10.548076000	-6.771694000	-4.235294000
H	10.941976000	-7.474317000	-4.973684000
C	11.565541000	-0.855608000	3.036541000
H	12.270665000	-1.622363000	2.678155000
H	11.936261000	-0.477241000	4.003957000
H	11.568180000	-0.018245000	2.320603000
C	12.610981000	-0.729785000	-3.265926000
H	13.404621000	-0.222317000	-3.819799000
C	9.124232000	-6.356808000	1.702430000
H	9.924853000	-6.681520000	1.020187000
H	9.247639000	-6.917977000	2.643868000
H	9.289714000	-5.289888000	1.927725000
C	5.996043000	-6.029569000	-4.945009000
H	5.638217000	-6.930901000	-4.441435000
C	6.030127000	0.627494000	-5.453527000
H	5.022438000	1.044794000	-5.387938000
C	8.607032000	-0.226970000	3.707353000
H	8.511362000	0.523363000	2.906608000
H	8.941381000	0.287025000	4.623841000
H	7.607465000	-0.646174000	3.901744000
C	9.798968000	-2.993743000	4.436102000
H	8.795265000	-3.447802000	4.479501000
H	10.059824000	-2.659165000	5.453803000
H	10.516655000	-3.777201000	4.143635000
C	5.824066000	-5.877510000	-6.320895000
H	5.335888000	-6.664425000	-6.901795000
C	6.184588000	-6.268743000	2.438192000
H	6.410885000	-5.305252000	2.923342000
H	6.271294000	-7.050301000	3.211722000
H	5.136625000	-6.255231000	2.097734000
C	6.881370000	-3.706103000	-6.216285000
H	7.215174000	-2.794927000	-6.718996000
C	7.162190000	-8.413103000	0.463140000
H	6.141443000	-8.579765000	0.080937000
H	7.333318000	-9.121043000	1.290825000
H	7.868812000	-8.661901000	-0.345716000
C	6.264933000	-4.715107000	-6.954232000
H	6.123670000	-4.588200000	-8.030585000
C	8.611885000	-0.429532000	-5.586010000
H	9.626920000	-0.824678000	-5.643968000
C	6.998584000	1.244280000	-6.247655000
H	6.748039000	2.144531000	-6.815000000
C	8.287383000	0.717154000	-6.310818000
H	9.050643000	1.200809000	-6.925584000
N	5.294398000	-3.319689000	1.052883000
H	7.222301000	-6.145128000	-1.388226000
B	5.614329000	-1.906206000	1.009998000
H	5.937713000	-5.329149000	-0.484024000
H	5.089454000	-3.806277000	1.921539000
H	6.240350000	-1.511058000	2.014859000
H	5.156104000	-1.132703000	0.217325000
H	4.726488000	-3.670210000	0.277803000

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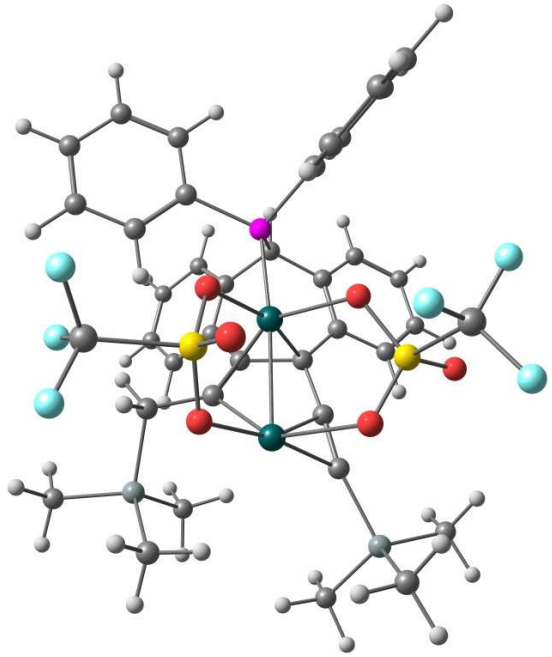


E(RPBE1PBE) = -4492.20140921

- Thermochemistry -

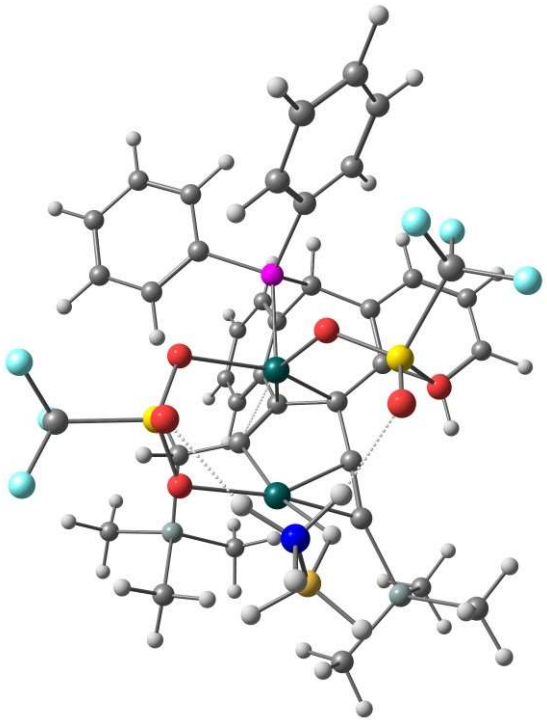
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.708058 (Hartree/Particle)
Thermal correction to Energy= 0.769012
Thermal correction to Enthalpy= 0.769957
Thermal correction to Gibbs Free Energy= 0.609308
Sum of electronic and zero-point Energies= -4491.493351
Sum of electronic and thermal Energies= -4491.432397
Sum of electronic and thermal Enthalpies= -4491.431453
Sum of electronic and thermal Free Energies= -4491.592102

Rh	7.288243000	-2.863090000	0.605419000
Rh	7.516090000	-2.574232000	-1.876423000
S	4.463062000	-2.858259000	-0.912658000
S	7.095026000	0.199046000	-0.340135000
P	7.993007000	-2.630867000	-4.083496000
Si	9.480863000	-1.699237000	3.137797000
Si	7.456287000	-6.439852000	1.168597000
F	3.985067000	-5.355640000	-1.611936000
O	6.544406000	-0.590320000	0.794935000
O	5.289291000	-2.822514000	-2.151973000
O	5.241925000	-3.363114000	0.273528000
F	5.949733000	2.317715000	0.655095000
O	6.912686000	-0.446324000	-1.685891000
F	4.676809000	1.184700000	-0.663655000
F	2.466296000	-3.942142000	-2.187500000
F	2.638381000	-4.562251000	-0.128838000
O	8.398696000	0.814389000	-0.124396000
O	3.595153000	-1.723047000	-0.665502000
F	6.258122000	2.399485000	-1.477691000
C	7.128395000	-5.620456000	-0.543148000
C	8.950229000	-4.060203000	-1.490974000
C	9.482175000	-2.706806000	-1.256616000
C	7.834535000	-4.331576000	-0.617155000
C	9.275535000	-2.375381000	0.127092000
C	9.555993000	-5.001028000	-2.462749000
C	9.174746000	-2.200883000	1.365608000
C	10.694138000	-2.238310000	-3.424566000
C	9.812265000	-6.325533000	-2.079723000
H	9.594627000	-6.635487000	-1.058604000
C	9.919481000	-4.591066000	-3.763880000
C	10.560834000	-2.054367000	-2.030070000
C	5.909942000	1.613574000	-0.468467000
C	11.447855000	-1.192656000	-1.369202000
H	11.336384000	-1.039500000	-0.293268000
C	10.452329000	-5.528045000	-4.654636000
H	10.711417000	-5.206776000	-5.667053000
C	7.104972000	-3.899402000	-5.044511000
C	3.313181000	-4.277005000	-1.229884000
C	9.780613000	-3.154899000	-4.206105000
H	10.054720000	-3.099608000	-5.269375000
C	11.718867000	-1.569929000	-4.101389000
H	11.826248000	-1.721894000	-5.179031000
C	10.359173000	-7.244280000	-2.969912000
H	10.546706000	-8.270197000	-2.643699000
C	6.460558000	-4.934357000	-4.355298000
H	6.453918000	-4.933574000	-3.263270000
C	6.644533000	-0.337796000	-4.761438000
H	5.921353000	-0.690338000	-4.021711000
C	7.808509000	-1.080425000	-5.010220000
C	12.456558000	-0.528649000	-2.059034000
H	13.133330000	0.139491000	-1.520924000
C	10.663387000	-6.849363000	-4.271227000
H	11.078088000	-7.565194000	-4.985229000
C	10.954313000	-0.541433000	3.113542000
H	11.852820000	-1.044568000	2.721771000
H	11.181042000	-0.187557000	4.133137000
H	10.746255000	0.338068000	2.483674000
C	12.596062000	-0.719618000	-3.432475000
H	13.384346000	-0.203953000	-3.986399000
C	9.268675000	-6.308276000	1.655557000
H	9.917216000	-6.989738000	1.082306000
H	9.389472000	-6.564893000	2.721131000
H	9.640879000	-5.280194000	1.513740000
C	5.818034000	-5.948914000	-5.062375000

H	5.310652000	-6.749341000	-4.517939000
C	6.422181000	0.856671000	-5.441393000
H	5.515646000	1.432644000	-5.239447000
C	7.933539000	-0.849838000	3.759559000
H	7.667510000	0.003695000	3.118506000
H	8.087325000	-0.487554000	4.789637000
H	7.075102000	-1.540993000	3.770896000
C	9.828948000	-3.261030000	4.117200000
H	8.977516000	-3.958768000	4.066424000
H	10.001033000	-3.017032000	5.178926000
H	10.723229000	-3.782302000	3.739991000
C	5.815514000	-5.933875000	-6.457211000
H	5.308798000	-6.728292000	-7.011467000
C	6.410537000	-5.568348000	2.465128000
H	6.736277000	-4.523029000	2.608909000
H	6.503121000	-6.080580000	3.437579000
H	5.345617000	-5.548713000	2.185774000
C	7.093703000	-3.881582000	-6.445256000
H	7.581909000	-3.068796000	-6.990369000
C	6.928684000	-8.234891000	1.007794000
H	5.870797000	-8.311395000	0.706985000
H	7.045256000	-8.766615000	1.966837000
H	7.534565000	-8.763154000	0.253404000
C	6.451754000	-4.899954000	-7.147185000
H	6.443812000	-4.883692000	-8.240107000
C	8.747606000	-0.611314000	-5.936571000
H	9.660444000	-1.174283000	-6.139896000
C	7.360781000	1.322306000	-6.363657000
H	7.188629000	2.264576000	-6.890501000
C	8.521536000	0.589042000	-6.609485000
H	9.259423000	0.953338000	-7.328806000
H	7.367982000	-6.316749000	-1.361831000
H	6.041554000	-5.463995000	-0.525237000

11



E(RPBE1PBE) = -4575.30832211

- Thermochemistry -

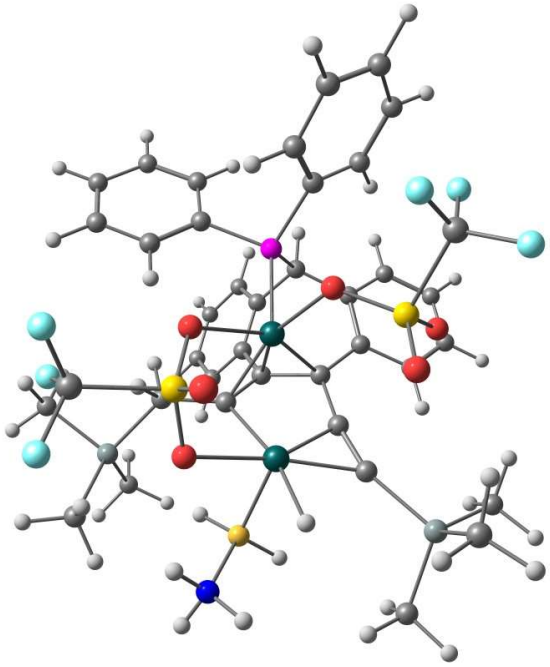
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.780858 (Hartree/Particle)
Thermal correction to Energy= 0.846013
Thermal correction to Enthalpy= 0.846957
Thermal correction to Gibbs Free Energy= 0.679217
Sum of electronic and zero-point Energies= -4574.527465
Sum of electronic and thermal Energies= -4574.462309
Sum of electronic and thermal Enthalpies= -4574.461365
Sum of electronic and thermal Free Energies= -4574.629105

Rh	4.192814000	-9.116511000	1.022360000
Rh	3.101084000	-10.932497000	-0.492516000
S	2.787544000	-11.581162000	2.621398000
S	0.412974000	-9.095975000	-0.423346000
P	2.635784000	-12.534185000	-2.013867000
Si	5.129462000	-5.767777000	0.022157000
Si	7.539612000	-10.419836000	1.537109000
F	4.608571000	-13.386949000	3.197735000
O	-0.043946000	-8.502696000	0.842941000
O	2.649822000	-12.265833000	1.311833000
O	3.861902000	-10.538806000	2.645028000
F	-1.864822000	-8.374603000	-1.478544000

O	0.991633000	-10.474999000	-0.254136000
F	-1.902081000	-10.338516000	-0.593349000
F	2.614462000	-13.870144000	3.852591000
F	3.763702000	-12.378534000	4.904901000
O	1.136920000	-8.223749000	-1.341036000
O	1.546056000	-11.178064000	3.281223000
F	-0.916082000	-10.024948000	-2.485586000
C	6.090264000	-11.455712000	0.813563000
C	4.992637000	-10.676726000	-1.372673000
C	4.026928000	-9.663656000	-1.834779000
C	5.151795000	-10.603942000	0.052422000
C	4.184221000	-8.514317000	-0.985410000
C	5.706897000	-11.585345000	-2.299659000
C	4.570750000	-7.511649000	-0.330871000
C	3.265790000	-10.655564000	-4.029849000
C	7.095421000	-11.742607000	-2.183362000
H	7.633672000	-11.174045000	-1.426420000
C	5.034017000	-12.270273000	-3.332961000
C	3.520835000	-9.528995000	-3.217012000
C	-1.168689000	-9.490280000	-1.299678000
C	3.251519000	-8.249999000	-3.723069000
H	3.428918000	-7.382666000	-3.084148000
C	5.748978000	-13.132870000	-4.168983000
H	5.213291000	-13.672886000	-4.954394000
C	3.276750000	-14.197497000	-1.627388000
C	3.493921000	-12.894374000	3.718485000
C	3.557687000	-12.066222000	-3.566899000
H	3.235614000	-12.771437000	-4.346339000
C	2.773695000	-10.459814000	-5.324630000
H	2.591532000	-11.332189000	-5.958605000
C	7.800092000	-12.591945000	-3.030668000
H	8.881993000	-12.695389000	-2.916990000
C	4.200105000	-14.354352000	-0.588004000
H	4.483420000	-13.492149000	0.017172000
C	0.044313000	-13.141683000	-1.367731000
H	0.441720000	-13.185877000	-0.350161000
C	0.892500000	-12.812713000	-2.436120000
C	2.754294000	-8.072610000	-5.009002000
H	2.550573000	-7.064632000	-5.378515000
C	7.122072000	-13.304484000	-4.018408000
H	7.662897000	-13.985250000	-4.680480000
C	6.293774000	-5.299272000	-1.375317000
H	7.182991000	-5.949978000	-1.389215000
H	6.636379000	-4.257082000	-1.260232000
H	5.792946000	-5.385924000	-2.353187000
C	2.514823000	-9.183251000	-5.816832000
H	2.124110000	-9.058721000	-6.829814000
C	8.198049000	-9.172764000	0.288670000
H	8.799215000	-9.633809000	-0.510980000
H	8.845658000	-8.442847000	0.802663000
H	7.371492000	-8.614918000	-0.182552000
C	4.742934000	-15.610205000	-0.320665000
H	5.459680000	-15.725693000	0.496417000
C	-1.303489000	-13.394663000	-1.600980000
H	-1.959250000	-13.646008000	-0.763839000
C	3.613586000	-4.666482000	0.032148000
H	3.093973000	-4.712978000	-0.938518000
H	3.890681000	-3.616892000	0.226092000
H	2.905241000	-4.987082000	0.811642000
C	6.022244000	-5.757147000	1.669659000
H	5.352456000	-6.060427000	2.489347000
H	6.390773000	-4.742683000	1.894982000
H	6.889498000	-6.436524000	1.657752000
C	4.366883000	-16.711525000	-1.089084000
H	4.792330000	-17.696328000	-0.878631000
C	6.935208000	-9.481543000	3.047587000
H	6.188250000	-8.719950000	2.766222000
H	7.775374000	-8.961094000	3.537588000
H	6.464498000	-10.149290000	3.785774000
C	2.891916000	-15.307461000	-2.391791000
H	2.158444000	-15.195795000	-3.195604000
C	8.877717000	-11.648098000	2.019820000
H	8.494707000	-12.387983000	2.742117000
H	9.734492000	-11.134532000	2.487050000
H	9.252243000	-12.196774000	1.139982000
C	3.440356000	-16.559544000	-2.123009000
H	3.139613000	-17.423318000	-2.721506000
C	0.374423000	-12.724917000	-3.732298000
H	1.013829000	-12.456734000	-4.574450000
C	-1.817709000	-13.309969000	-2.896593000
H	-2.878603000	-13.501789000	-3.077206000
C	-0.979726000	-12.973692000	-3.958209000
H	-1.379583000	-12.900541000	-4.972708000
H	6.490741000	-12.305585000	0.238019000
H	5.608102000	-11.853302000	1.716559000
N	1.526539000	-8.259322000	3.190358000
H	0.851606000	-8.205590000	2.408830000
H	1.097808000	-7.826364000	4.010412000
B	2.887007000	-7.559504000	2.804464000
H	2.722891000	-6.346753000	2.802866000
H	1.615386000	-9.263428000	3.392400000
H	3.058480000	-7.804472000	1.576299000
H	3.791468000	-7.904924000	3.548123000

11-oxad



E(RPBE1PBE) = -4575.24975360

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.780053 (Hartree/Particle)
Thermal correction to Energy= 0.844575
Thermal correction to Enthalpy= 0.845519
Thermal correction to Gibbs Free Energy= 0.681003
Sum of electronic and zero-point Energies= -4574.469700
Sum of electronic and thermal Energies= -4574.405179
Sum of electronic and thermal Enthalpies= -4574.404235
Sum of electronic and thermal Free Energies= -4574.568751

Rh	7.361969000	-3.446362000	1.181552000
Rh	7.422538000	-3.660100000	-1.516361000
S	4.490750000	-3.963494000	0.098272000
S	7.042057000	-0.468701000	-1.516357000
P	7.898175000	-4.020753000	-3.683628000
Si	9.358101000	-0.725545000	2.557420000
Si	7.036622000	-7.841976000	1.080526000
F	3.788995000	-6.498963000	-0.173081000
O	6.338414000	-0.038126000	-0.310019000
O	5.144764000	-4.170173000	-1.223903000
O	5.382181000	-4.335728000	1.259575000
F	6.551588000	1.943634000	-2.393299000
O	6.534859000	-1.774817000	-2.084456000
F	5.174864000	0.461819000	-3.136705000
F	2.267688000	-5.068713000	-0.695970000
F	2.738820000	-5.431958000	1.376115000
O	8.496483000	-0.327272000	-1.542269000
O	3.717841000	-2.747574000	0.272929000
F	7.174609000	0.573067000	-3.931768000
C	7.148604000	-6.404823000	-0.176775000
C	9.032990000	-4.879503000	-0.936505000
C	9.429215000	-3.472403000	-0.914657000
C	7.859088000	-5.098227000	-0.132244000
C	9.093777000	-2.839300000	0.334839000
C	9.726630000	-5.896587000	-1.758862000
C	8.944284000	-2.097430000	1.361059000
C	10.582113000	-3.266231000	-3.157324000
C	10.105167000	-7.103988000	-1.158578000
H	9.904440000	-7.247996000	-0.097138000
C	10.031266000	-5.682734000	-3.117388000
C	10.448461000	-2.876798000	-1.807243000
C	6.444772000	0.693398000	-2.831484000
C	11.302470000	-1.889268000	-1.299058000
H	11.193166000	-1.580890000	-0.259266000
C	10.655389000	-6.697694000	-3.849131000
H	10.875442000	-6.530679000	-4.906990000
C	7.147248000	-5.535621000	-4.370475000
C	3.241526000	-5.335392000	0.155565000
C	9.731770000	-4.356349000	-3.772129000
H	9.976542000	-4.433115000	-4.841482000
C	11.578468000	-2.672531000	-3.940146000
H	11.691598000	-2.989081000	-4.981025000
C	10.737887000	-8.102670000	-1.891716000
H	11.024706000	-9.037253000	-1.403202000
C	6.198505000	-6.248284000	-3.630587000
H	5.882282000	-5.882806000	-2.652081000
C	6.113303000	-2.474575000	-5.078132000
H	5.369138000	-3.012518000	-4.484684000
C	7.479941000	-2.739485000	-4.899904000
C	12.280889000	-1.300764000	-2.091280000
H	12.932996000	-0.533075000	-1.667512000
C	11.001454000	-7.904420000	-3.247034000
H	11.486634000	-8.686955000	-3.835699000
C	10.964791000	0.062396000	1.984046000
H	11.795493000	-0.661420000	1.977405000
H	11.241877000	0.885895000	2.663733000
H	10.859919000	0.485414000	0.972214000
C	12.422109000	-1.694482000	-3.420962000
H	13.187596000	-1.241704000	-4.055970000
C	8.650062000	-8.543328000	1.757394000
H	9.205097000	-9.098796000	0.984946000
H	8.401825000	-9.260547000	2.558624000
H	9.315213000	-7.781505000	2.191200000
C	5.648573000	-7.421199000	-4.149564000

H	4.907629000	-7.973439000	-3.565720000
C	5.703136000	-1.522460000	-6.004759000
H	4.637522000	-1.318223000	-6.134865000
C	7.969403000	0.526836000	2.530264000
H	7.729889000	0.821757000	1.497553000
H	8.249099000	1.422739000	3.109497000
H	7.052057000	0.102515000	2.968499000
C	9.564720000	-1.451327000	4.276148000
H	8.637551000	-1.937431000	4.618473000
H	9.805925000	-0.645124000	4.989341000
H	10.378465000	-2.192310000	4.312380000
C	6.042979000	-7.882708000	-5.403984000
H	5.614111000	-8.803332000	-5.808315000
C	5.827769000	-7.523483000	2.496747000
H	6.344682000	-7.327176000	3.447716000
H	5.205385000	-8.422168000	2.642247000
H	5.151358000	-6.683780000	2.280088000
C	7.530288000	-5.992319000	-5.639695000
H	8.256675000	-5.430264000	-6.233668000
C	6.258524000	-9.178981000	-0.003359000
H	5.279900000	-8.852474000	-0.393740000
H	6.097822000	-10.107626000	0.569326000
H	6.900034000	-9.423331000	-0.866506000
C	6.981239000	-7.165145000	-6.150385000
H	7.284836000	-7.520576000	-7.138405000
C	8.427302000	-2.028875000	-5.643346000
H	9.494695000	-2.203382000	-5.504976000
C	6.650576000	-0.823587000	-6.756199000
H	6.326795000	-0.072792000	-7.481664000
C	8.008318000	-1.075434000	-6.572139000
H	8.753882000	-0.524018000	-7.150550000
N	6.810405000	-4.647280000	3.873728000
H	7.450486000	-6.937165000	-1.095281000
B	7.987731000	-4.702809000	2.813641000
H	6.075678000	-6.202700000	-0.293613000
H	6.744777000	-3.730357000	4.322774000
H	6.973809000	-2.518935000	2.435890000
H	8.092819000	-5.838620000	2.406389000
H	6.935722000	-5.348179000	4.611315000
H	9.002936000	-4.241218000	3.302779000
H	5.903482000	-4.827392000	3.432624000

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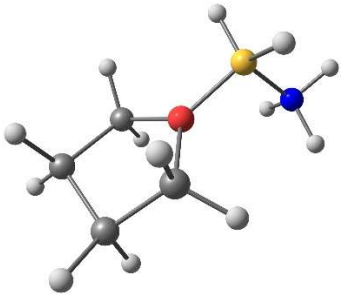


E(RPBE1PBE) = -314.373825902

- Thermochemistry -

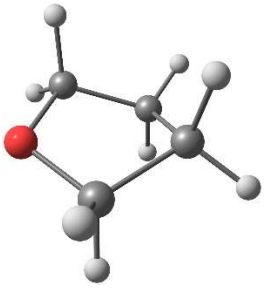
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.184126 (Hartree/Particle)
Thermal correction to Energy= 0.192260
Thermal correction to Enthalpy= 0.193204
Thermal correction to Gibbs Free Energy= 0.151410
Sum of electronic and zero-point Energies= -314.189700
Sum of electronic and thermal Energies= -314.181566
Sum of electronic and thermal Enthalpies= -314.180622
Sum of electronic and thermal Free Energies=-314.222416

Charge = 1 Multiplicity = 1

N	-0.622632000	-0.012473000	-1.045340000
B	-1.133605000	-0.149414000	0.445358000
H	-1.170388000	0.645180000	-1.608714000
H	-1.197370000	0.953472000	0.946826000
H	-0.441139000	-0.959783000	1.026473000
H	-0.596001000	-0.903491000	-1.551281000
H	0.338885000	0.344922000	-1.041006000
C	-4.321628000	-2.218970000	0.182327000
C	-2.837659000	-2.151585000	0.456864000
O	-2.550249000	-0.719326000	0.374584000
C	-3.773371000	0.084256000	0.381029000
C	-4.836643000	-0.912351000	0.780632000
H	-4.774130000	-3.110346000	0.637106000
H	-4.510642000	-2.249546000	-0.902162000
H	-2.208319000	-2.663713000	-0.282534000
H	-2.565329000	-2.481032000	1.470184000
H	-3.914175000	0.480920000	-0.635604000
H	-3.619411000	0.909156000	1.087328000
H	-5.824736000	-0.622257000	0.399028000
H	-4.896366000	-0.986292000	1.877423000

THF



E(RPBE1PBE) = -232.020116043

- Thermochemistry -

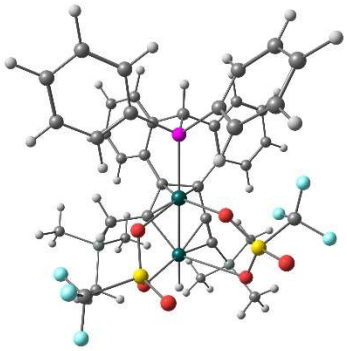
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.117087 (Hartree/Particle)
Thermal correction to Energy= 0.121877
Thermal correction to Enthalpy= 0.122821
Thermal correction to Gibbs Free Energy= 0.089278
Sum of electronic and zero-point Energies= -231.903029
Sum of electronic and thermal Energies= -231.898239
Sum of electronic and thermal Enthalpies= -231.897295
Sum of electronic and thermal Free Energies=-231.930838

Charge = 0 Multiplicity = 1

C	-4.327514000	-2.221877000	0.187519000
C	-2.833917000	-2.096362000	0.453043000
O	-2.534378000	-0.713277000	0.375997000
C	-3.730865000	0.046964000	0.381353000
C	-4.842752000	-0.914163000	0.778646000
H	-4.769876000	-3.121618000	0.639648000
H	-4.523351000	-2.252787000	-0.897332000
H	-2.216122000	-2.645562000	-0.277764000
H	-2.578428000	-2.482594000	1.460044000
H	-3.914869000	0.466743000	-0.627714000
H	-3.622111000	0.895793000	1.077751000
H	-5.828916000	-0.609915000	0.398422000
H	-4.909559000	-0.992431000	1.876591000

10-H$^-$



E(RPBE1PBE) = -4492.90037062

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.713661 (Hartree/Particle)
Thermal correction to Energy= 0.775226
Thermal correction to Enthalpy= 0.776170
Thermal correction to Gibbs Free Energy= 0.615320
Sum of electronic and zero-point Energies= -4492.186710
Sum of electronic and thermal Energies= -4492.125145
Sum of electronic and thermal Enthalpies= -4492.124200
Sum of electronic and thermal Free Energies=-4492.285051

Charge = -1 Multiplicity = 1

Rh	0.365462000	0.031197000	-0.167478000
Rh	0.172421000	0.157658000	2.465848000
S	-1.492670000	2.408922000	0.870529000
S	-2.816059000	-1.208833000	1.697719000
P	0.452576000	0.041692000	4.760468000
Si	1.097574000	-2.996845000	-2.075853000
Si	3.145239000	2.479098000	-0.644993000
F	-0.148257000	4.687697000	0.810493000
O	-4.228709000	-1.078765000	2.041838000
O	-0.864727000	2.200299000	2.206105000
O	-0.631814000	1.957013000	-0.273286000
F	-3.369129000	-3.778420000	1.634342000
O	-1.929882000	-0.450587000	2.641929000
F	-2.424269000	-3.138108000	3.462752000
F	-2.152202000	4.833927000	1.584762000
F	-1.828108000	4.595377000	-0.533287000
O	-2.444641000	-1.118744000	0.284850000
O	-2.910613000	2.110627000	0.758281000
F	-1.261157000	-3.357836000	1.663307000
C	2.149101000	2.171776000	0.960112000
C	2.187083000	-0.115574000	2.137823000
C	1.489598000	-1.409420000	2.052752000
C	1.651980000	0.784004000	1.137220000

C	1.152713000	-1.651047000	0.675500000
C	3.294206000	0.159577000	3.082254000
C	1.042849000	-1.947504000	-0.553544000
C	1.917974000	-2.335185000	4.373949000
C	4.466682000	0.779045000	2.624452000
H	4.563613000	1.010691000	1.564342000
C	3.209770000	-0.197385000	4.445582000
C	1.681542000	-2.534860000	2.994749000
C	-2.439543000	-2.972545000	2.143169000
C	1.618697000	-3.848510000	2.505216000
H	1.429946000	-4.003375000	1.441063000
C	4.258094000	0.137167000	5.309434000
H	4.171380000	-0.122386000	6.368207000
C	0.900007000	1.611250000	5.593951000
C	-1.394385000	4.247942000	0.669224000
C	2.025915000	-0.957383000	4.988019000
H	2.176845000	-1.072181000	6.070252000
C	2.094376000	-3.450975000	5.200224000
H	2.291129000	-3.291912000	6.264176000
C	5.509445000	1.093865000	3.490431000
H	6.407989000	1.580728000	3.102814000
C	1.266395000	2.699342000	4.791408000
H	1.209357000	2.605664000	3.703510000
C	-2.115378000	-0.419072000	5.648634000
H	-2.381947000	0.228535000	4.811397000
C	-0.767167000	-0.733349000	5.879794000
C	1.785425000	-4.946573000	3.341817000
H	1.727261000	-5.957202000	2.929674000
C	5.398101000	0.788162000	4.845951000
H	6.201554000	1.045348000	5.540859000
C	1.796356000	-4.675615000	-1.586219000
H	2.794887000	-4.573901000	-1.130894000
H	1.893548000	-5.327918000	-2.470703000
H	1.139074000	-5.186671000	-0.864022000
C	2.027660000	-4.748800000	4.700016000
H	2.163145000	-5.600831000	5.370989000
C	4.061741000	0.939952000	-1.221446000
H	4.773622000	0.549582000	-0.476904000
H	4.630479000	1.155323000	-2.141481000
H	3.337627000	0.139723000	-1.445162000
C	1.686369000	3.893111000	5.377035000
H	1.970468000	4.736609000	4.742340000
C	-3.112917000	-0.963910000	6.454264000
H	-4.159304000	-0.717896000	6.255782000
C	-0.653847000	-3.188910000	-2.719982000
H	-1.309568000	-3.615340000	-1.943613000
H	-0.689839000	-3.846534000	-3.604721000
H	-1.065088000	-2.207321000	-3.003716000
C	2.207552000	-2.182063000	-3.352408000
H	1.834612000	-1.177493000	-3.606732000

H	2.242361000	-2.781328000	-4.277873000
H	3.237264000	-2.083138000	-2.972856000
C	1.733598000	4.011464000	6.766089000
H	2.058508000	4.949043000	7.225192000
C	1.992438000	3.062707000	-2.006813000
H	1.261285000	2.275966000	-2.248803000
H	2.559047000	3.309250000	-2.920355000
H	1.433056000	3.960267000	-1.696965000
C	0.940266000	1.737888000	6.988665000
H	0.640833000	0.900637000	7.625301000
C	4.373962000	3.852416000	-0.239696000
H	3.849791000	4.754063000	0.119551000
H	4.960386000	4.138782000	-1.128940000
H	5.083112000	3.542351000	0.545926000
C	1.355999000	2.934403000	7.570642000
H	1.382513000	3.027629000	8.659670000
C	-0.439413000	-1.601911000	6.930059000
H	0.600304000	-1.859273000	7.139434000
C	-2.779679000	-1.833303000	7.493378000
H	-3.564420000	-2.268596000	8.117931000
C	-1.442157000	-2.150273000	7.729710000
H	-1.173550000	-2.830195000	8.542633000
H	2.761480000	2.492302000	1.818859000
H	1.304676000	2.868530000	0.887668000
H	0.380208000	-0.008230000	-1.803371000

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