Supporting Information

Iridium(III) hydride complexes for the catalytic dehydrogenation of hydrazine borane

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Experimental Details

General:

All manipulations were carried out in an oxygen- and moisture-free argon atmosphere using standard Schlenk- and glovebox techniques. All solvents were dispensed from a solvent purification system (PureSolv, Innovative Technology) or dried over sodium/benzophenone and freshly distilled prior to use. Resorcinol starting materials, (*t*-Bu)$_2$PCl, NaH, NaO*t*-Bu, and [(COD)IrCl] were purchased from Sigma-Aldrich and used as received. Resorcinol ligand 1,3-(OP*t*Bu$_2$)-4,6-COOMe-C$_6$H$_2$[1], complexes **1-Cl**[2], **1-H**[3], and **2-Cl**[4] as well as hydrazine borane[5] were prepared according to published procedures.

NMR spectroscopy:

NMR spectra were recorded on a Bruker AV 300 or AV 400 spectrometer. All ^{1}H NMR spectra are referenced using the chemical shifts of residual protio solvent resonances (THF-d_8: δH 1.73, 3.58, δC 25.4, 67.6). Chemical shifts are reported in ppm (δ) relative to tetramethylsilane. The ^{31}P{^{1}H} NMR spectra were referenced to external H_3PO_4, the ^{11}B NMR spectra were referenced to $BF_3{\cdot}Et_2O$ in chloroform.

Mass spectrometry:

Mass spectra were recorded on a Finnigan MAT 95-XP (Thermo Electron) instrument using chemical or electronic ionisation.

X-ray analysis:

X-ray analysis was performed on a Bruker Kappa APEX II Duo diffractometer. The structures were solved by direct methods (SHELXS-97)[6] and refined by full-matrix least-squares procedures on F^2 (SHELXL-2014).[7] Diamond was used for graphical representations.[8] CCDC 1431007-1431009 and CCDC 1454019 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Vibrational spectroscopy:

ATR-IR spectra were recorded on a Bruker Alpha spectrometer. Raman spectra were recorded on a Renishaw inVia Raman spectrometer using a 633 nm HeNe laser with a laser power of 10%.

Elemental analysis:

For determination of the B/N ratio, CHN and ICP analysis were performed on a Leco TruSpec Micro CHNS analyser and a Varian/Agilent 715-ES, respectively.

Synthesis and catalytic studies

Preparation of 3-Cl: 1,3-(*t*-Bu$_2$PO)-4,6-COOMe-C$_6$H$_2$ (267.5 mg, 0.55 mmol) and [(COD)IrCl]$_2$ (167.9 mg, 0.25 mmol) were heated in toluene at 150 °C for 8 hours. The reaction mixture was cooled to room temperature and all volatiles were removed in vacuum. The dark red residue was washed twice with pentane to yield the product complex. Yield: 345 mg (0.46 mmol). Single crystalline material

suitable for an X-ray analysis was obtained by slow evaporation of a THF solution. ^{1}H NMR (THF-d_8, 300 MHz, 297 K): δ 8.16 (s, 1H, Ar-H), 3.83 (s, 6H, $COOCH_3$), 1.40/1.38 (2 t, 36H, P(*t*-Bu)$_2$, -40.59 (t, $^{2}J_{PH}$= 12.9 Hz, 1H, IrH). ^{13}C NMR (THF-d_8, 75 MHz, 297 K): δ 169.3 ($\underline{C}_{Ar}$-O-P), 165.0 ($\underline{C}OOCH_3$), 132.6 (*p*-C_{Ar}), 123.7 (Ir-C), 110.7 ($\underline{C}_{Ar}$-$COOCH_3$), 51.6 ($COO\underline{C}H_3$), 43.8 ($\underline{C}(CH_3)_3$), 40.3 ($\underline{C}(CH_3)_3$), 27.7 ($C(\underline{C}H_3)_3$), 27.6 ($C(\underline{C}H_3)_3$). ^{31}P NMR (THF-d_8, 121 MHz, 297 K): δ 181.5. CHN analysis (anal. calcd. for $C_{26}H_{44}O_6P_2IrCl$): C, 42.33 (42.07); H, 5.78 (5.98). MS (EI, 70 eV): *m/z* 742.19 $[M]^+$.

General procedure for the preparation of complexes 2-H and 3-H: One equivalent of the hydride chloride complex (**2-Cl**/**3-Cl**) and 1.1 equiv. of NaO*t*Bu were dissolved in benzene under Ar. The Ar atmosphere was removed and replaced with hydrogen followed by stirring at room temperature until a colour change from red to orange was observed. After removal of the solvent in vacuum, pentane was added and the solution was filtered. The solution was evaporated to dryness and the residue was dissolved in benzene, followed by removal of the solvent in vacuum at 0 °C.

Complex **2-H**: ^{1}H NMR (THF-d_8, 300 MHz, 297 K): δ 7.06 (s, 1H, Ar-H), 1.44 (s, 18H, *t*-Bu), 1.35 (t, 36H, P(*t*-Bu)$_2$), -18.06 (t, $^{2}J_{PH}$= 8.5 Hz, 2H, IrH_2). ^{13}C NMR (C_6D_6, 75 MHz, 297 K): δ 166.2 ($\underline{C}_{Ar}$-O-P), 160.1 (Ir-$\underline{C}$), 126.8 ($\underline{C}_{Ar}$-H), 125.7 ($\underline{C}_{Ar}$- *t*-Bu), 40.8 (P-$\underline{C}CH_3$), 35.2 (Ph-$\underline{C}CH_3$), 30.9 ($PhC\underline{C}H_3$), 29.3 ($PC\underline{C}H_3$). ^{31}P NMR (THF-d_8, 121 MHz, 297 K): δ 206.5. CHN analysis (anal. calcd. for $C_{30}H_{57}O_2P_2Ir$): C, 51.26 (51.19); H, 8.19 (8.16). MS (EI, 70 eV): *m/z* 702 $[M-2H]^+$.

Complex **3-H**: ^{1}H NMR (THF-d_8, 300 MHz, 297 K): δ 8.37 (s, 1H, H-Ar), 3.82 (s, 6H, $COOCH_3$), 1.32 (t, 36H, P(*t*-Bu)$_2$), -17.29 (t, $^{2}J_{PH}$= 8.8 Hz, 2H, IrH_2). ^{13}C NMR (THF-d_8, 75 MHz, 297 K): δ 172.0 ($\underline{C}_{Ar}$-O-P), 165.6 ($\underline{C}OOCH_3$), 159.0 (Ir-$\underline{C}$), 137.5 ($\underline{C}_{Ar}$-H), 109.8 ($\underline{C}_{Ar}$-$COOCH_3$), 51.4 ($COO\underline{C}H_3$), 41.0 ($\underline{C}(CH_3)_3$), 28.6 ($C(\underline{C}H_3)_3$). ^{31}P NMR (THF-d_8, 121 MHz, 297 K): δ 210.6. CHN analysis (anal. calcd. for $C_{26}H_{45}O_6P_2Ir$): C, 43.62 (44.12); H, 6.09 (6.41). MS (CI, *i*-butane): *m/z* 708 $[M]^+$.

NMR data of complex 4 isolated from catalytic HB dehydrogenation experiments: ^{1}H NMR (THF-d_8, 300 MHz, 297 K): δ 7.88 (s, 1H, H-Ar), 5.18 (s, 2H, -NH_2), 3.92 (t, 2H, Ir-NH_2, $^{3}J_{PH}$ = 4.2 Hz), 3.74 (s, 6H, $COOCH_3$), 1.46 (t, 36H, $^{3}J_{PH}$ = 6.9 Hz), -9.22 (t, $^{2}J_{PH}$ = 16.2 Hz, 2H, IrH_2). ^{31}P NMR (THF-d_8, 121 MHz, 297 K): δ 177.9. Due to the limited amount of analytically pure material, no ^{13}C NMR, MS and CHN data were collected.

General procedure for dehydrogenation experiments: Hydrazine borane (HB, 50 mg, 1.09 mmol) and the corresponding Ir catalyst (0.5, 1.0, 2.0, or 5.0 mol%, respectively) were weighed in the glovebox and transferred to a three-necked dehydrogenation vessel and a Schlenk flask, respectively. Then, the HB containing dehydrogenation flask was connected to the gas buret and subsequently equipped with a dropping funnel with pressure compensation under Ar atmosphere. The gas buret was initialised and HB and Ir catalyst were dissolved in 5 mL of THF, respectively. The catalyst solution was transferred to the dropping funnel, the data acquisition was started and the catalyst solution was quickly added to the HB solution via the dropping funnel. After completion of the dehydrogenation reaction, a gas sample was taken and analysed by TCD-GC. The reaction solution was filtered and the BN residue as well as the filtrate were further analysed. Details of the experimental setup were published before.[9,10]

X-ray crystallography

Crystallographic data for complex **2-H**: $C_{30}H_{57}IrO_2P_2$, M_r = 703.89, red prism, monoclinic, a = 15.3157(11), b = 12.5538(9), c = 17.5443(12) Å, β = 105.3035(18)°, V = 3253.6(4) Å^3, T = 150(2) K, space group $P\,2_1/n$, Z = 4, 7099 independent reflections, 6481 reflections observed, final R values: R_1 ($I > 2\sigma(I)$) = 0.0202, wR_2 (all data) = 0.0472, 342 parameters, CCDC 1431007. The H1 and H2 atoms were found from a difference Fourier map and SADI instruction was used to equalize both Ir-H distances.

Crystallographic data for complex **3-Cl**: $C_{26}H_{44}ClIrO_6P_2$, M_r = 742.20, red plate, monoclinic, a = 8.1246(4), b = 33.5291(15), c = 11.6849(5) Å, β = 107.5091(13)°, V = 3035.6(2) Å^3, T = 150(2) K, space group $P\,2_1/c$, Z = 4, 7332 independent reflections, 5472 reflections observed, final R values: R_1 ($I > 2\sigma(I)$) = 0.0342, wR_2 (all data) = 0.0662, 340 parameters, CCDC 1431008. One COOMe group is disordered, which could not be fully resolved. Therefore the distances C23-O3 and C23-O4 are equalized (SADI instruction) and the methyl group C24 is half occupied at two positions. H1 could be found from the difference Fourier map and was refined with Ir-H = 1.55 Å and U_{iso}(H) fixed at 1.5 U_{eq}(Ir).

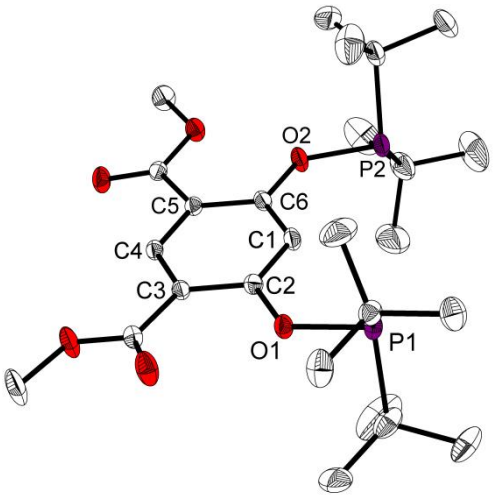


Figure S1. Molecular structure of the POCOP ligand 1,3-(*t*-Bu_2PO)-4,6-COOMe-C_6H_2. Thermal ellipsoids correspond to 30% probability at 150 K. Hydrogen atoms are omitted for clarity.

Crystallographic data for the POCOP ligand 1,3-(*t*-Bu_2PO)-4,6-COOMe-C_6H_2: $C_{26}H_{44}O_6P_2$, M_r = 514.55, colourless rod, monoclinic, a = 10.5142(5), b = 18.0091(9), c = 16.4272(9) Å, β = 107.797(2) °, V = 2961.7(3) Å^3, T = 150(2) K, space group $P\,2_1/n$, Z = 4, 5983 independent reflections, 4877 reflections observed, final R values: R_1 ($I > 2\sigma(I)$) = 0.0399, wR_2 (all data) = 0.1118, 321 parameters, CCDC 1454019.

Crystallographic data for complex **4** (Figure 7): $C_{26}H_{49}IrN_2O_6P_2$, M_r = 739.81, red plate, trigonal, a = b = 40.862(2), c = 11.1596(7) Å, V = 16137(2) Å^3, T = 150(2) K, space group $R\bar{3}$, Z = 18, 8643 independent

reflections, 7370 reflections observed, final *R* values: R_1 ($I > 2\sigma(I)$) = 0.0301, wR_2 (all data) = 0.0831, 366 parameters, CCDC 1431009. The estimated diffraction contributions of disordered solvent molecules were removed from the observed diffraction data using the SQUEEZE procedure in PLATON.[11] The Ir bound H atoms were found from difference Fourier map and refined with Ir-H = 1.55 Å. Additionally AFIX 2 instruction was used for H2C to fix s.o.f. and U.

NMR spectroscopy

Further characterization of the hydrides

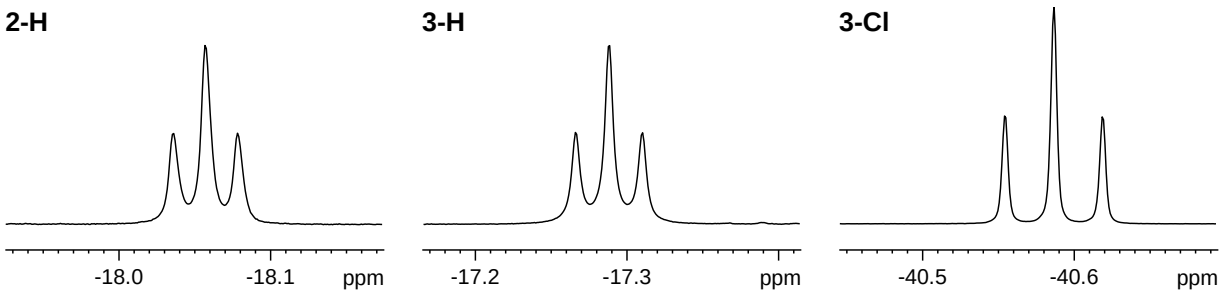


Figure S2. ^{1}H NMR spectra (THF-d_8, 400.1 MHz, 297 K) of the iridium complexes **2-H**, **3-H** and **3-Cl** (hydride region). It is evident that the dihydride complexes differ from the monohydride complex with respect to chemical shift, P-H-coupling constant and linewidth. The larger linewidth observed for the signals of **2-H** and **3-H** is an intrinsic property and not due to field inhomogeneity.

Table S1. Compilation of NMR properties

compound	**2-H**	**3-H**	**3-Cl**
$\delta(^{1}H)$/ppm	–18.06	–17.29	–40.59
$^{2}J(^{31}P,^{1}H)$/Hz	8.6	8.8	12.9
linewidth (fwhm)/Hz	2.6	2.5	1.6
T_1/s	0.24 AREA fit : Inversion-Recovery (T1) : I[t]=I[0](1-2*A*exp(-t/T1)) 12 points for Integral 2, Integral Region from -17.968 to -18.157 ppm Converged after 81 iterations! Results Comp. 1 I[0] = 1.001e+000 A = 8.992e-001 **T1 = 242.264m** RSS = 2.391e-004 SD = 4.464e-003	0.25 AREA fit : Inversion-Recovery (T1) : I[t]=I[0](1-2*A*exp(-t/T1)) 12 points for Integral 2, Integral Region from -17.226 to -17.351 ppm Converged after 68 iterations! Results Comp. 1 I[0] = 9.915e-001 A = 9.032e-001 **T1 = 252.286m** RSS = 9.277e-004 SD = 8.793e-003	1.0 AREA fit : Inversion-Recovery (T1) : I[t]=I[0](1-2*A*exp(-t/T1)) 12 points for Integral 1, Integral Region from -40.532 to -40.633 ppm Converged after 66 iterations! Results Comp. 1 I[0] = 9.953e-001 A = 8.950e-001 **T1 = 1.020s** RSS = 4.540e-004 SD = 6.151e-003

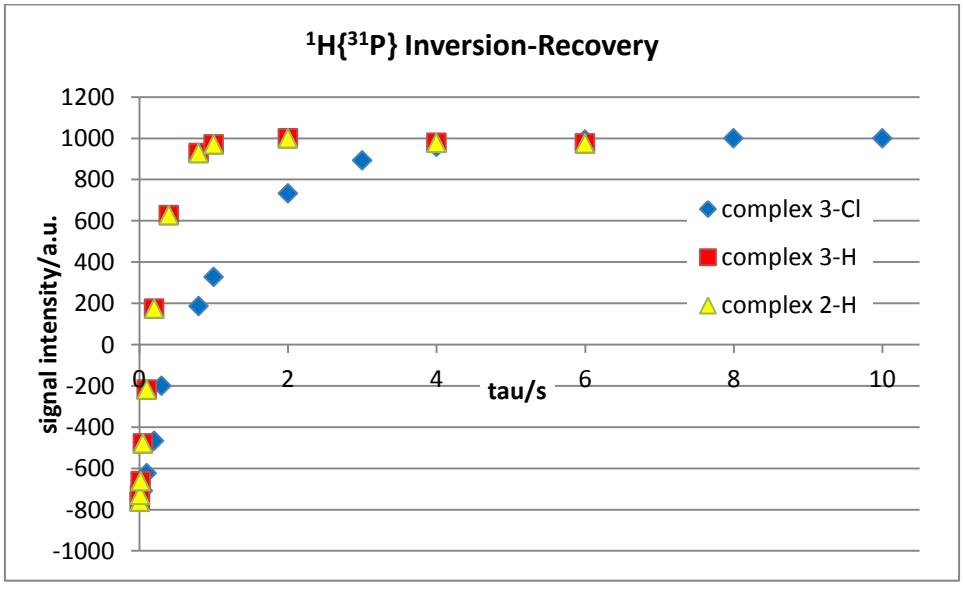


Figure S3. Estimation of the longitudinal relaxation time T_1 for the hydride atoms by the Inversion-Recovery sequence (under phosphorus decoupling). B_0 = 9.4 T (400.1 MHz ^{1}H), THF-d_8 solution, T = 297 K

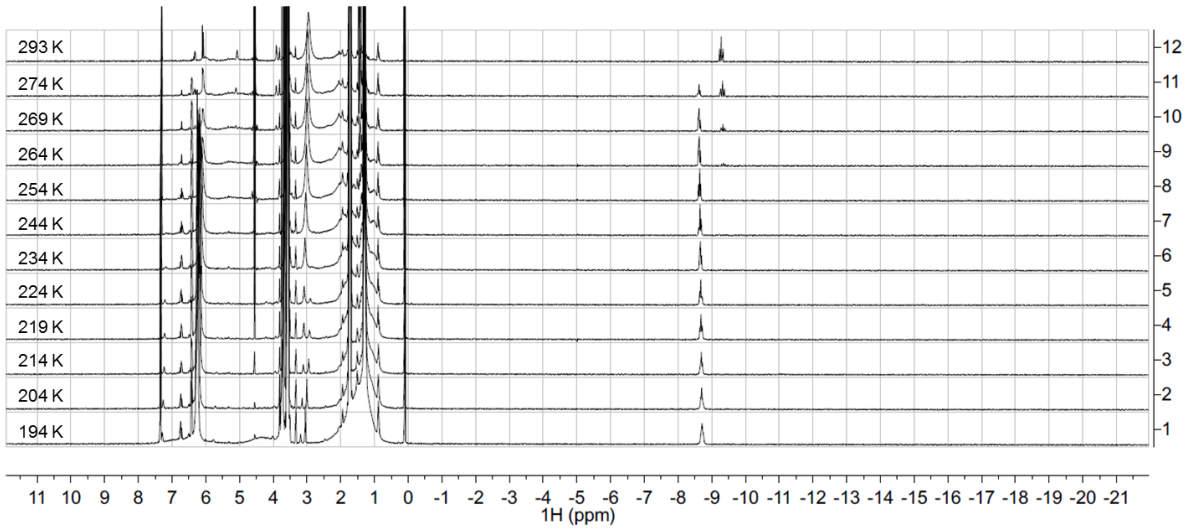


Figure S4. Complete view of the in situ ^{1}H NMR spectrum of HB dehydrogenation with complex **1-H** in THF-d_8 (300 MHz, c(**1-H**) = 1.4·10^{-6} mol·l^{-1}, c(HB) = 2.7·10^{-5} mol·l^{-1}).

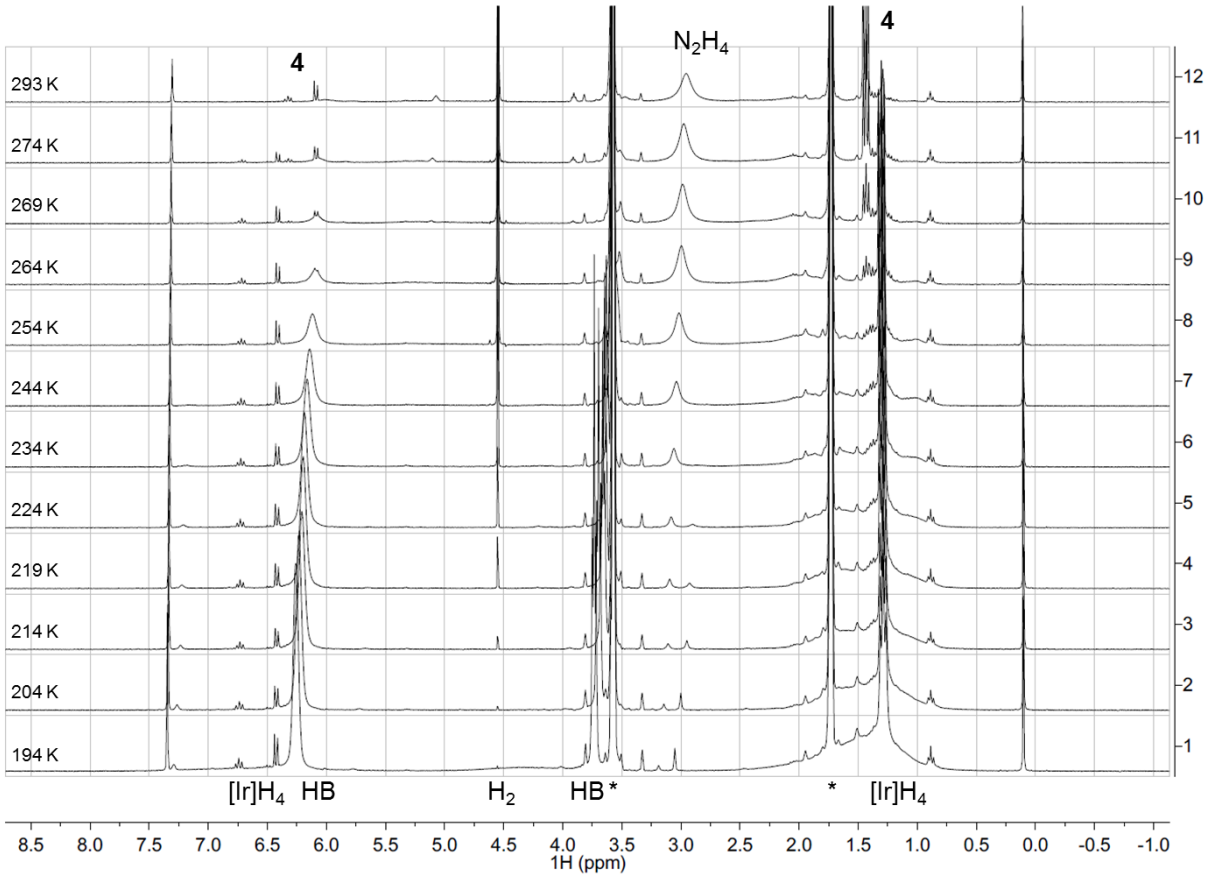


Figure S5. In situ ^{1}H NMR spectrum of HB dehydrogenation with complex **1-H** in THF-d_8 (300 MHz, c(**1-H**) = 1.4·10^{-6} mol·l^{-1}, c(HB) = 2.7·10^{-5} mol·l^{-1}).

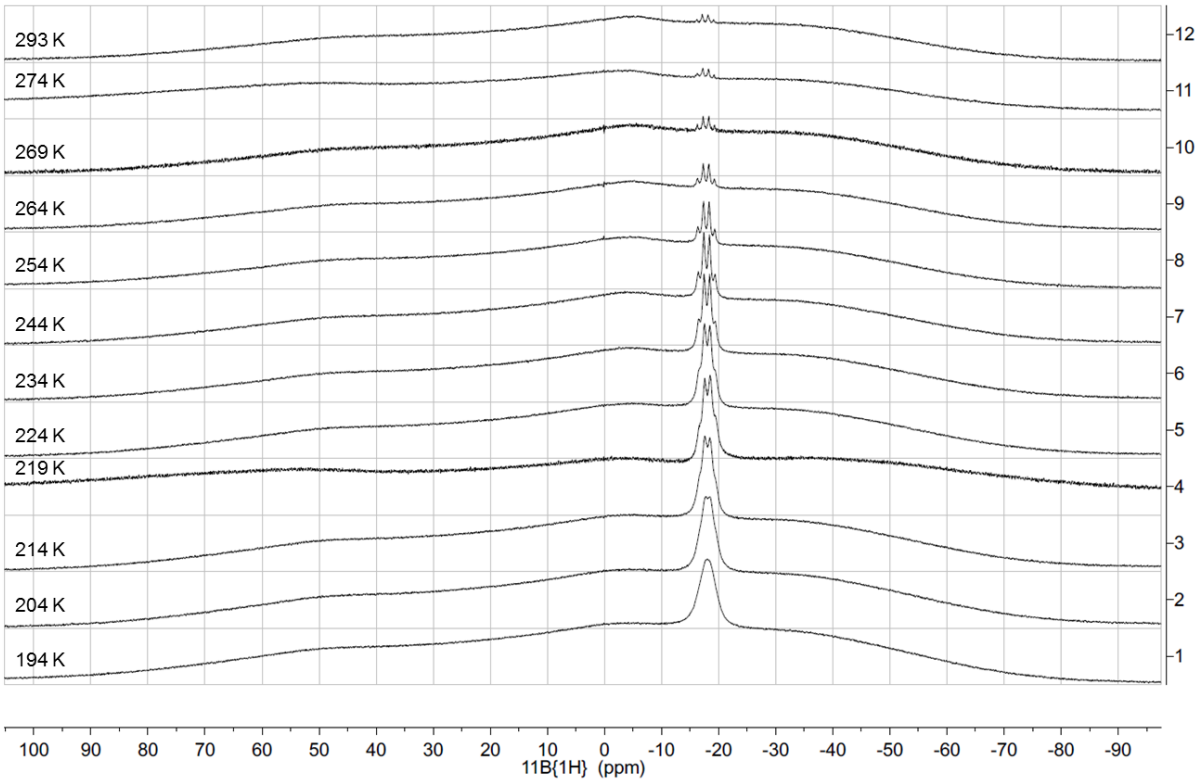


Figure S6. In situ $^{11}B\{^{1}H\}$ NMR spectrum of HB dehydrogenation with complex **1-H** in THF-d_8 (96 MHz, c(**1-H**) = $1.4 \cdot 10^{-6}$ mol·l^{-1}, c(HB) = $2.7 \cdot 10^{-5}$ mol·l^{-1}).

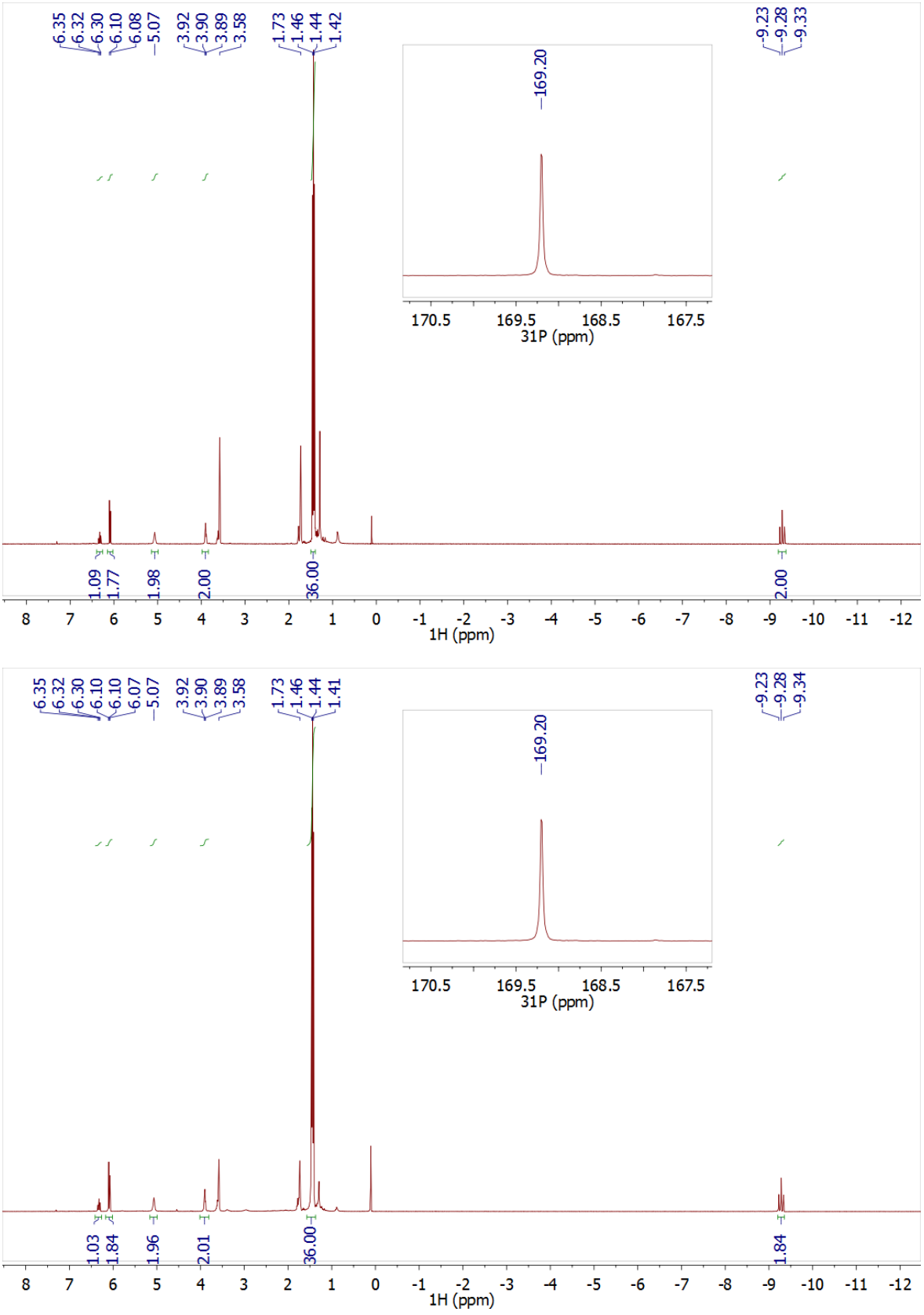


Figure S7. ^{1}H (THF-d_8, 300 MHz, 298 K) and ^{31}P NMR spectra (THF-d_8, 121 MHz, 298 K; inset) of the residue obtained from the filtrate after dehydrogenation of HB with complexes **1-Cl** (top) and **1-H** (bottom).

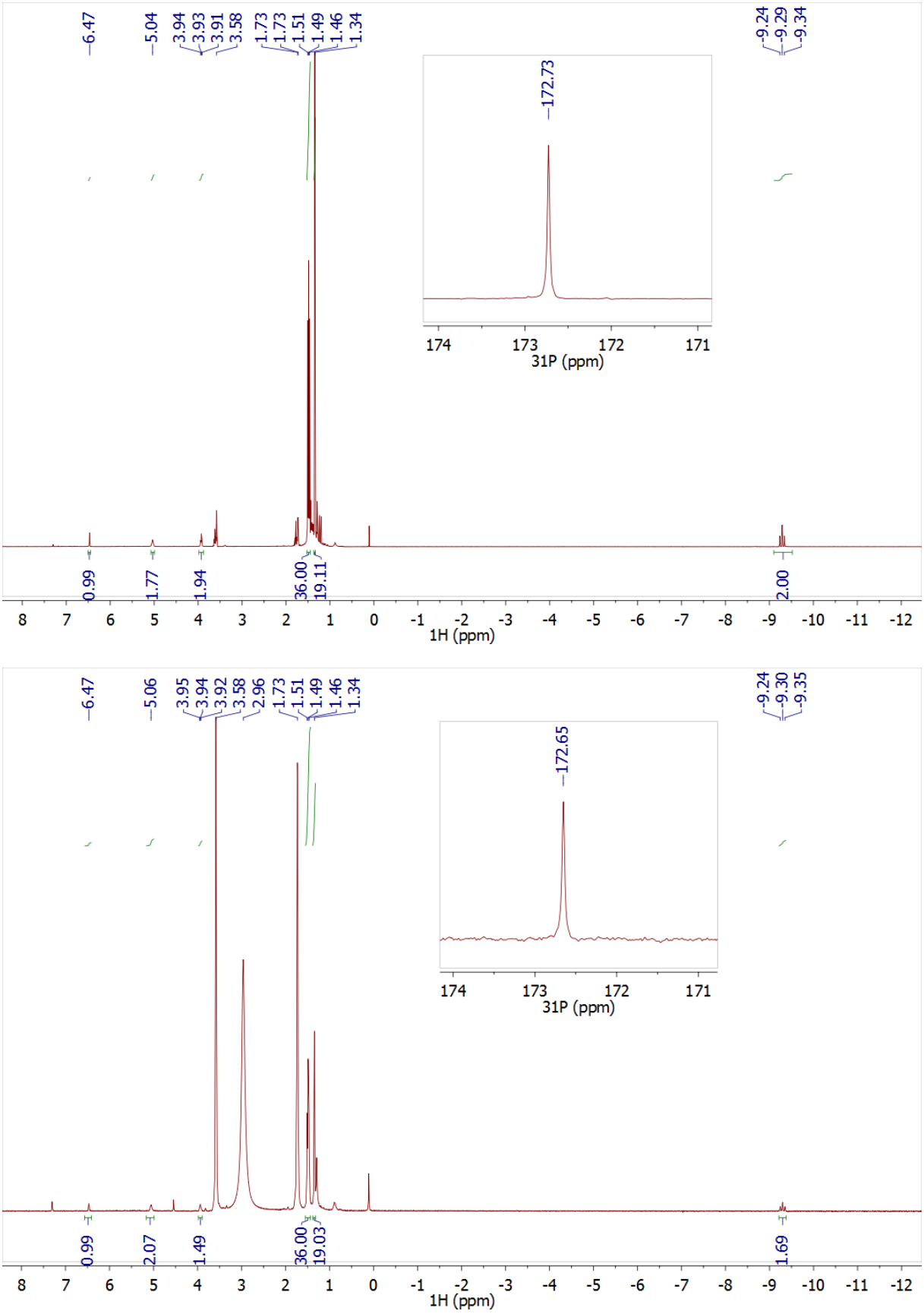


Figure S8. ^{1}H (THF-d_8, 300 MHz, 298 K) and ^{31}P NMR spectra (THF-d_8, 121 MHz, 298 K; inset) of the residue obtained from the filtrate after dehydrogenation of HB with complexes **2-Cl** (top) and **2-H** (bottom).

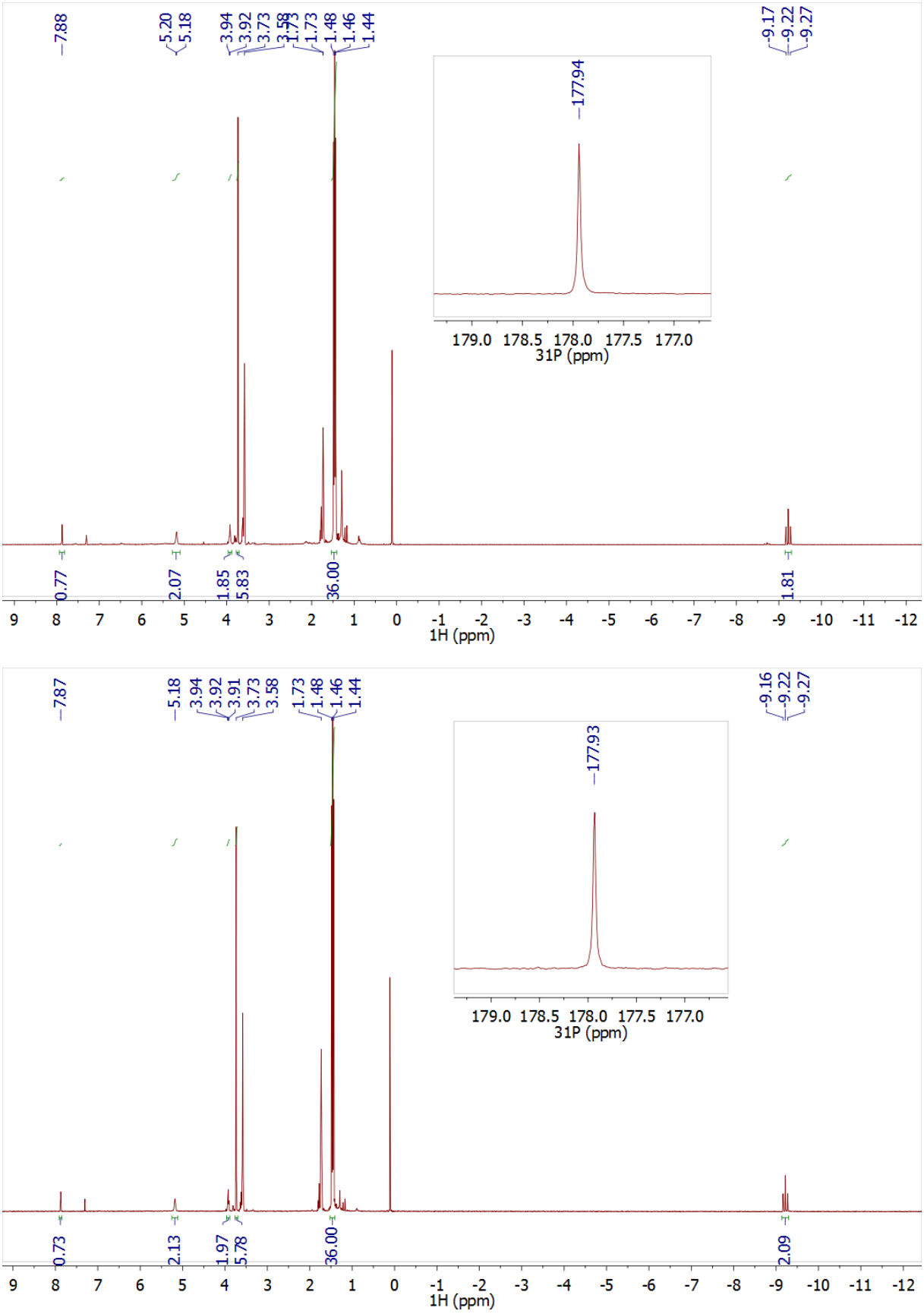


Figure S9. ^{1}H (THF-d_8, 300 MHz, 298 K) and ^{31}P NMR spectra (THF-d_8, 121 MHz, 298 K; inset) of the residue obtained from the filtrate after dehydrogenation of HB with complex **3-Cl** (top) and **3-H** (bottom).

Mass spectrometry

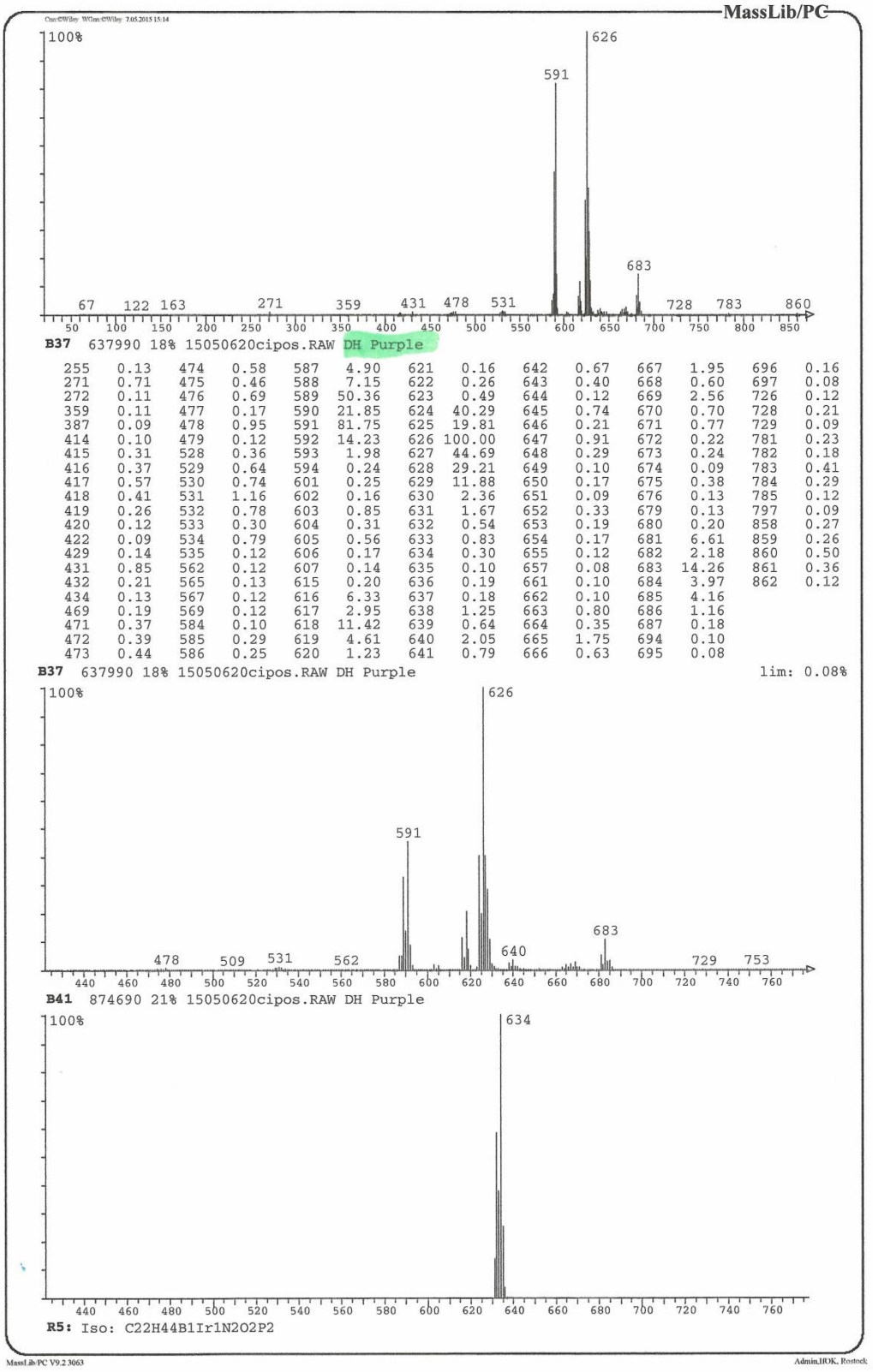


Figure S10. CI-MS of the residue obtained from the filtrate after dehydrogenation of HB with complex **1-H**.

Solid state NMR spectroscopy

^{11}B-MAS-NMR studies were conducted on Bruker Avance III 300 and Bruker DSX 500 spectrometers operating at 96.3 and 160.4 MHz, respectively, using short excitation pulses (0.6 µs) and sample rotation frequencies of 12.5 and 10.0 kHz, respectively.

^{11}B{^{1}H}-CPMAS- and CPHETCOR-experiments were conducted at 160.4 MHz at a MAS rotation speed of 29.8 kHz. The ramped version was used, varying the ^{1}H excitation power from 50-100% to a maximum nutation frequency of 100 kHz. The overall cross-polarization contact time was 1.0 ms. Signal acquisition was done under proton decoupling (TPPM15 scheme with 10/12-π-pulses at the nutation frequency of 100 kHz). The indirect dimension in the CPHETCOR-experiments was incremented in a rotor synchronized fashion (increment 33.6 µs) and 128 data points were acquired.

^{11}B{^{1}H}-REDOR experiments were conducted at 160.4 MHz using a MAS rotation frequency of 29.8 kHz and π-pulses of 4.1 and 3.2 µs for ^{11}B and ^{1}H, respectively. Signal acquisition was done under proton decoupling (TPPM15 scheme with 10/12-π-pulses). ^{1}H{^{11}B}REAPDOR experiments were conducted at 160.4 MHz using a MAS frequency of 29.8 kHz. The ^{11}B nutation frequency was 161 kHz.

All experiments were done with relaxation delays between 5-10 seconds, which was found to be sufficient for observing quantitatively representative spectra.

Table S2. ^{1}H chemical shifts of the four spectral components observed in the ^{1}H spin echo and ^{1}H{^{11}B} REAPDOR spectra.

δ / ppm REAPDOR	δ / ppm ECHO
4.01	4.10
3.35	3.73
2.12	2.12
1.46	1.38

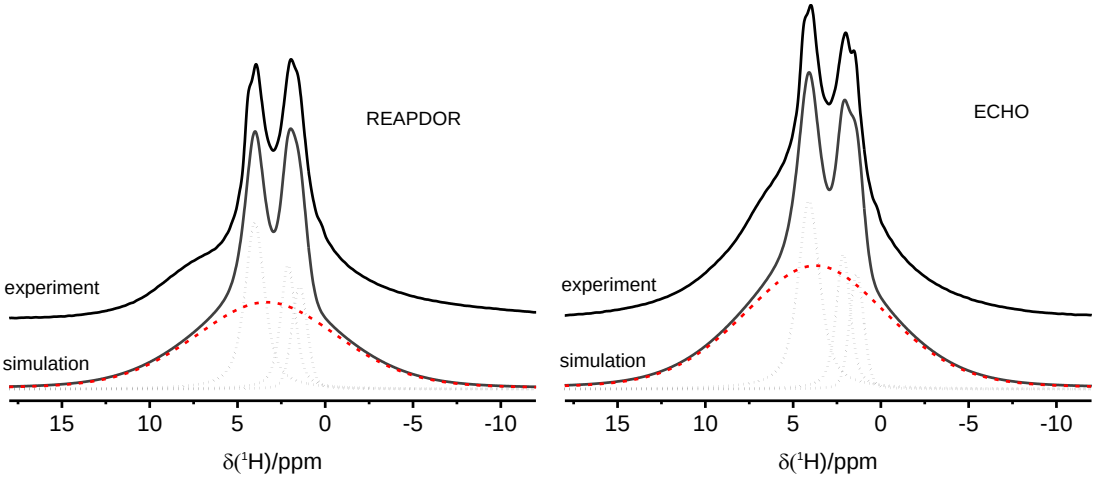


Figure S11. ^{1}H MAS-NMR spectrum (rotor synchronized spin echo, right) and ^{1}H {^{11}B} REAPDOR spectrum (using a dipolar evolution time of 67.2 µs, left) and their deconvolutions into different signal components. The proton signal with strongest ^{11}B dipolar dephasing effect is highlighted (dashed red).

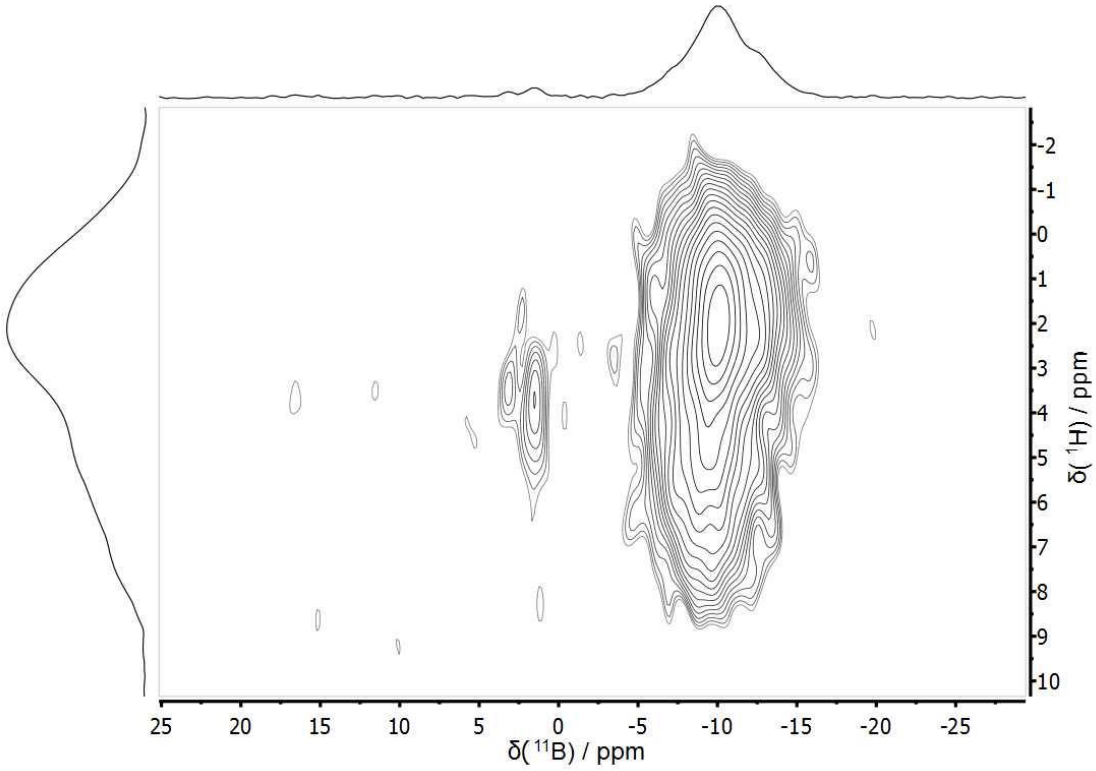


Figure S12. Solid-state ^{1}H/^{11}B heteronuclear correlation experiment obtained via ^{11}B{^{1}H} CPMAS.

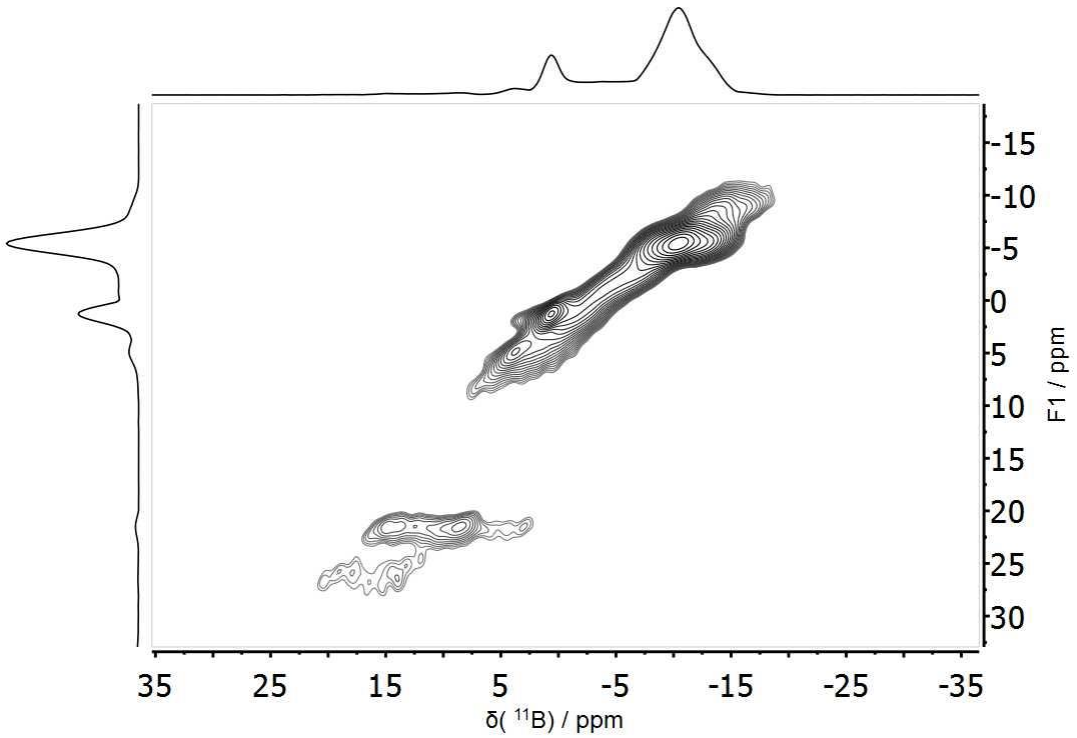


Figure S13. 2D ^{11}B-TQ-MAS NMR spectrum of the dehydrogenation reaction product obtained with **1-H** as catalyst (*c* = 10 mol%, cf. Fig 4a) recorded at a spinning speed of 29.8 kHz and a field strength of 11.7 T. High power proton decoupling was used during the pulse sequence and acquisition.

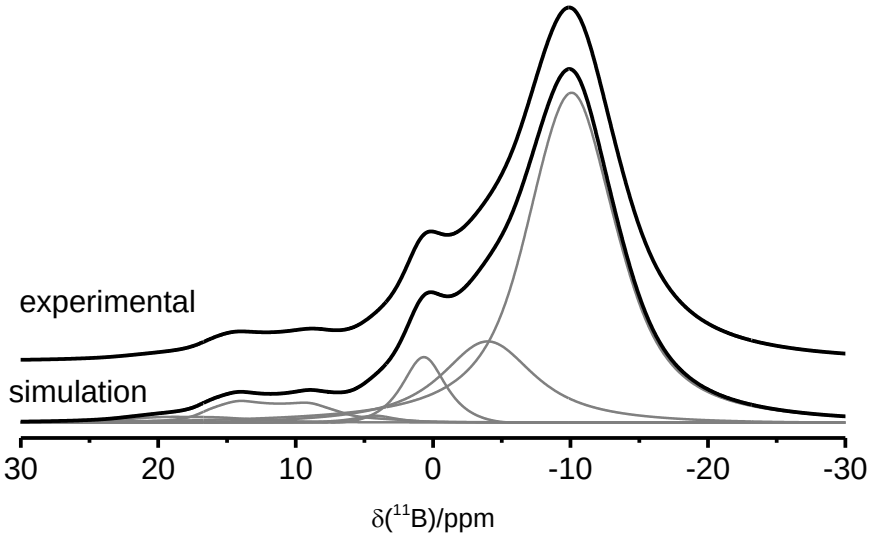


Figure S14. Experimental (top) and simulated (bottom) ^{11}B -MAS NMR spectrum of the dehydrogenation reaction product obtained with **1-H** as catalyst (*c* = 10 mol%, cf. Fig 4b) recorded at a spinning speed of 29.8 kHz and a field strength of 11.7 T. High power proton decoupling was used during acquisition.

Table S3. Isotropic chemical shift and quadrupolar coupling parameters of ^{11}B species in dehydrogenated HB determined by analysis of ^{11}B TQ-MAS (grey) and ^{11}B MAS (white) NMR spectra. Dehydrogenation of HB with different amounts of catalyst **1-H** led to the highlighted values (10 mol%) and those in parenthesis (2 mol%, only four species). Values in brackets marked with * are calculated using formula S1, η_Q of the deconvolution and SOQE of ^{11}B TQ-MAS.

^{11}B resonance	1	2	3	4	5	6
F2 /ppm	**-10.4** (-10.1)	**-3.7** (-2.37)	**0.7** (1.2)	**3.84**	**12.0** (12.3)	**17.6**
F1 /ppm	**-5.5** (-5.1)	**-1.0** (-6.7)	**1.2** (1.7)	**4.8**	**21.7** (23.1)	**26.6**
δ^{CS} /ppm	**-7.3** (-6.9)	**-2.0** (-4.0)	**1.0** (1.5)	**4.4**	**18.1** (19.1)	**23.3**
SOQE /MHz	**1.80** (1.80)	**1.32** (1.67)	**0.57** (0.57)	**0.81**	**2.51** (2.65)	**2.4**
δ^{CS} /ppm	**-6.7** (-7.1)	**-2.2** (-3.3)	**1.1** (1.4)	**4.8**	**18.0** (18.29)	**23.5**
η_Q	**0.90** (0.77)	**>0.7** (---)	---	---	**0.25** **(0.28)**	---
C_Q /MHz	**1.64 [1.57]*** (1.63 [1.66]*)	**1.20 [<1.22]*** (---)	---	---	**2.55 [2.47]*** (2.53 [2.62]*)	---

$$SOQE = C_Q\sqrt{1+\frac{{\eta_Q}^2}{3}} \qquad \text{(S1)}$$

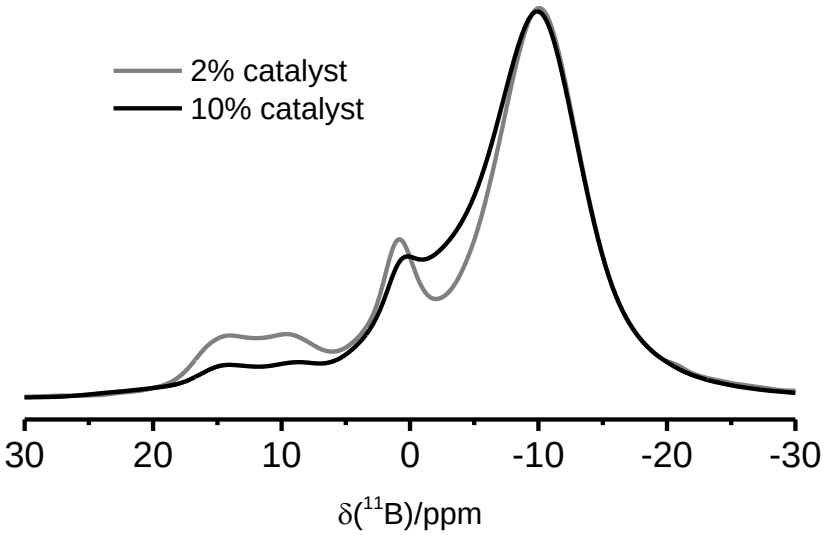


Figure S15. ^{11}B -MAS NMR spectrum of the dehydrogenation reaction product obtained with 2 mol% (grey curve) respectively 10 mol% (black curve) of **1-H** as catalyst recorded at a spinning speed of 29.8 kHz and a field strength of 11.7 T. High power proton decoupling was used during acquisition.

Vibrational spectroscopy

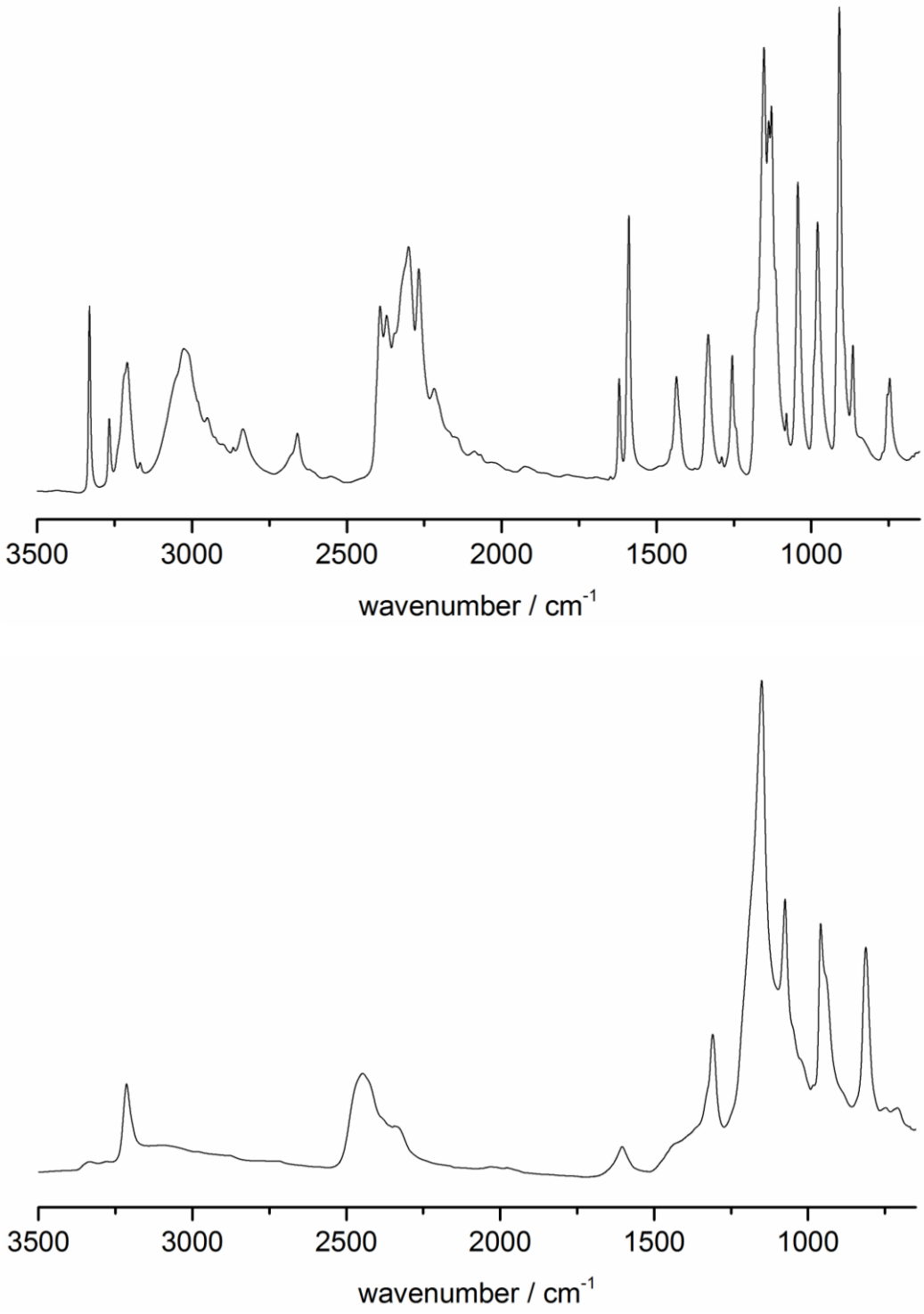


Figure S16. Comparison of IR spectra of HB (top) and the dehydrogenated solid residue obtained after dehydrogenation with 2mol% **1-H** as catalyst (bottom).

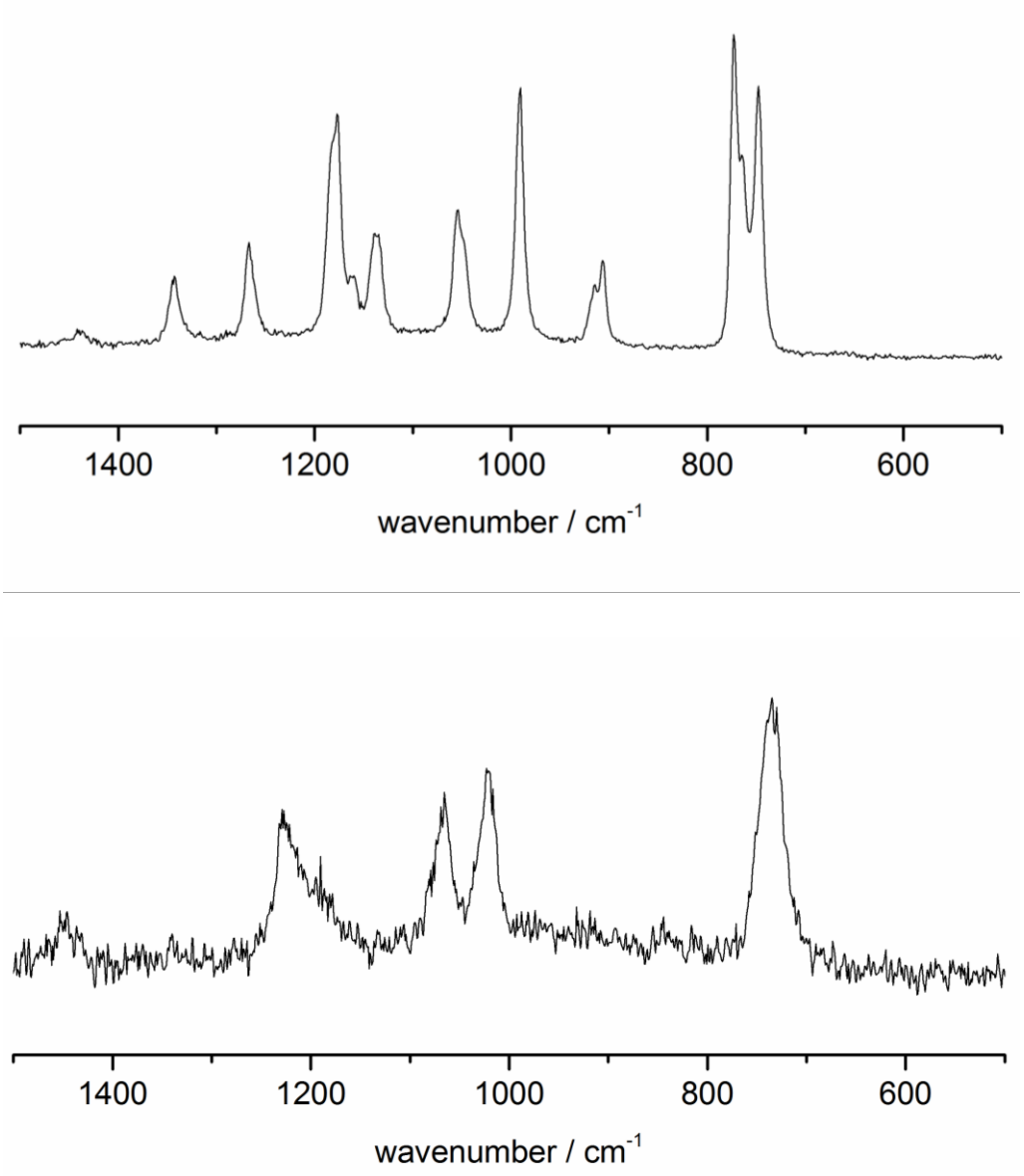


Figure S17. Comparison of Raman spectra of HB (top) and the dehydrogenated residue obtained after dehydrogenation with 2mol% **1-H** as catalyst (bottom).

Volumetric data

The amount of gas evolved during dehydrogenation was determined using an automatically operating gas buret.[9,10] After completion of the reaction, the composition of the gas was determined using TCD-GC. For graphical presentation the amount of hydrogen was related to the amount of HB used. Data points recorded prior to addition of the catalyst solution (see Experimental Section) are not shown.

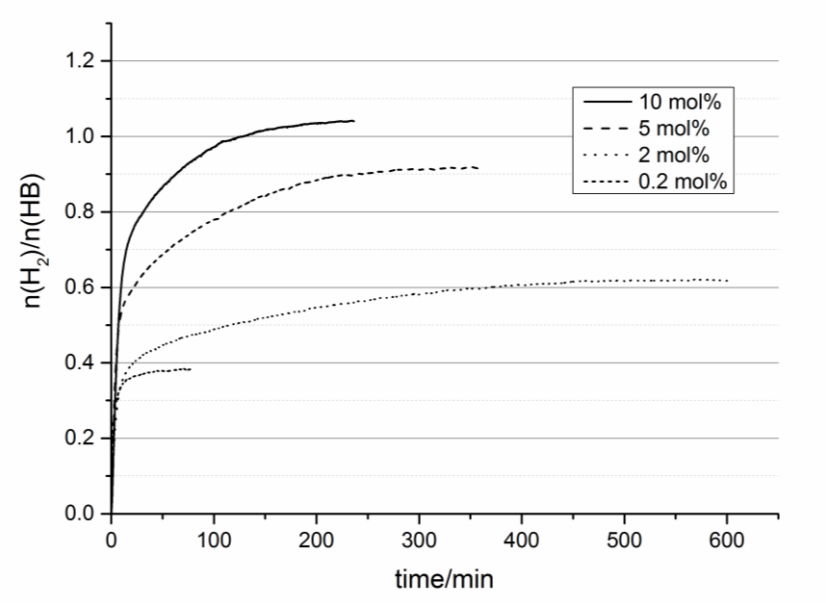


Figure S18. Summary of volumetric data obtained from HB dehydrogenation with **1-Cl** (THF, *T* = 25 °C).

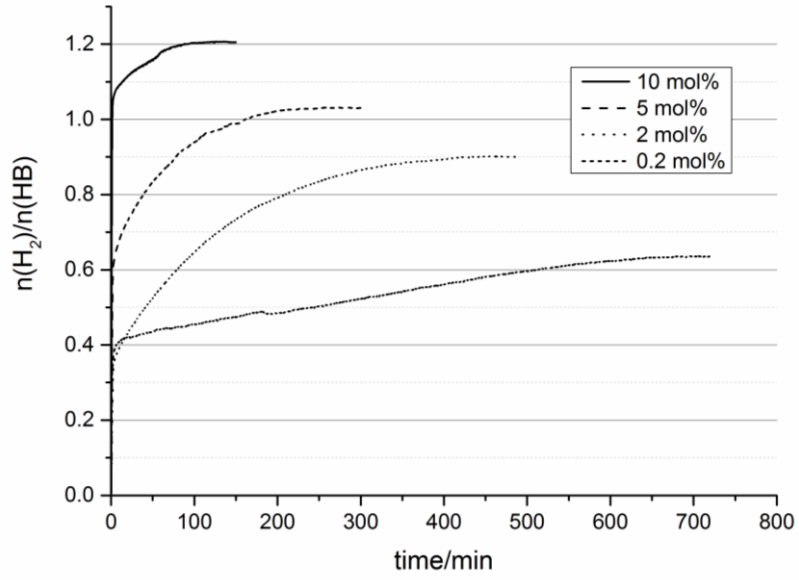


Figure S19. Summary of volumetric data obtained from HB dehydrogenation with **1-H** (THF, *T* = 25 °C)

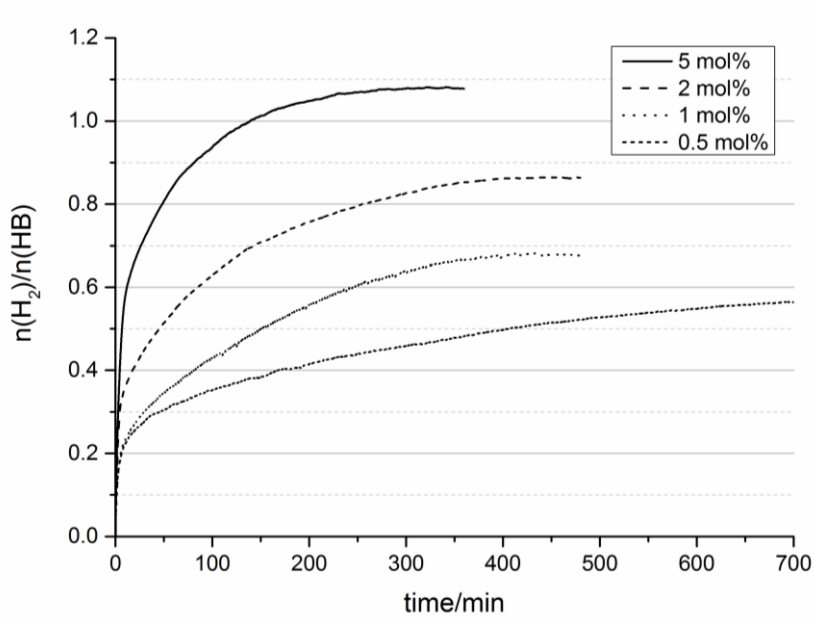


Figure S20. Summary of volumetric data obtained from HB dehydrogenation with **2-Cl** (THF, *T* = 25 °C).

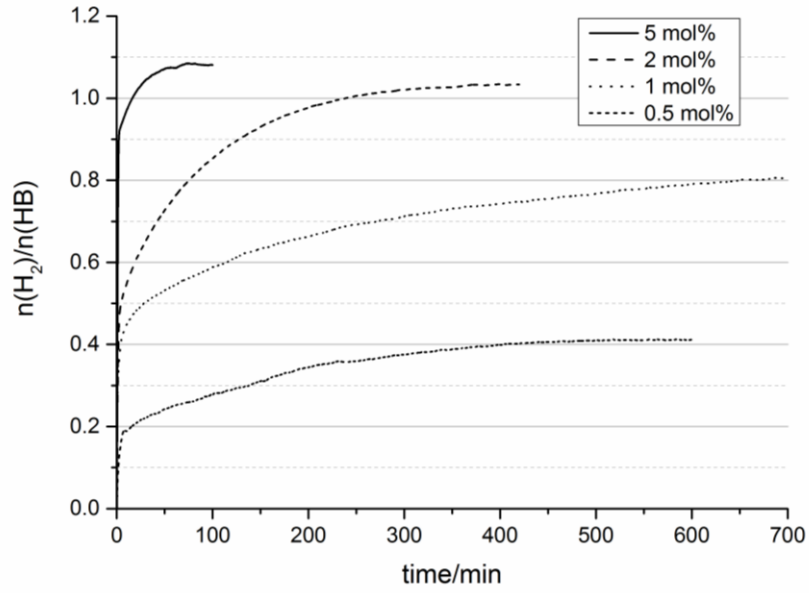


Figure S21. Summary of volumetric data obtained from HB dehydrogenation with **2-H** (THF, *T* = 25 °C).

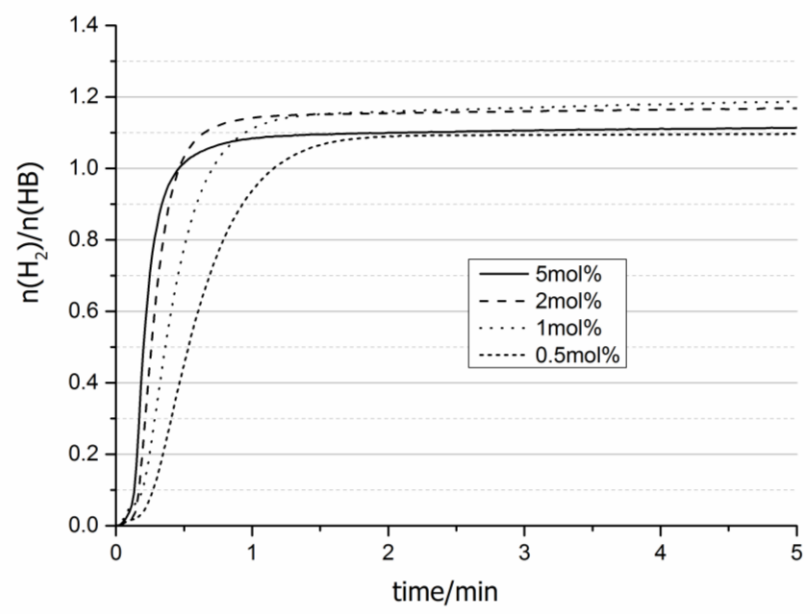


Figure S22. Summary of volumetric data obtained from HB dehydrogenation with **3-Cl** (THF, *T* = 25 °C).

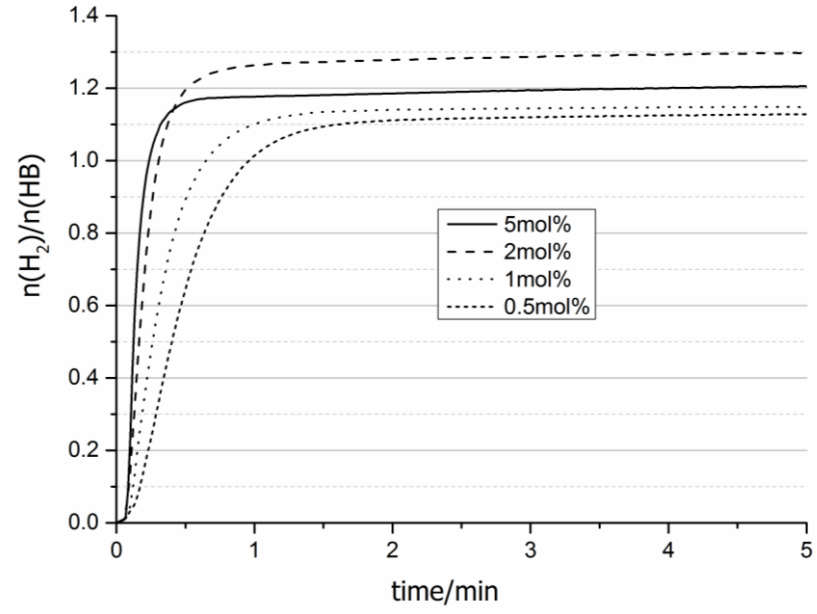


Figure S23. Summary of volumetric data obtained from HB dehydrogenation with **3-H** (THF, *T* = 25 °C).

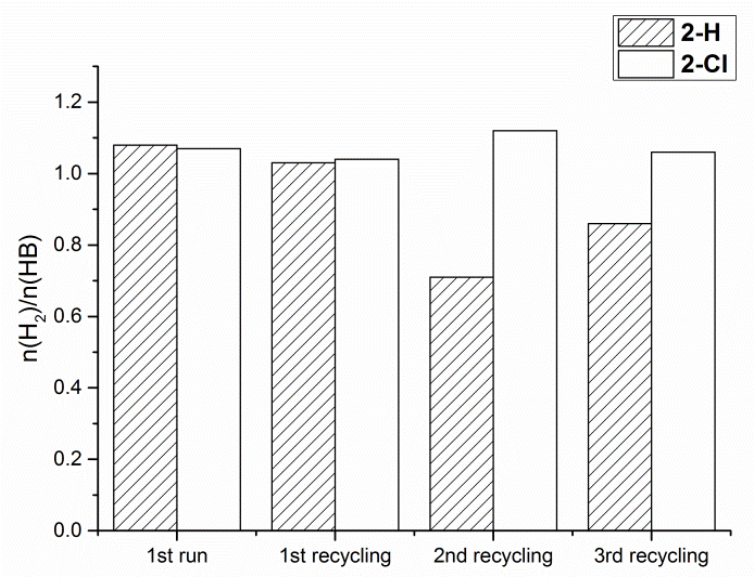


Figure S24. Summary of volumetric data obtained from HB dehydrogenation recycling experiments with **2-Cl** and **2-H**. Note that for each run, a fresh 50 mg portion of HB was added (THF, T = 25 °C, initial Ir concentration c = 5 mol%)

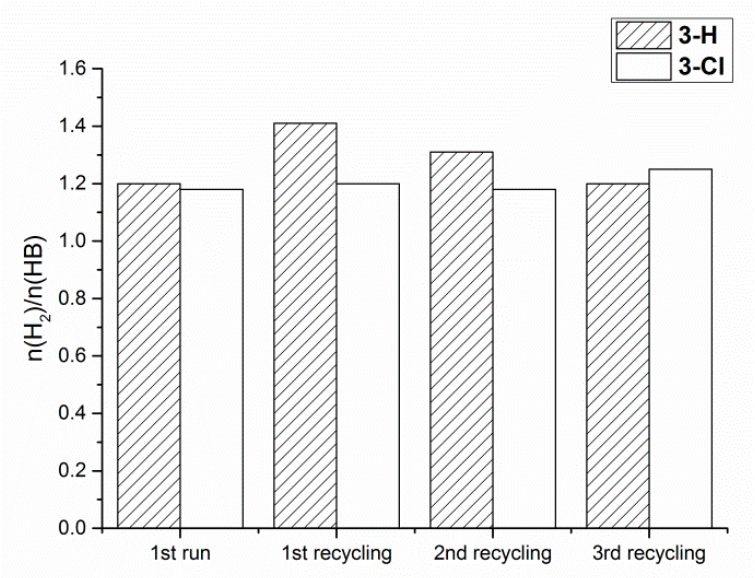


Figure S25. Summary of volumetric data obtained from HB dehydrogenation recycling experiments with **3-Cl** and **3-H**. Note that for each run, a fresh 50 mg portion of HB was added (THF, T = 25 °C, initial Ir concentration c = 5 mol%)

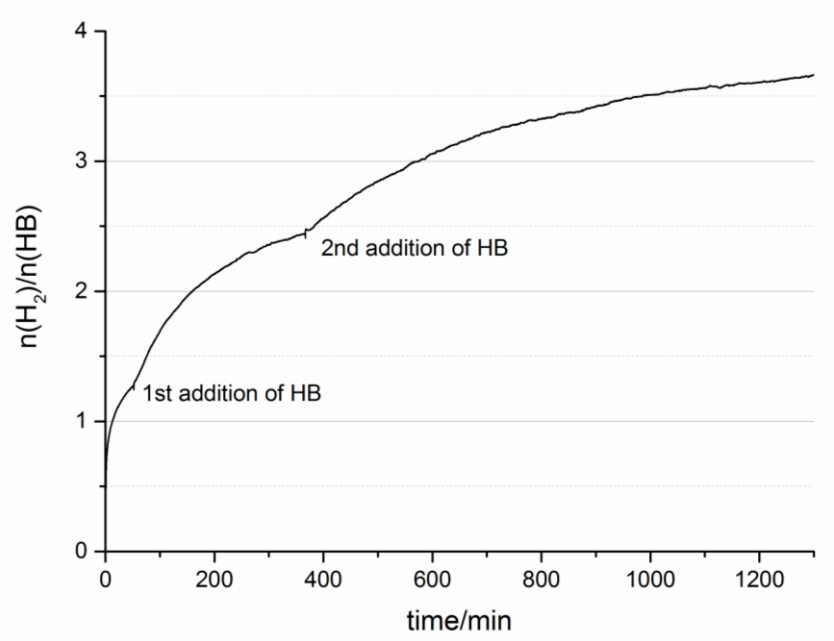


Figure S26. Volumetric data obtained from consecutive HB addition without removal of the catalyst species (10 mol% **1-H**, 50 mg of HB were added in each step). A relatively high catalyst loading was chosen as lower concentrations resulted in very long reaction times after addition of the third portion of HB. Note that the Ir dihydrido hydrazine complex was isolated at the end of this experiment. ^{1}H and ^{31}P NMR spectra resemble those shown in Figure S7.

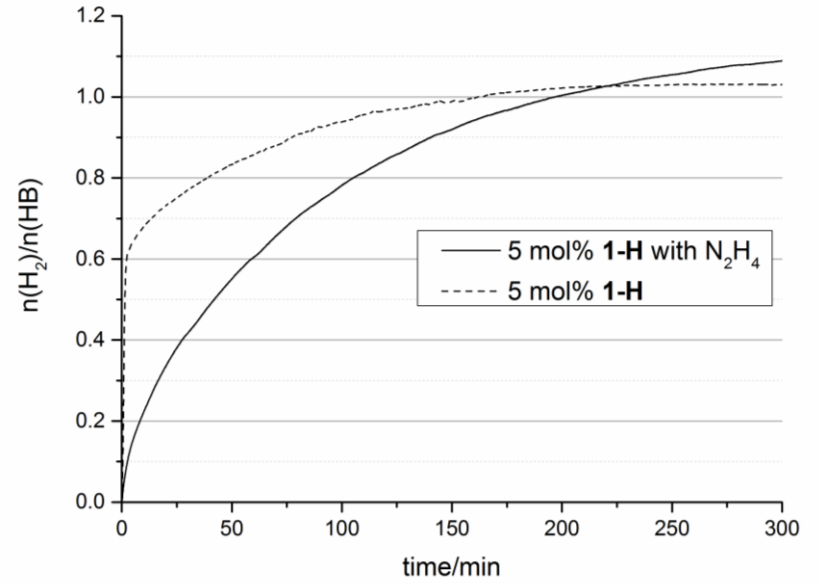
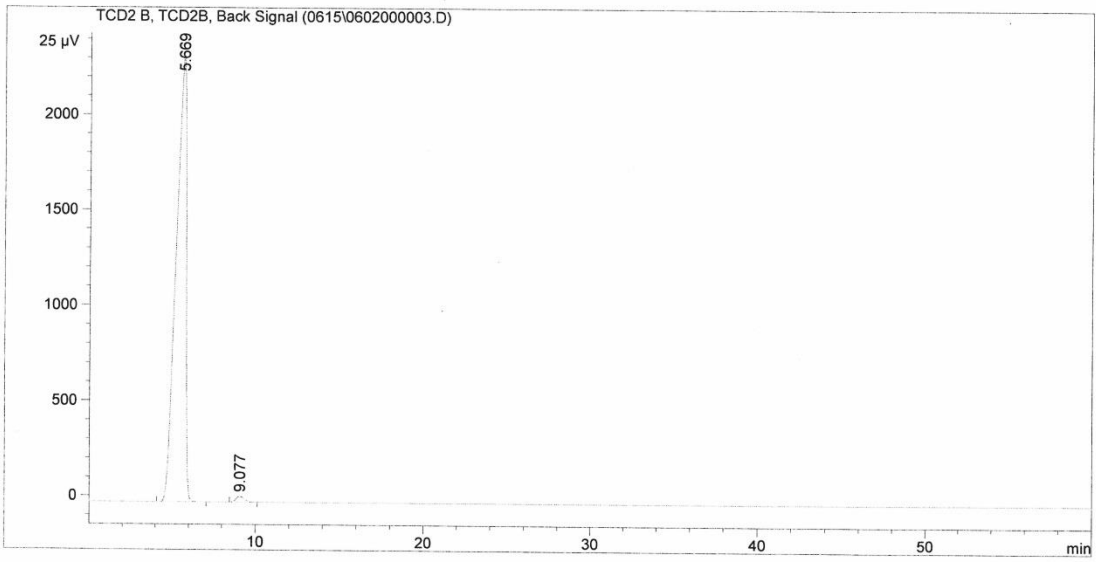


Figure S27. Comparison of volumetric data of HB dehydrogenation with and without addition of free hydrazine.

Gas chromatography

Data File C:\CHEM32\1\DATA\0615\0602000003.D
Sample Name: DH84

```
Acq. Operator   : L2H
Acq. Instrument : Instrument 1                    Location :   -
Injection Date  : 6/2/2015 1:09:33 PM
                                                  Inj Volume : Manually
Acq. Method     : C:\CHEM32\1\METHODS\GASGEMISCH1.M
Last changed    : 6/2/2015 12:38:42 PM by L2H
Analysis Method : C:\CHEM32\1\METHODS\GASGEMISCH1.M
Last changed    : 6/2/2015 2:09:34 PM by L2H
Sample Info     : DH84 5%
```




```
                          Area Percent Report

Calculated By             :      Signal
Multiplier:                      :      1.0000
Dilution:                        :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: TCD2 B, TCD2B, Back Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  [25 µV*s]   [25 µV]      %
----|-------|----|-------|----------|----------|--------|
   1   5.669 BB    0.6988 9.85830e4  2343.42529 99.03520
   2   9.077 BB    0.5359  960.39020   28.88872  0.96480

Totals :                  9.95434e4  2372.31401
```

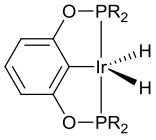
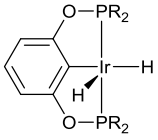
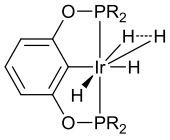
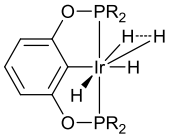
Instrument 1 6/2/2015 2:09:34 PM L2H Page 1 of 1

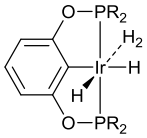
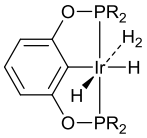
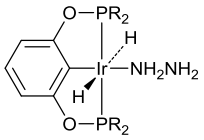
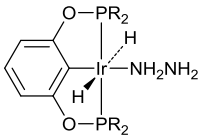
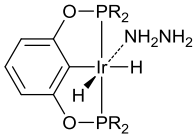
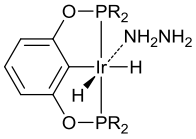
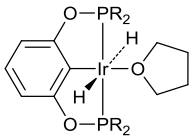
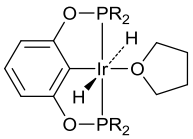
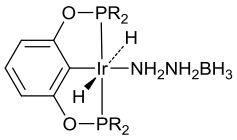
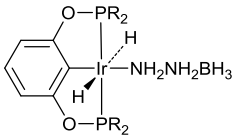
Figure S28. Representative gas chromatograph recorded after dehydrogenation of HB using **1-H** as the catalyst. The minor peak at 9.077 corresponds to residual air.

Computational details

Computational procedure: To study to reaction mechanisms, we used both B3PW91 functional[12] and B3PW91 functional including dispersion correction (EmpiricalDispersion=GD3BJ[13]) and solvation effect of THF using self-consistent reaction field (SCRF,[14]). In our study we used TZVP basis set[15] (LANL2DZ for Ir[16]) for structure optimization and frequency calculation. The corresponding frequency calculation was used to characterize the nature of the optimized structures; i.e.; energy minimums without imaginary frequencies or transition states with only one imaginary frequency; and the imaginary model connects the initial and the final states. The thermal corrections to Gibbs free energy at 298 K from the frequency analysis were added to the total electronic energies, and we therefore used the corrected Gibbs free energy (ΔG) at 298 K for our energetic discussion and comparison. All calculations were carried out by using the Gaussian 09 program.[17]

Table S4. Computed energetic data.

B3PW91	B3PE91-D3-SCRF (THF)
	
1-H	**1-H**
HF=-1800,9670798 ZPE=368.34080´; NImag=0 Htot=-1800.344907 Gtot=-1800,441864	HF=-1801.1691769 ZPE=369.73750; NImag=0 Htot=-1800,545511 Gtot= -1800,640838
	B3PW91-D3-SCRF//B3PW91//SP HF=-1801.1647327 ZPE=367.43429; NImag=0 Htot=-1800,543659 Gtot= -1800,641611
	
1-H-H_2	**1-H-H_2**
HF=-1802,1584766 ZPE= 379.96741; NImag=0 Htot= -1801.517600 Gtot= -1801,614685	HF=-1802.3661212 ZPE= 380.22806; NImag=0 Htot= -1801.724962 Gtot= -1801,822595

 **1-H-H_2-TS** HF=-1802,1315249 ZPE= 377.07953; NImag=1 (-336.4853) Htot= -1801.494076 Gtot= -1801,592679	 **1-H-H_2-TS** HF=-1802.3423304 ZPE= 377.77065; NImag=1 (-543.8211) Htot= -1801.705289 Gtot= -1801,799696
 **1-H-N_2H_4-Eq** HF=-1912.8524379 ZPE= 405.04461; NImag=0 Htot= -1912.169043 Gtot= -1912,270989	 **1-H-N_2H_4-Eq** HF=-1913,0801601 ZPE= 405.96774; NImag=0 Htot= -1912.395640 Gtot= -1912,497373
 **1-H-N_2H_4-Axial** HF=-1912.8481854 ZPE=406.63639; NImag= 0 Htot=-1912.162746 Gtot= -1912,262658	 **1-H-N_2H_4-Axial** HF=-1913,0777715 ZPE= 407.01480; NImag=0 Htot= -1912.391865 Gtot= -1912,492116
 **1-H-THF-Eq** HF=-2033.3991334 ZPE=443.00864; NImag=0 Htot= -2032.652931 Gtot= = -2032,760437	 **1-H-THF-Eq** HF=-2033.6417348 ZPE= 444.36721; NImag=0 Htot= -2032.893260 Gtot= -2033,001303
 **1-H-$NH_2NH_2NH_3$-Eq**	 **1-H-$NH_2NH_2NH_3$-Eq**

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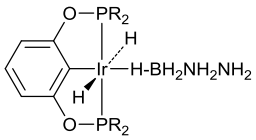
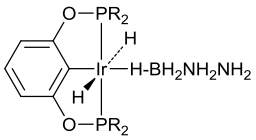
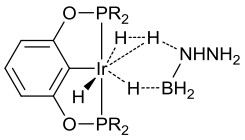
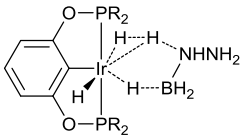
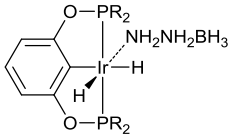
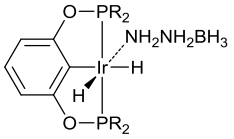
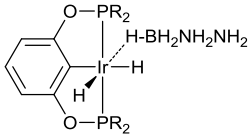
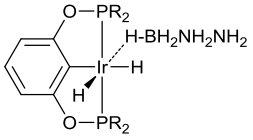
 **1-H-HBH$_2$NH$_2$NH$_2$-Eq** HF=-1939.5055654 ZPE= 424.98323; NImag=0 Htot= -1938.787878 Gtot= -1938,895879	 **1-H-HBH$_2$NH$_2$NH$_2$-Eq** HF=-1939.7445809 ZPE= 426.14329; NImag=0 Htot= -1939.025609 Gtot= -1939,132099
 **Ir-2H-P-2H-BH$_3$-N$_2$H$_4$-Eq-TS** HF=-1939.4838367 ZPE=421.72716; NImag=1 (-702.4597) Htot= -1938.771914 Gtot= -1938,878099	 **Ir-2H-P-2H-BH$_3$-N$_2$H$_4$-Eq-TS** HF=-1939.7220467 ZPE= 421.58304; NImag=1 (-629.9189) Htot= -1939.010435 Gtot= -1939,116825
 **1-H-NH$_2$NH$_2$NH$_3$-Axial** HF=-1939.5047719 ZPE= 427.05133; NImag=0 Htot= -1938.784327 Gtot= -1938,890824	 **1-H-NH$_2$NH$_2$NH$_3$-Axial** HF=-1939.746972 ZPE= 427.99072; NImag=0 Htot= -1939.025523 Gtot= -1939,131687
 **1-H-HBH$_2$NH$_2$NH$_2$-Axial** HF=-1939.5009047 ZPE= 425.94259; NImag=0 Htot= -1938.781922 Gtot= -1938,889218	 **1-H-HBH$_2$NH$_2$NH$_2$-Axial** HF=-1939.7396844 ZPE= 426.88494; NImag=0 Htot= -1939.019454 Gtot= -1939,127234

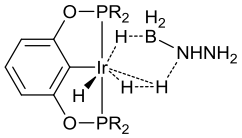
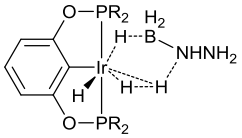
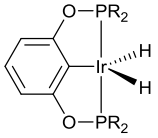
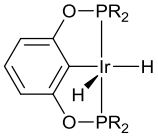
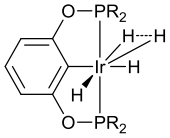
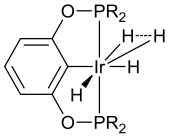
 **1-H-HBH$_2$NH$_2$NH$_2$-Axial-TS** HF=-1939.4757011 ZPE= 421.38724; NImag=(-441.8196) Htot= -1938.764401 Gtot= -1938,870702	 **1-H-HBH$_2$NH$_2$NH$_2$-Axial-TS** HF=-1939.7128888 ZPE=421.84403; NImag=1 (-535.1720) Htot=-1939.002212 Gtot= -1939,104133
H$_2$ HF=-1.1786359 ZPE=6.31541; NImag=0 Htot=-1.165267 Gtot= -1,180065	**H$_2$** HF=-1.1788966 ZPE=6.30078; NImag=0 Htot=-1.165551 Gtot= -1,180350
N$_2$H$_4$-BH$_3$ HF=-138.5333206 ZPE=55.14575; NImag=0 Htot=-138.439775 Gtot= -138,471257	**N$_2$H$_4$-BH$_3$** HF=-138.5550952 ZPE=55.11325; NImag=0 Htot=-138.461582 Gtot= -138,493144
H$_2$B=NH-NH$_2$ HF=-137.3500808 ZPE=41.01400; NImag=0 Htot=-137.279332 Gtot= -137,310524	**H$_2$B=NH-NH$_2$** HF=-137.3604899 ZPE=40.93317; NImag=0 Htot=-137.289899 Gtot= -137,320846
NH$_2$-NH$_2$ HF=-111.8706654 ZPE=33.62064; NImag=0 Htot=-111.812898 Gtot= -111,839003	**NH$_2$-NH$_2$** HF=-111.8807246 ZPE=33.66095; NImag=0 Htot=-111.822879 Gtot=-111,849026
C$_4$H$_8$O-THF HF=-232.4459247 ZPE= 73.27263; NImag=0 Htot= -232.323267 Gtot= -232,356983	**C$_4$H$_8$O-THF** HF=-232.4648469 ZPE= 73.26992; NImag=0 Htot= -232.342222 Gtot= -232,375681

Table S5. Optimized Cartesian Coordinates

B3PW91	B3PE91-D3-SCRF (THF)
	
1-H	**1-H**
H,0,-5.7823844667,-0.3213314566,0.	H,0,0.7542435223,0.0359126192,-0.5160830906
C,0,-4.699147105,-0.2619927243,0.	Ir,0,0.3600289276,-0.0065469984,0.9623275308
C,0,-1.917159131,-0.1116578113,0.	H,0,2.0066060912,-0.0118411262,1.1694082893
C,0,-4.026621337,-0.22486304,1.2175898829	C,0,-1.7009449965,-0.0050957722,0.7976776689
C,0,-4.026621337,-0.22486304,-1.2175898829	C,0,-4.4897269557,-0.004450888,0.6039604997
C,0,-2.6386222505,-0.1495805111,-1.1954748221	C,0,-2.4229022655,-1.195306444,0.724905125
C,0,-2.6386222505,-0.1495805111,1.1954748221	C,0,-2.4251974664,1.185452186,0.7649592734
H,0,-4.5647842492,-0.2528029276,2.1568645481	C,0,-3.8119472094,1.2109186864,0.6705275912
H,0,-4.5647842492,-0.2528029276,-2.1568645481	C,0,-3.8096219513,-1.2201107283,0.6299004813
O,0,-1.9597084726,-0.1089562444,2.3882893795	H,0,-4.3473996686,2.15214204,0.6462794039
O,0,-1.9597084726,-0.1089562444,-2.3882893795	H,0,-4.3433785361,-2.1609250792,0.5736217222
P,0,-0.2621471077,-0.0011926644,2.2545872738	H,0,-5.5714375441,-0.0042241489,0.5302904898
P,0,-0.2621471077,-0.0011926644,-2.2545872738	O,0,-1.7364845,2.3773647287,0.8247983987
C,0,0.2093484247,-1.5526634285,3.2319335927	O,0,-1.7320968338,-2.3877217168,0.7432697949
C,0,0.2093484247,-1.5526634285,-3.2319335927	P,0,-0.0368683021,-2.2506936109,0.8199690535
C,0,0.0319020119,1.6154342446,3.1918306736	P,0,-0.0435804898,2.2394690515,0.9405656278
C,0,0.0319020119,1.6154342446,-3.1918306736	C,0,0.2809926164,-3.2482775842,2.3735948566
C,0,-0.6027183753,-1.7472286504,4.5134631384	C,0,0.4456122831,-3.1250609512,-0.760828014
C,0,-0.6027183753,-1.7472286504,-4.5134631384	C,0,0.4784354556,3.2171012116,-0.5641239476
H,0,-0.3803215858,-2.7389934457,4.9212914588	C,0,0.2211631259,3.1284255838,2.5682466386
H,0,-0.3803215858,-2.7389934457,-4.9212914588	C,0,-0.0554492557,-2.2821745384,3.5166200379
H,0,-1.6743632367,-1.6971469963,4.3180143025	H,0,0.0484451503,-2.8062806302,4.4710258189
H,0,-1.6743632367,-1.6971469963,-4.3180143025	H,0,-1.0800924368,-1.9107104293,3.445573232
H,0,-0.3576170628,-1.0164245234,5.2826195406	H,0,0.6286479447,-1.4292030209,3.5295908494
H,0,-0.3576170628,-1.0164245234,-5.2826195406	C,0,1.7623881631,-3.6108257899,2.4388563826
C,0,1.7088231484,-1.5286555924,3.5356949216	H,0,2.0273539274,-4.3772904245,1.7091878743
C,0,1.7088231484,-1.5286555924,-3.5356949216	H,0,1.9896879964,-4.0075320068,3.4324588044
H,0,2.0131986559,-2.5121412519,3.9076641509	H,0,2.3935572904,-2.7348239972,2.27172862
H,0,2.0131986559,-2.5121412519,-3.9076641509	C,0,-0.599382968,-4.4885633081,2.4982958989
H,0,1.961953352,-0.7976257202,4.3059457056	H,0,-0.3636108416,-5.2442477053,1.7519410053
H,0,1.961953352,-0.7976257202,-4.3059457056	H,0,-1.6550427718,-4.2324589381,2.4093861748
H,0,2.2985574831,-1.3128473093,2.6415290681	H,0,-0.4372488787,-4.9337678937,3.4847079525
H,0,2.2985574831,-1.3128473093,-2.6415290681	C,0,1.9452540344,-2.927116924,-0.9841068176
C,0,-0.0917046875,-2.7176891709,2.2782024172	H,0,2.5457782254,-3.4264009591,-0.2236222895
C,0,-0.0917046875,-2.7176891709,-2.2782024172	H,0,2.2049245141,-1.8680330131,-0.9795975467
H,0,0.1698065756,-3.6583608039,2.7741817797	H,0,2.2159920976,-3.3502525858,-1.9557100435
H,0,0.1698065756,-3.6583608039,-2.7741817797	C,0,-0.3278824595,-2.4171687334,-1.8780500492
H,0,0.4863514431,-2.633939491,1.3563987155	H,0,-0.0154230794,-2.836222859,-2.8384274689
H,0,0.4863514431,-2.633939491,-1.3563987155	H,0,-0.124815604,-1.3454632491,-1.889612234
H,0,-1.1500336266,-2.7590019913,2.0126075338	H,0,-1.4035589258,-2.5595195951,-1.773046447
H,0,-1.1500336266,-2.7590019913,-2.0126075338	C,0,0.0897464728,-4.6075235908,-0.763768287
C,0,-0.4427622945,1.592874108,4.6440629356	H,0,0.7008763735,-5.1758292809,-0.0621620974
C,0,-0.4427622945,1.592874108,-4.6440629356	H,0,0.274937057,-5.0134669208,-1.762708681
H,0,0.2013422608,0.9820971336,5.2783183416	H,0,-0.9627432183,-4.7686511097,-0.526598679
H,0,0.2013422608,0.9820971336,-5.2783183416	C,0,-0.6541154791,4.365855829,2.7441688073
H,0,-1.468792695,1.2319394583,4.7325681155	H,0,-0.375676135,5.1725822932,2.0693606654
H,0,-1.468792695,1.2319394583,-4.7325681155	H,0,-0.5367960538,4.7340320068,3.7679800849
H,0,-0.4128359053,2.6129220563,5.0413644193	H,0,-1.7062554571,4.1296280897,2.5856563095

H,0,-0.4128359052,2.6129220563,-5.0413644193 C,0,-0.7642379416,2.6743067868,2.4160385659 C,0,-0.7642379416,2.6743067868,-2.4160385659 H,0,-1.8385231242,2.491666515,2.4667424441 H,0,-1.8385231242,2.491666515,-2.4667424441 H,0,-0.4688190157,2.6985567739,1.3651285325 H,0,-0.4688190157,2.6985567739,-1.3651285325 H,0,-0.5641786125,3.656926912,2.8552651841 H,0,-0.5641786125,3.656926912,-2.8552651841 C,0,1.5198563489,1.9722453121,3.1199395711 C,0,1.5198563489,1.9722453121,-3.1199395711 H,0,2.146694992,1.2745796406,3.6769013873 H,0,2.146694992,1.2745796406,-3.6769013873 H,0,1.665881434,2.9656174046,3.5562872207 H,0,1.665881434,2.9656174046,-3.5562872207 H,0,1.8698205084,1.9983094739,2.0868934113 H,0,1.8698205084,1.9983094739,-2.0868934113 Ir,0,0.1391750777,0.0070292053,0. H,0,1.5993257668,-0.6485565681,0. H,0,1.4356696236,0.922485191,0.	C,0,-0.1719814674,2.0873189048,3.6241393046 H,0,-0.0933228135,2.5373987432,4.6179540815 H,0,0.4967084572,1.2224503624,3.598214264 H,0,-1.1990235532,1.7416226308,3.4899154229 C,0,1.7009500947,3.470145521,2.7199233114 H,0,2.0031033595,4.2781251688,2.052226013 H,0,2.3324072114,2.6003991875,2.5248368119 H,0,1.888146913,3.8012813633,3.7454251016 C,0,0.1177013607,4.6960803301,-0.4799349378 H,0,0.3270750053,5.1661781157,-1.4454019487 H,0,0.7096542731,5.2181830503,0.2722320786 H,0,-0.9407734273,4.8403986981,-0.2592687249 C,0,1.9849990408,3.0378309346,-0.7551284913 H,0,2.2832016904,3.5284970902,-1.686077065 H,0,2.2494057767,1.9817078392,-0.8164908001 H,0,2.5603146837,3.4843500221,0.0561733438 C,0,-0.2594511202,2.5819101171,-1.7471581438 H,0,0.082970865,3.0594479479,-2.6692550319 H,0,-1.3378715831,2.7192661463,-1.6666975008 H,0,-0.0556467518,1.5125970522,-1.8196763597
 **1-H-H_2**	 **1-H-H_2**
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H,0,2.2532759034,-0.726884419,-4.4719531691	H,0,-1.6031309489,-1.3512735248,-4.3770983715
H,0,2.6207648693,-1.5226049114,2.9323627906	H,0,-0.1409107181,-1.9539283603,-5.1670991128
H,0,2.6207648693,-1.5226049114,-2.9323627906	C,0,0.7692108301,2.8724495793,-2.770879321
C,0,0.177923863,-2.8500833144,2.6904267592	H,0,1.6179754609,2.3786009836,-3.2458226574
C,0,0.177923863,-2.8500833144,-2.6904267592	H,0,0.9584612957,2.9170872427,-1.6989449181
H,0,0.2445883579,-3.6912000644,3.3871354847	H,0,0.7131325981,3.8922663949,-3.1624748455
H,0,0.2445883579,-3.6912000644,-3.3871354847	C,0,-1.6973173133,2.9180740859,-2.3810657966
H,0,0.8852888749,-3.0331843651,1.8834656569	H,0,-1.690522268,3.9491913708,-2.7450076664
H,0,0.8852888749,-3.0331843651,-1.8834656569	H,0,-1.5857565237,2.9376478181,-1.2972228825
H,0,-0.832611117,-2.8395145926,2.2761244342	H,0,-2.6650351875,2.476675994,-2.620249402
H,0,-0.832611117,-2.8395145926,-2.2761244342	C,0,-0.820869482,2.1364039028,-4.5625718956
C,0,0.3428416026,1.6510123358,4.5605198097	H,0,0.0104200846,1.713646748,-5.126309576
C,0,0.3428416026,1.6510123358,-4.5605198097	H,0,-0.9552544587,3.1666815411,-4.9047887765
H,0,1.0113412727,1.0119704301,5.1383277445	H,0,-1.7315110588,1.5860179935,-4.8020075424
H,0,1.0113412727,1.0119704301,-5.1383277445	C,0,-0.2433985679,-0.8303112253,4.7661055705
H,0,-0.6901598407,1.4092505625,4.8153584997	H,0,0.3916396346,-0.0929195547,5.2560964399
H,0,-0.6901598407,1.4092505625,-4.8153584997	H,0,-0.0373000056,-1.7984622165,5.2321318283
H,0,0.5286379808,2.681674179,4.8796017381	H,0,-1.2883566575,-0.5850286539,4.958909219
H,0,0.5286379808,2.681674179,-4.8796017381	C,0,-0.7634010108,-2.1196716632,2.7202843272
C,0,-0.281265256,2.6178139944,2.3704191593	H,0,-0.4143825836,-3.0366103364,3.2025583244
C,0,-0.281265256,2.6178139944,-2.3704191593	H,0,-0.6455697382,-2.2412747893,1.6442856244
H,0,-1.3358703876,2.4845524212,2.614685371	H,0,-1.8257923525,-2.001648336,2.9334879272
H,0,-1.3358703876,2.4845524212,-2.614685371	C,0,1.5393480331,-1.1940170122,3.0517542634
H,0,-0.175209661,2.5997737071,1.2861551962	H,0,2.155530764,-0.3819385661,3.438085655
H,0,-0.175209661,2.5997737071,-1.2861551962	H,0,1.774597419,-1.3199130647,1.9958432532
H,0,0.0290764264,3.6057957076,2.7246650342	H,0,1.8241814465,-2.1097994844,3.5774591134
H,0,0.0290764264,3.6057957076,-2.7246650342	C,0,-1.0647266882,2.2925887914,4.4464141787
C,0,2.0705301283,1.85672914,2.7552711785	H,0,-0.9392139326,3.2978147781,4.8587025934
C,0,2.0705301283,1.85672914,-2.7552711785	H,0,-0.7981546755,1.5830941159,5.2242012997
H,0,2.7451630337,1.1585534442,3.2545447873	H,0,-2.1175027102,2.1574507344,4.1983768939
H,0,2.7451630337,1.1585534442,-3.2545447873	C,0,1.2970105763,2.2778401209,3.5545118039
H,0,2.3097659312,2.8620761002,3.1169329113	H,0,1.5017895328,3.2829765874,3.9332315101
H,0,2.3097659312,2.8620761002,-3.1169329113	H,0,1.9278493124,2.1140559486,2.6775475014
H,0,2.2743324919,1.8134660664,1.6852240869	H,0,1.5871055206,1.5683834551,4.3305919291
H,0,2.2743324919,1.8134660664,-1.6852240869	C,0,-0.5592580226,3.3147767858,2.2519996112
Ir,0,0.5693989028,-0.299347882,0.	H,0,-0.4955326902,4.255402126,2.8061323138
H,0,0.6559530121,1.2826199898,0.	H,0,-1.5790200527,3.211027802,1.8759527492
H,0,2.2121345033,-0.1600669698,0.	H,0,0.1156127111,3.367205091,1.3998695317
H,0,1.1326243261,-1.9131658153,0.	H,0,0.9035682782,-0.9618310149,0.0427477638
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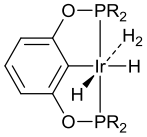	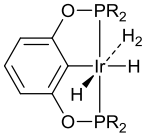
1-H-H_2-TS	**1-H-H_2-TS**
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C,0,1.216668993,-2.2072059621,-1.0635378124	Ir,0,-0.0086625022,0.0149527834,-0.0000390326
C,0,1.2475948198,-3.4638181636,-1.656320422	P,0,0.4193307477,0.2264542985,2.2490968623
C,0,0.0342913293,-4.0843263439,-1.9397979467	P,0,0.4194633142,0.226506879,-2.2491316617
H,0,0.0391957415,-5.0642758222,-2.4046937118	H,0,-1.6684510426,-0.0510431633,-0.0001225652
C,0,-1.1851106305,-3.483222455,-1.6410784384	H,0,-0.2261935035,1.5271583503,-0.0000039984
C,0,-1.1668031578,-2.2262181129,-1.0486084871	H,0,0.5674611918,-2.7168122891,-0.0004568014
C,0,3.5566447788,0.901942126,-0.9145247479	H,0,1.0928724957,-2.1736119526,0.0006575682
C,0,3.9965524211,2.111930683,-0.0866186119	C,0,2.7914905425,-0.0318657887,-1.1897069623
H,0,4.6343772556,1.8332266878,0.7531949567	C,0,2.7914116617,-0.0319430799,1.1898221339

H,0,3.1398055777,2.6731255315,0.2950162032	C,0,4.1801091263,-0.0896075327,-1.2153467557
H,0,4.5750048945,2.786260418,-0.7259223446	C,0,4.1800285002,-0.0896828896,1.2155534011
C,0,4.7661481785,0.0763486522,-1.3633655711	C,0,4.8605212707,-0.1155787205,0.0001252547
H,0,5.3891066616,0.7023583412,-2.0108649337	H,0,5.9437158039,-0.1605304175,0.0001598655
H,0,4.4578900453,-0.7995732605,-1.9343315296	C,0,-0.1876750455,-1.0310946821,-3.5045067283
H,0,5.3876344524,-0.2570095851,-0.535018351	C,0,-0.1879805366,-1.0310495008,3.5044932756
C,0,2.8390072655,1.4126643993,-2.166434278	C,0,-1.6212682238,-0.6790333007,-3.8974950081
H,0,3.553348091,1.9762818907,-2.7753410982	C,0,-1.621576845,-0.6788477772,3.8973495906
H,0,2.0118135207,2.0742164544,-1.9097010316	H,0,-1.6733290125,0.2189744388,-4.5132061239
H,0,2.4528167584,0.5944463287,-2.7767467375	H,0,-1.6735986678,0.2191757489,4.5130392416
C,0,2.9593525042,-0.5988234731,1.7686328615	H,0,-2.2536973423,-0.5367967687,-3.0184746779
C,0,2.1019115948,-1.7765576573,2.2453394782	H,0,-2.2539232441,-0.5365627478,3.0182768725
H,0,2.2129058744,-2.6489233911,1.600184593	H,0,-2.0398237252,-1.5040338701,-4.4806916745
H,0,1.046773976,-1.5104821411,2.2783810799	H,0,-2.0402606717,-1.5037971305,4.4805261532
H,0,2.4209994989,-2.0565345549,3.2542914773	C,0,0.7100480175,-1.1520823297,-4.7346303305
C,0,2.7929821164,0.562580916,2.7549104964	C,0,0.7096322496,-1.1520292522,4.7346996146
H,0,3.0874388691,0.2201645674,3.7523470551	H,0,0.3563635337,-1.9944607245,-5.3367580023
H,0,1.7577669932,0.9016660512,2.8052877053	H,0,0.3559369824,-1.9944520922,5.3367591367
H,0,3.417008264,1.4210978177,2.5057229419	H,0,1.7434981948,-1.3488400454,-4.4500248295
C,0,4.4193598675,-1.0544456516,1.7402584434	H,0,1.7431222326,-1.3487203675,4.4501927939
H,0,5.1103628704,-0.2349759844,1.5402666673	H,0,0.6882104498,-0.2657874014,-5.3637661928
H,0,4.5846987631,-1.8452623343,1.0066301758	H,0,0.6876753407,-0.2657609588,5.3638689922
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C,0,-3.5544138456,0.8450693703,-0.8687829974	C,0,-0.1909726015,-2.375434296,2.7749627477
C,0,-2.8612451727,1.3675302646,-2.1295951806	H,0,-0.5454078377,-3.1482943555,-3.4625896636
H,0,-3.5922685394,1.9199273812,-2.7289089621	H,0,-0.5460987108,-3.1481721541,3.4626680755
H,0,-2.4700706879,0.5557218404,-2.7452721818	H,0,-0.8530251143,-2.3581942273,-1.9083555593
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C,0,-4.7561162602,0.0001874283,-1.3024459771	H,0,0.8104310062,-2.6533477954,-2.4424228118
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H,0,-5.3612048798,-0.3437731272,-0.4663336107	C,0,0.2858445948,1.9880369792,-2.8960127268
H,0,-4.4411550016,-0.8702354277,-1.8781415256	C,0,0.285797805,1.9880082986,2.8959429107
C,0,-4.003144948,2.0476314658,-0.0348133697	C,0,1.2948348944,2.8189884373,-2.0982671722
H,0,-3.1507523271,2.6224841857,0.3360940373	C,0,1.2948588587,2.8188807389,2.0982022671
H,0,-4.6256250534,1.7585023044,0.8129501072	H,0,2.3199888629,2.5079906223,-2.2992983934
H,0,-4.6005117614,2.7126800994,-0.6663970969	H,0,2.3199965285,2.5079225143,2.299378026
C,0,-2.8986317499,-0.6464157676,1.8058830686	H,0,1.1236732765,2.7435084883,-1.0259520626
C,0,-4.3513014334,-1.1256696988,1.7959955607	H,0,1.123805837,2.7432659905,1.0258796701
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H,0,-5.0580219579,-0.3174682898,1.6052802178	H,0,1.1895233849,3.8673162421,2.3897827729
H,0,-4.5885885455,-1.5339272124,2.7840347055	C,0,-1.1246548102,2.5147180646,-2.6306826007
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H,0,-3.0146581486,0.1700913077,3.7913559815	H,0,-1.1757676938,3.5592344144,-2.9514427975
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H,0,-1.7083583006,0.8731482456,2.8276910652	H,0,-1.372616663,2.4673501182,-1.5704035485
C,0,-2.0161973194,-1.8101600852,2.2711987016	H,0,-1.3726296519,2.467322886,1.5702944276
H,0,-0.9652503779,-1.526810056,2.2915190961	H,0,-1.8848886834,1.9593209892,-3.1793616534
H,0,-2.1207431123,-2.6839181577,1.6268505651	H,0,-1.8849361305,1.9595246724,3.179319021
H,0,-2.3182767443,-2.0958583659,3.283777749	C,0,0.6298724357,2.116987756,-4.3771559252
Ir,0,0.0113133108,0.3529464371,0.0408492447	C,0,0.6298048406,2.1169659762,4.3770894439
O,0,2.4101149748,-1.5816791211,-0.7682794643	H,0,-0.1136393447,1.6464677627,-5.0197127123
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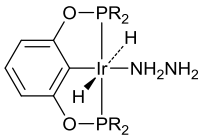
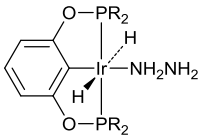
P,0,2.2748276679,-0.10418187,0.0644698189	H,0,1.6102575819,1.694341569,-4.6008125279
P,0,-2.2440998467,-0.1404863027,0.0932585564	H,0,1.6101183727,1.6941787436,4.6007912218
H,0,0.000061619,1.9665807087,0.3016952021	H,0,0.6579932388,3.1798001694,-4.6350002823
H,0,-0.0114400319,0.8486390748,-2.8730964291	H,0,0.6580825249,3.1797845897,4.6348920442
H,0,-0.0094356519,1.1540947658,-2.1841350969	O,0,2.0970232613,-0.0251629306,-2.3826015525

H,0,0.0181700958,0.6955147528,1.5486399618 H,0,2.1903691536,-3.9444962193,-1.8868969686 H,0,-2.1229131277,-3.9789020269,-1.8598669084	O,0,2.0968630669,-0.0253272696,2.3826728259 H,0,4.7150069263,-0.1117578869,-2.1569393719 H,0,4.7148624402,-0.1118941522,2.1571808014
 **1-H-N_2H_4-Eq**	 **1-H-N_2H_4-Eq**
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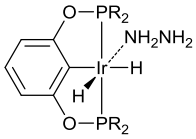
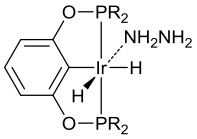
C,0,-0.5011435113,18.3902200992,9.2664175455 H,0,0.2120832888,18.5258543339,10.0803750285 H,0,-1.3989280649,17.9096811582,9.6584231861 H,0,-0.7953686141,19.3863507082,8.9189833241 C,0,-0.9627009205,17.4040668984,7.0167062754 H,0,-1.4039320584,18.3661988792,6.7369821861 H,0,-1.7800880063,16.7664606279,7.3669547862 H,0,-0.5176289019,16.9683351013,6.1198458168 C,0,1.2316197324,18.4875161147,7.4938141061 H,0,1.7408828299,17.9687431865,6.6805572248 H,0,1.9688751069,18.7581708542,8.2503816535 H,0,0.7939845131,19.4091873325,7.0961234182 Ir,0,1.6871156305,14.7167803967,6.7062787856 O,0,4.6975060798,14.1375229834,5.8985789824 O,0,2.2792518304,16.4163215729,9.318691884 P,0,3.2038757151,13.7856645201,5.2181972449 P,0,0.8960817823,15.9372095745,8.5020820207 N,0,-0.2191511426,14.0963501192,5.7682285603 H,0,-0.148169107,14.2898594913,4.7760365666 H,0,-0.9457510752,14.6998383414,6.1400915279 N,0,-0.5501393709,12.7080708787,5.9171778202 H,0,-1.5556058249,12.5846422622,5.9855746603 H,0,-0.1072136789,12.4132814185,6.7804451255 H,0,1.6795843774,13.32777231,7.6031964419 H,0,1.638129494,16.0879392251,5.7672832734 H,0,6.8124763137,14.9597367078,7.1636110906 H,0,4.6272363929,17.0214472528,10.2565986081	C,0,-0.4595756357,18.3595235429,9.2022734324 H,0,0.2398927453,18.4869591857,10.0289967261 H,0,-1.3699529857,17.8901678454,9.5758825191 H,0,-0.7323060565,19.3560015277,8.8413987571 C,0,-0.885012103,17.350918552,6.9552735477 H,0,-1.300144751,18.3145914933,6.6464044668 H,0,-1.717323085,16.7331038354,7.3005835475 H,0,-0.4235078475,16.8847664435,6.0831925584 C,0,1.3150568964,18.4050531432,7.4676884795 H,0,1.8411189616,17.8493664115,6.6901789632 H,0,2.0279341746,18.683817044,8.2438819019 H,0,0.9058973205,19.3195444508,7.0284079635 Ir,0,1.7159095698,14.6810978633,6.735363852 O,0,4.7162737566,14.1413127137,5.906606523 O,0,2.2889999483,16.3836621435,9.3354492243 P,0,3.2077802402,13.7876596739,5.2357699108 P,0,0.9050989451,15.9057470496,8.4970842773 N,0,-0.1649221754,13.999103419,5.8425893245 H,0,-0.0881110728,14.0861745676,4.8360695023 H,0,-0.8987355431,14.6390293681,6.1296016509 N,0,-0.5196282704,12.6370659392,6.1286444743 H,0,-1.5288471523,12.5470363308,6.192701759 H,0,-0.1085332727,12.4310731329,7.0312903455 H,0,1.7766951541,13.3154759256,7.6603892456 H,0,1.5898050183,16.0249252492,5.7711071608 H,0,6.8363541725,15.0334775081,7.1351070244 H,0,4.6380226977,17.0653408346,10.2413622624
 **1-H-N_2H_4-Axial** H,0,0.8649278952,-0.0165129703,0.0652201578 Ir,0,0.3037620944,-0.0356272596,1.516877285 H,0,1.9068480011,-0.0497880778,1.9476608876 C,0,-1.7340384797,-0.0239270771,1.0822379478 C,0,-4.496918215,-0.0132625609,0.6485544793 C,0,-2.4510775682,-1.2069429564,0.9442945698 C,0,-2.4467580354,1.1655067246,0.9807302709 C,0,-3.8213656823,1.1975406705,0.7711806833 C,0,-3.8245117717,-1.2296287566,0.7315397463 H,0,-4.3465945411,2.1422981137,0.6978906649 H,0,-4.3520966484,-2.1701013806,0.626696686 H,0,-5.5687032561,-0.009120451,0.4834328201 O,0,-1.7577167654,2.361029225,1.0983011314 O,0,-1.7643906499,-2.4096172983,1.0293375354 P,0,-0.0710884347,-2.2736130759,1.07825385 P,0,-0.0649731409,2.2269214199,1.183401494 C,0,0.2753975741,-3.7214809176,2.2776228554 C,0,0.4006170626,-2.8002953298,-0.6968323873 C,0,0.393750181,2.9481697429,-0.5316910313 C,0,0.2935519984,3.5320598464,2.5373167755 C,0,-0.0127598029,-3.213192954,3.6932215279 H,0,0.1730996227,-4.0224927782,4.4065536427 H,0,-1.0629428153,-2.926127177,3.8064914684	 **1-H-N_2H_4-Axial** H,0,0.8877364771,-0.0097865863,0.0997002099 Ir,0,0.2998952779,-0.0331275444,1.5416754434 H,0,1.880463239,-0.049074828,2.0670543032 C,0,-1.7249332696,-0.022695343,1.0673171328 C,0,-4.4822098231,-0.01586449,0.6037621308 C,0,-2.437825239,-1.2090861967,0.9299823615 C,0,-2.4381919412,1.1674613825,0.9698867731 C,0,-3.8102751131,1.1967508728,0.7412059782 C,0,-3.8087511958,-1.2321794169,0.6984732866 H,0,-4.3371374775,2.140403137,0.6664158806 H,0,-4.3346087788,-2.1730198439,0.5892556318 H,0,-5.5514450163,-0.0133100438,0.4243389363 O,0,-1.7539086192,2.3573901359,1.1162953333 O,0,-1.7523471123,-2.4046442369,1.0386130659 P,0,-0.0543408903,-2.2593315586,1.0899687728 P,0,-0.0564824211,2.2142799198,1.1980332181 C,0,0.3144367375,-3.6850138037,2.2681459817 C,0,0.393535509,-2.7468780767,-0.6804683085 C,0,0.3764862183,2.8937246342,-0.5150439729 C,0,0.3267464786,3.5032858645,2.5242335262 C,0,0.0324776422,-3.1694407922,3.6786994789 H,0,0.2563460467,-3.961561669,4.3983182231 H,0,-1.0235444113,-2.9132318836,3.8034883821

H,0,0.6427410364,-2.383865423,3.9621704235	H,0,0.661604551,-2.3140103098,3.9225754035
C,0,1.759117335,-4.0874400509,2.1975876106	C,0,1.8016800885,-4.016089461,2.1626791545
H,0,2.0127707226,-4.5811490386,1.259387163	H,0,2.0493269805,-4.4980943147,1.2175759122
H,0,2.0051532315,-4.7805366188,3.0086903086	H,0,2.0737301207,-4.7047260415,2.9675508511
H,0,2.3948173792,-3.2043899974,2.3045121197	H,0,2.4159033081,-3.1180332909,2.2651900552
C,0,-0.6162160946,-4.947318684,2.0520985972	C,0,-0.5548319244,-4.9230628441,2.0482117445
H,0,-0.3802795101,-5.4860066375,1.1386407095	H,0,-0.3121080693,-5.456281116,1.1342143393
H,0,-1.6700142779,-4.667895018,2.0238272052	H,0,-1.6124736361,-4.6596438274,2.0255728042
H,0,-0.4715589256,-5.6421901585,2.886621857	H,0,-0.3932171692,-5.6108686035,2.8839680433
C,0,1.8849745077,-2.4997245677,-0.9328437532	C,0,1.8649481701,-2.4181361241,-0.936882037
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C,0,-0.4525026169,-1.9457347681,-1.6430645644	C,0,-0.4883979375,-1.8892519565,-1.5920872261
H,0,-0.1241259944,-2.1340221467,-2.6703240938	H,0,-0.1623530705,-2.0331858077,-2.6261089616
H,0,-0.3506362184,-0.8823818109,-1.4383731607	H,0,-0.4127010738,-0.8334056077,-1.3462989737
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C,0,1.7674415554,3.4123696921,2.9407240035	C,0,1.7923176761,3.3186634965,2.9238207654
H,0,2.4449906489,3.7328149443,2.1484411297	H,0,2.4776854084,3.5986014461,2.1232638997
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H,0,2.0884254245,4.2142305351,0.0547564083	H,0,2.0925654158,4.1352038049,0.0345240299
C,0,0.1603128355,1.8669066044,-1.5931330487	C,0,0.0975023178,1.7969810954,-1.5458774734
H,0,0.2939318846,2.322744624,-2.5794689379	H,0,0.1706122428,2.2374580298,-2.544153201
H,0,-0.8499055147,1.455470802,-1.5486496605	H,0,-0.902624628,1.3750386626,-1.4310644339
H,0,0.87102074,1.0483590321,-1.5011640541	H,0,0.8192606669,0.9867417614,-1.476578535
N,0,-0.3607874552,-0.0593857803,3.6773715655	N,0,-0.4600570915,-0.0625267034,3.6492951821
H,0,-0.8070807449,-0.9579880926,3.818343917	H,0,-0.9172121941,-0.9575768227,3.7798411219
H,0,-1.077685721,0.6496918954,3.7872658322	H,0,-1.1824306206,0.6451321278,3.7259434298
N,0,0.6676326685,0.1827611022,4.6403488211	N,0,0.5162247878,0.1791041297,4.6656107372
H,0,0.5169843023,-0.363076015,5.4821824205	H,0,0.302735532,-0.3563867338,5.5003159534
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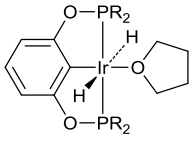	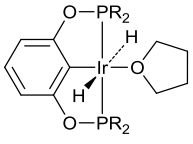
1-H-THF-Eq	**1-H-THF-Eq**

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Ir,0,-0.116419895,0.0035097228,0.004632963
H,0,0.0156418106,-0.2049251949,1.6464797774
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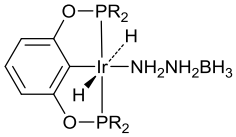	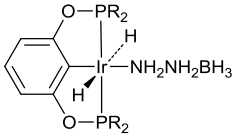
1-H-$NH_2NH_2BH_3$-Eq	**1-H-$NH_2NH_2BH_3$-Eq**
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C,0,5.8605707127,16.0244327743,8.7923911328	C,0,5.8718504613,16.0659932755,8.780492094
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H,0,1.7398096245,13.2924009963,7.6169859969	H,0,1.7528930125,13.2817220707,7.6226947007
H,0,1.6027779848,16.0351935688,5.7581764032	H,0,1.6358814098,16.0280881642,5.7821211441
H,0,6.8235158956,14.9610316125,7.1745544905	H,0,6.8422163833,15.0171776478,7.1563835255
H,0,4.6100876283,16.989438732,10.2690468372	H,0,4.6199033051,17.0106850057,10.2702979886
H,0,0.0788223117,12.0577832233,6.0315644927	H,0,0.1410454005,12.0835671224,6.1271912906
H,0,-2.3426856999,11.1906148972,5.9654848486	H,0,-2.2691559894,11.1879047999,6.0895305406
H,0,-2.8639211799,13.1445061984,5.8264885559	H,0,-2.8158129425,13.1236221933,5.8651254347
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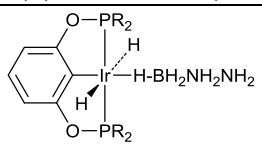	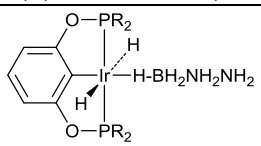

1-H-HBH$_2$NH$_2$NH$_2$-Eq	**1-H-HBH$_2$NH$_2$NH$_2$-Eq**
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C,0,2.6325469815,-1.1870678659,0.2170817953	C,0,2.6478909107,-1.1897146674,0.2051999688
C,0,4.016110652,-1.1857789983,0.3301906647	C,0,4.0338123847,-1.187201583,0.2959251349
C,0,4.6794567663,0.0348209221,0.3659798685	C,0,4.6979363533,0.0356852695,0.3174638258
H,0,5.7597081574,0.0568630341,0.4532064944	H,0,5.7793363814,0.057280498,0.3869798614
C,0,3.970756409,1.2270523947,0.283113883	C,0,3.9885381254,1.2307683693,0.2477890783
C,0,2.5875779524,1.1729706283,0.1725555907	C,0,2.6029360244,1.1784474453,0.1587227339
C,0,-0.2318770936,-3.5461805764,1.2455469463	C,0,-0.265347402,-3.4981810563,1.2329283776
C,0,-1.7079833225,-3.8911523016,1.0336073088	C,0,-1.7525559627,-3.7565021272,0.9951155532
H,0,-1.8579380606,-4.5455716642,0.1731102344	H,0,-1.9180447318,-4.4149881423,0.1414846146
H,0,-2.3235550934,-3.0011651369,0.8724324219	H,0,-2.30325523,-2.8319478509,0.8028102016
H,0,-2.0937508471,-4.4144293445,1.9142365281	H,0,-2.1891968834,-4.2365845568,1.8749302549
C,0,0.6133804868,-4.8245446052,1.3109108088	C,0,0.5188899043,-4.8105884796,1.2907973371
H,0,0.3721295486,-5.3528866248,2.2391840966	H,0,0.2554774806,-5.3297321475,2.2170061579
H,0,1.6785204874,-4.5914924461,1.3279987378	H,0,1.5932859659,-4.6247483516,1.305245762
H,0,0.4193544375,-5.508630671,0.489154121	H,0,0.2908899779,-5.478699573,0.4659282767
C,0,-0.0507359342,-2.8267033427,2.5868831505	C,0,-0.0573490954,-2.7910412514,2.5738010389
H,0,-0.4036495527,-3.4828838119,3.3889257699	H,0,-0.4455109037,-3.4311831605,3.3707297373
H,0,-0.5888814044,-1.8812317257,2.6292171642	H,0,-0.5495099645,-1.8217201208,2.6132260317
H,0,1.0003544438,-2.5983368271,2.7737496924	H,0,1.0037201402,-2.6156797564,2.7617328703
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C,0,1.2497094743,-2.4177113376,-2.7130614502	C,0,1.2719774603,-2.3677657241,-2.6657664086
H,0,2.2644667873,-2.6767553783,-2.4077356042	H,0,2.2767714147,-2.6620670247,-2.360809232
H,0,1.141850893,-1.333564482,-2.6784238935	H,0,1.1860794379,-1.283646439,-2.5897091968
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H,0,-0.5289546879,1.7316980192,2.7224868031	H,0,-0.4851398509,1.6824001255,2.704202025
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C,0,0.16081213,4.5691770176,-1.8208051395	C,0,0.1377400263,4.5190292091,-1.8115930318
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H,0,0.9345586948,1.3404100111,-2.7381408951	H,0,0.9800446067,1.2910017676,-2.6586252702
H,0,2.0132440357,2.7186616394,-2.4673642398	H,0,2.0217651745,2.7056911288,-2.4295807579
H,0,0.7922657958,2.7875821279,-3.7482898282	H,0,0.8050427217,2.701835445,-3.7179469298
Ir,0,-0.1509475332,-0.0668969298,-0.0043460094	Ir,0,-0.1306609424,-0.0669274763,0.005086766
O,0,1.9818438172,-2.4058374995,0.1739711551	O,0,1.9902671352,-2.4023381484,0.1858922747
O,0,1.8918051257,2.3606989204,0.0909011865	O,0,1.8996385704,2.3590396539,0.1001348161
P,0,0.3298493699,-2.3307082678,-0.1092461213	P,0,0.3308049079,-2.3137588457,-0.0985437513
P,0,0.2246002159,2.2298474089,-0.084166351	P,0,0.2235700506,2.2117567164,-0.0741565353
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H,0,4.5552154609,-2.1236467713,0.3850539923	H,0,4.5761048144,-2.1235498926,0.3451135995
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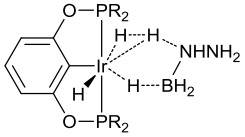	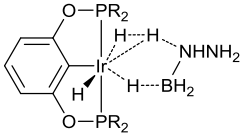
Ir-2H-P-2H-BH_3-N_2H_4-Eq-TS	**Ir-2H-P-2H-BH_3-N_2H_4-Eq-TS**
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C,0,1.2106909065,-2.1627462682,-1.1040864876	C,0,1.220056378,-2.1680526295,-1.0889728586
C,0,1.2497639399,-3.4062309056,-1.7218723637	C,0,1.265521531,-3.425562737,-1.6782790112
C,0,0.0473321385,-4.0374571656,-2.0168841468	C,0,0.0647695596,-4.064197685,-1.9717555777
H,0,0.0575648691,-5.0077766198,-2.5000960523	H,0,0.0810131498,-5.0455298384,-2.4314252154
C,0,-1.1678738359,-3.4485844848,-1.6880734783	C,0,-1.1566340509,-3.4675966651,-1.6742354566
C,0,-1.1546450978,-2.2042090378,-1.0715539494	C,0,-1.152594194,-2.2097065023,-1.0850995977
C,0,3.5136180448,0.916294598,-0.9706228331	C,0,3.4834583082,0.9308277969,-0.9518083169
C,0,3.9100234821,2.1837327757,-0.2101718281	C,0,3.8611229577,2.1960125773,-0.1852080902
H,0,4.5661891642,1.9703108818,0.6355017185	H,0,4.4956141297,1.9804666988,0.6752639607
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C,0,2.775619835,1.2991122308,-2.2598362529	C,0,2.7492767405,1.3052058724,-2.2421626498
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H,0,1.9540247681,1.9887503342,-2.0804276748	H,0,1.9413132371,2.0097102613,-2.0635018889
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C,0,3.0528175201,-0.5940383946,1.7532715487	C,0,2.9801072271,-0.5579748465,1.7496734343
C,0,2.3792856279,-1.9027699523,2.185702454	C,0,2.3001239735,-1.8672705239,2.1605702896
H,0,2.6410012314,-2.7291931839,1.5235189339	H,0,2.5917522864,-2.6900564121,1.5072997474
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H,0,-2.5929710043,0.1204504231,-2.8083104017	H,0,-2.6289132435,0.1565937403,-2.8027883463
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H,0,-5.3517468935,0.5907975034,-2.0246854212	H,0,-5.3550064829,0.697103468,-1.9463815609
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H,0,-1.5568355532,0.6215428875,2.8519233255	H,0,-1.4512482851,0.5520375414,2.8062102678
C,0,-2.3347350309,-1.941062744,2.2378709396	C,0,-2.2644793631,-1.9720125645,2.1484499531
H,0,-1.247266466,-1.8736567519,2.2235271529	H,0,-1.1786429096,-1.9113453844,2.0831916763
H,0,-2.6344452217,-2.775252299,1.6021963112	H,0,-2.6017621019,-2.7877540113,1.5086513313
H,0,-2.6449152664,-2.1636542615,3.2634627252	H,0,-2.5298236217,-2.2113193244,3.1816643266
Ir,0,-0.0010469471,0.3131560343,0.1337139012	Ir,0,-0.0120743101,0.3155692981,0.0944758672
O,0,2.4064506273,-1.5482198889,-0.7894438279	O,0,2.4042054093,-1.5367634293,-0.7812351729
O,0,-2.3642044323,-1.6309101141,-0.7250313917	O,0,-2.3611568864,-1.620840275,-0.7727611862
P,0,2.3012900849,-0.1082245375,0.0742389553	P,0,2.2767332456,-0.0831483336,0.0707867838
P,0,-2.279705655,-0.1729425797,0.1062145076	P,0,-2.2692269426,-0.1703595096,0.0796605215
H,0,-0.1304686704,1.7810683074,1.0768496461	H,0,-0.2524633241,1.7693062579,1.0211403065
B,0,0.1954751283,3.0922997253,0.8800657383	B,0,0.2297881657,3.0167345937,0.8201544996
H,0,1.2371679813,3.2106627648,1.4740305476	H,0,1.2928468135,3.0627771794,1.3820149291
H,0,-0.762341568,3.5720612773,1.4472702463	H,0,-0.6685440535,3.5663192546,1.4314820129
N,0,0.278813538,3.4766781252,-0.6028737499	N,0,0.2981648461,3.4311465033,-0.651605309
N,0,-0.7414839438,4.3161908219,-1.1591229178	N,0,-0.7722038184,4.2195021572,-1.1877882624
H,0,0.1388169838,1.9789724871,-1.0632097437	H,0,0.1589354165,1.9096768996,-1.1385692919
H,0,-0.0241068997,1.1697859779,-1.4462177735	H,0,-0.0370033136,1.0955583732,-1.5244401473
H,0,0.0053339025,-0.505143544,1.4762232233	H,0,-0.0090718894,-0.4709454514,1.4509995369
H,0,2.2011216307,-3.8657150752,-1.9602208438	H,0,2.2186126361,-3.891508865,-1.895773948
H,0,-2.1088959725,-3.941029816,-1.9001067835	H,0,-2.0937040437,-3.9663140859,-1.8883442999
H,0,1.1618978122,3.9095759405,-0.8400778027	H,0,1.1602679917,3.9076416642,-0.8804767887
H,0,-1.4234076819,3.7251276939,-1.6219577134	H,0,-1.430370794,3.5908766754,-1.6357812626
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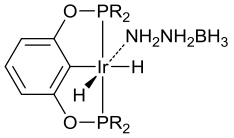	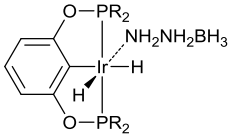

1-H-$NH_2NH_2NH_3$-Axial	**1-H-$NH_2NH_2NH_3$-Axial**
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Ir,0,0.2731758033,-0.0305088809,1.5604808018	Ir,0,0.2873934118,-0.0311508878,1.5596293186
H,0,1.8786602776,-0.0446033846,1.9969010264	H,0,1.8769763398,-0.0386530886,2.0513372678
C,0,-1.7577403509,-0.0269190773,1.0885185719	C,0,-1.7387929618,-0.0337323562,1.086896724
C,0,-4.5126289642,-0.0248914376,0.600943988	C,0,-4.4928589617,-0.0424400083,0.6096611945
C,0,-2.4738590256,-1.2119788551,0.9617573083	C,0,-2.4518516751,-1.2239075049,0.986657786
C,0,-2.4664914779,1.1583139567,0.9306742315	C,0,-2.447886746,1.1515492805,0.9260827189
C,0,-3.8358697044,1.18744985,0.6936634773	C,0,-3.8184212368,1.1735144506,0.6910420067
C,0,-3.8429286779,-1.2386271874,0.7258358918	C,0,-3.8213078914,-1.2548880264,0.7525586594
H,0,-4.357000627,2.1304090752,0.5808981895	H,0,-4.3429962052,2.1135455171,0.5707951264
H,0,-4.3699419695,-2.1810163749,0.6382321007	H,0,-4.3476485009,-2.1986269128,0.6774431246
H,0,-5.5817890501,-0.0241169736,0.4206353506	H,0,-5.561799857,-0.0456393049,0.4293420868
O,0,-1.7763606749,2.3587003761,1.0080452105	O,0,-1.7602456844,2.3477411685,1.0026953234
O,0,-1.7884793156,-2.41278417,1.0715003584	O,0,-1.7625136465,-2.4156787908,1.121871463
P,0,-0.0982401985,-2.2795705122,1.1004468803	P,0,-0.0671259851,-2.2649984963,1.1060182405
P,0,-0.0951094803,2.227976815,1.1705000022	P,0,-0.0744750957,2.2121232531,1.174431939
C,0,0.2620224264,-3.7467365539,2.2642392505	C,0,0.3590458308,-3.6985868067,2.2521574489
C,0,0.3621562712,-2.7624167729,-0.6894377556	C,0,0.3204921361,-2.7237824282,-0.6852467957
C,0,0.45026334,2.919288043,-0.5287018091	C,0,0.4626171406,2.8738979891,-0.5116032101
C,0,0.1976961475,3.5645962999,2.517243619	C,0,0.2311216432,3.5138066568,2.5172735277
C,0,-0.0190519299,-3.2726289648,3.6911265924	C,0,0.1471167744,-3.2016039463,3.6806251555
H,0,0.1287711107,-4.1051978164,4.3846317986	H,0,0.379458251,-4.0078922516,4.3803678008
H,0,-1.05408746,-2.9407556002,3.8124478474	H,0,-0.8937417053,-2.9174367666,3.8579511611
H,0,0.6722025968,-2.4868133359,3.9942322235	H,0,0.8180460703,-2.374872951,3.9099929254
C,0,1.7454928592,-4.1133611458,2.1653639165	C,0,1.839474369,-4.0306439319,2.071323773
H,0,1.9915961582,-4.6008075891,1.2216001064	H,0,2.0387051093,-4.5138318914,1.1153970851
H,0,1.9971373113,-4.8130452413,2.9685914684	H,0,2.1504598352,-4.7197069146,2.8613846782
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C,0,-0.6286519673,-4.9701908615,2.0156626592	C,0,-0.5198214081,-4.9348332231,2.0594473775
H,0,-0.4202211789,-5.4693444977,1.0737341932	H,0,-0.342980397,-5.4370645476,1.113540852
H,0,-1.6851490131,-4.701260073,2.0366451149	H,0,-1.5772928714,-4.6789699227,2.1242540846
H,0,-0.4478857865,-5.6950209157,2.8164323051	H,0,-0.2912489282,-5.6455599944,2.8592675749
C,0,1.8409236372,-2.4442569876,-0.9347436969	C,0,1.7811056304,-2.3920961712,-0.9927509361
H,0,2.5053885202,-3.07985879,-0.3472716615	H,0,2.4762240306,-3.0005801498,-0.4141728909
H,0,2.0761140145,-1.4068412908,-0.697668669	H,0,2.0007427286,-1.344179399,-0.7916876514
H,0,2.0681450085,-2.6178208547,-1.9915697671	H,0,1.9681457583,-2.5880063306,-2.0524986049
C,0,-0.5125531555,-1.9036122851,-1.6116823657	C,0,-0.5944560026,-1.8597346105,-1.558374174
H,0,-0.1826583617,-2.0574498934,-2.6440376663	H,0,-0.3119017406,-2.0066707826,-2.6045607401
H,0,-0.4372589015,-0.8440852263,-1.3800961616	H,0,-0.5043585692,-0.8038361675,-1.3189629746
H,0,-1.5628866379,-2.1914262795,-1.5467987821	H,0,-1.6397791733,-2.1480526031,-1.4439776848
C,0,0.0897304954,-4.2245963161,-1.048171173	C,0,0.0388137195,-4.1843204239,-1.0274690415
H,0,0.7559513144,-4.9196401856,-0.5369723483	H,0,0.7351769886,-4.8701154177,-0.5465872863
H,0,0.2620274411,-4.3483847533,-2.1223468721	H,0,0.1560313578,-4.3088536192,-2.1080191826
H,0,-0.9448898836,-4.5075054524,-0.8491225321	H,0,-0.981451193,-4.4705909871,-0.7699578062
C,0,-0.0626056273,5.0093073352,2.0845533825	C,0,0.0417243082,4.9670431389,2.090074817
H,0,0.6529142563,5.3580171708,1.3413852525	H,0,0.7894012167,5.2845401459,1.3656536899
H,0,0.0480121633,5.6558521956,2.9615096065	H,0,0.1600488439,5.6006742498,2.974144605
H,0,-1.0737043175,5.1463477225,1.6989703736	H,0,-0.9531743525,5.1475751656,1.6825123893
C,0,-0.7680025392,3.2718879949,3.6744198777	C,0,-0.7706548768,3.2460713618,3.6449446206
H,0,-0.7210164739,4.099645145,4.3878471798	H,0,-0.6801708454,4.0426166074,4.3873392921
H,0,-0.5041133874,2.3826617737,4.2441958168	H,0,-0.5843560477,2.3195121346,4.1811591189
H,0,-1.7997817283,3.1802794797,3.3339279631	H,0,-1.7971719842,3.2315082783,3.2805167851
C,0,1.6454094799,3.4420651473,3.0084825698	C,0,1.6628141875,3.321606029,3.0243757899
H,0,2.3564445883,3.8661409163,2.2981719815	H,0,2.3948766435,3.7260171299,2.3247592963
H,0,1.9417942015,2.400473387,3.1571160364	H,0,1.9137504468,2.266665771,3.1561603606

H,0,1.7602624158,3.9835800339,3.9525160316	H,0,1.7876897268,3.8440524142,3.9765762175
C,0,-0.3907639217,4.1246528471,-0.9738206736	C,0,-0.3243788099,4.1172964259,-0.9380610955
H,0,-0.131392706,4.3551881187,-2.011676524	H,0,-0.0798902468,4.3307875943,-1.9821431572
H,0,-0.2121357319,5.0240953523,-0.3929494359	H,0,-0.0828050387,5.0041654206,-0.3626769067
H,0,-1.4568578345,3.8972763386,-0.9391836346	H,0,-1.3986301333,3.9418073063,-0.8740250916
C,0,1.9401183974,3.2664954449,-0.4863453458	C,0,1.9648444186,3.1435466818,-0.4764771885
H,0,2.2846965428,3.4908049607,-1.5008003578	H,0,2.3159276036,3.3591925206,-1.4895757505
H,0,2.5346114904,2.430305259,-0.109772079	H,0,2.5114626907,2.2719686116,-0.1083947689
H,0,2.1475174164,4.1446178275,0.1271608695	H,0,2.2169114045,4.0017387457,0.1477674448
C,0,0.2314241792,1.8324709229,-1.5876125416	C,0,0.1685792205,1.7957926495,-1.5578421761
H,0,0.4031644165,2.2771501293,-2.5728476043	H,0,0.3133888852,2.233011003,-2.5492900468
H,0,-0.7871307762,1.4402318155,-1.5715638897	H,0,-0.8596656462,1.43547689,-1.4946761203
H,0,0.9248519144,1.0028602996,-1.4703656274	H,0,0.8384024968,0.9451910135,-1.4636013468
N,0,-0.3168272592,-0.0771007071,3.7324291257	N,0,-0.392244981,-0.0862017166,3.677036491
H,0,-0.703828044,-0.9747496573,4.0121692446	H,0,-0.7613830662,-0.9975445083,3.9321807128
H,0,-1.0411091537,0.5942111305,3.979011886	H,0,-1.1576049345,0.5580463409,3.8628262609
N,0,0.767198052,0.1525533849,4.6687346227	N,0,0.6224068407,0.191257499,4.6708132725
B,0,0.3760519529,0.0134250476,6.2248950134	B,0,0.1311634534,0.0642138642,6.1895524541
H,0,1.5070854553,-0.4796590742,4.3628035129	H,0,1.3985490548,-0.4264561197,4.4343469199
H,0,1.1300108524,1.0766189036,4.4396113043	H,0,0.9761631892,1.1215296638,4.4500067875
H,0,1.3994951593,0.235473558,6.8341446839	H,0,1.0974453018,0.3223355242,6.8757605491
H,0,-0.4845110473,0.8500261439,6.4123674571	H,0,-0.7656827151,0.8752892647,6.3113420022
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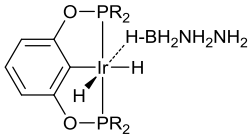	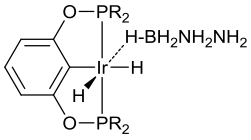
1-H-HBH$_2$NH$_2$NH$_2$-Axial	**1-H-HBH$_2$NH$_2$NH$_2$-Axial**
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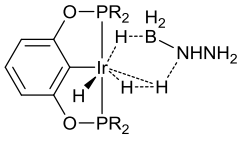
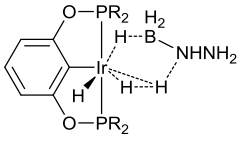
Ir,0,-0.1392846602,0.1979114709,0.0532935388	Ir,0,-0.1693286314,0.1939525501,0.0617752426
H,0,0.0469342682,-1.4669974131,0.1130182687	H,0,-0.0300538974,-1.4695914826,0.1304065809
C,0,-0.149274804,2.285136418,0.0298428897	C,0,-0.1652604836,2.2786436626,0.0305174018
C,0,-0.1290261172,5.0945393658,0.0064963062	C,0,-0.1223644795,5.084649242,-0.0065730841
C,0,-0.1513119292,3.0109441405,-1.155548658	C,0,-0.1565023959,2.9943027749,-1.1622669451
C,0,-0.0662552647,3.0285648564,1.2018879498	C,0,-0.0928282631,3.0234927023,1.2031749687
C,0,-0.0673321521,4.4182845008,1.2196942107	C,0,-0.0819676288,4.4141183277,1.2126508294
C,0,-0.1525218191,4.3993849622,-1.1977011518	C,0,-0.1443156923,4.3834533181,-1.2092107776
H,0,-0.0139834377,4.953459882,2.1599491489	H,0,-0.033073458,4.9554694108,2.1496015525
H,0,-0.1645997633,4.9194575189,-2.1478398865	H,0,-0.1428499247,4.9008663792,-2.1608635628
H,0,-0.1336019345,6.1787968751,-0.0016497631	H,0,-0.1153034284,6.1686514512,-0.0203225637
O,0,0.058817235,2.3594202811,2.4043715087	O,0,0.0035170659,2.3545995846,2.4041165449
O,0,-0.1160943539,2.3171287479,-2.3532051913	O,0,-0.1287780667,2.2906810479,-2.3490110903
P,0,0.1125976797,0.6522526654,-2.2211297822	P,0,0.1110541846,0.62041221,-2.1937082732
P,0,0.1226778039,0.6769922319,2.3187915675	P,0,0.112573071,0.6674065777,2.3045229975
C,0,-1.0924261488,0.1652653794,-3.6168375589	C,0,-1.0597999355,0.0940571799,-3.569517882
C,0,1.9229767623,0.4480159049,-2.8037955446	C,0,1.9160432061,0.4464402821,-2.7248563949
C,0,1.8480713889,0.3783386787,3.0817350862	C,0,1.8467179776,0.4249256066,3.0073485383
C,0,-1.2424744311,0.2781771518,3.5808963113	C,0,-1.2057991126,0.2022194952,3.5594297015
C,0,-2.4951845116,0.440447127,-3.0692466042	C,0,-2.4591864415,0.4313417245,-3.0523223787
H,0,-3.2358702198,0.1311755033,-3.8139905191	H,0,-3.2056489178,-0.0076011334,-3.7202351544
H,0,-2.6372910703,1.5056125312,-2.8777897691	H,0,-2.6092227802,1.5118520994,-3.037841686
H,0,-2.709565677,-0.0753591146,-2.1373309896	H,0,-2.6436172303,0.0811041311,-2.0414993391
C,0,-0.9190490018,-1.3197697829,-3.9417471477	C,0,-0.8883126193,-1.4086344148,-3.7863054791
H,0,0.0003469326,-1.5105497717,-4.4986738447	H,0,0.0353710924,-1.6295837206,-4.323207576
H,0,-1.7532734762,-1.6639051864,-4.5613487784	H,0,-1.7189546861,-1.7959896865,-4.3824012346

H,0,-0.8802063225,-1.9452062703,-3.0449534967	H,0,-0.8473650587,-1.9664139563,-2.8473949727
C,0,-0.9556619592,1.0074146234,-4.8925220753	C,0,-0.8931664306,0.8460726352,-4.8926640959
H,0,-0.0782031657,0.7594322328,-5.482904215	H,0,-0.0334287968,0.5162742172,-5.467567326
H,0,-0.9346138552,2.0726224966,-4.6615084509	H,0,-0.8187818363,1.9212151669,-4.7291867705
H,0,-1.8334724855,0.8197236034,-5.5200378917	H,0,-1.7841403464,0.6616049204,-5.5005831674
C,0,2.3858351163,-0.9728902577,-2.4637506332	C,0,2.400175021,-0.9544776455,-2.3479849394
H,0,1.8411035449,-1.7309928246,-3.0313395135	H,0,1.8460840533,-1.7330526301,-2.8755873019
H,0,2.2592451094,-1.1957389711,-1.4045142548	H,0,2.3009353313,-1.1369282523,-1.2789609241
H,0,3.4462613513,-1.072008308,-2.7181274981	H,0,3.454536955,-1.0496598473,-2.6238494343
C,0,2.7618801168,1.469573266,-2.0258895222	C,0,2.7096354449,1.5014295426,-1.9470211078
H,0,3.8176466764,1.3054831238,-2.2646377666	H,0,3.7746287359,1.3407417169,-2.1365180145
H,0,2.6405030003,1.376115873,-0.9480977788	H,0,2.5397043192,1.4408479548,-0.8737906183
H,0,2.5059269276,2.4919970577,-2.3068815687	H,0,2.4518109401,2.5091547687,-2.2741972763
C,0,2.1564547339,0.7101070156,-4.2921170802	C,0,2.1634882017,0.6823930897,-4.2110937762
H,0,1.7065714453,-0.0535644276,-4.9271352847	H,0,1.7612124452,-0.1205193845,-4.827892732
H,0,3.2351475589,0.6867289964,-4.4789576849	H,0,3.2443596451,0.7079176147,-4.3786603137
H,0,1.791120838,1.6906327921,-4.5994730096	H,0,1.7517515429,1.6333834499,-4.548697646
C,0,-0.9522934903,0.7129085704,5.0186411578	C,0,-0.9020581871,0.5569759416,5.011826086
H,0,-0.1806621318,0.1051943221,5.4928951719	H,0,-0.1143200821,-0.0657314772,5.4353526123
H,0,-1.8686608594,0.582618371,5.6044160565	H,0,-1.8076440376,0.3778051347,5.5999261051
H,0,-0.6696924063,1.7646151233,5.0810699788	H,0,-0.6334667514,1.6070612615,5.1297188741
C,0,-2.4725691264,1.0650492682,3.1046218717	C,0,-2.4468078135,0.9993600058,3.1380147204
H,0,-3.3471587862,0.7244461767,3.6674708958	H,0,-3.3206598171,0.589022197,3.6513490985
H,0,-2.6798488031,0.9224263782,2.046546626	H,0,-2.6313130928,0.9508035724,2.0678230234
H,0,-2.3411609865,2.1322177695,3.286222594	H,0,-2.3370511276,2.0466872884,3.419149945
C,0,-1.512556392,-1.2290929488,3.5571669131	C,0,-1.4394818867,-1.3053591701,3.4470166708
H,0,-0.7101426018,-1.79342872,4.0345128497	H,0,-0.6127285523,-1.8694680643,3.8799876864
H,0,-1.6331702796,-1.5959820682,2.5400749355	H,0,-1.5587422164,-1.614222616,2.4113855298
H,0,-2.4365250144,-1.4372456343,4.1061412214	H,0,-2.3487505369,-1.5697357621,3.994430625
C,0,2.1436136087,1.3234760849,4.2531003316	C,0,2.1159461492,1.316339188,4.2221582514
H,0,3.1887251852,1.1864669057,4.5489521682	H,0,3.1717018847,1.2185370437,4.4906658822
H,0,1.5316871402,1.1298721894,5.1297883714	H,0,1.5312999418,1.0402951037,5.0937890523
H,0,2.0095782853,2.3659990815,3.9631823504	H,0,1.9213955945,2.3636114735,3.9902151249
C,0,1.9689174744,-1.0844695109,3.5145501594	C,0,2.0346377773,-1.0506085426,3.3519433707
H,0,3.010708215,-1.2968105865,3.775293381	H,0,3.0877097254,-1.2353931937,3.5828089398
H,0,1.6816479778,-1.7655245083,2.7094563558	H,0,1.7562825517,-1.6908010352,2.5112507817
H,0,1.3626556865,-1.3078317689,4.3936211088	H,0,1.4498753822,-1.3462209975,4.223886648
C,0,2.9063268971,0.6578756949,2.0077363118	C,0,2.8577833246,0.8223363053,1.9277628378
H,0,3.8935837495,0.6177514471,2.4791137163	H,0,3.8515903549,0.8550695871,2.3826131151
H,0,2.7894469676,1.648016347,1.5625361355	H,0,2.6438605228,1.8079979525,1.5096028979
H,0,2.8839030691,-0.0873078831,1.2135360251	H,0,2.884422044,0.0996243653,1.1143946361
H,0,-2.0712539346,0.0529070758,0.0637361407	H,0,-2.0446105337,0.1872275935,0.0555947834
B,0,-2.9599428916,-0.8537497751,0.1457356484	B,0,-2.9465026366,-0.7070104859,0.1587810969
H,0,-3.9173413792,-0.4713197279,-0.483182437	H,0,-3.9061373235,-0.2354132667,-0.4046323622
H,0,-3.2169294061,-1.1243861376,1.2858347042	H,0,-3.1595771541,-1.0021675982,1.2982357087
N,0,-2.3938087766,-2.1804521906,-0.5217236258	N,0,-2.5022788262,-2.0333463598,-0.5822910106
N,0,-3.1796956123,-3.3809845431,-0.3432044556	N,0,-3.3655922541,-3.1790111429,-0.4109522182
H,0,-2.255586061,-2.0701306219,-1.5239703598	H,0,-2.396464562,-1.8969053006,-1.5851505128
H,0,-1.4356104259,-2.3123425621,-0.1609263883	H,0,-1.5518871453,-2.2555420124,-0.2576006391
H,0,-3.2293629156,-3.5181847042,0.6630094567	H,0,-3.448316147,-3.3023922816,0.5950017914
H,0,-4.1258650899,-3.1254161258,-0.6181721177	H,0,-4.2868363916,-2.8752020097,-0.7177743688
	
1-H-HBH$_2$NH$_2$NH$_2$-Axial-TS	**1-H-HBH$_2$NH$_2$NH$_2$-Axial-TS**

H,0,-0.0538823427,-0.4746616367,1.52979999	H,0,-0.087780422,-0.4461004274,1.4780856795
Ir,0,-0.0145937754,0.3127140528,0.1722826265	Ir,0,-0.0367984877,0.3164592484,0.1137619864
H,0,0.1270917161,1.7276793277,1.1940645589	H,0,0.0726864657,1.7278980157,1.1282233324
C,0,-0.0452970035,-1.6146066376,-0.5195998108	C,0,-0.0407807168,-1.6141570659,-0.5603085072
C,0,-0.0800204766,-4.3086811979,-1.3305993805	C,0,-0.0390060089,-4.3100339851,-1.3533525986
C,0,-1.2299239246,-2.3394662362,-0.6233556348	C,0,-1.2245220921,-2.3229251676,-0.7575137059
C,0,1.1253008159,-2.3305473976,-0.7515340871	C,0,1.1396504756,-2.3439282128,-0.6797197557
C,0,1.1347706351,-3.6547136678,-1.1705772284	C,0,1.1675622666,-3.6708098913,-1.0902601251
C,0,-1.2749541243,-3.6644022263,-1.0363544349	C,0,-1.2487428918,-3.6498134555,-1.1674432042
H,0,2.0762985062,-4.1574125223,-1.3537979926	H,0,2.1139253873,-4.1879646747,-1.1874355891
H,0,-2.2272678192,-4.173705875,-1.1165710101	H,0,-2.1957026414,-4.1510323998,-1.3240215904
H,0,-0.094062822,-5.3414842946,-1.6594182975	H,0,-0.0374701572,-5.3442538973,-1.6771921201
O,0,2.3360375276,-1.7225205142,-0.5033385923	O,0,2.3249031258,-1.7466273547,-0.3258602048
O,0,-2.4136025587,-1.7346365166,-0.2597665298	O,0,-2.4218528993,-1.7006820751,-0.4914912575
P,0,-2.3265102344,-0.1057637057,0.1313668843	P,0,-2.3231839879,-0.1170049732,0.0677403141
P,0,2.2853351516,-0.1604286201,0.1092433924	P,0,2.2469683958,-0.1308884653,0.1467927155
C,0,-3.4564647894,0.5305950473,-1.2565446683	C,0,-3.4597302414,0.6631670704,-1.1972617275
C,0,-3.167197138,-0.0659858654,1.838241818	C,0,-3.072997956,-0.2445025572,1.7890959123
C,0,3.1964030403,-0.4164637119,1.7686236092	C,0,3.0955784405,-0.2299776687,1.8259103419
C,0,3.4112500668,0.6659234923,-1.1760679876	C,0,3.3693438836,0.5839503011,-1.1773152762
C,0,-2.6731473595,0.2861057624,-2.5548004278	C,0,-2.7587655234,0.4282174474,-2.5407899373
H,0,-3.2424084227,0.7145725134,-3.3856055673	H,0,-3.2766898627,1.0097807451,-3.3081994512
H,0,-2.5584813794,-0.7827573502,-2.7446341666	H,0,-2.8102822089,-0.6256062181,-2.8166956808
H,0,-1.6906983095,0.7498691837,-2.5465589915	H,0,-1.7180973025,0.7379794587,-2.5255994276
C,0,-3.7430459847,2.0180258472,-1.0565809328	C,0,-3.5754321653,2.1487975652,-0.8687235102
H,0,-4.3672351073,2.1971588661,-0.177854908	H,0,-4.1636904767,2.3117369757,0.036871396
H,0,-4.2849936761,2.3998033121,-1.9272218854	H,0,-4.0771016635,2.6664553409,-1.6906153043
H,0,-2.8258188092,2.5977290011,-0.9640088699	H,0,-2.5949980542,2.6026842882,-0.7344849752
C,0,-4.7701855626,-0.2525431913,-1.3765152492	C,0,-4.8423823986,0.0161775624,-1.2935017471
H,0,-5.4990779133,0.0080780256,-0.6131332085	H,0,-5.5016361676,0.2975095564,-0.4774571116
H,0,-4.6016353029,-1.3297205341,-1.3543911296	H,0,-4.7741642849,-1.0715735766,-1.3379472682
H,0,-5.2156009443,-0.008195678,-2.3460691147	H,0,-5.3055690566,0.3576032715,-2.2237385221
C,0,-2.8395430273,1.2810081356,2.492378193	C,0,-2.6558465714,1.0073769226,2.564632248
H,0,-3.2096705163,2.1301641346,1.9133441184	H,0,-2.9870797712,1.9265888028,2.0768558258
H,0,-1.7657978377,1.4064353797,2.6304346635	H,0,-1.5743267373,1.0566199115,2.6828682213
H,0,-3.3157059878,1.3214104702,3.4768897244	H,0,-3.1105044873,0.9739988247,3.5584828798
C,0,-2.5593495292,-1.1996057154,2.6725127265	C,0,-2.4713284187,-1.4880209904,2.4492849367
H,0,-2.9638780519,-1.1382397735,3.6877078894	H,0,-2.7999592195,-1.5168375223,3.4917174011
H,0,-1.4737036703,-1.1247772923,2.7368748749	H,0,-1.3815417538,-1.473244788,2.4390200495
H,0,-2.8111403725,-2.1783989219,2.262678658	H,0,-2.8069752849,-2.4007897768,1.9565909277
C,0,-4.6836429192,-0.26040626,1.8086476263	C,0,-4.5925559745,-0.3771385727,1.8133142173
H,0,-5.2006536486,0.5794191512,1.3440081406	H,0,-5.0891752138,0.5385795469,1.4935687893
H,0,-5.040780644,-0.3284593051,2.8412652619	H,0,-4.9018671903,-0.572068473,2.8441649308
H,0,-4.9727335009,-1.1803884671,1.2994305451	H,0,-4.9429246622,-1.2059562507,1.1984038029
C,0,4.8175527149,0.0635471463,-1.2176798205	C,0,4.7705809318,-0.0197397249,-1.153778764
H,0,5.4129355019,0.3309388154,-0.3438300215	H,0,5.350910679,0.3293193314,-0.2999606592
H,0,5.3342940806,0.4669568454,-2.0944239641	H,0,5.296079613,0.3018869207,-2.0577245548
H,0,4.7956927703,-1.0225428214,-1.3176535728	H,0,4.7453473972,-1.1097689908,-1.1499531587
C,0,2.7403885611,0.4115352774,-2.5335627966	C,0,2.6946977761,0.2193031362,-2.5047505819
H,0,3.318715215,0.9306370559,-3.3040821468	H,0,3.2669954286,0.6758790293,-3.3167860176
H,0,1.7221763791,0.7951388884,-2.564118086	H,0,1.6739327958,0.5948521564,-2.5542415263
H,0,2.7265570678,-0.65108787,-2.7784640996	H,0,2.6818733914,-0.8597416469,-2.6602710206
C,0,3.4995853758,2.1709867897,-0.9223276104	C,0,3.4499904212,2.0998134292,-1.0427837166
H,0,4.0377900736,2.4112638807,-0.0051559952	H,0,3.9885539002,2.4128642076,-0.1496568642
H,0,2.513045074,2.6294912268,-0.8860962768	H,0,2.4585928086,2.5432796434,-1.0338390322
H,0,4.0424051899,2.6336526373,-1.7525877689	H,0,3.9819196572,2.5004463984,-1.9104379526

C,0,4.2952801698,-1.4804350554,1.6641403858 H,0,4.714564117,-1.6381423846,2.6629388199 H,0,5.1127138696,-1.1905471969,1.0085576763 H,0,3.8960628836,-2.4314975081,1.3121001639 C,0,3.782511493,0.9090527626,2.2616261888 H,0,4.1415722639,0.7772595556,3.2870363481 H,0,3.0381003564,1.7094594137,2.278158832 H,0,4.6308541684,1.2363966903,1.659900326 C,0,2.174385053,-0.910868838,2.798578063 H,0,2.7054313504,-1.1424254227,3.7275345085 H,0,1.6656970668,-1.8185641197,2.4680176798 H,0,1.4188557098,-0.156674341,3.016016644 H,0,0.0395081592,1.3907576194,-1.3189075389 B,0,-0.1199781477,2.7549346412,-1.6662895759 H,0,-1.0806850335,2.6959515882,-2.3866707503 H,0,0.9248152289,2.9528994178,-2.2394270286 N,0,-0.3366265281,3.608344117,-0.4381740592 N,0,0.6868428878,4.4824253528,0.0334519588 H,0,-1.2043583769,4.124881209,-0.4226600826 H,0,-0.2148994338,2.2124054235,0.5281897119 H,0,1.2458506219,3.9861228623,0.7224311968 H,0,1.3081451431,4.709663753,-0.7381425046	C,0,4.2269094531,-1.2595579083,1.8419226851 H,0,4.6107576727,-1.3282010369,2.8637087851 H,0,5.057561533,-0.9902865608,1.1954023482 H,0,3.8658332195,-2.24438333,1.54659391 C,0,3.6128241157,1.1540811688,2.2122652978 H,0,3.9182957681,1.1370486178,3.2618884096 H,0,2.8417796077,1.9213403046,2.1060530265 H,0,4.4804693756,1.446456809,1.6214209894 C,0,2.0486100207,-0.6736426876,2.8504930787 H,0,2.5522142362,-0.8300819752,3.8086223872 H,0,1.5709592167,-1.6118541778,2.5618438681 H,0,1.2725225447,0.0779047473,2.9895250054 H,0,0.0524514353,1.3350187014,-1.4146620953 B,0,-0.0898278964,2.6830852646,-1.7665444783 H,0,-1.062858524,2.6526639594,-2.4735122035 H,0,0.9506256502,2.8586598098,-2.3603440267 N,0,-0.2892624492,3.5597715292,-0.5509082112 N,0,0.801672668,4.2889501031,0.0067798498 H,0,-1.0910392259,4.1720066818,-0.5846847307 H,0,-0.2906988637,2.1925257854,0.4421718393 H,0,1.2847295482,3.6765046597,0.660968762 H,0,1.4724043048,4.4935893293,-0.7299579579
H_2 H,0,0.,0.,-0.3703590277 H,0,0.,0.,0.3748169527	**H_2** H,0,0.,0.,-0.370550263 H,0,0.,0.,0.375008188
N_2H_4-BH_3 H,0,-0.0986554841,-0.1158083297,0.1483673604 B,0,0.1668676169,-0.2224081212,1.3274488209 H,0,0.0759355738,-1.3615868264,1.7388101082 H,0,-0.4078219296,0.5897086043,2.0241648439 N,0,1.7329433392,0.147584508,1.4523318183 H,0,1.9151995661,1.0849293392,1.100961298 H,0,2.3001880853,-0.4679692374,0.8738675653 N,0,2.3108108974,0.0960017071,2.7847121974 H,0,1.7056495191,0.6984604189,3.3398789368 H,0,2.0873861105,-0.8413211066,3.1147034235	**N_2H_4-BH_3** H,0,-0.1028242877,-0.116630672,0.1469233426 B,0,0.1758983243,-0.2199868691,1.3262015809 H,0,0.0631807263,-1.3604492727,1.734129245 H,0,-0.4189214075,0.5841690212,2.0185075255 N,0,1.7314391794,0.147069861,1.4533010673 H,0,1.9171970857,1.0837355919,1.1008659492 H,0,2.3014058495,-0.4660177455,0.8742321719 N,0,2.3071440801,0.0950471767,2.7850231099 H,0,1.7152722142,0.7036517608,3.3461211383 H,0,2.098711526,-0.8429978969,3.1199412389
H_2B=NH-NH_2 B,0,-0.034583155,1.1208043262,1.6889852661 H,0,-0.1617099958,2.1716357419,1.1306613508 H,0,0.0678853885,1.022059472,2.8759092938 N,0,-0.0028495379,-0.044322336,0.9385060974 H,0,0.1026206866,-0.9527033044,1.3638493722 N,0,-0.1050213352,-0.1710435734,-0.4729691444 H,0,-0.9843737242,0.2356077724,-0.7701983402 H,0,0.6409706899,0.3661036872,-0.8994810237	**H_2B=NH-NH_2** B,0,0.007469467,1.1222383103,1.686831717 H,0,0.0238232713,2.1782907547,1.1229974493 H,0,0.0485476119,1.0190504265,2.8776254362 N,0,-0.048474535,-0.0400672526,0.9392506952 H,0,-0.0197377116,-0.9533635498,1.3671598865 N,0,-0.0166510368,-0.1527991845,-0.4775016815 H,0,-0.9673030672,-0.071071953,-0.8261548476 H,0,0.4952650173,0.6458642345,-0.834945783
NH_2-NH_2 N,0,-0.1306227772,-0.0657473638,1.003028009 H,0,-0.8323106384,-0.700810114,1.3694549877 H,0,0.7647380191,-0.3058583599,1.4064648023 N,0,-0.0137184497,-0.125084052,-0.4115376194 H,0,-0.2425635545,-1.0385404497,-0.7899112567 H,0,-0.6432765445,0.5573547154,-0.8115619015	**NH_2-NH_2** N,0,-0.121460665,-0.0484756621,1.0069818109 H,0,-0.835640321,-0.6829275569,1.3531628319 H,0,0.7619972039,-0.3427525038,1.4035182277 N,0,-0.0027423753,-0.1088433811,-0.4152328769 H,0,-0.2253221358,-1.0332721992,-0.7734404949 H,0,-0.674585652,0.537585679,-0.8090524772
C_4H_8O-THF	**C_4H_8O-THF**

C,0,-0.1137144081,0.1517954302,1.1180544902	C,0,-0.1095097525,0.1495301998,1.1180359871
H,0,0.8418338744,0.3415487888,1.6149333214	H,0,0.8494771909,0.3324920762,1.6097819562
H,0,-0.8238243139,0.9137333929,1.4434749109	H,0,-0.8156468406,0.912780671,1.4465323328
C,0,0.0763830019,0.1034735856,-0.3971874333	C,0,0.0722658353,0.1010595135,-0.3970087287
H,0,0.7579645043,0.8673612881,-0.7748463019	H,0,0.7498322199,0.8658971062,-0.7778209782
H,0,-0.8849479306,0.223002018,-0.9046548928	H,0,-0.8922543436,0.2140396365,-0.8988866225
C,0,0.6111055468,-1.311288832,-0.5909583114	C,0,0.6137921866,-1.3081022366,-0.5922283583
H,0,1.7042080908,-1.3352260925,-0.4889901299	H,0,1.7051350991,-1.326690974,-0.4822982042
H,0,0.3507897422,-1.7419162221,-1.5614156977	H,0,0.3579323113,-1.7391925098,-1.5627966711
C,0,-0.5954880394,-1.2653851264,1.4087802885	C,0,-0.5982934057,-1.2622216951,1.4098329347
H,0,-1.686803398,-1.3370344712,1.3100846275	H,0,-1.6880398827,-1.3290174166,1.3028260186
H,0,-0.3205160434,-1.6186359148,2.4060746722	H,0,-0.3277570875,-1.6160927483,2.4072753278
O,0,0.0231381136,-2.1082192002,0.4369806269	O,0,0.0231952102,-2.1112729782,0.4370851766

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