

Homogeneous Catalytic Transfer Dehydrogenation of Alkanes with a Group 10 Metal Center

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General

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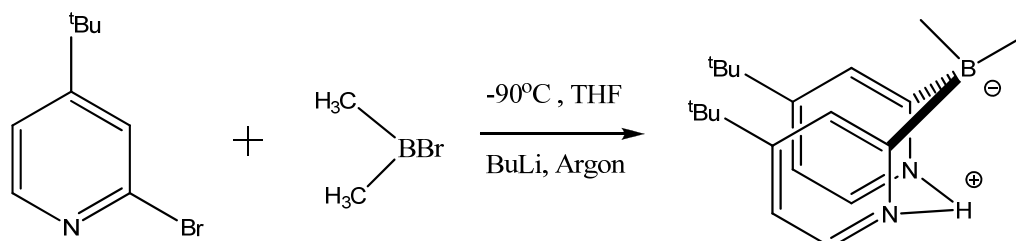
General. All manipulations were carried out under purified argon using standard Schlenk and glove-box techniques. Solvents were dried and distilled following standard protocols and stored in gas-tight bulbs under argon. All reagents for which a synthesis is not given are commercially available from Aldrich, Acros, Alfa Aesar or Pressure Chemicals and were used as received without further purification. Deuterated solvents from Cambridge Isotope Laboratories were dried, vacuum-transferred and stored in an argon-filled glove box.

^1H (400.132 MHz) and ^{13}C NMR (100.625 MHz) spectra were recorded on a Bruker Avance 400 spectrometer. Chemical shifts are reported in ppm and referenced to residual solvent resonance peaks. Elemental analyses were carried out by Chemisar Laboratories Inc., Guelph, Canada.

Computational details. Theoretical calculations in this work have been performed using density functional theory (DFT) method,¹ specifically functional PBE,² implemented in an original program package “Priroda”.³ In PBE calculations relativistic Stevens-Basch-Krauss (SBK) effective core potentials (ECP)⁴ optimized for DFT-calculations have been used. Basis set was 311-split for main group elements with one additional polarization *p*-function for hydrogen, additional two polarization *d*-functions for elements of higher periods. Full geometry optimization has been performed without constraints on symmetry. For all species under investigation frequency analysis has been carried out. All minima have been checked for the absence of imaginary frequencies. All transition states possessed just one imaginary frequency. Using method of Intrinsic Reaction Coordinate, reactants, products and the corresponding transition states were proven to be connected by a single minimal energy reaction path.

1. Synthesis of ligands and complexes

Hydrogen dimethyldi(4-*tert*-butyl-2-pyridyl)borate, H(dpb^{tBu})



The known compound, 2-bromo-4-*t*-butyl-pyridine, was prepared via Chichibabin amination⁵ of 4-*t*-butyl-pyridine followed by its subsequent bromination following the method of Adams and Miyano.⁶ After amine purification via column chromatography or recrystallization, bromination usually affords pure product via the published procedure (>95%), and no further purification is required. Pure by ¹H NMR 2-bromo-4-*t*-butyl-pyridine is a dark red solid/liquid dual phase mixture at room temperature. The procedure for the preparation of the title compound is similar to the published procedure of Hodgkins.⁷ 9.60 grams (4.48e-2 mol) of the Bromide were put into a flame dried flask under an argon atmosphere and 150 mL of dry diethyl ether were added. The temperature was lowered to -90°C and 17.9 mL of 2.5 M solution of *n*-BuLi (4.48e-2 mol) were added dropwise with vigorous stirring. The temperature was allowed to slowly rise to -80°C over the span of the next half an hour. Raising the temperature further usually results in the decomposition of the metallated pyridine and subsequent lower yields. After half an hour, the temperature was again lowered to -90°C and 2.19 mL of dimethylbromoborane (2.24e-2 mol) were added dropwise to the solution, which took on a dark black color. The reaction was continued for a further 18 hours, during which time it was allowed to come to room temperature. It was quenched with water and the organic layer washed with 2x100 mL of 1M acetic acid. To the aqueous washings, 100 mL of 6M NaOH were added and a black solid formed at the top of

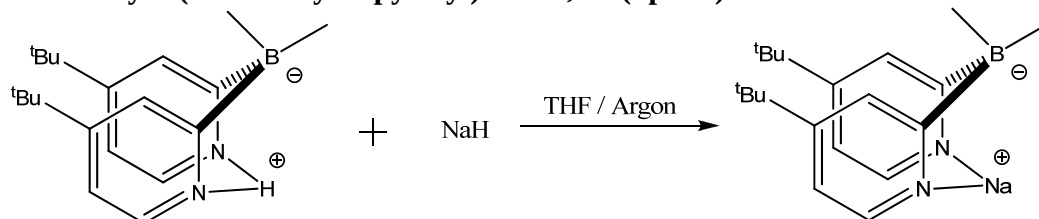
the liquid after a few hours. The black solid was collected and washed with cold water, then recrystallized from hexane, to obtain 1.40g of the title compound (10.1% yield).

^1H NMR (22°C, acetone- d_6 , 400MHz), δ : 14.31 (bs, 1H, NH), 8.45 (d, $J=5.9\text{Hz}$, 2H, pyC6-H), 7.79 (s, 2H, pyC3-H), 7.26 (dd, $J=5.92, 2.17\text{Hz}$, 2H, pyC5-H), 1.35 (s, 18H, CMe_3), 0.05 (bs, 6H, BMe_2).

^{13}C NMR (22°C, acetone- d_6 , 400MHz), δ : 191.7 (quartet, $J_{\text{C-B}}=47.2\text{Hz}$), 161.2, 141.5, 125.8, 117.4, 35.7, 30.8, 14.65 (quartet, $J_{\text{C-B}}=40.85\text{ Hz}$).

Anal. Found (Calcd for $\text{C}_{20}\text{H}_{31}\text{BN}_2$): C, 77.42 (77.42); H, 10.36 (10.07); N, 9.11 (9.03).

Sodium dimethyldi(4-*tert*-butyl-2-pyridyl)borate, Na(dpb^{tBu})



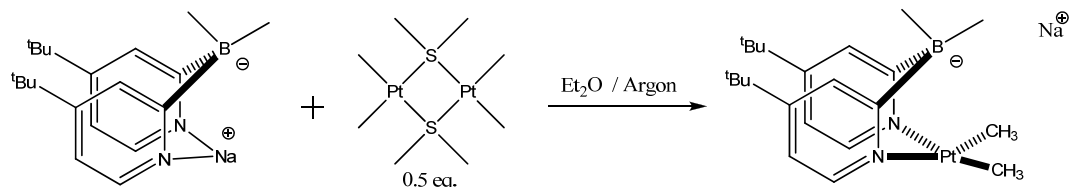
100 mg of H(dpb^{tBu}), (3.22e-4 mol), was dissolved in 3-4mL of THF in a small vial in the glove box and 50 mg of dry NaH (3.5x excess) was added slowly accompanied by vigorous evolution of hydrogen gas. The reaction was allowed to stir overnight, after which time it was filtered through Celite and washed two times with 1mL of THF. The solution was dried under vacuum and the residue washed two times with a minimum amount of benzene. After the washings, the remaining solids were once again dried under high vacuum to give 61.2 mg of the title compound as a flaky, white solid (57.2% yield). The benzene washings can be omitted to obtain yellowish title compound in quantitative yield that is >95% pure. The product is highly hydrolysable and thus should be stored and used under a dry atmosphere.

¹H NMR (22°C, THF-d₈, 500MHz), δ: 8.19 (d, *J*=5.5Hz, 2H, pyC6-H), 7.59 (s, 2H, pyC3-H), 6.69 (d, *J*=5.5Hz, 2H, pyC5-H), 1.24 (s, 18H, CMe₃), 0.42 (bs, 6H, BMe₂).

¹³C NMR (22°C, THF-d₈, 125MHz), δ: 194.06 (quartet, *J*_{C-B}=50.7Hz), 155.65, 147.52, 123.61, 114.62, 35.02, 31.26, 13.56 (quartet, *J*_{C-B}=42.3Hz).

Anal. Found (Calcd for C₂₀H₃₀BN₂Na): C, 72.05(72.30); H, 9.39 (9.10); N, 7.99 (8.43).

**Sodium dimethyldi(4-*tert*-butyl-2-pyridyl)borato dimethylplatinate(II),
Na[(d**pb**^{*t*Bu})PtMe₂], 4**



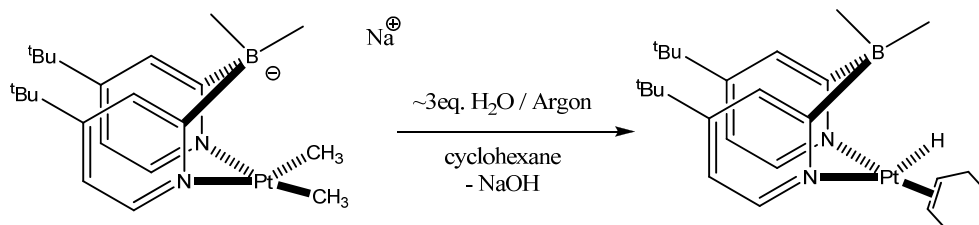
Inside the glove box, 100 mg of **Na(d**pb**^{*t*Bu})** (3.01e-4 mol), and 86.5 mg of Pt₂Me₄(μ-SMe₂)₂ (1.50e-4 mol) were added to a vial containing 4 mL of diethyl ether. The reaction mixture was stirred overnight, then dried under high vacuum, washed with heptanes and further dried under high vacuum 12 hours to obtain the title compound (163.7 mg; 99.0% yield) as an air sensitive white solid.

¹H NMR (22°C, THF-d₈, 500MHz), δ: 8.52 (d, *J*_{H-H}=6.3Hz, *J*_{Pt-H}=22.0Hz, 2H, pyC6-H), 7.58 (d, *J*_{H-H}=2.4Hz, 2H, pyC3-H), 6.71 (dd, *J*_{H-H}=6.3, 2.4Hz, 2H, pyC5-H), 1.25 (s, 18H, CMe₃), 0.46 (bs, 6H, BMe₂), 0.24-0.46 (bs, 6H, PtMe₂).

¹³C NMR (22°C, THF-d₈, 125MHz), δ: 189.15 (quartet, *J*_{C-B}=51.8Hz), 155.40, 149.54, 124.60, 116.74 (*J*_{Pt-C}=24.5Hz), 35.18, 30.96, 13.0-15.0 (bs), -20.61 (*J*_{Pt-C}=768.0Hz).

Anal. Found (Calcd for C₂₂H₃₆BN₂NaPt): C, 47.46 (47.40); H, 6.94 (6.51); N, 4.85 (5.03).

**Cyclohexene hydrido dimethyldi(4-*tert*-butyl-2-pyridyl)borato platinum(II),
(dpb^{tBu})PtH(cyclo-C₆H₁₀), **3****



40.2 mg of **4** (7.21e-5 mol) was added to a reaction vial in the glove box and 4 mL of cyclohexane were added to the vial and the contents stirred vigorously. Most of the dimethyl complex dissolved, with the rest forming a fine, light-yellow suspension. 5 μ L of H₂O were added to the solution, after which a vigorous evolution of methane gas occurred. The suspension became a clear, yellow liquid with large particulates after five minutes. After half an hour, the contents of the vial were filtered through Celite and washed two times with 1mL of cyclohexane. The clear, yellow liquid was dried overnight under high vacuum to obtain **3** (42.0 mg, quantitative yield). The product is stable in cyclohexane solutions at room temperature for at least 24 h.

¹H NMR (22°C, acetone-d₆, 400MHz), δ : 8.68 (d, $J_{\text{H-H}}=6.16\text{Hz}$; $J_{\text{Pt-H}}=61.2\text{Hz}$, 1H, pyC6-H), 8.06 (d, $J_{\text{H-H}}=6.06\text{Hz}$; $J_{\text{Pt-H}}=23.8\text{Hz}$, 1H, pyC6'-H), 7.73 (brn, 2H, pyC3-H and pyC3'-H), 7.06 (dd, $J_{\text{H-H}}=6.16$, 2.33Hz, 1H, pyC5-H), 6.96 (dd, $J_{\text{H-H}}=6.16$, 2.33 Hz, 1H, pyC5'-H), 4.92 (brn, $J_{\text{Pt-H}}=72\text{Hz}$, 2H, CH=CH), 2.40-2.62 (brn, 4H, cyclohexene CH₂'s), 1.73-1.84 (brn, 2H, cyclohexene CH₂'s), 1.38-1.29 (brn, 2H, cyclohexene CH₂'s), 1.26 (s, 9H, CMe₃), 1.25 (s, 9H, CMe₃), 0.46 (br, 6H, BMe₂), -21.27 (s, $J_{\text{Pt-H}}=1269.35\text{Hz}$, 1H, PtH).

See a ¹H NMR spectrum of **3** in cyclohexane-*d*₁₂ in Figure 1 below.

¹³C NMR (22°C, cyclohexane-*d*₁₂, 125.77MHz), δ : 190 (very broad, C2, C2', py), 159.0, 158.0 (C4, C4', py), 154.8, 144.4 (C6, C6', py), 126.6, 126.0 (C3, C3', py), 117.5, 116.7 (C5, C5', py),

78.3 (br, $J_{\text{PtC}}=160\text{Hz}$, CH=, cyclohexene), 35.3, 35.2 ($\underline{\text{C}}\text{Me}_3$, $\underline{\text{C}}'\text{Me}_3$), 30.9, 30.8 ($\text{C}\underline{\text{Me}}_3$, $\text{C}'\underline{\text{Me}}_3$), 30.5 (br, α -C's, cyclohexene), 22.2 (β -C's, cyclohexene), 15 (brm, BMe_2).

See a ^{13}C NMR spectrum of **3** in cyclohexane- d_{12} in Figure 2 below.

Anal. Found (Calcd for $\text{C}_{26}\text{H}_{41}\text{BN}_2\text{Pt}$): C, 53.47 (53.15); H, 7.17 (7.03); N, 4.71 (4.77).

Figure S1. ^1H NMR spectrum of cyclohexene hydrido dimethyldi(4-*tert*-butyl-2-pyridyl)borato platinum(II), $(\text{dpb}^{\text{tBu}})\text{PtH}(\text{cyclo-}\text{C}_6\text{H}_{10})$, **3**, in cyclohexane- d_{12} , 500MHz.

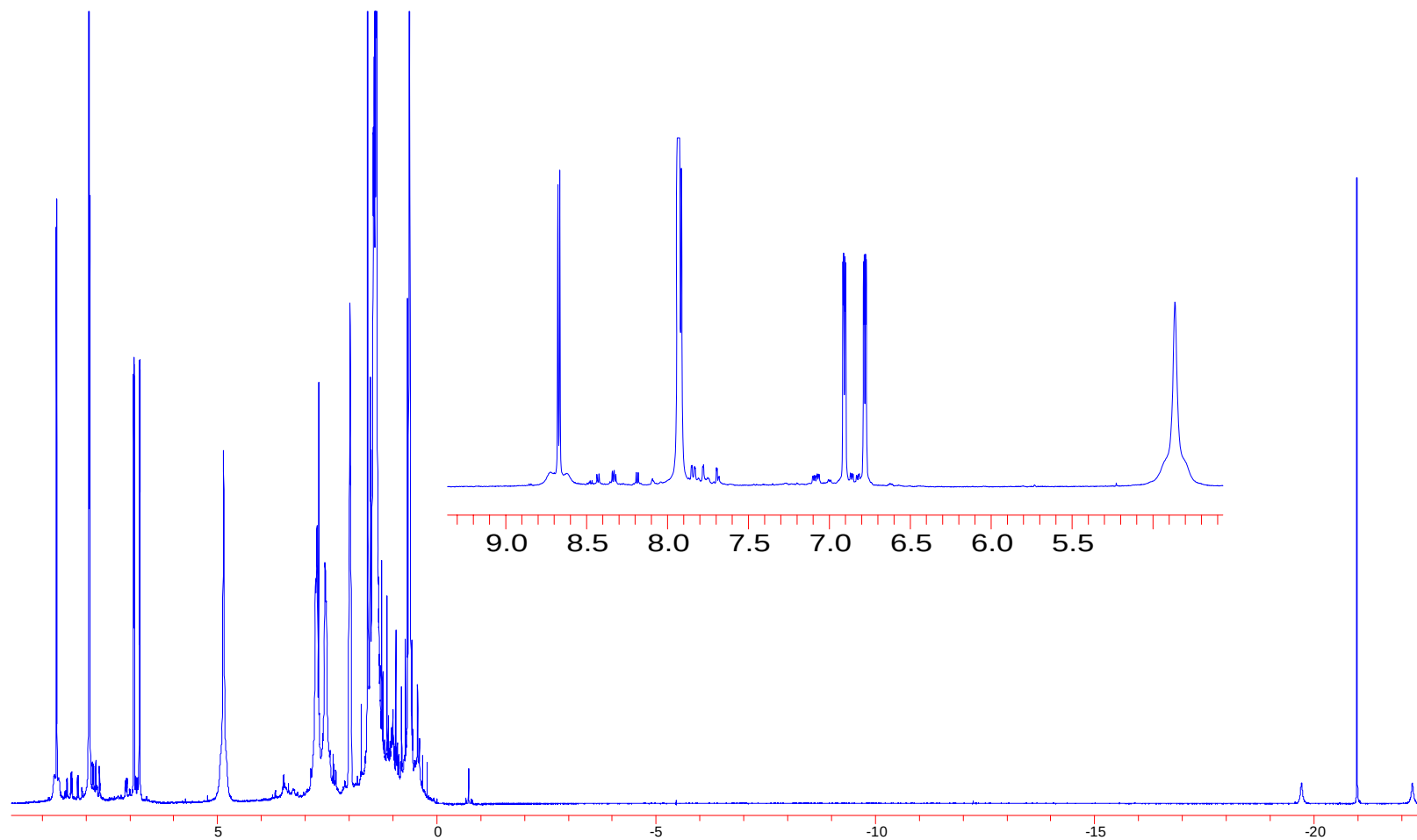
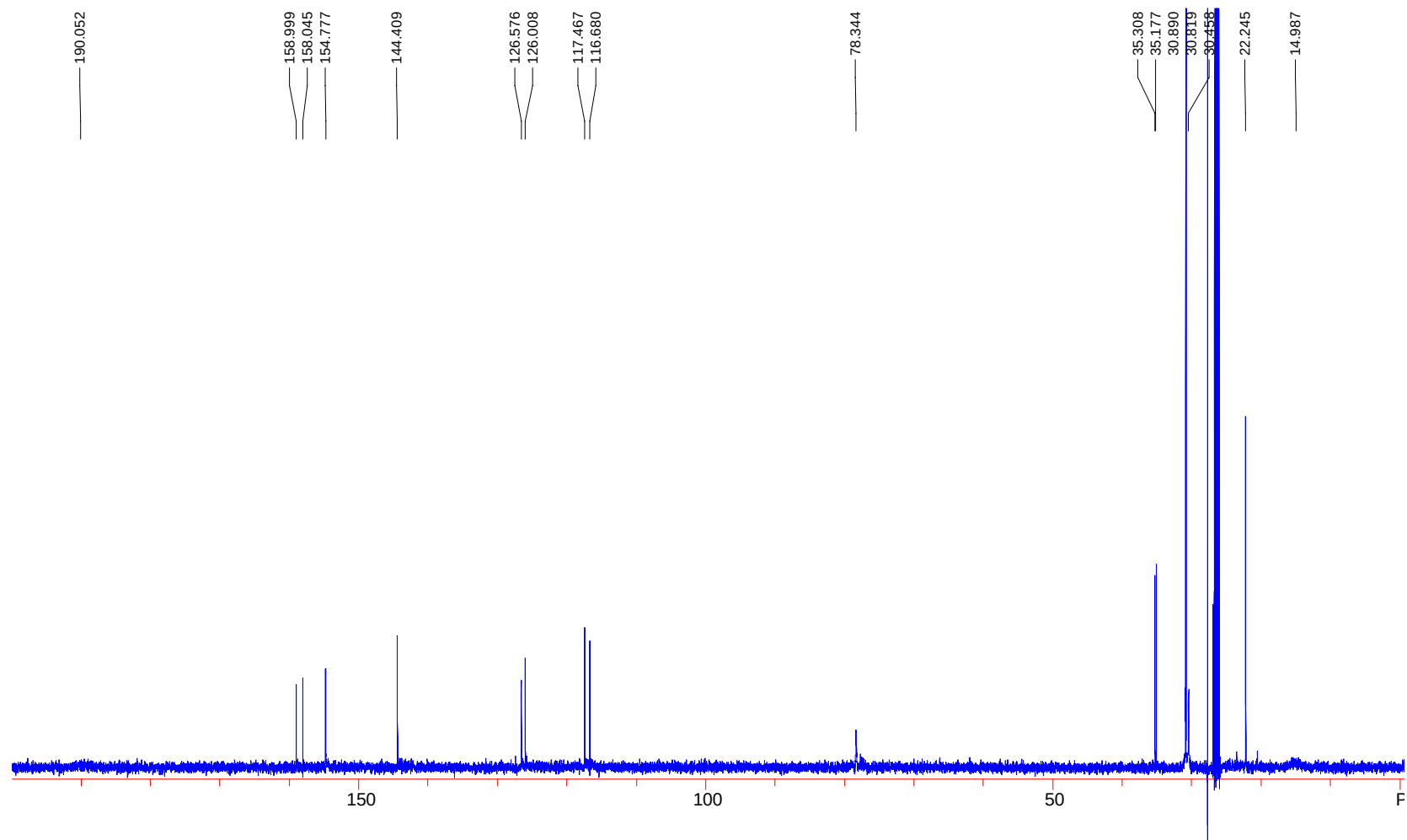
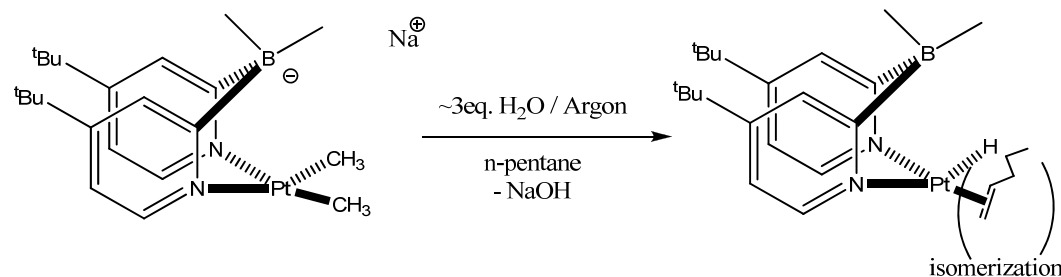


Figure S2. ^{13}C NMR spectrum of cyclohexene hydrido dimethyldi(4-*tert*-butyl-2-pyridyl)borato platinum(II), (dpb^{tBu})PtH(*cyclo*- C_6H_{10}), **3**, in cyclohexane- d_{12} , 125.8MHz.



1-Pentene hydrido dimethyldi(4-*tert*-butyl-2-pyridyl)borato platinum(II), (dpb^{tBu})PtH(1-C₅H₁₀), 5 and its isomers



The reaction with *n*-pentane was performed in the same manner as with the formation of complex 3 detailed above. When stopping the reaction after half an hour, a complex spectrum containing a number of Pt hydride signals was observed. However, when the reaction was stopped after 3-5 minutes, a single major PtH signal (up to 95%) was seen along with signals of five other minor PtH species accounting for the rest of the total integral intensity of the PtH signals. Based on the ¹H NMR data and olefin exchange experiments (see below), the predominant complex was assigned as a 1-pentene hydrido Pt^{II} complex (one of the two possible diastereomers). For this complex, the metal hydride signal appears at -20.98 ppm with $J_{\text{Pt-H}}=1189.0$ Hz.

Thereafter, a solution of the complex in cyclo-C₆D₁₂ was observed by ¹H NMR in the course of few days. After three days the signal at -20.98 ppm still remains to be the major (40%). It is seen along with other five PtH resonances; two other major signals are at -20.58 ppm (14%) and -21.45 ppm with $J_{\text{Pt-H}}=1278$ Hz (38%).

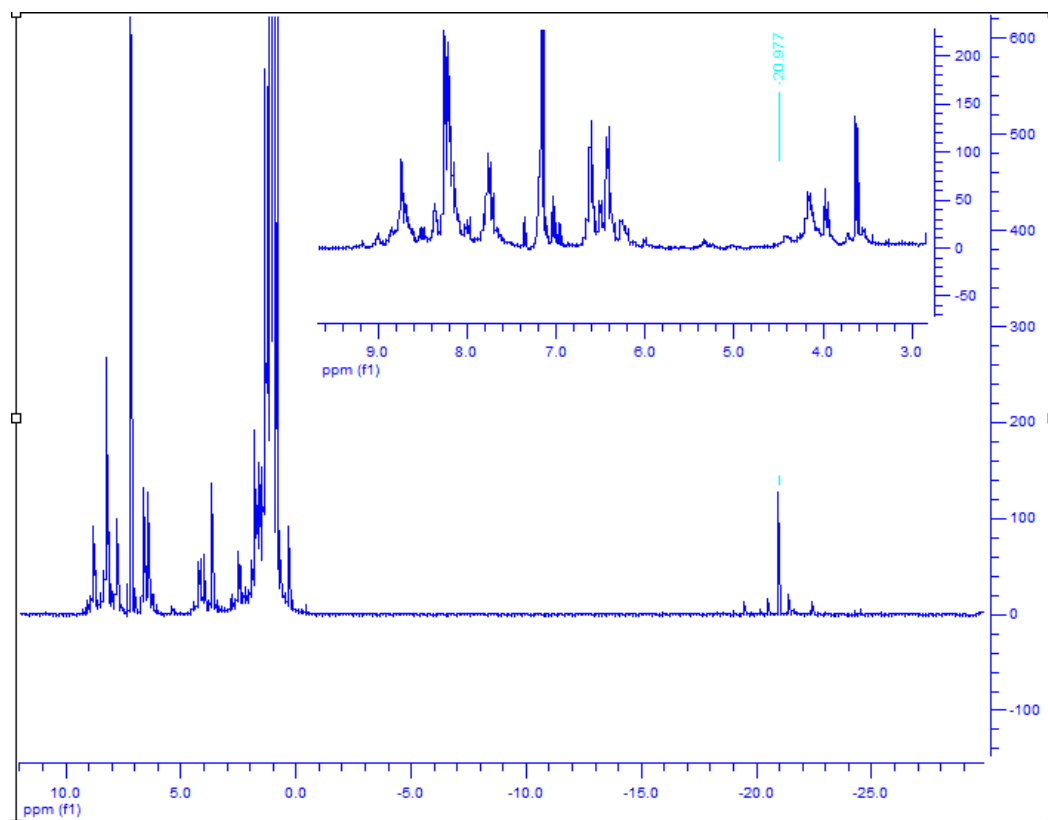
¹H NMR (22°C, C₆D₆), δ : 8.73 (d, $J_{\text{H-H}}=6.7\text{Hz}$, 1H, pyC6-H), 8.20-8.25 (m, 2H), 7.72-7.80 (m, 1H), 6.61 (m, 1H), 6.41 (m, 1H), 4.13 (vdd, $J_{\text{H-H}}=13.5\text{Hz}$, 8.4Hz, $J_{\text{Pt-H}}=65\text{Hz}$, 1H, *n*-PrCH,), 3.95 (d, $J_{\text{H-H}}=13.5\text{Hz}$, $J_{\text{Pt-H}}=56\text{Hz}$, 1H, *trans*-*n*-PrC=CH), 3.62 (d, $J_{\text{H-H}}=8.4\text{Hz}$; $J_{\text{Pt-H}}=72\text{Hz}$, 1H, *cis*-*n*-PrC=CH), 1.09 (s, 9H), 1.00 (s, 9H), 0.764 (t, $J_{\text{H-H}}=7.3\text{Hz}$, 3H, penteneCH₃), -20.98 (s, $J_{\text{Pt-H}}=1189.0\text{Hz}$, 1H).

Not all NMR signals could be assigned due to large overlap of signals in the aliphatic region and some isomerization that had already taken place. See spectrum in Figure S3 below.

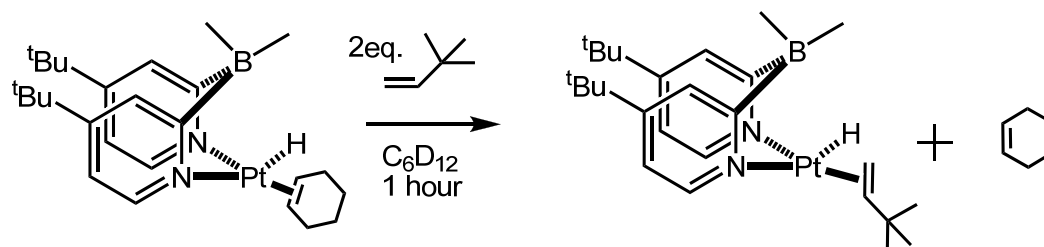
Upon addition of 1 equivalent TBE to a freshly prepared solution of LPtH(1-pentene) complex (fraction 95%) in *cyclo*-C₆D₁₂ formation of **6** and free 1-pentene was evident according to a ¹H NMR spectroscopy. In particular, observed were the following signals of free 1-pentene: a characteristic multiplet of the *n*-PrCH= proton at 5.73 ppm with $J_{HH} = 10\text{Hz}$, 17 Hz, a doublet of the =CH_{cis}(H) proton at 4.94 ppm with $J_{HH} = 17\text{ Hz}$.

Similarly, addition of 5 equivalents of TBE to an aged (7 days) solution of LPtH(1-pentene) complex in *cyclo*-C₆D₁₂ led to the formation of **6** and isomeric pentenes among which 1-pentene, *cis*-2-pentene and *trans*-2-pentene could be identified based on their very characteristic standing alone multiplets of their vinylic hydrogens at 5.73 ppm (1-pentene), 5.30-5.45 ppm (*trans*-2-pentene) and 5.10-5.25 ppm (*cis*-2-pentene). The amount of the olefins liberated was equivalent to the amount of complex **6** formed.

Figure S3. Spectrum of one of the diastereomeric 1-pentene Pt-H complexes when quenching the reaction after a short time.



***tert*-Butylethene hydrido dimethyldi(4-*tert*-butyl-2-pyridyl)borato platinum(II),
(d**pb**^{tBu})PtH(*tert*-BuCH=CH₂), **6****



Complex **3** (5.0 mg, 8.5e-5 mmol) was dissolved in 0.5 mL of deuterated cyclohexane in a Young tube under Argon and 2 eq. of TBE (2.3 μ L) were added to ensure an excess of TBE. Although the reaction was relatively slow at room temperature and both the starting material and the product could be observed even half an hour after mixing at room temperature, complete olefin exchange took place 90 minutes after addition. One of the two possible diastereomeric complexes formed.

¹H NMR (22°C, *cyclo*-C₆D₁₂), δ : 8.58 (d, $J_{H-H}=6.1$ Hz; $J_{Pt-H}=56.7$ Hz, 1H, pyC6-H), 7.86 (bd, $J_{H-H}=6.1$ Hz, 1H, pyC6'-H), 7.81 (bs, 2H, pyC3-H, pyC3'-H), 6.82 (m, 1H, pyC5-H), 6.70 (m, 1H, pyC5'-H), 4.32 (dd, $J_{H-H}=13.5$, 8.2Hz; $J_{Pt-H}=60$ Hz, 1H, *t*-BuCH), 3.66 (d, $J_{H-H}=13.5$ Hz; $J_{Pt-H}=50$ Hz, 1H, *trans*-*t*-BuC=CH), 3.49 (d, $J_{H-H}=8.2$ Hz; $J_{Pt-H}=64$ Hz, 1H, *cis*-*t*-BuC=CH), 1.26 (s, 18H, CMe₃), 1.20 (s, 9H, CMe₃), 0.43 (bs, 3H, BMe), 0.46 (bs, 3H, BMe), -21.81 (s, $J_{Pt-H}=1152$ Hz, 1H, PtH).

See a ¹H NMR spectrum of **6** in *cyclo*-C₆D₁₂ solution in Fig. 4 below.

¹³C NMR (22°C, cyclohexane-*d*₁₂, 125.77MHz), δ : 159.3, 158.1 (C4, C4', py), 154.3, 143.9 (C6, C6', py), 126.5, 126.1 (C3, C3', py), 117.4, 116.7 (C5, C5', py), 35.3, 35.2, 35.1 (CMe₃, C'Me₃,

C''Me₃), 30.9, 30.8, 30.8 (CMe₃, C'Me₃, C''Me₃), 16 (brn, BMe₂). Normally very broad signals of the B-bound aromatic carbons could not be seen. Signals of olefinic carbons could not be detected either.

See a ¹³C NMR spectrum of **6** in *cyclo*-C₆D₁₂ solution in Fig. 5 below.

Figure S4. ^1H NMR spectrum of the *tert*-butylethylene Pt-H complex $(\text{dpb}^{\text{tBu}})\text{PtH}(\text{tert-BuCH=CH}_2)$, **6**, in *cyclo*- C_6D_{12} solution.

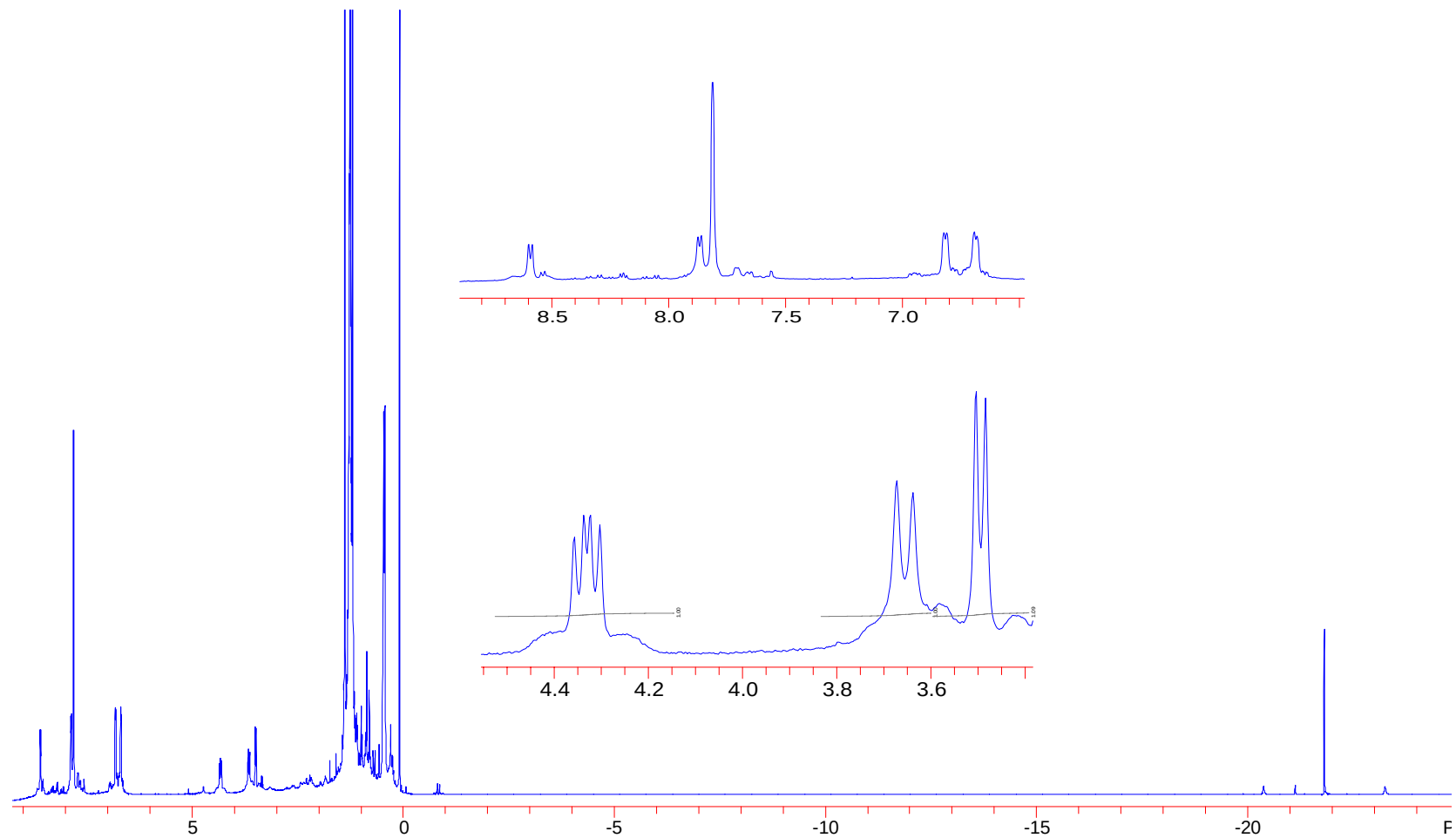
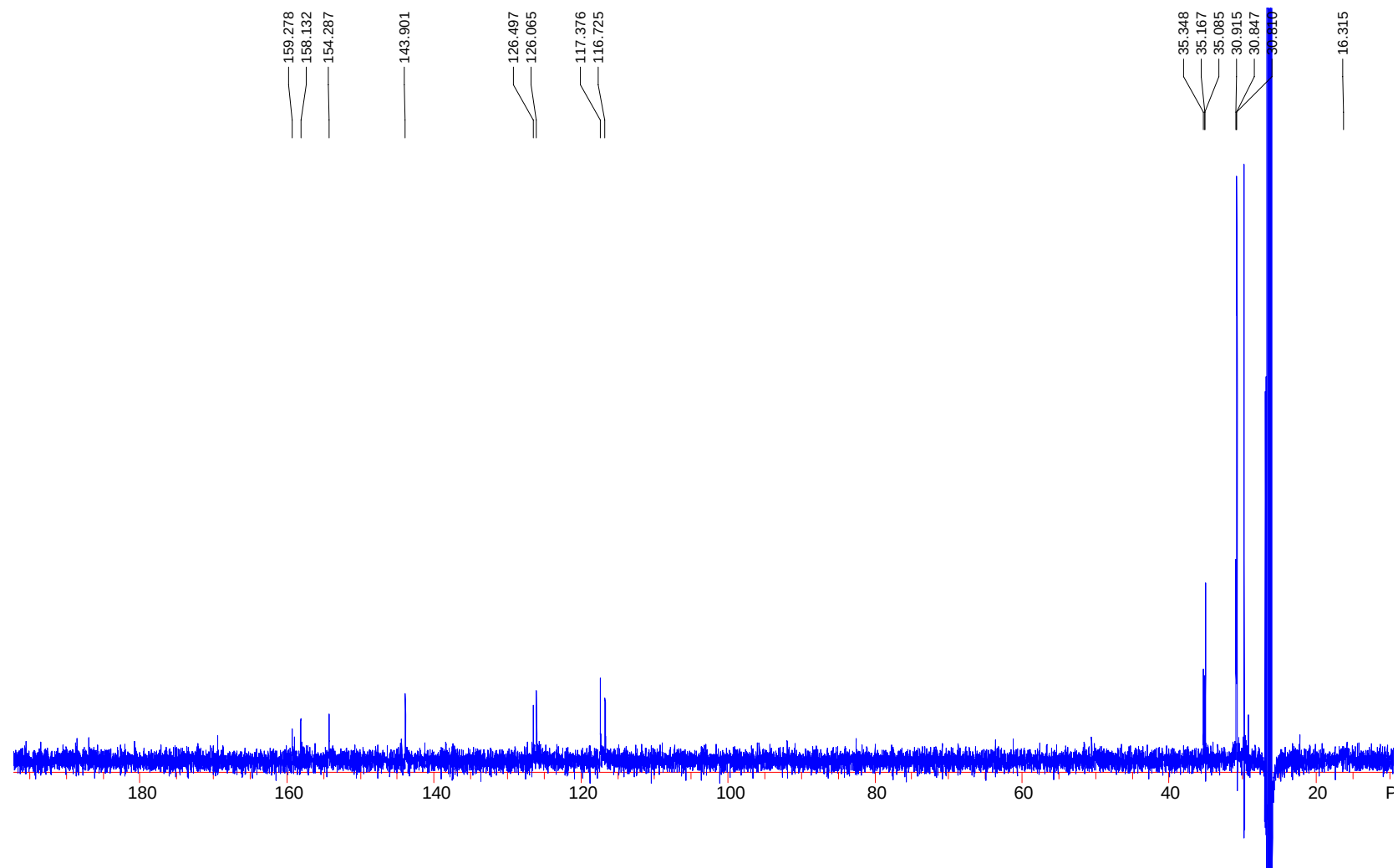


Figure S5. ^{13}C NMR spectrum of the *tert*-butylethylene Pt-H complex $(\text{dpb}^{\text{tBu}})\text{PtH}(\text{tert-BuCH=CH}_2)$, **6**, in *cyclo*- C_6D_{12} solution.



2. Catalytic dehydrogenation

Transfer dehydrogenation experiments with **3** as catalyst; sample procedure for cyclohexane dehydrogenation with TBE as the sacrificial olefin

In a 50 mL Schlenk flask under an inert atmosphere, 5.0 mg of **3** (8.5×10^{-5} mol) were added to 3 mL of cyclohexane. 23 μ L of TBE (1.7×10^{-4} mol, 20eq.) were then added and the flask sealed. The contents were heated in an oil bath at 100°C for 24 hours, after which time the flask was opened, 10 equivalents of anisole internal standard were added, and an NMR spectrum was obtained in CDCl₃ or acetone-*d*₆. Conversion was based on the integration of remaining TBE and TON is based on the signals of olefinic protons of the cycloalkene formed. The runs were found to give catalytic turnover at least three times for each olefin; results summarized in the manuscript are an average of 2 best runs.

A large excess of sacrificial olefin was found to be detrimental for the reaction. For example, 100 eq. of 3,3-dimethylbutene gave no catalysis with the same amount of substrate and catalyst.

An experiment was set up to determine the fate of the catalyst. After 24 hours of reaction at 100°C, all the volatiles were removed under high vacuum, and the resulting dark orange solid was dissolved in acetone-*d*₆ and an NMR spectrum was taken. A large number of complex decomposition products, many of them still containing Pt (as evidenced by ¹⁹⁵Pt – pyridine *ortho*-CH couplings), and one hydride peak at ~-17ppm were observed. The presumed catalyst, or catalytic precursor, does not survive under the reaction conditions. This explains why higher yields were not observed, when the reaction was stopped after >24 hours.

An attempt to identify the catalyst resting state has been made but no single complex such as **VI** (Scheme 3) was not found.

In transfer dehydrogenation reactions with cyclohexane as substrate and tetramethylethylene or trimethylethylene, no catalytic (tetramethylethylene), or poor in the case of 2-methyl-2-butene (~2eq.), turnover was observed when using 20 equivalents of these olefins. Isomerization of the free olefins to 1-butenes was also observed at the end of these reactions.

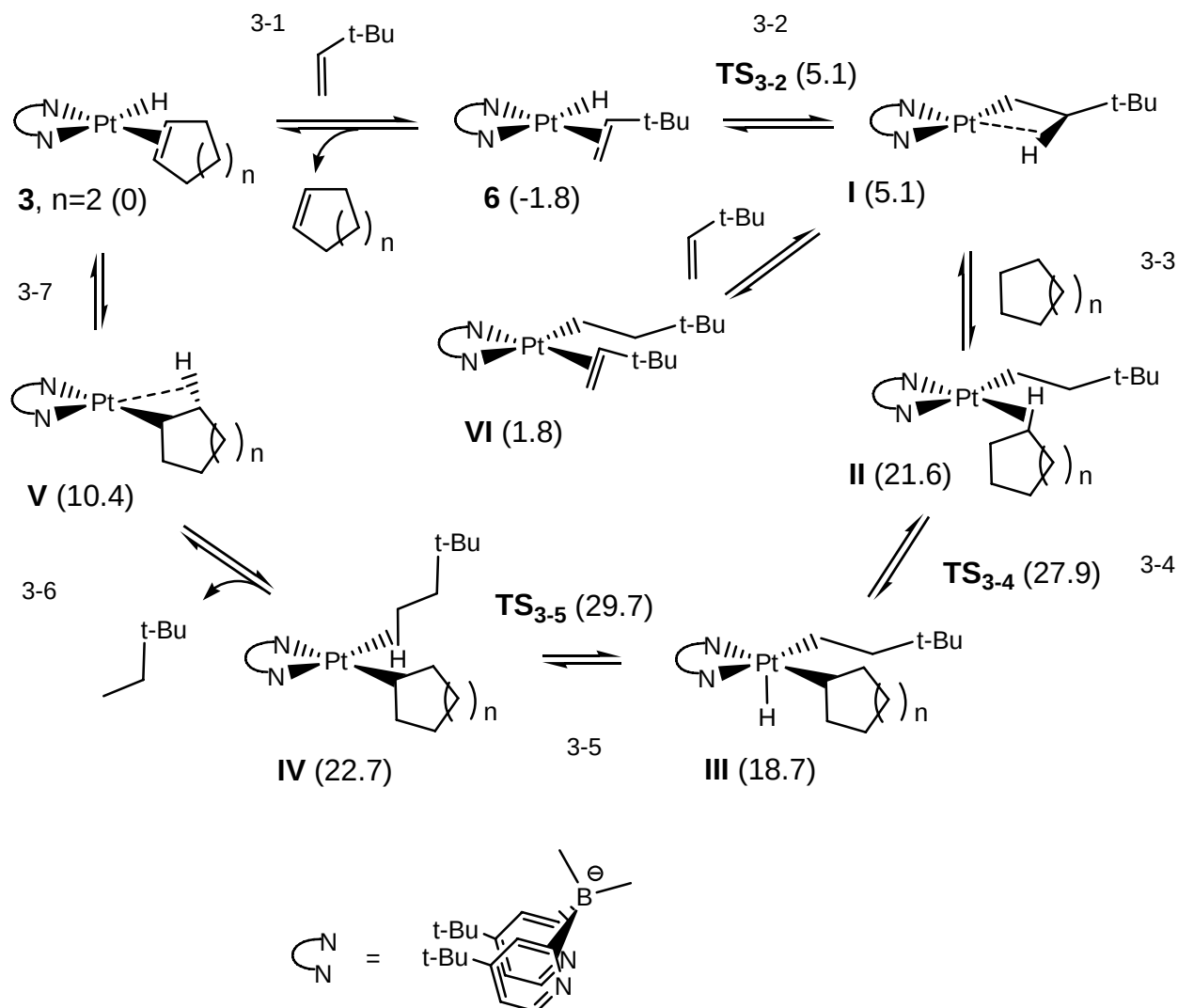
Transfer dehydrogenation of *n*-pentane. In an experiment set up as described above but with *n*-pentane as a solvent and a substrate, a mixture of isomeric 1- and 2-pentenenes formed in an yield corresponding to about four catalyst turnovers.

Attempted transfer dehydrogenation of diethyl ether. In an experiment set up as described above but with Et₂O as a solvent and a substrate, no change in the amount of TBE was detected after 1 day of heating at 100°C.

3. Olefin-for-olefin exchange in complex 3

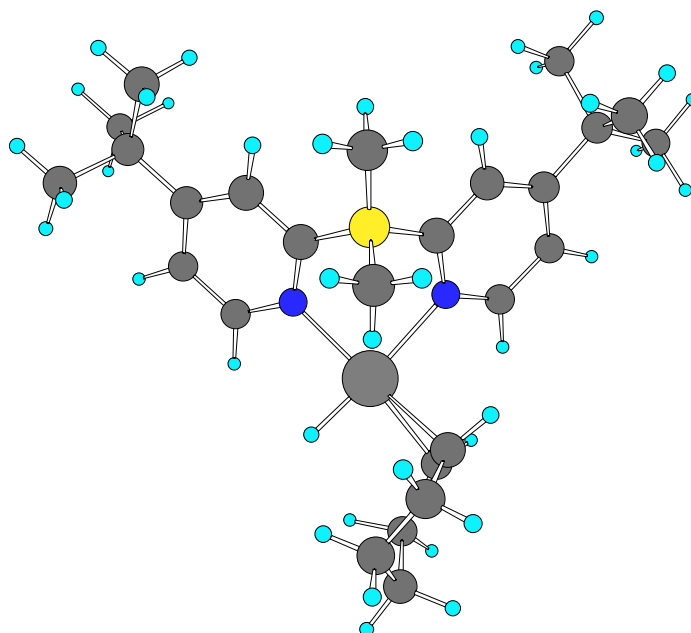
6.6 mg of **3** (1.1×10^{-5} mol) were added to a Teflon valve NMR tube in the glove box and dissolved in acetone- d_6 . 5 Equivalents of 2-methyl-2-butene were added to the NMR tube, after which it was sealed. The system comes to a steady state after two days, after which the apparent K_{eq} was calculated, 0.36 for 2-methyl-2-butene and $2.1 \cdot 10^{-4}$ for 2,3-dimethyl-2-butene. It is reported here as an average of two runs. For tetramethylethylene, 10 equivalents of olefin were used.

4. DFT calculations: optimized geometries and energies of intermediates in Scheme 3



Below are given the DFT optimized geometries and potential energies without (*E*) and with (*E*₀) zero-point energy correction in Hartrees for all complexes listed in Scheme 3 ($n = 2$; see above). The reaction Gibbs energies in Scheme 3 are given in kcal/mol.

3



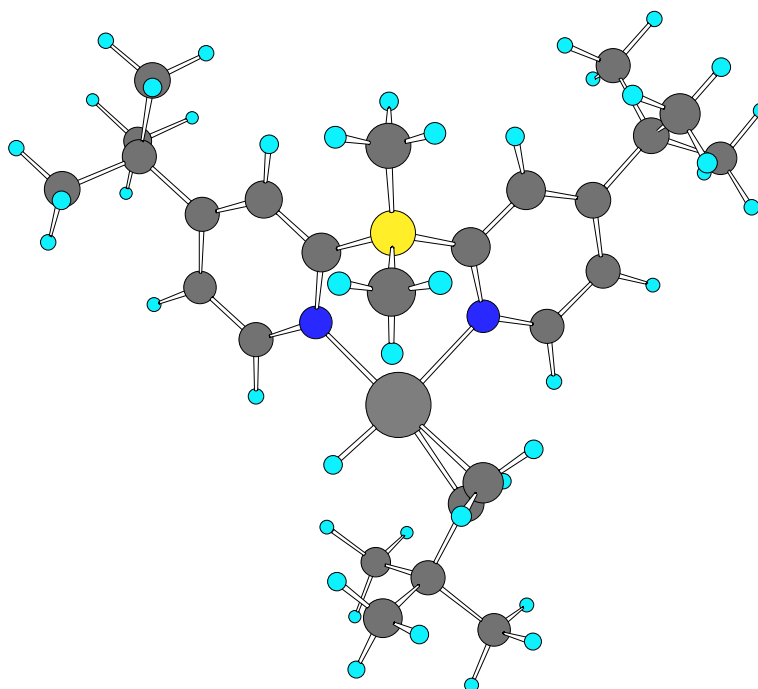
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C 2.69711589 0.23926104 -3.76771607
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H -0.10037770 -1.57371673 -3.03177102
C 2.94945676 0.37566821 2.06145354
C 3.72328829 0.46764775 -4.88888641
C 2.72780724 0.91964753 -2.54699375
C 1.92358623 0.38391472 1.09483093
C 3.05294375 -0.58888287 3.07392625
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H -1.52292460 -2.34602903 1.49205673
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H -5.01432547 -1.52825917 1.22557253
H -5.22118879 0.59074452 -0.11706212
H -3.85490704 0.08526425 -1.12159014
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C 4.45893183 -0.86387590 -5.17905525
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C 5.55139707 -0.62619929 3.35529564
C 4.12358775 0.81111850 4.86586328
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6



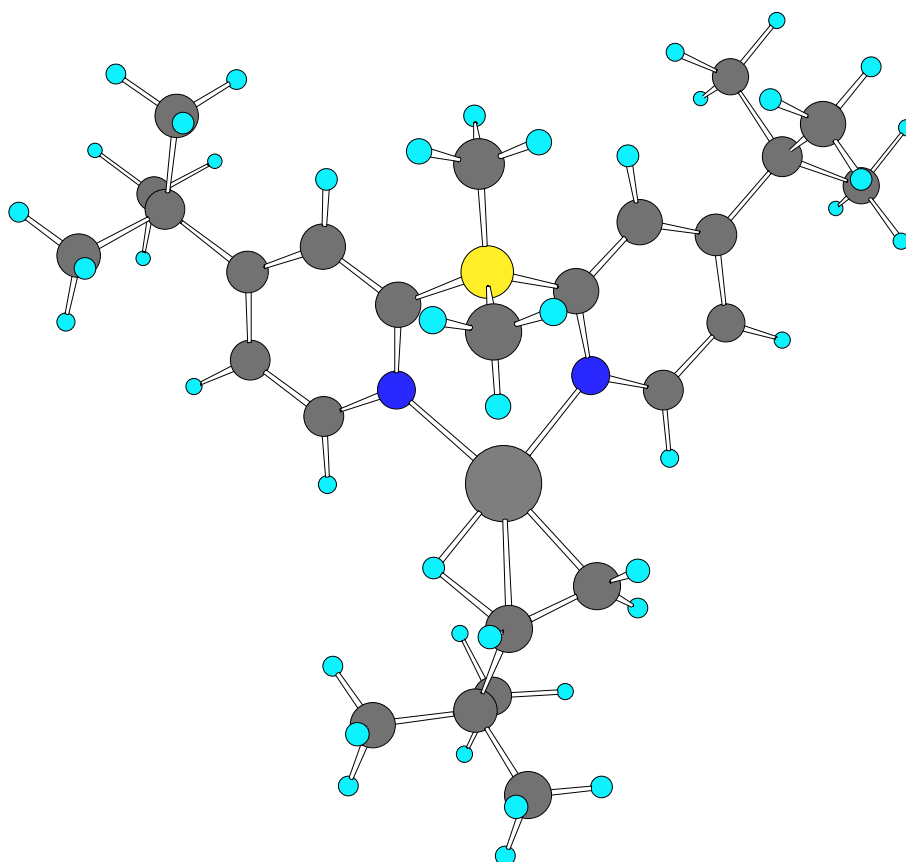
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C 0.59578593 2.96489958 0.29216107

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H -4.75731277 -3.34891581 0.75644339
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H -4.26015602 -2.26347686 2.07884295
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TS₃₋₂



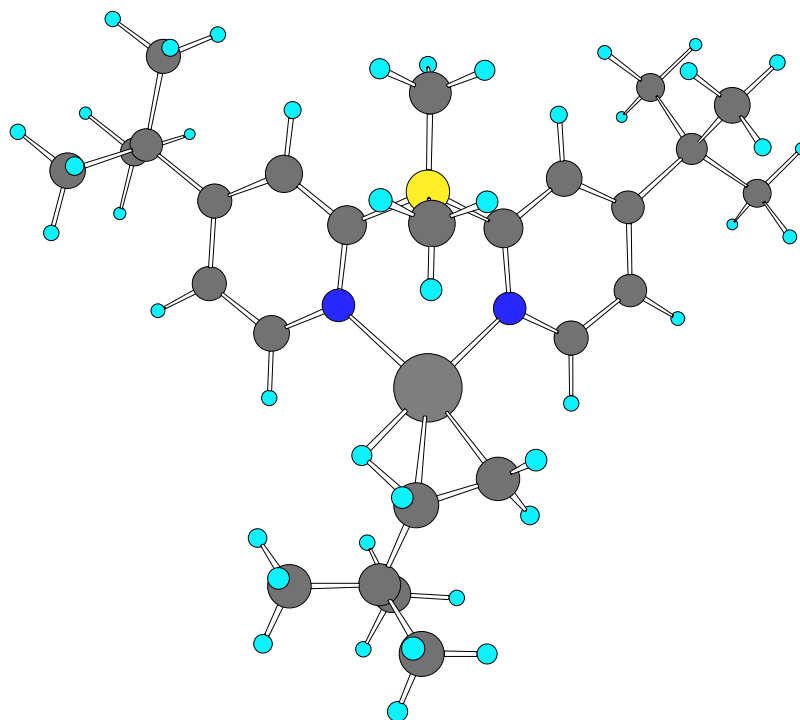
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C 2.14302960 -1.55543977 0.51565861
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C 1.67890903 -3.72658454 -1.20246278
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Pt -0.48234978 -0.17673209 -0.05693747
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H 3.26098423 5.57713228 0.99112441
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I



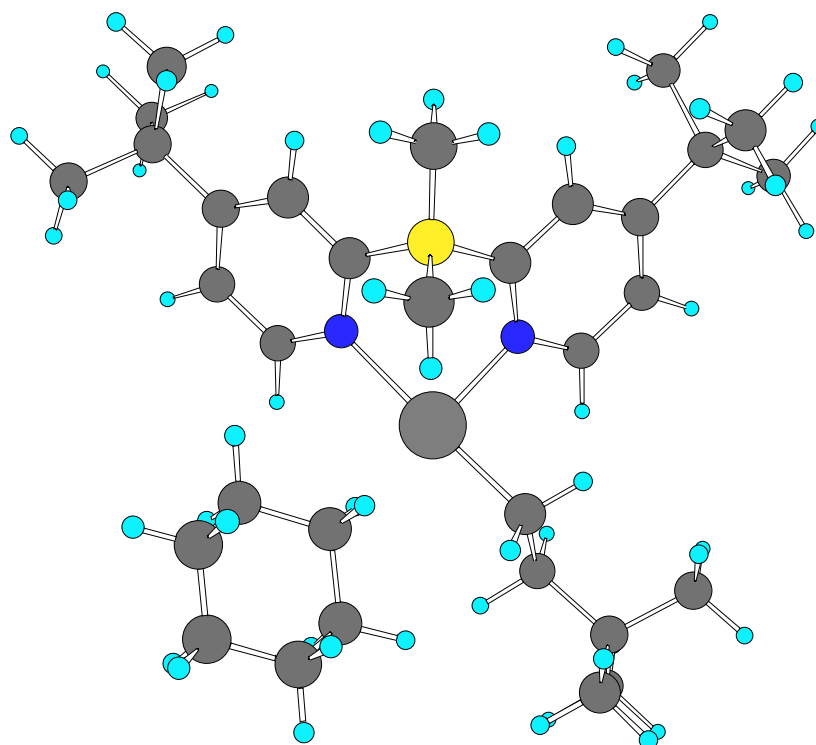
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H -0.38292038 1.63913913 2.65542755
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II



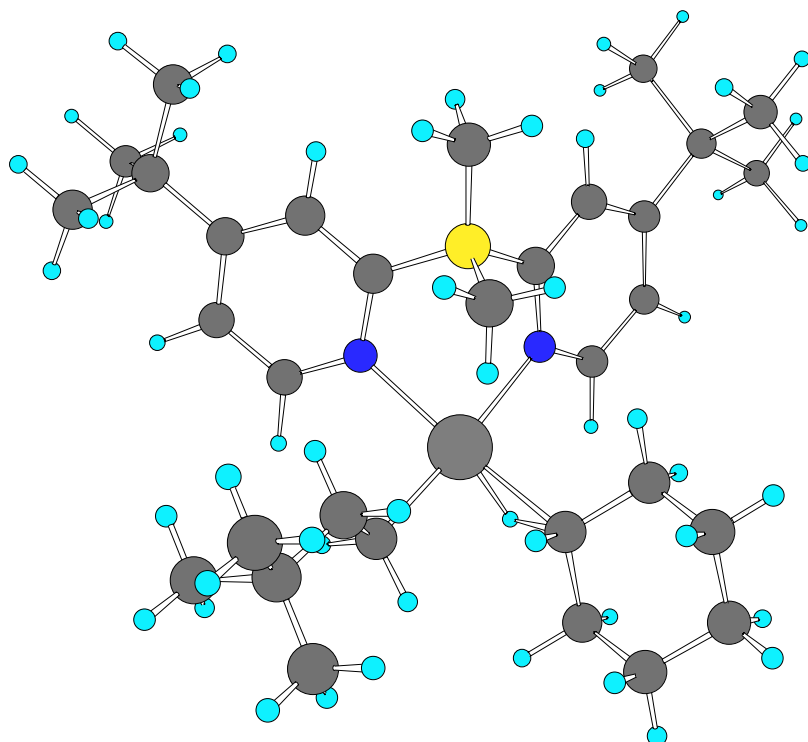
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TS₃₋₄



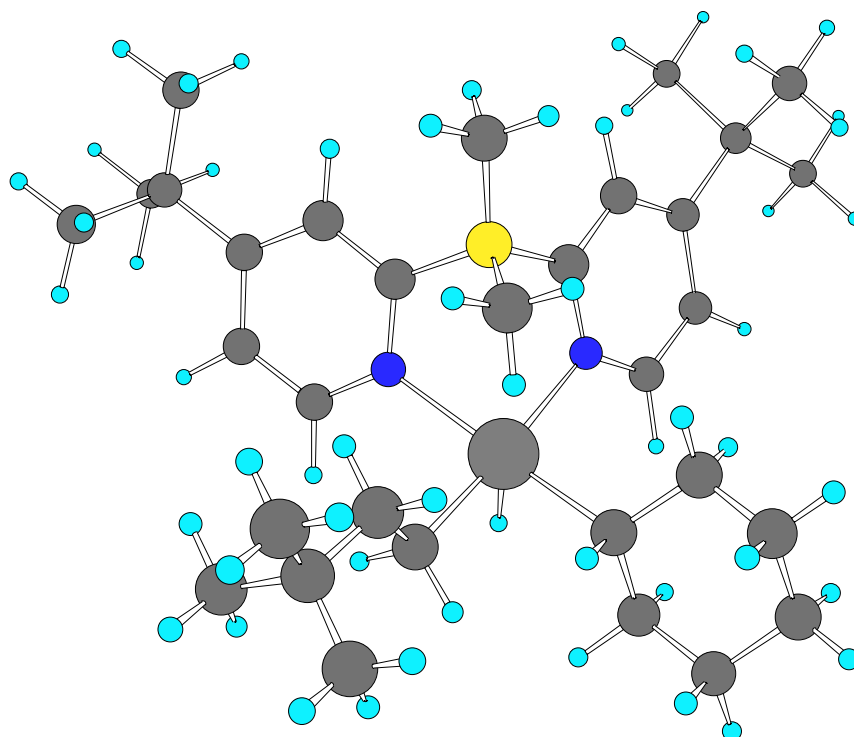
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Pt -0.03500487 -0.88232563 -0.27676992
C 2.15072922 -0.61430322 -0.05046437
C -0.13205429 -0.85197654 1.81561740
C 3.08852001 -1.66406265 0.59013710
H 2.01739677 0.20078150 0.67946251
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H 3.22612519 -2.51707986 -0.09975262
H 4.58999686 0.93515905 -1.98097575
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H 5.12630162 -1.80562689 1.33766157
H 4.34367302 -0.24900739 1.64860939
H 6.06425957 0.02538866 -0.13482428
H 5.32174266 -1.26825884 -1.08521521
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C -1.06541601 2.10481758 4.23778928
C -1.83627794 -0.27539464 4.41123445
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C -6.87804942 0.99434974 -1.62439930
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H 0.55560390 -2.06045782 -8.52257296
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III



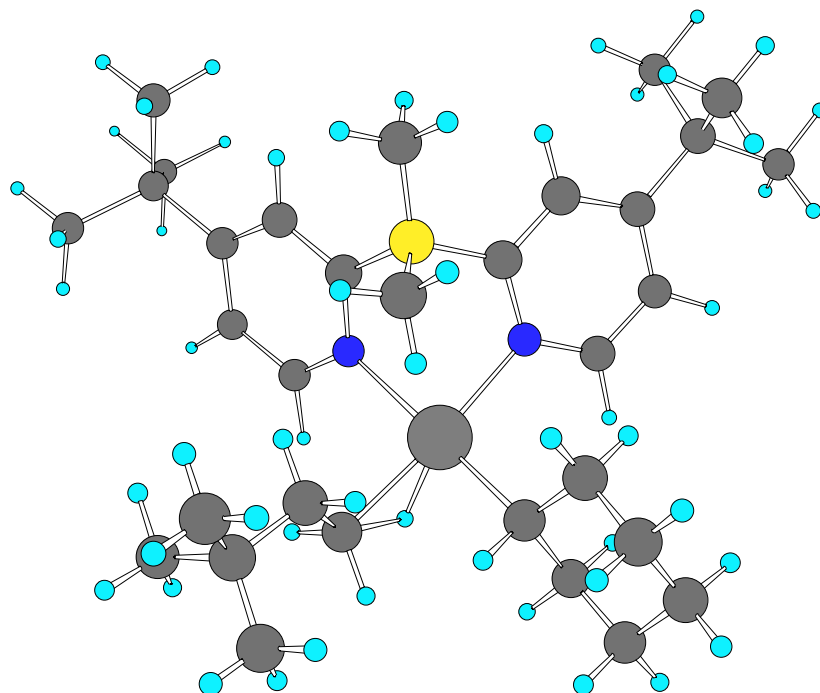
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H -2.51606923 -1.94685966 -1.38557156
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C -2.41052222 1.32206967 -3.34058039
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C 2.96405005 0.43587430 -4.37752121
C -1.37400962 0.98529686 -2.44533436
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N 1.45372628 -0.18748329 -2.08706924
B -0.03975791 1.90295033 -2.18683696
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C 2.81870640 0.99732333 -6.82442070
C 4.51150104 2.16055382 -5.35150955
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H 5.20353736 2.06605012 -4.50166266
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TS₃₋₅



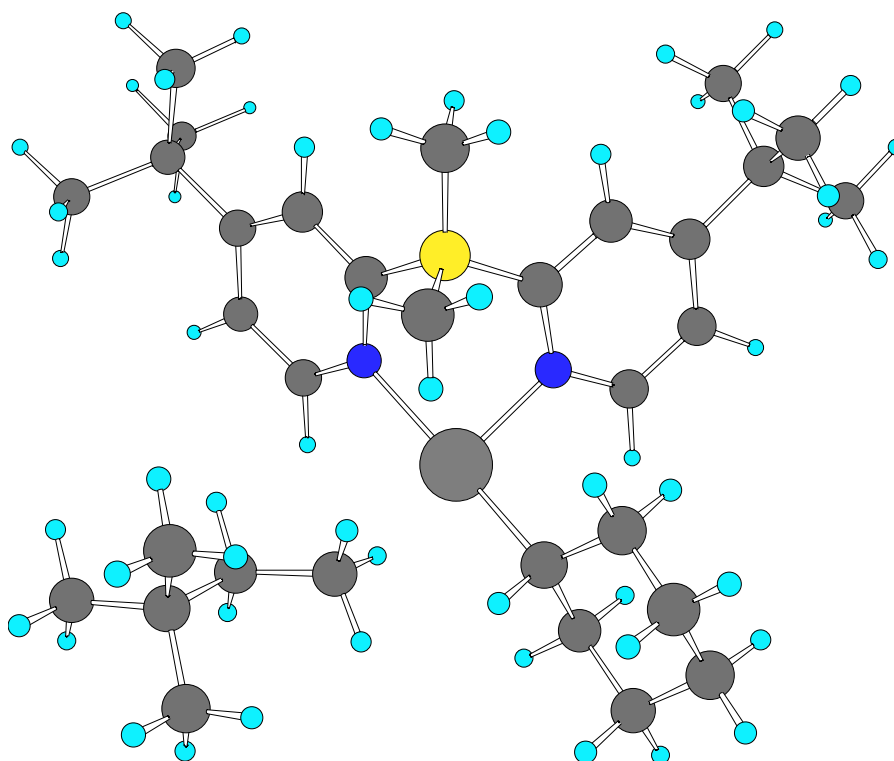
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C 2.81910029 0.64588197 -1.09099981
C 5.16149332 -0.04099776 -0.67271341
C 0.85082088 0.64340183 -2.80183234
H 1.17394535 1.80103833 -4.57010548
N 2.39194011 -0.41523582 -0.33326745
B 1.73034602 1.63339689 -1.82132288
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C 3.28550131 -1.27686918 0.20515107
H 4.53542860 1.67728869 -1.82394389
C 6.66496490 0.21416522 -0.86706634
H 5.31055499 -1.86954495 0.52067649
H 2.86886495 -2.10729460 0.77403095
C 0.77629860 2.35114292 -0.67896821

C 2.47612639 2.81078219 -2.68376550
Pt 0.33688956 -0.81871197 -0.14444530
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C -1.86650018 -1.03894947 -0.04902314
C 0.56303123 -2.45457072 2.47749887
H -0.68299683 -0.73237432 2.24172376
C 1.28672423 -0.03411447 2.68137784
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H -2.22789026 -1.58095829 0.83888143
H -2.29492603 -1.52164694 -0.94112872
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H -0.03584615 2.93523931 -1.14447509
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H 3.09107045 3.45332991 -2.02931915
C 1.11788377 -0.11414795 4.21338853
H 2.34069042 -0.25244145 2.43971196
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H 2.39633009 -1.83223995 4.53778709
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H -4.38272513 -1.12064278 1.32137194
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H -3.72268133 2.64752878 -0.76600865
H -5.63822418 0.28455156 -1.18472188
H -4.12744145 0.47728603 -2.10443115
H -4.46814892 -1.04554450 -1.24451926
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C 0.45857620 -0.83775810 -7.35793096
C -1.67620072 0.42757261 -6.88149274
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H -2.21066917 -0.50111984 -6.63567972
H -2.14783449 1.24870841 -6.32173663
C 7.53152775 -0.85242986 -0.17039401
C 6.99103618 0.20154929 -2.38093823
C 7.02107947 1.60075353 -0.27623622
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IV



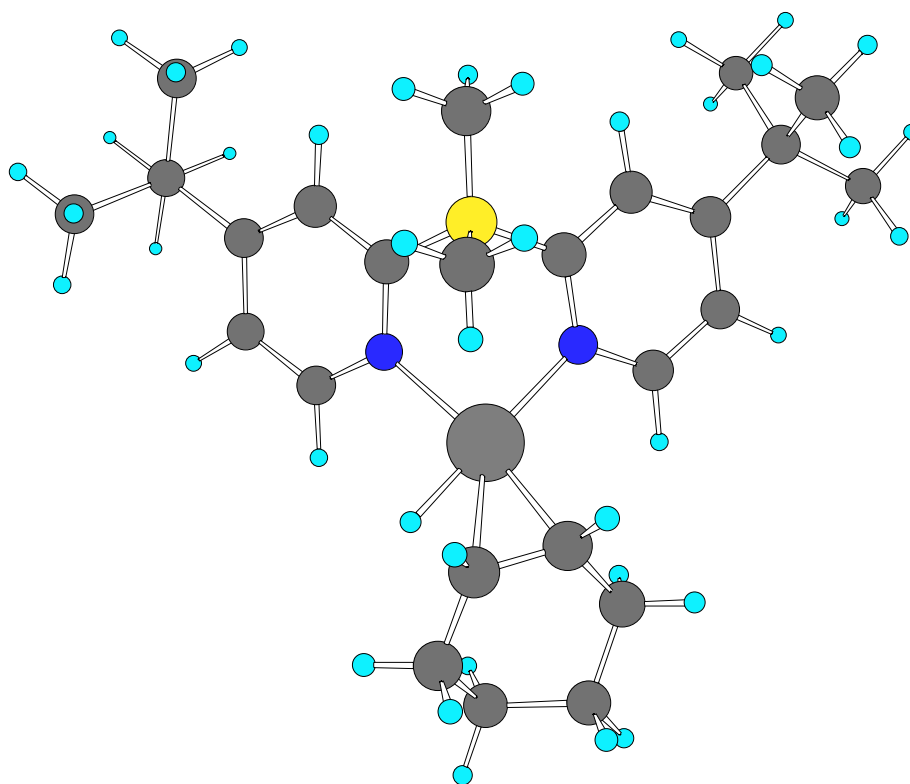
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H 2.62858686 -0.75139991 2.50692933
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V



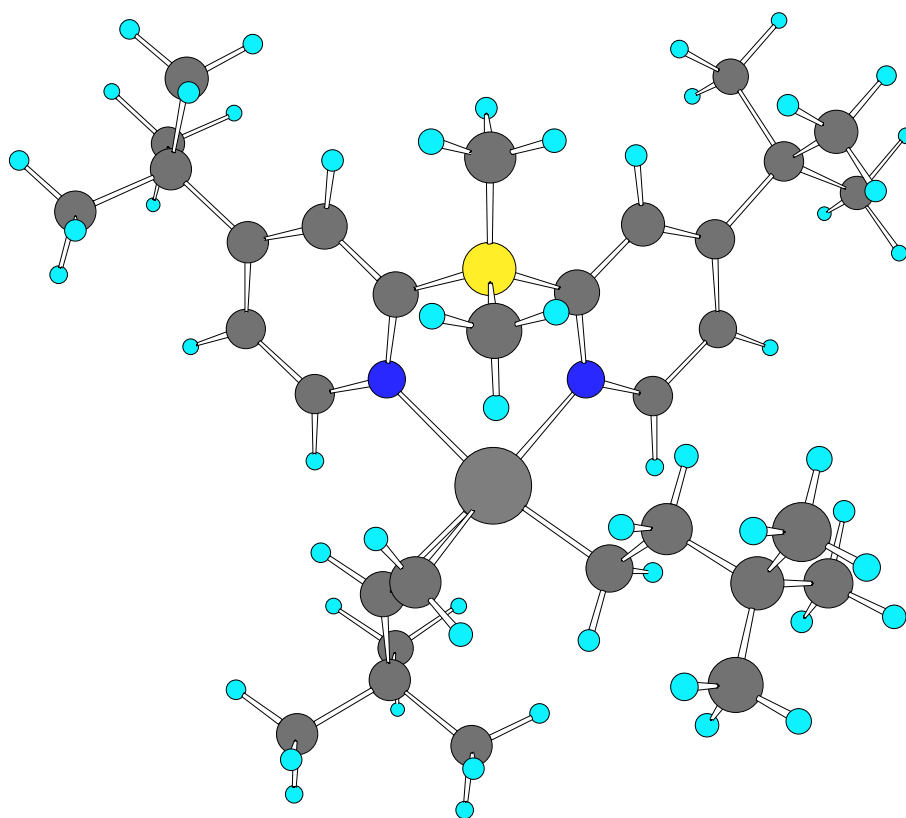
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