Electronic Supplementary Material (ESI) for Chemical Communications

Room Temperature Reversible C–H Activation Mediated by a Pt(0) center, and Stoichiometric Biphenyl Formation via Solvent Activation

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1 Experimental Details

1.1 Generalities

All reactions were routinely performed under an inert atmosphere of argon or nitrogen using Schlenk and glovebox techniques and dry deoxygenated solvents. Solvents were purified with an MBraun Solvent Purifying System SPS 800. Nuclear magnetic resonance spectra were recorded on a Bruker AC-300 SY spectrometer operating at 300.13 MHz for ^{1}H, 75.5 MHz for ^{13}C and 121.5 MHz for ^{31}P. Solvent peaks were used as an internal reference relative to Me_4Si for ^{1}H and ^{13}C chemical shifts (ppm); ^{31}P chemical shifts are relative to an 85% H_3PO_4 external reference. Coupling constants are given in Hertz. The following abbreviations are used: s, singlet; d, doublet; t, triplet; m, multiplet. Unless otherwise specified, all reagents and chemicals were obtained commercially and used as received. $CODPtCl_2$[1], $CODPtI_2$[2], and the diphosphine DCPP[3] (1,3-bis(dicyclohexylphosphino)propane) were synthesized according to previously published procedures.

1.2 1_{Cl}: Bis[dicyclohexylphosphino]propane Platinum (II) Chloride ($dcppPtCl_2$)

18.65 mL of a 0.24M solution of DCPP (44.7 mmol, 1 eq.) in petroleum ether were evaporated, then dissolved in 30mL of dichloromethane. 1.675g of $(COD)PtCl_2$ (44.7 mmol, 1 eq.) were then added and stirred for 30 minutes. The solution was then evaporated, and the remaining solid washed with petroleum ether to remove all remaining cyclooctadiene. 2.66 g of a white solid were then collected.

Yield: 85%

$^{31}P\{^{1}H\}$ NMR (121.5 MHz, CD_2Cl_2): δ = 7.92 ($J_{Pt\text{-}P}$= 3460 Hz) ppm

Found C: 46.24%, H: 7.16%. $C_{27}H_{50}Cl_2P_2Pt$ requires C: 46.15%, H: 7.17%.

1.3 1_I: 1,3-bis(dicyclohexylphosphino)propane Platinum (II) Iodide ($dcppPtI_2$)

15 mL of a 0.12M solution of DCPP in hexane were evaporated under vacuum, then redissolved in 30mL of dichloromethane. 1g of $(COD)PtI_2$ were then added, the solution became yellow after about half an hour. The solution was then evaporated under vacuum, and the remaining solid was washed three times with hexane and centrifugation. The remaining solid was redissolved in dichloromethane and evaporated, then dried under vacuum. 880 mg of a light orange solid were collected.

Yield: 56%

^{1}H (300 MHz, CD_2Cl_2) : δ = 1.07-2.07 (44H, br, all cyclohexyls) 2.52 (4H, P-C**H$_2$**), 2.84 (2H, $PCH_2C\mathbf{H_2}CH_2P$) ppm
^{13}C (75.5 MHz, CD_2Cl_2) : δ = 27.29 – 30.47 (m, All cyclohexyls), 31.95 (t, ^{2}J(P-C) = 15.1 Hz, $PCH_2\mathbf{C}H_2CH_2P$), 40.63 (d, ^{1}J(P-C) = 35.7 Hz, P-**C**H_2) ppm
$^{31}P\{^{1}H\}$ NMR (121.5 MHz, CD_2Cl_2): δ = 11.73 ($J_{Pt\text{-}P}$=3317 Hz) ppm

1.4 Potassium graphite (KC_8)

5 g (0.13 mol, 1 eq.) of potassium were weighed in a shlenk flask with 12.3 g (1.0 mol, 8 eq.) of graphite powder. The flask was put under static vacuum, and then heated under vigorous stirring to

120°C for two hours. Upon melting of the potassium, it gradually incorporated into the graphite powder, yielding quantitatively 17.3 g of an highly air sensitive bronze powder.

1.5 3_H: Bis[dicyclohexylphosphino]propane Platinum (II) Hydrido Meta Toluene

200 mg of dcppPtCl$_2$ (284 µmol, 1 eq.) were dissolved in 5 mL of toluene. 76.8 mg of potassium graphite (568 µmol, 2 eq.) were then added. After 48h, the solution is centrifugated to remove the salts and graphite, the solid residue are washed with small amounts of Toluene until the washings are colorless. After mixing of the washings, a pure solution of the title compound in toluene was obtained.

^{1}H (300 MHz, Tol-D^8) : δ = 8.16-6.64 (m, All aromatic Protons), 2.65 – 0.62 (m, All aliphatic H), -1.53 (dd, J(P_{trans}-H)=179.3 Hz, J(P_{cis}-H)=21.2 Hz, J(Pt-H)= 579 Hz, 1H) ppm
^{13}C (75.5 MHz, Tol-D^8) : δ = 130.7 – 125.5 (m, all aromatic C), 31.0-22.3 (m, all aliphatic C) ppm
^{31}P{^{1}H} NMR (121.5 MHz, Tol-D^8): δ = 16.3 (d, J(P-P) = 20 Hz, J(Pt-P) = 1785 Hz), 4.0 (d, J(P-P) = 20 Hz, J(Pt-P) = 1800 Hz) ppm

1.6 4_H: Bis[dicyclohexylphosphino]propane Platinum (II) Hydrido Benzene

50 mg of dcppPtCl$_2$ (71 µmol, 1 eq.) were dissolved in 2 mL of benzene. 20 mg of potassium graphite (142 µmol, 2 eq.) were then added. The solution starts to darken within a few hours. After 48h, the solution is centrifugated to remove the salts and graphite. The liquid phase is collected, and the remaining solid is washed with portions of 2 mL of benzene until the washings are colorless. All liquid portions are united, then evaporated to dryness, a dark brown solid is collected.

^{1}H (300 MHz, C_6D_6) : δ = 7.96 (m, J_{H-Pt}=59 Hz, 2H) 7.36 (m, 2H) 7.06 (1H), 2.65 – 0.62 (m, All aliphatic H), -1.59 (dd, $J_{P(trans)-H}$=178.8 Hz, $J_{P(cis)-H}$=21.0 Hz, J_{H-Pt}= 1152 Hz, 1H) ppm
^{13}C (75.5 MHz, C_6D_6) : δ = 130.7 – 125.5 (m, all aromatic C), 31.0-22.3 (m, all aliphatic C) ppm
^{31}P{^{1}H} NMR (121.5 MHz, C_6D_6): δ = 16.18 (d, J_{P-P} = 20 Hz, J_{Pt-P} = 1794 Hz, P trans to C) , 3.75 (d, J_{P-P} = 20 Hz, J_{Pt-P} = 1808 Hz, P trans to H) ppm

1.7 4_D: Bis[dicyclohexylphosphino]propane Platinum (II) Deutero Benzene

50 mg of dcppPtCl$_2$ (71 µmol, 1 eq.) were dissolved in 2 mL of Benzene-d^6. 20 mg of potassium graphite (142 µmol, 2 eq.) were then added. After 48h, the solution is centrifugated to remove the salts and graphite. The filtrate is collected, and the remaining solid is washed with portions of 2 mL of benzene-d^6 until the washings are colorless. All liquid portions are united, then evaporated to dryness, a dark brown solid is collected.

^{1}H (300 MHz, C_6D_6) : 2.65 – 0.62 (m, All aliphatic H) ppm
^{13}C (75.5 MHz, C_6D_6) : δ = 130.7 – 125.5 (m, all aromatic C), 31.0-22.3 (m, all aliphatic C) ppm
^{31}P{^{1}H} NMR (121.5 MHz, C_6D_6): δ = 16.92 (d, J_{P-P} = 20 Hz, J_{Pt-P} = 1791 Hz, P trans to C) , 4.59 (m, J_{P-P} = 20 Hz, J_{Pt-P} = 1784 Hz, J_{P-D} = 27 Hz, P trans to D) ppm

1.8 5: Bis[dicyclohexylphosphino]propane Platinum (0)-η^2-Diphenylacetylene

To a solution of 71µmol of dcppPt-Benzene in 3mL of Toluene, 12.6 mg of diphenylacetylene (71 µmol, 1 eq.) are added, yielding after few minutes the complex. Evaporation of the volatiles gave the title compound as a yellow powder.

Yield : 91 %

^{1}H (300 MHz, Tol-d^{8}) : δ = 7.7 – 6.9 (all aromatic H), 2.3 – 1.0 (broad, all aliphatic H) ppm
^{13}C (75.5 MHz, Tol-d^{8}) : δ = 133-123 (all aromatic CH) 90.4 (C≡C) 39 – 27 (m, all aliphatic carbons) ppm
^{31}P{^{1}H} NMR (121.5 MHz, Tol-d^{8}): δ = 16.93 ($^{1}J_{P\text{-}Pt}$ = 3133 Hz) ppm

1.9 6: [(DCPP)Pt(H)]$_2$

A solution of **3$_H$** was heated for two hours at 80°C in an NMR tube. The formation of **6** was subsequently observed by NMR, and the analysis of the reaction mixture by GC-MS confirmed the formation of the various isomers of dimethylbiphenyl.

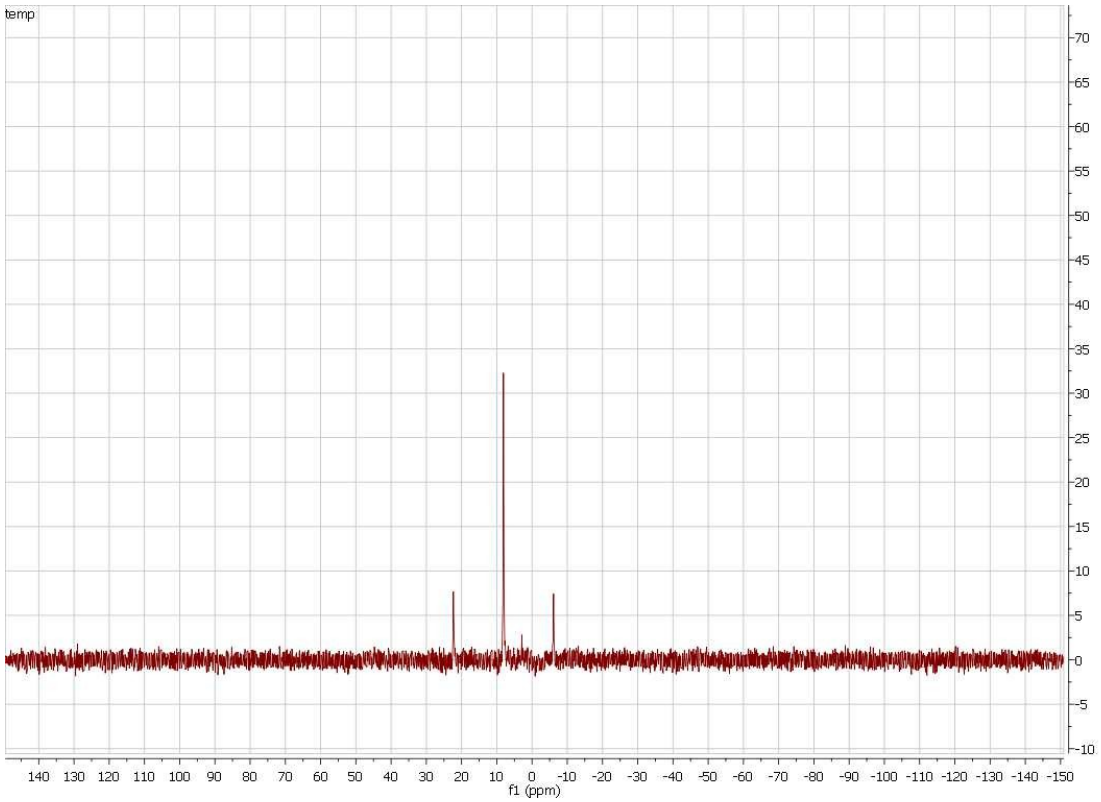
The corresponding complex crystallized spontaneously from the reaction mixture. The NMR spectrum was consistent with the X-Ray structure, since the hydrides, although unsymmetrical in the solid state, can readily exchange at room temperature in solution, making the P atoms magnetically equivalent.

^{31}P{^{1}H} NMR (121.5 MHz, Tol): δ = 37.5 ($^{1}J_{P\text{-}Pt}$ = 2510 Hz, $^{2}J_{P\text{-}Pt}$ = 415 Hz) ppm

2 NMR Spectra

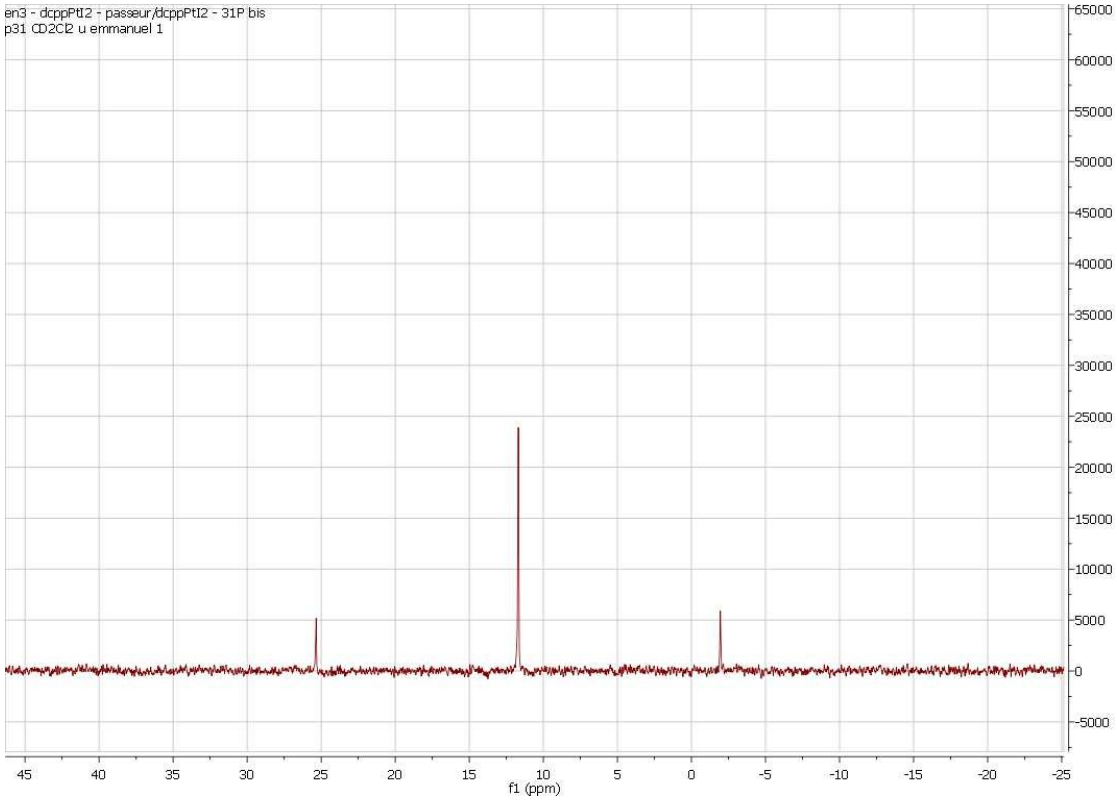
2.1 1_{Cl}: DCPPPtCl$_2$

2.1.1 $^{31}P\{1H\}$

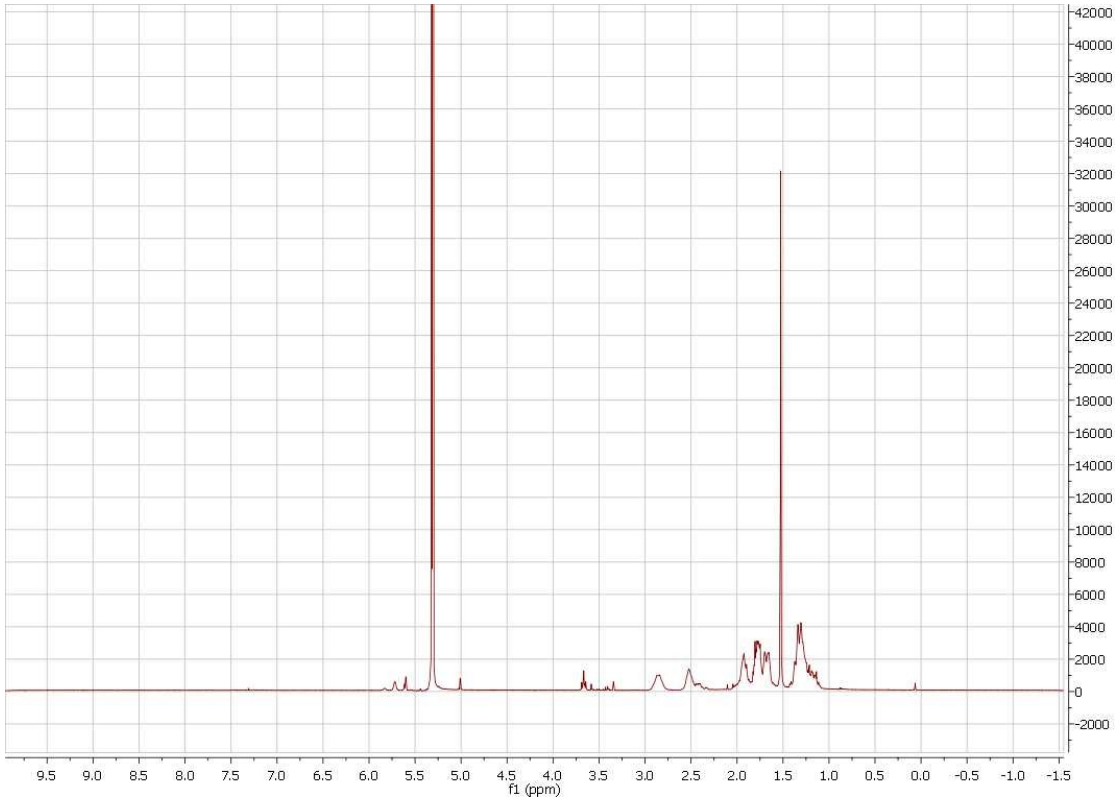


2.2 1_I: DCPPPtI$_2$

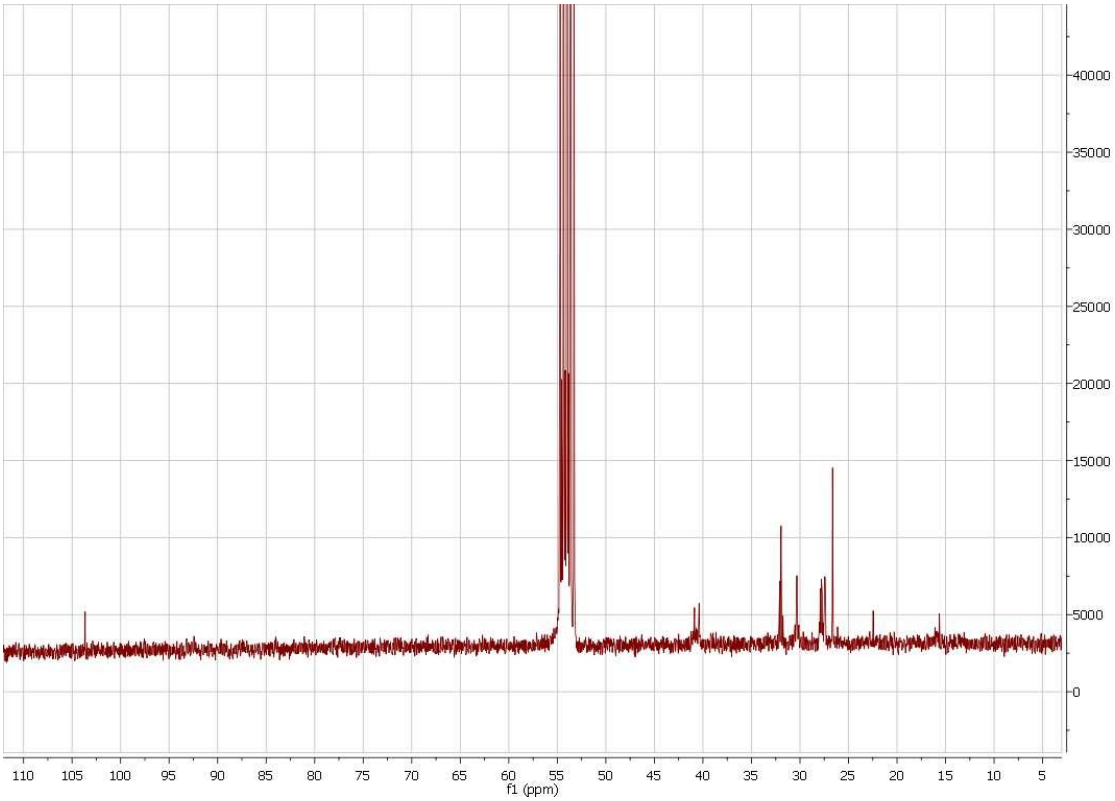
2.2.1 $^{31}P\{^1H\}$



2.2.2 ^1H

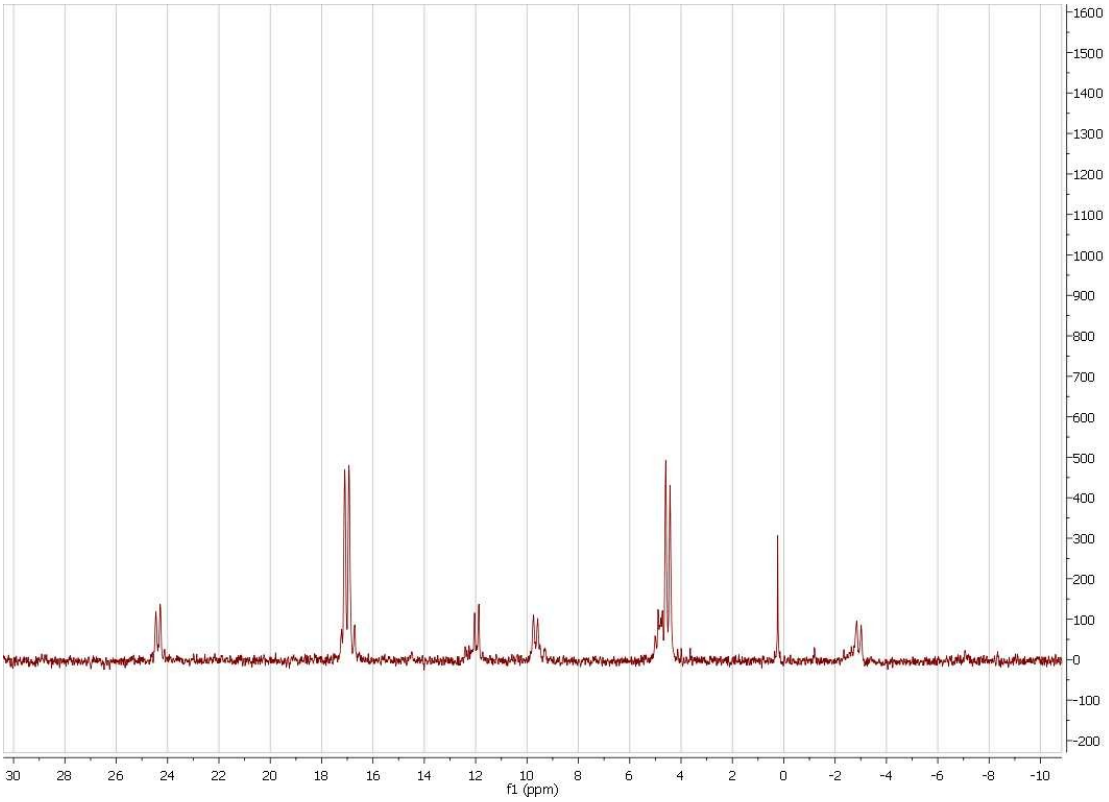


2.2.3 ^{13}C

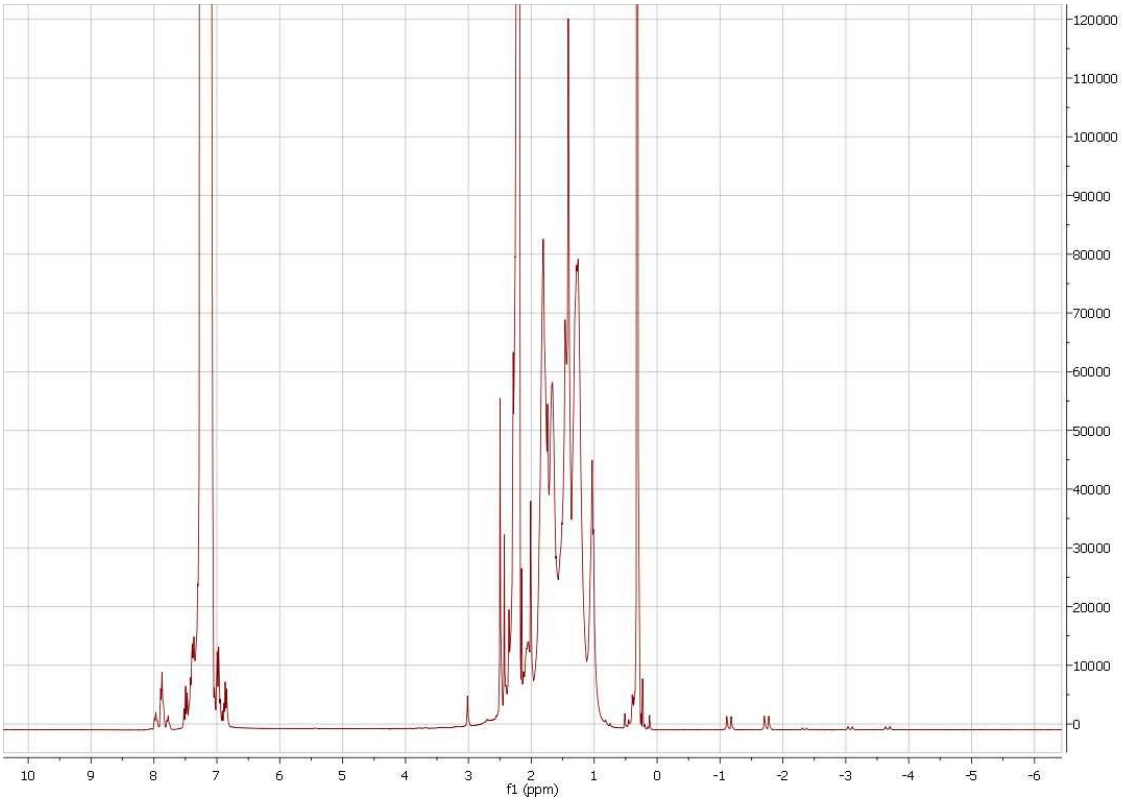


2.3 3_H: Bis[dicyclohexylphosphino]propane Platinum (II) Hydrido Meta Toluene

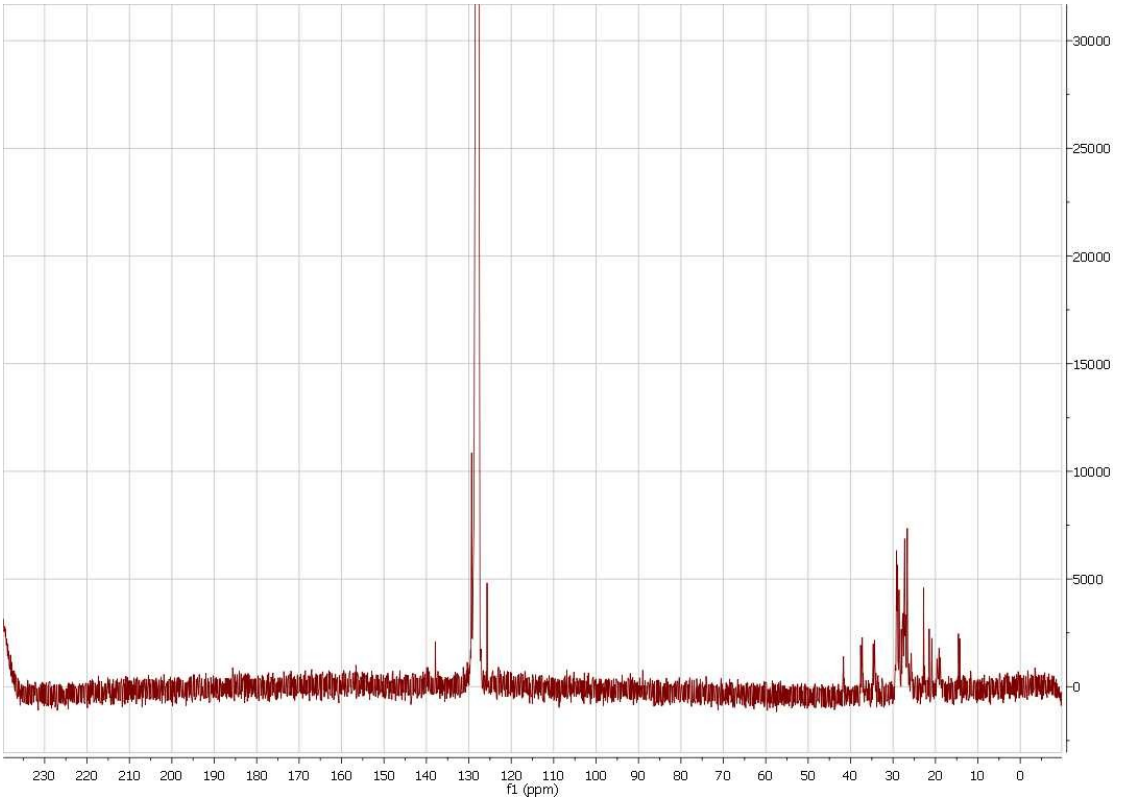
2.3.1 $^{31}P\{1H\}$



2.3.2 ^{1}H

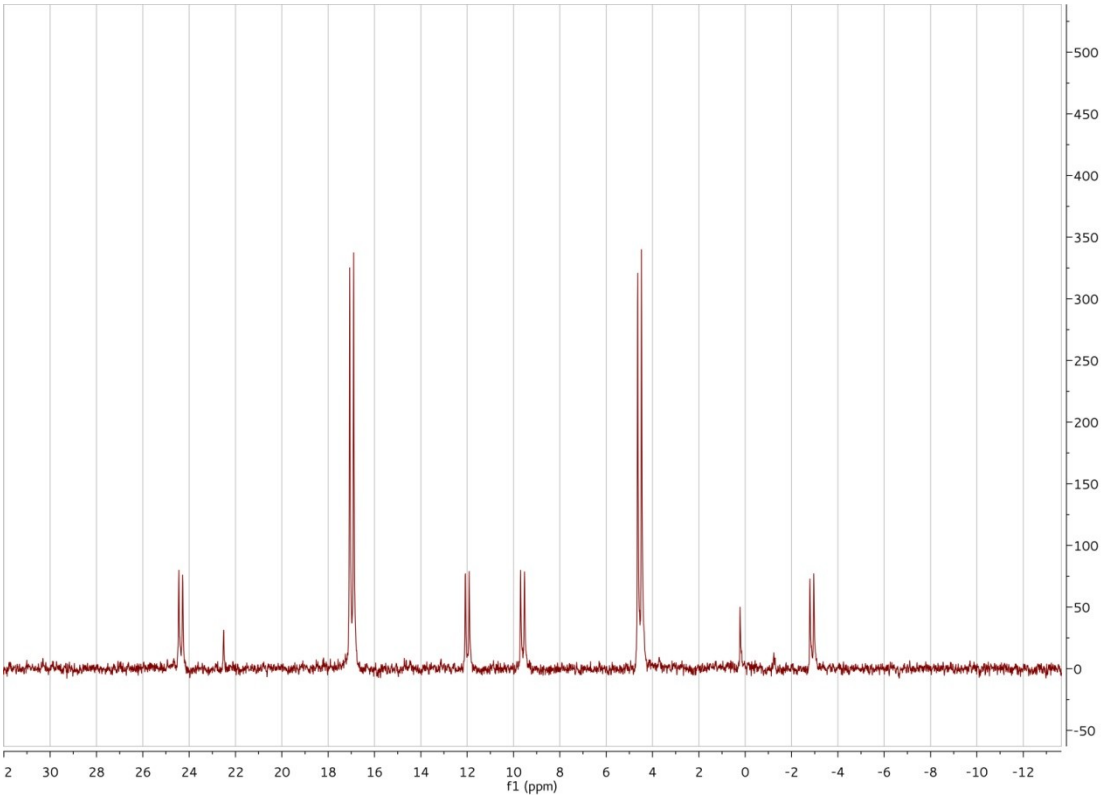


2.3.3 ^{13}C

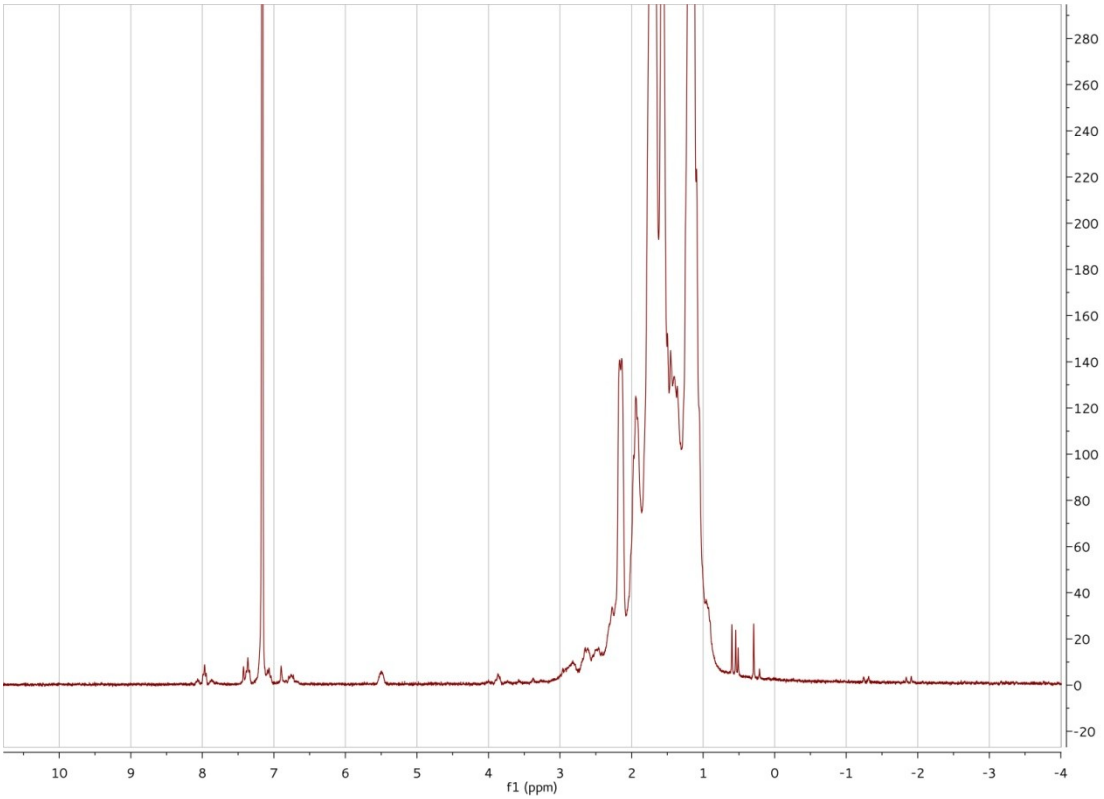


2.4 4_H: Bis[dicyclohexylphosphino]propane Platinum (II) Hydrido Benzene

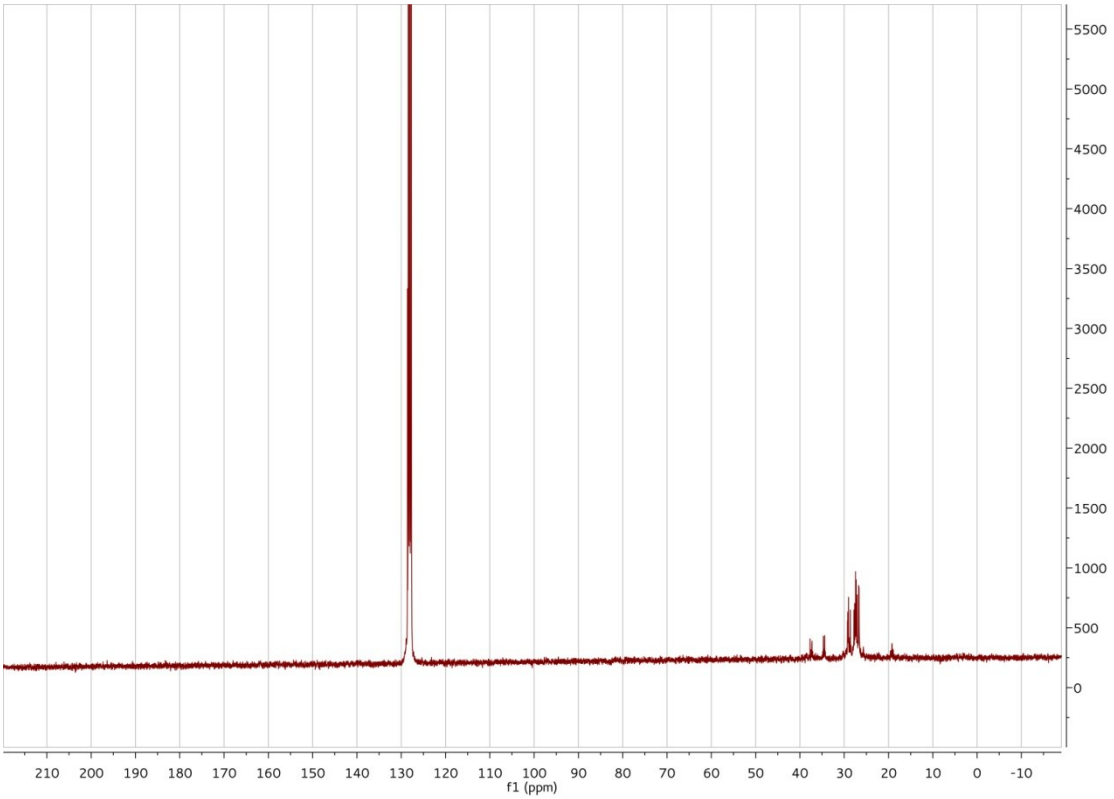
2.4.1 $^{31}P\{1H\}$



2.4.2 ^{1}H

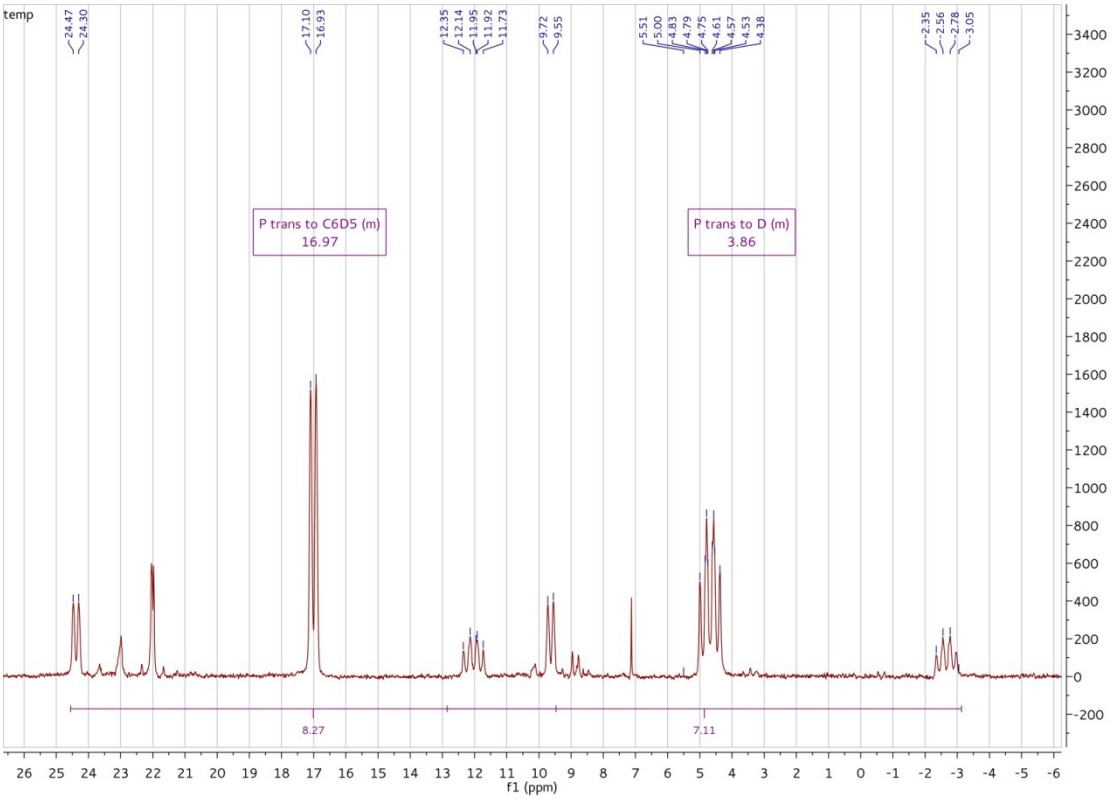


2.4.3 ^{13}C

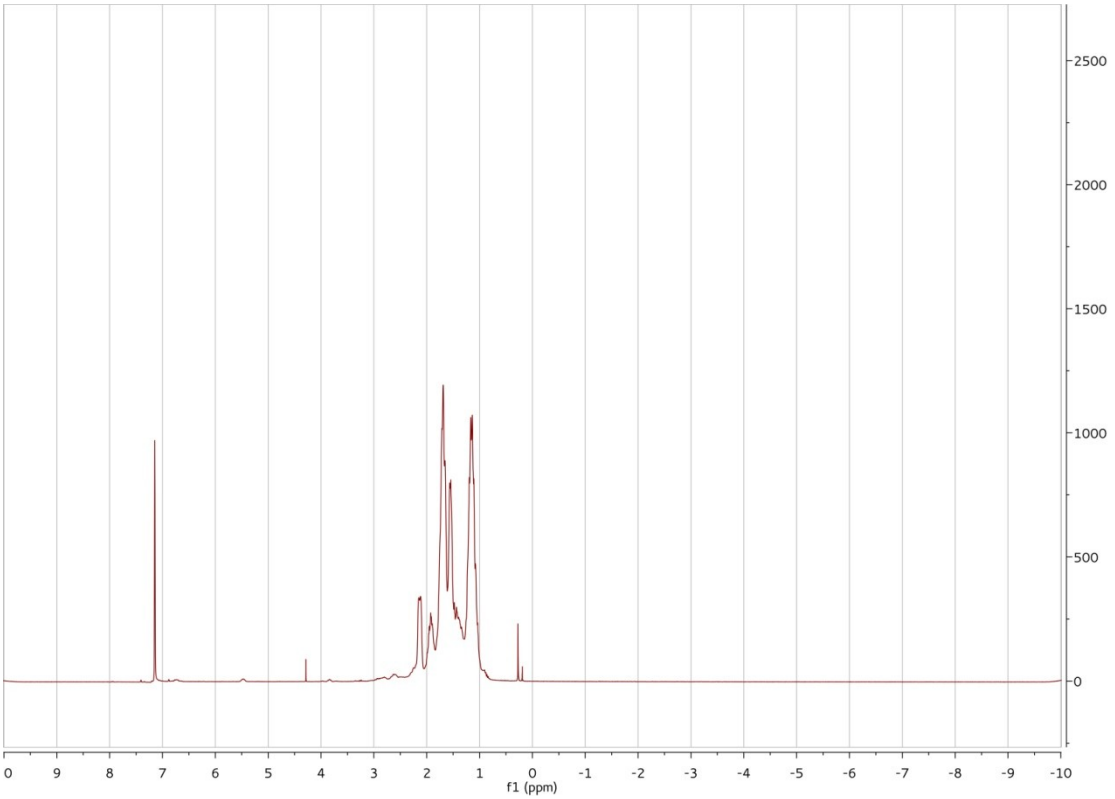


2.5 4_D: Bis[dicyclohexylphosphino]propane Platinum (II) Deutero Benzene

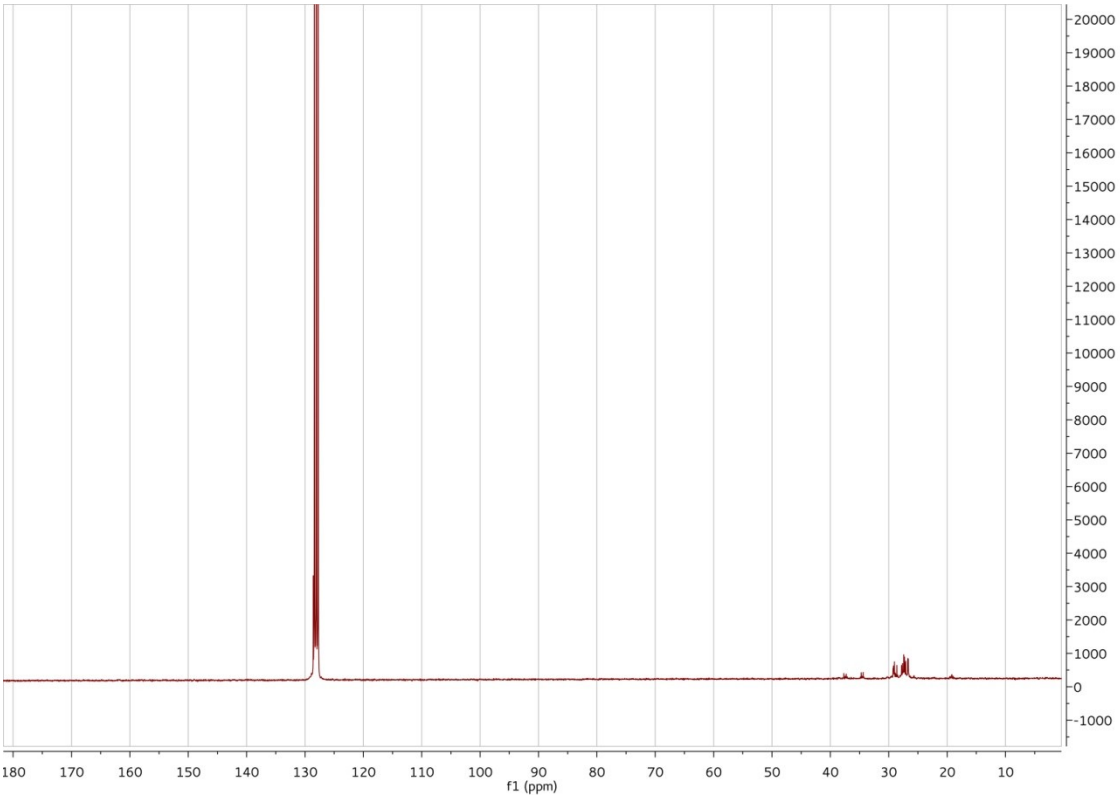
2.5.1 $^{31}P\{1H\}$



2.5.2 ^{1}H

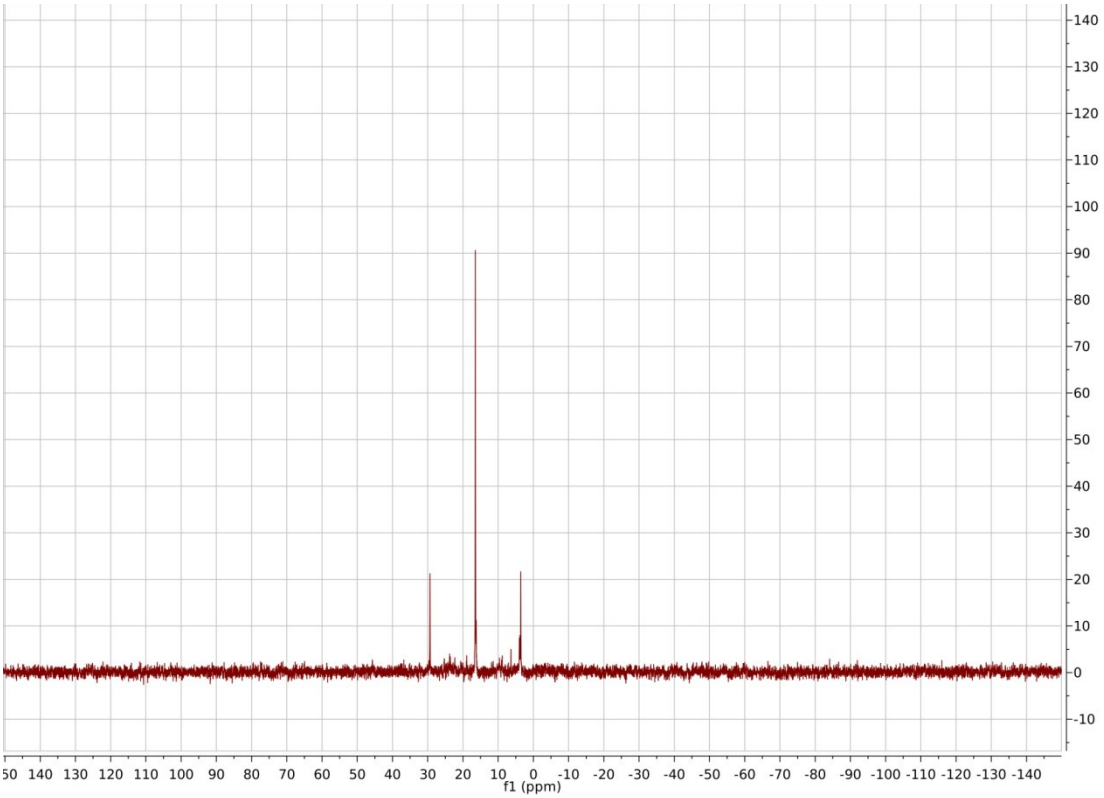


2.5.3 ^{13}C

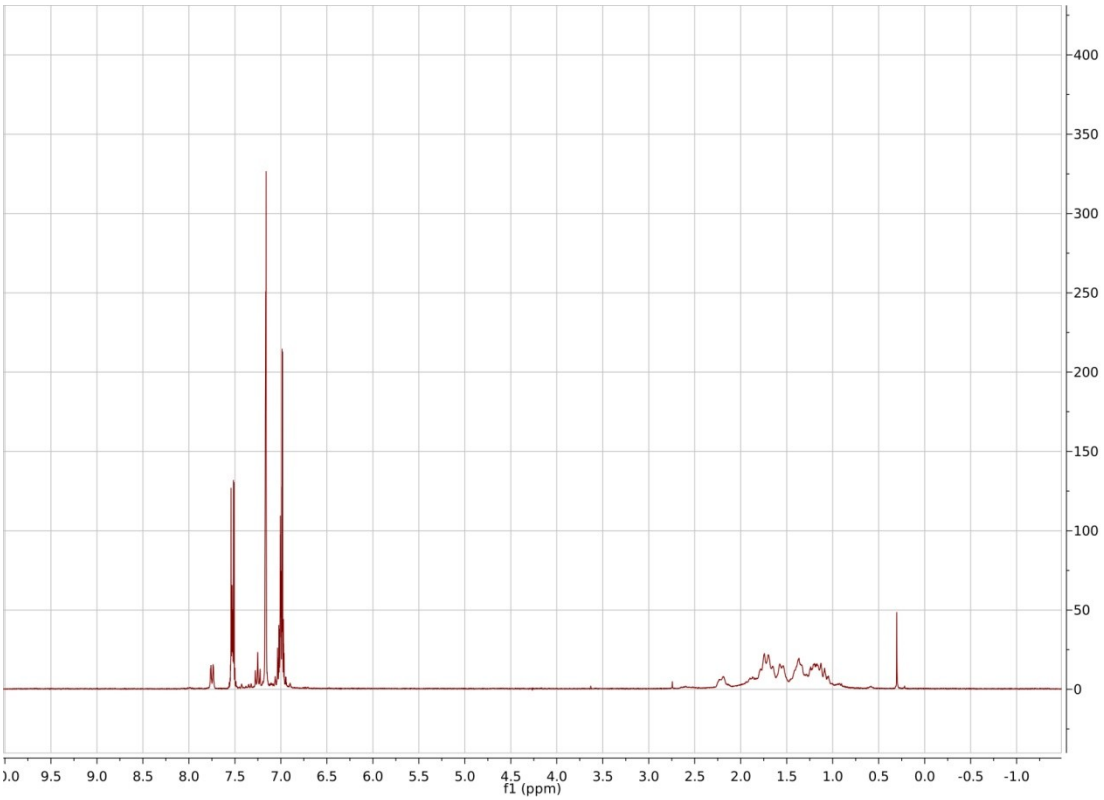


2.6 5: Bis[dicyclohexylphosphino]propane Platinum (0)-η²-Diphenylacetylene

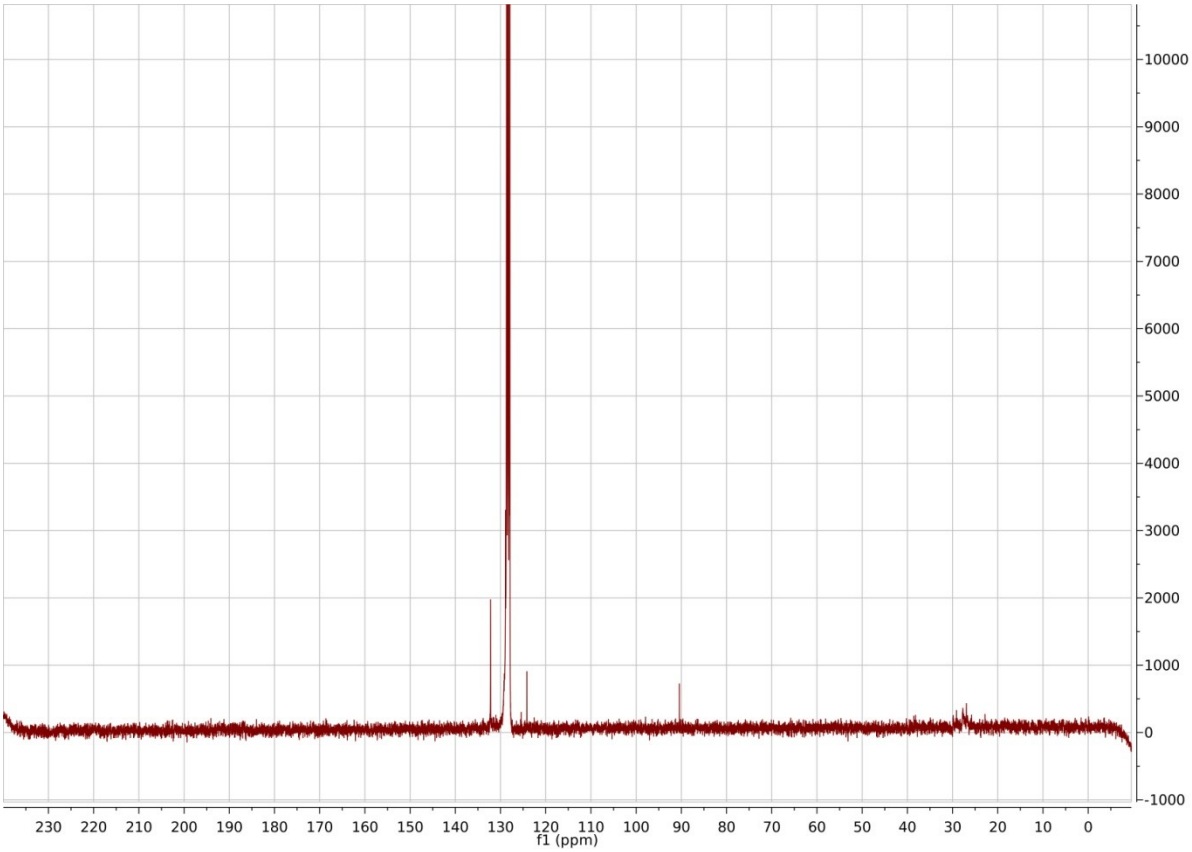
2.6.1 $^{31}P\{1H\}$



2.6.2 ^{1}H

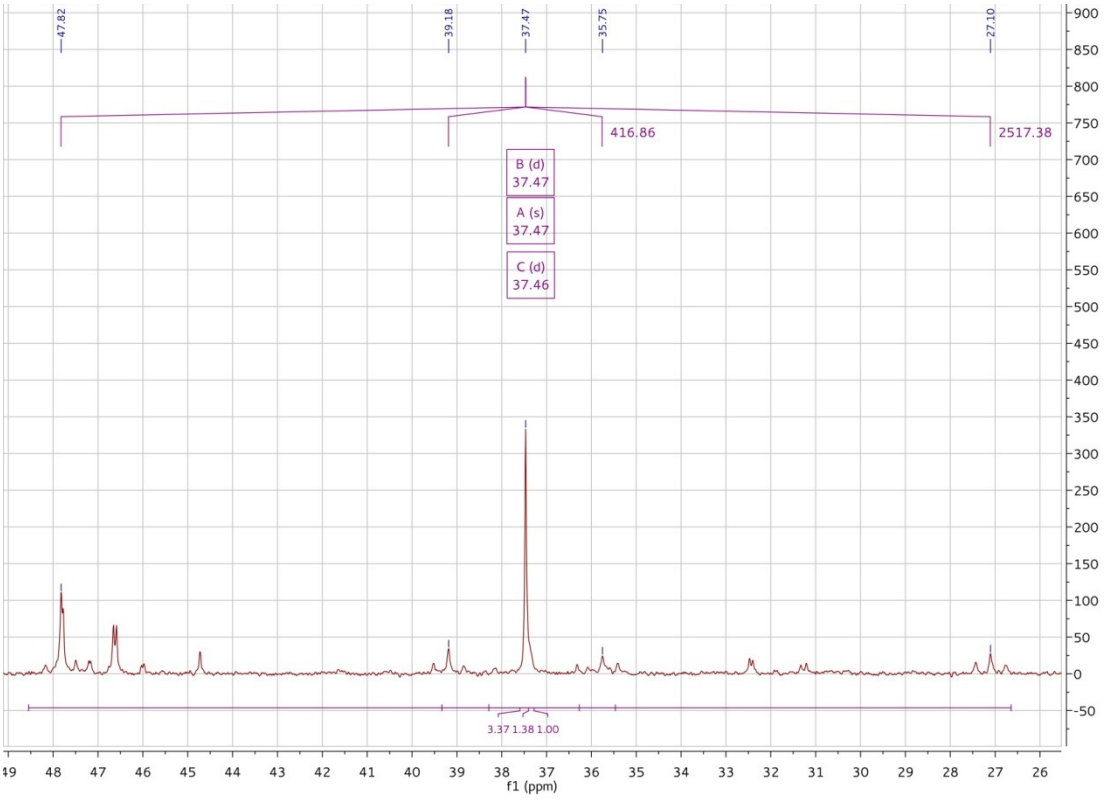


2.6.3 ^{13}C



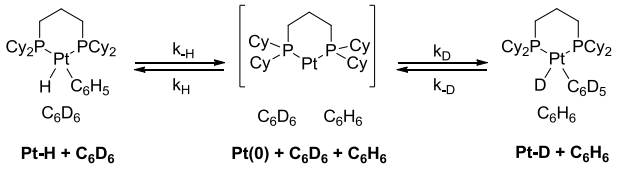
2.7 6: $[(DCPP)Pt(H)]_2$

2.7.1 $^{31}P\{1H\}$



3 Kinetic Study

3.1 Equation Details



Let us consider the system described in the equation *supra*. Since we never observe the formation of Pt(0), we can consider this species as transient, and thus apply to it the steady state approximation:

$$SSA \Rightarrow \frac{d[Pt(0)]}{dt} = 0 = k_{-H}[Pt-H] - k_H[Pt(0)][C_6H_6] + k_{-D}[Pt-D] - k_D[Pt(0)][C_6D_6]$$

$$\Leftrightarrow [Pt(0)] = \frac{k_{-H}[Pt-H] + k_{-D}[Pt-D]}{k_H[C_6H_6] + k_D[C_6D_6]}$$

$$Pt-H \Rightarrow \frac{d[Pt-H]}{dt} = k_H[Pt(0)][C_6H_6] - k_{-H}[Pt-H]$$

$$\Leftrightarrow \frac{d[Pt-H]}{dt} = k_H[C_6H_6]\frac{k_{-H}[Pt-H] + k_{-D}[Pt-D]}{k_H[C_6H_6] + k_D[C_6D_6]} - k_{-H}[Pt-H]$$

$$C_0 = [Pt(0)] + [Pt-H] + [Pt-D] \approx [Pt-H] + [Pt-D]$$

$$\Rightarrow \frac{d[Pt-H]}{dt} = k_H[C_6H_6]\frac{k_{-H}[Pt-H] + k_{-D}(C_0 - [Pt-H])}{k_H[C_6H_6] + k_D[C_6D_6]} - k_{-H}[Pt-H]$$

$$\Leftrightarrow \frac{d[Pt-H]}{dt} + \left(k_{-H} - \frac{k_H(k_{-H} - k_{-D})[C_6H_6]}{k_H[C_6H_6] + k_D[C_6D_6]}\right)[Pt-H] = \frac{k_{-D}k_H C_0[C_6H_6]}{k_H[C_6H_6] + k_D[C_6D_6]}$$

$$Pt-D \Rightarrow \frac{d[Pt-D]}{dt} = k_D[Pt(0)][C_6D_6] - k_{-D}[Pt-D]$$

$$\Leftrightarrow \frac{d[Pt-D]}{dt} = k_D\frac{k_{-H}[Pt-H] + k_{-D}[Pt-D]}{k_H[C_6H_6] + k_D[C_6D_6]}[C_6D_6] - k_{-D}[Pt-D]$$

$$C_0 = [Pt(0)] + [Pt-H] + [Pt-D] \approx [Pt-H] + [Pt-D]$$

$$\Rightarrow \frac{d[Pt-D]}{dt} = k_D\frac{k_{-H}(C_0 - [Pt-D]) + k_{-D}[Pt-D]}{k_H[C_6H_6] + k_D[C_6D_6]}[C_6D_6] - k_{-D}[Pt-D]$$

$$\Leftrightarrow \frac{d[Pt-D]}{dt} + \left(k_{-D} - \frac{k_D(k_{-D} - k_{-H})[C_6D_6]}{k_H[C_6H_6] + k_D[C_6D_6]}\right)[Pt-D] = \frac{k_D k_{-H} C_0[C_6D_6]}{k_H[C_6H_6] + k_D[C_6D_6]}$$

$$\Rightarrow \begin{cases} \frac{d[Pt-H]}{dt} + \left(k_{-H} - \frac{k_H(k_{-H} - k_{-D})[C_6H_6]}{k_H[C_6H_6] + k_D[C_6D_6]}\right)[Pt-H] = \frac{k_{-D}k_H C_0[C_6H_6]}{k_H[C_6H_6] + k_D[C_6D_6]} \\ \frac{d[Pt-D]}{dt} + \left(k_{-D} - \frac{k_D(k_{-D} - k_{-H})[C_6D_6]}{k_H[C_6H_6] + k_D[C_6D_6]}\right)[Pt-D] = \frac{k_{-H}k_D C_0[C_6D_6]}{k_H[C_6H_6] + k_D[C_6D_6]} \end{cases}$$

We thus have a general system of differential equations, which is *a priori* insoluble, since the terms $[C_6D_6]$ and $[C_6H_6]$ are dependent on the variable [Pt-H].

However, simple approximations can lead us to a simpler equation, for example if we consider the study of the disappearance of the [Pt-H] complex in C_6D_6. (The reverse case will lead to a symmetrical solution) In this case, $[C_6D_6]$ can be considered as constant, and we have $[C_6H_6]=[Pt\text{-}D]=C_0-[Pt\text{-}H]$ and $[C_6H_6]<<[C_6D_6]$.

$$\Rightarrow \begin{cases} \dfrac{d[Pt-H]}{dt} + \left(k_{-H} - \dfrac{k_H (C_0 - [Pt-H])(k_{-H} - k_{-D})}{k_H (C_0 - [Pt-H]) + k_D [C_6D_6]} \right)[Pt-H] = \dfrac{k_{-D} k_H C_0 (C_0 - [Pt-H])}{k_H (C_0 - [Pt-H]) + k_D [C_6D_6]} \\ \dfrac{d[Pt-D]}{dt} + \left(k_{-D} - \dfrac{k_D (k_{-D} - k_{-H})[C_6D_6]}{k_H (C_0 - [Pt-H]) + k_D [C_6D_6]} \right)[Pt-D] = \dfrac{k_{-H} k_D C_0 [C_6D_6]}{k_H (C_0 - [Pt-H]) + k_D [C_6D_6]} \end{cases}$$

$$[C_6H_6] = O([Pt-H]) = O(C_0) = o([C_6D_6])$$

$$\Rightarrow \begin{cases} \dfrac{d[Pt-H]}{dt} + \left(k_{-H} - \dfrac{k_H (k_{-H} - k_{-D})(C_0 - [Pt-H])}{k_D [C_6D_6]} \right)[Pt-H] = \dfrac{k_{-D} k_H C_0 (C_0 - [Pt-H])}{k_D [C_6D_6]} \\ \dfrac{d[Pt-D]}{dt} + k_{-H}[Pt-D] = k_{-H} C_0 \end{cases}$$

$$\Leftrightarrow \begin{cases} \dfrac{d[Pt-H]}{dt} + \left(k_{-H} - \dfrac{k_H (k_{-H} - k_{-D})(C_0 - [Pt-H])}{k_D [C_6D_6]} \right)[Pt-H] = \dfrac{k_{-D} k_H C_0 (C_0 - [Pt-H])}{k_D [C_6D_6]} \\ \dfrac{d[Pt-D]}{dt} + k_{-H}[Pt-D] = k_{-H} C_0 \end{cases}$$

$$\Leftrightarrow \begin{cases} \dfrac{d[Pt-H]}{dt} + \left(k_{-H} - \dfrac{k_H (k_{-H} - 2k_{-D}) C_0 - k_H (k_{-H} - k_{-D})[Pt-H]}{k_D [C_6D_6]} \right)[Pt-H] = \dfrac{k_{-D} k_H C_0^2}{k_D [C_6D_6]} \\ \dfrac{d[Pt-D]}{dt} + k_{-H}[Pt-D] = k_{-H} C_0 \end{cases}$$

$$\Leftrightarrow \begin{cases} \dfrac{d[Pt-H]}{dt} + \dfrac{k_H (k_{-H} - k_{-D})}{k_D [C_6D_6]}[Pt-H]^2 + \left(k_{-H} - \dfrac{k_H (k_{-H} - 2k_{-D}) C_0}{k_D [C_6D_6]} \right)[Pt-H] = \dfrac{k_{-D} k_H C_0^2}{k_D [C_6D_6]} \\ \dfrac{d[Pt-D]}{dt} + k_{-H}[Pt-D] = k_{-H} C_0 \end{cases}$$

At this point, we can consider several approximations, thanks to the experimental observations :

- $k_{-H}<<k_H$ and $k_{-D}<<k_D$ since we never observe the Pt(0) species.
- Being in C_6D_6, we can consider that $C_0<<C6D6$.

The equations thus simplify themselves into:

$$\begin{cases} \dfrac{d[Pt-H]}{dt} + \overbrace{\dfrac{k_H (k_{-H} - k_{-D})}{k_D [C_6D_6]}[Pt-H]^2}^{o\left(C_0^2 / [C_6D_6]\right)} + k_{-H} \overbrace{\left(1 - \dfrac{k_H (k_{-H} - 2k_{-D}) C_0}{k_{-H} k_D [C_6D_6]} \right)}^{O(1)}[Pt-H] = \overbrace{\dfrac{k_{-D} k_H C_0^2}{k_D [C_6D_6]}}^{\approx 0} \\ \dfrac{d[Pt-D]}{dt} + k_{-H}[Pt-D] = k_{-H} C_0 \end{cases}$$

$$\begin{cases} \dfrac{d[Pt-H]}{dt} + k_{-H}[Pt-H] = 0 \\ \dfrac{d[Pt-D]}{dt} + k_{-H}[Pt-D] = k_{-H} C_0 \end{cases}$$

This means that the hypothesis of a transient Pt(0) species can be confirmed through a kinetic study, if the rate of disappearance of the Pt-H species in C_6D_6 follows a first order kinetics, with a constant which will be k_{-H}. The reverse study will lead to the k_{-D} constant.

At the equilibrium in a mixture of C_6H_6 and C_6D_6, we have:

$$\begin{cases} \left(k_{-1} - \dfrac{k_H\left(k_{-1} - k_{-2}\right)[C_6H_6]}{k_H[C_6H_6] + k_D[C_6D_6]}\right)[Pt-H] = \dfrac{k_{-2}k_H C_0[C_6H_6]}{k_H[C_6H_6] + k_D[C_6D_6]} \\ \left(k_{-2} - \dfrac{k_D\left(k_{-2} - k_{-1}\right)[C_6D_6]}{k_H[C_6H_6] + k_D[C_6D_6]}\right)[Pt-D] = \dfrac{k_{-1}k_D C_0[C_6D_6]}{k_H[C_6H_6] + k_D[C_6D_6]} \end{cases}$$

$$\Rightarrow \frac{[Pt-H]}{[Pt-D]} = \frac{k_{-2}k_H[C_6H_6]}{k_{-1}k_D[C_6D_6]} \underbrace{\left(\frac{k_{-2}k_H[C_6H_6] + k_D[C_6D_6] - k_D\left(k_{-2} - k_{-1}\right)[C_6D_6]}{k_{-1}k_H[C_6H_6] + k_D[C_6D_6] - k_H\left(k_{-1} - k_{-2}\right)[C_6H_6]}\right)}_{=1}$$

$$\Leftrightarrow \frac{[Pt-H][C_6D_6]}{[Pt-D][C_6H_6]} = \frac{k_{-2}k_H}{k_{-1}k_D} = K_{eq}$$

We can thus retrieve the KIE of the reaction through the kinetics of the disappearance and the equilibrium isotope effect:

$$KIE = K_{eq}\frac{k_{-1}}{k_{-2}}$$

3.2 H/D exchange kinetics experiments

A typical synthesis of dcppPt-Benzene-H[6] was performed, yielding 71 µmol of the complex. The volatile were evaporated, and the solid dissolved in 0.5 mL of C_6D_6, then placed in a J. Young NMR tube. The disappearance of the hydride was monitored with ^{1}H NMR. Integrations were performed using MestReNova 7.3.1.

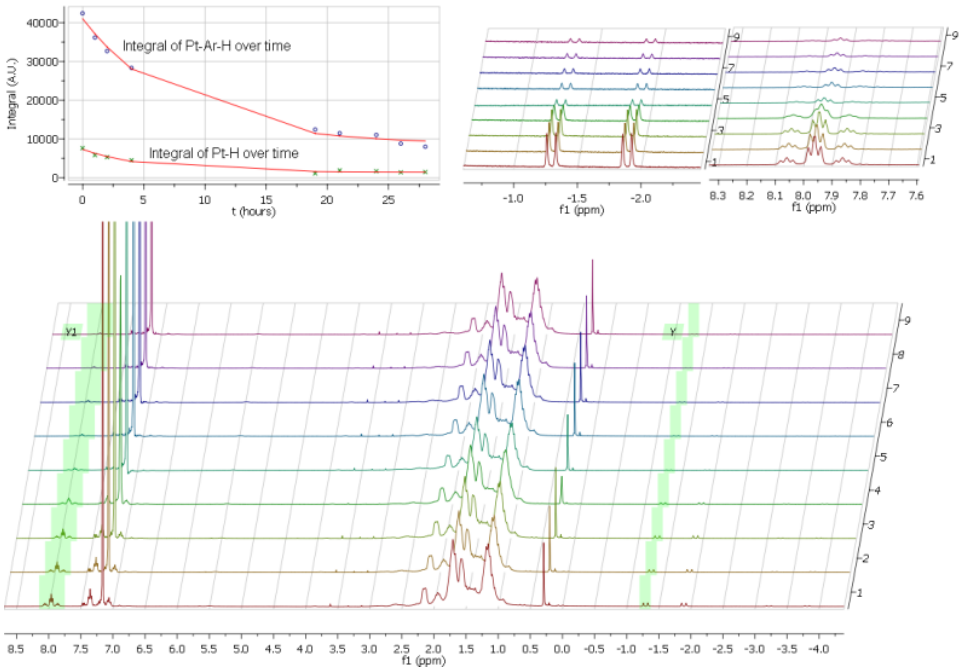


Figure 1: Evolution of Pt-H in C_6D_6

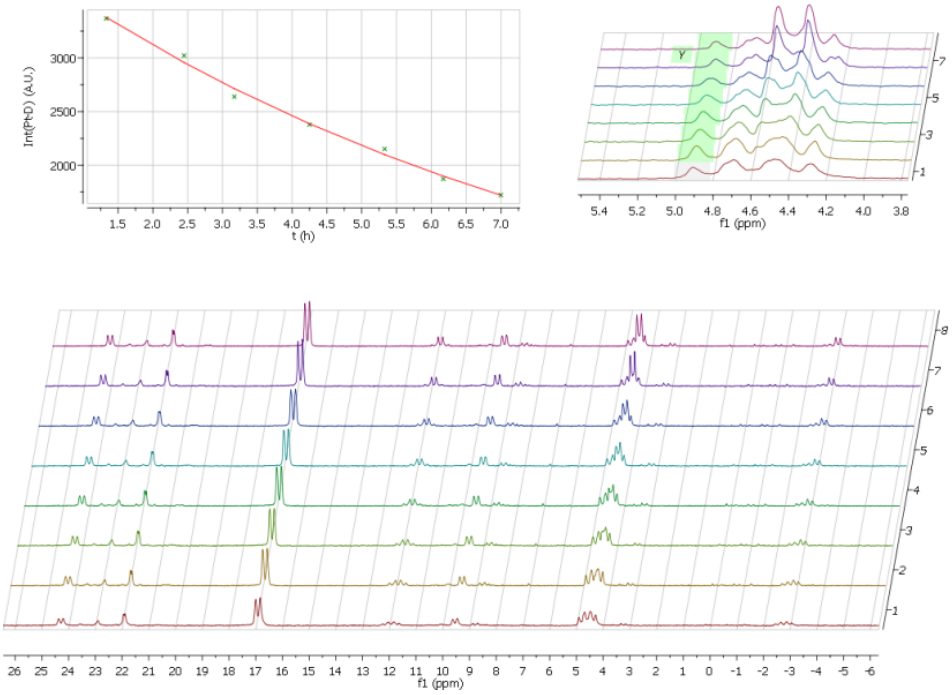


Figure 2: Evolution of Pt-D in C_6H_6

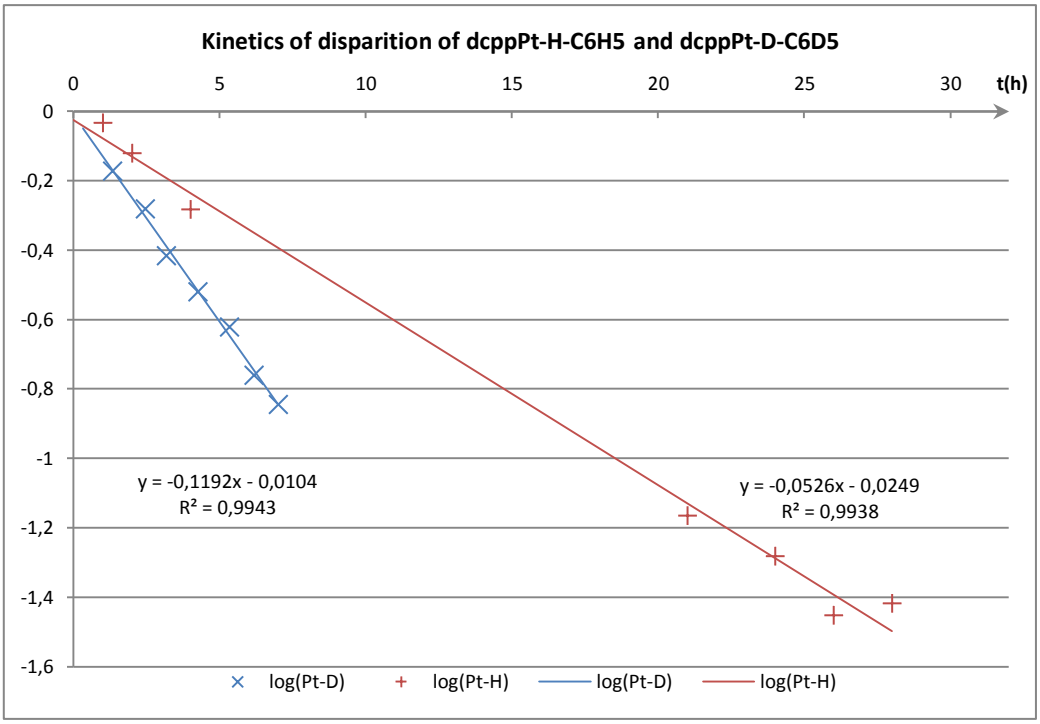


Figure 3: Graph of log(Pt-X/C_0) over time

From these graphs, we can see that we can retrieve the k_{-H} and k_{-D} constants:

k_{-H}= 0.053 L.mol^{-1}.h^{-1}

k_{-D}= 0.12 L.mol^{-1}.h^{-1}

3.3 Equilibrium Isotope Effect determination

A typical reduction of $dcppPtCl_2$ was performed in a mixture of 80% of C_6D_6 and 20% of C_6H_6. After full reduction and at equilibrium, a 31P{1H} NMR was performed. The analysis and integration of the coupling figures around 4 ppm gave the following EIE:

$$K_{EIE} = \frac{k_{-D}k_H}{k_{-H}k_D} = \frac{[Pt-H][C_6D_6]}{[Pt-D][C_6H_6]} = \frac{2.64\times 1.8}{6\times 1.2} = 1.76$$

3.4 Kinetic Isotope Effect determination

From the previous computations, we can deduce the KIE:

$$KIE = K_{eq}\frac{k_{-H}}{k_{-D}} = 1.76\times\frac{0.053}{0.12} = 1.78$$

3.5 Transition state energy determination

The Eyring-Polanyi equation gives: (where R is the gas constant, T the absolute temperature, k_{-H} the considered kinetic constant, ħ the Planck constant, and k_B the Boltzmann constant)

$$\Delta_r G^{\ddagger} = -RT\ln\left(\frac{k_{-H}\hbar}{k_B T}\right)$$

In our case, we have:

$$\Delta_r G^{\ddagger \leftarrow H} = 12.2\ kcal.mol^{-1}$$

$$\Delta_r G^{\ddagger \leftarrow D} = 12.7\ kcal.mol^{-1}$$

4 X-Ray Structures

4.1 Generalities

Data were collected at 150.0.(1) K on a Nonius Kappa CCD diffractometer using a Mo Kα (λ = 0.71070 Å) X.ray source and a graphite monochromator. All data were measured using phi and omega scans. The crystal structures were solved using SIR 97[4] and Shelxl97[5]. ORTEP drawings were made using ORTEP III for Windows[6] and POV-Ray[7] for Linux.

CCDC 882554 to 882557 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44.1223/336.033; E.mail: deposit@ccdc.cam.ac.uk

4.2 X-Ray Structure of $\mathbf{1}_{Cl}$ (dcpp Platinum (II) Chloride)

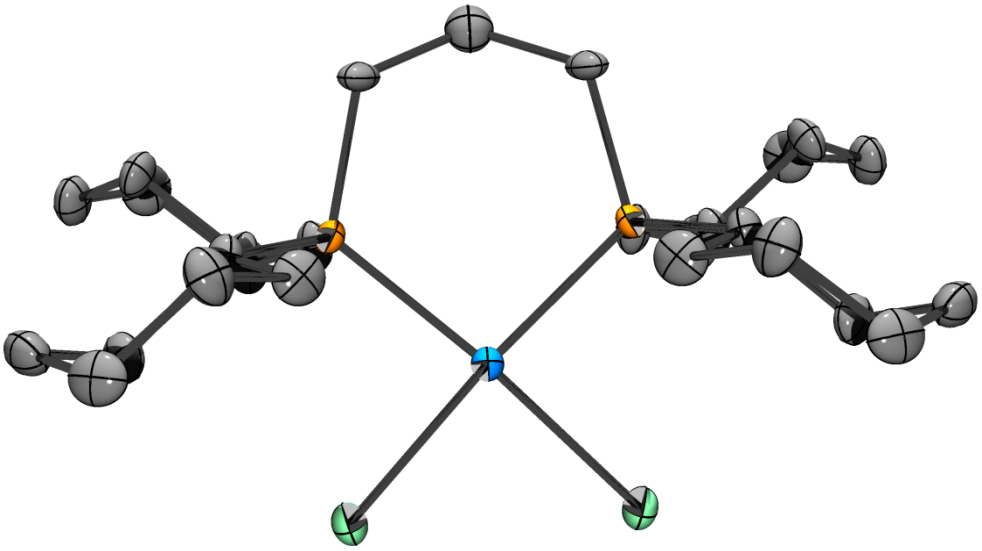


Table 1. Crystal data for $\mathbf{1}_{Cl}$

Compound	$\mathbf{1}_{Cl}$
Molecular formula	$C_{27}H_{48}Cl_2P_2Pt$, 2 (CH_2Cl_2)
Molecular weight	870.44
Crystal habit	Colorless Block
Crystal dimensions(mm)	0.40x0.24x0.14
Crystal system	Monoclinic
Space group	Cm
a(Å)	8.9590(10)
b(Å)	17.604(2)
c(Å)	11.9600(10)
α(°)	90.00
β(°)	110.056(2)
γ(°)	90.00
V(Å^3)	1771.9(3)
Z	2

d(g-cm^{-3})	1.631
F(000)	872
μ(cm^{-1})	4.521
Absorption corrections	multi-scan ; 0.2650 min, 0.5702 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	27.48
HKL ranges	-11 8 ; -20 22 ; -15 13
Reflections measured	3929
Unique data	2471
Rint	0.0418
Reflections used	2470
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	constr
Parameters refined	149
Reflections / parameter	16
wR2	0.1020
R1	0.0384
Flack's parameter	0.21(2)
Weights a, b	0.0747 ; 6.4213
GoF	1.066
difference peak / hole (e Å^{-3})	1.804(0.186) / -1.085(0.186)

Table 2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1Cl

atom	x	y	z	U(eq)
Pt(1)	77(2)	10000	260(2)	16(1)
Cl(1)	-1854(5)	10928(3)	211(4)	25(1)
P(1)	1774(4)	9045(3)	286(3)	16(1)
C(1)	3780(10)	9277(5)	370(10)	22(2)
C(2)	4060(20)	10000	-230(10)	30(3)
C(4)	2240(10)	8411(5)	1597(8)	20(2)
C(5)	2500(10)	8869(6)	2710(8)	28(2)
C(6)	3120(10)	8379(6)	3820(10)	29(2)
C(7)	2040(10)	7722(6)	3790(10)	30(2)
C(8)	1770(10)	7256(5)	2660(10)	27(2)
C(9)	1070(10)	7761(5)	1540(10)	25(2)
C(10)	950(10)	8441(5)	-1044(8)	22(2)
C(11)	2030(10)	7788(5)	-1100(10)	25(2)
C(12)	1230(10)	7294(5)	-2190(10)	30(2)
C(13)	800(20)	7745(7)	-3330(10)	36(2)
C(14)	-310(10)	8419(6)	-3303(8)	29(2)
C(15)	470(10)	8914(5)	-2189(8)	25(2)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table 3. Bond lengths (A) and angles (deg) for 1Cl

Pt(1)-P(1)#2	2.260(6)	Pt(1)-P(1)	2.260(6)
Pt(1)-Cl(1)	2.366(6)	Pt(1)-Cl(1)#2	2.366(6)
P(1)-C(1)	1.81(1)	P(1)-C(10)	1.84(1)
P(1)-C(4)	1.85(1)	C(1)-C(2)	1.52(1)
C(1)-H(1A)	0.9900	C(1)-H(1B)	0.9900
C(2)-C(1)#2	1.52(1)	C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900	C(4)-C(5)	1.50(1)
C(4)-C(9)	1.54(1)	C(5)-C(6)	1.52(1)
C(5)-H(5A)	0.9900	C(5)-H(5B)	0.9900
C(6)-C(7)	1.50(1)	C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900	C(7)-C(8)	1.53(1)
C(7)-H(7A)	0.9900	C(7)-H(7B)	0.9900
C(8)-C(9)	1.55(1)	C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900	C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900	C(10)-C(11)	1.52(1)
C(10)-C(15)	1.53(1)	C(10)-H(10)	1.0000
C(11)-C(12)	1.52(1)	C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900	C(12)-C(13)	1.51(1)
C(12)-H(12A)	0.9900	C(12)-H(12B)	0.9900
C(13)-C(14)	1.55(2)	C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900	C(14)-C(15)	1.54(1)
C(14)-H(14A)	0.9900	C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9900	C(15)-H(15B)	0.9900

P(1)#2-Pt(1)-P(1)	96.1(3)	P(1)#2-Pt(1)-Cl(1)	88.3(1)
P(1)-Pt(1)-Cl(1)	175.6(2)	P(1)#2-Pt(1)-Cl(1)#2	175.6(2)
P(1)-Pt(1)-Cl(1)#2	88.3(1)	Cl(1)-Pt(1)-Cl(1)#2	87.4(3)
C(1)-P(1)-C(10)	106.0(5)	C(1)-P(1)-C(4)	99.0(5)
C(10)-P(1)-C(4)	106.8(5)	C(1)-P(1)-Pt(1)	118.9(4)
C(10)-P(1)-Pt(1)	110.5(4)	C(4)-P(1)-Pt(1)	114.5(4)
C(2)-C(1)-P(1)	118.7(8)	C(2)-C(1)-H(1A)	107.6
P(1)-C(1)-H(1A)	107.6	C(2)-C(1)-H(1B)	107.6
P(1)-C(1)-H(1B)	107.6	H(1A)-C(1)-H(1B)	107.1
C(1)-C(2)-C(1)#2	113(1)	C(1)-C(2)-H(2A)	108.9
C(1)#2-C(2)-H(2A)	108.9	C(1)-C(2)-H(2B)	108.9
C(1)#2-C(2)-H(2B)	108.9	H(2A)-C(2)-H(2B)	107.7
C(5)-C(4)-C(9)	109.3(8)	C(5)-C(4)-P(1)	110.4(6)
C(9)-C(4)-P(1)	117.5(6)	C(4)-C(5)-C(6)	111.7(8)
C(4)-C(5)-H(5A)	109.3	C(6)-C(5)-H(5A)	109.3
C(4)-C(5)-H(5B)	109.3	C(6)-C(5)-H(5B)	109.3
H(5A)-C(5)-H(5B)	108.0	C(7)-C(6)-C(5)	112.2(8)
C(7)-C(6)-H(6A)	109.2	C(5)-C(6)-H(6A)	109.2
C(7)-C(6)-H(6B)	109.2	C(5)-C(6)-H(6B)	109.2
H(6A)-C(6)-H(6B)	107.9	C(6)-C(7)-C(8)	109.7(8)
C(6)-C(7)-H(7A)	109.7	C(8)-C(7)-H(7A)	109.7
C(6)-C(7)-H(7B)	109.7	C(8)-C(7)-H(7B)	109.7
H(7A)-C(7)-H(7B)	108.2	C(7)-C(8)-C(9)	110.4(8)
C(7)-C(8)-H(8A)	109.6	C(9)-C(8)-H(8A)	109.6
C(7)-C(8)-H(8B)	109.6	C(9)-C(8)-H(8B)	109.6
H(8A)-C(8)-H(8B)	108.1	C(4)-C(9)-C(8)	108.8(7)
C(4)-C(9)-H(9A)	109.9	C(8)-C(9)-H(9A)	109.9
C(4)-C(9)-H(9B)	109.9	C(8)-C(9)-H(9B)	109.9
H(9A)-C(9)-H(9B)	108.3	C(11)-C(10)-C(15)	111.0(8)
C(11)-C(10)-P(1)	113.8(7)	C(15)-C(10)-P(1)	111.3(6)
C(11)-C(10)-H(10)	106.7	C(15)-C(10)-H(10)	106.7
P(1)-C(10)-H(10)	106.7	C(10)-C(11)-C(12)	110.4(8)
C(10)-C(11)-H(11A)	109.6	C(12)-C(11)-H(11A)	109.6
C(10)-C(11)-H(11B)	109.6	C(12)-C(11)-H(11B)	109.6
H(11A)-C(11)-H(11B)	108.1	C(13)-C(12)-C(11)	111.6(8)
C(13)-C(12)-H(12A)	109.3	C(11)-C(12)-H(12A)	109.3
C(13)-C(12)-H(12B)	109.3	C(11)-C(12)-H(12B)	109.3
H(12A)-C(12)-H(12B)	108.0	C(12)-C(13)-C(14)	110.6(8)
C(12)-C(13)-H(13A)	109.5	C(14)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5	C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	108.1	C(15)-C(14)-C(13)	110.3(8)
C(15)-C(14)-H(14A)	109.6	C(13)-C(14)-H(14A)	109.6
C(15)-C(14)-H(14B)	109.6	C(13)-C(14)-H(14B)	109.6
H(14A)-C(14)-H(14B)	108.1	C(10)-C(15)-C(14)	111.8(7)
C(10)-C(15)-H(15A)	109.3	C(14)-C(15)-H(15A)	109.3
C(10)-C(15)-H(15B)	109.3	C(14)-C(15)-H(15B)	109.3
H(15A)-C(15)-H(15B)	107.9		

Estimated standard deviations are given in the parenthesis.
Symmetry operators ::

```
1: x, y, z                  2: x, -y, z                 3: x+1/2, y+1/2, z
4: x+1/2, -y+1/2, z
```

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1Cl

atom	U11	U22	U33	U23	U13	U12
Pt(1)	16(1)	14(1)	19(1)	0	7(1)	0
Cl(1)	24(2)	17(2)	34(2)	0(1)	10(2)	2(1)
P(1)	17(2)	12(2)	21(2)	2(1)	8(1)	3(1)
C(1)	13(4)	24(4)	29(4)	-6(3)	9(3)	-2(3)
C(2)	27(7)	31(7)	28(7)	0	5(6)	0
C(4)	22(4)	17(3)	19(4)	1(3)	5(3)	2(3)
C(5)	29(5)	33(5)	16(4)	-9(4)	1(3)	-2(4)
C(6)	33(5)	27(4)	23(4)	-5(4)	4(4)	-8(4)
C(7)	28(5)	40(5)	17(4)	10(4)	2(4)	3(4)
C(8)	25(5)	27(4)	30(5)	7(4)	10(4)	-2(4)
C(9)	28(5)	23(4)	22(4)	8(3)	4(4)	1(4)
C(10)	27(4)	18(4)	18(4)	-2(3)	4(3)	4(3)
C(11)	28(5)	19(4)	26(4)	-5(3)	9(4)	4(4)
C(12)	41(6)	21(4)	31(5)	-6(4)	18(4)	0(4)
C(13)	40(6)	39(5)	26(5)	-11(4)	9(4)	-3(5)
C(14)	44(6)	28(5)	11(4)	-2(3)	4(4)	-2(4)
C(15)	36(5)	20(4)	19(4)	2(3)	9(4)	-3(4)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table 5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1Cl

atom	x	y	z	U(eq)
H(1A)	4442	9308	1225	26
H(1B)	4188	8846	30	26
H(2A)	3338	10000	-1068	36
H(2B)	5163	10000	-226	36
H(5A)	1486	9108	2676	34
H(5B)	3273	9279	2752	34
H(6A)	4185	8182	3894	35
H(6B)	3234	8695	4529	35
H(7A)	1004	7914	3809	36
H(7B)	2514	7398	4502	36
H(8A)	1031	6832	2635	32
H(8B)	2791	7036	2674	32
H(9A)	892	7455	817	30
H(9B)	32	7973	1520	30
H(10)	-43	8208	-996	26
H(11A)	2290	7477	-372	30
H(11B)	3041	7993	-1149	30
H(12A)	1952	6875	-2217	35
H(12B)	255	7067	-2119	35
H(13A)	257	7411	-4013.0002	43
H(13B)	1780	7942	-3431	43
H(14A)	-511	8732	-4028	35
H(14B)	-1338	8221	-3295	35
H(15A)	1418	9168	-2256	30
H(15B)	-292	9312	-2148	30

4.3 X-Ray Structure of 1_I (dcpp Platinum (II) Iodide)

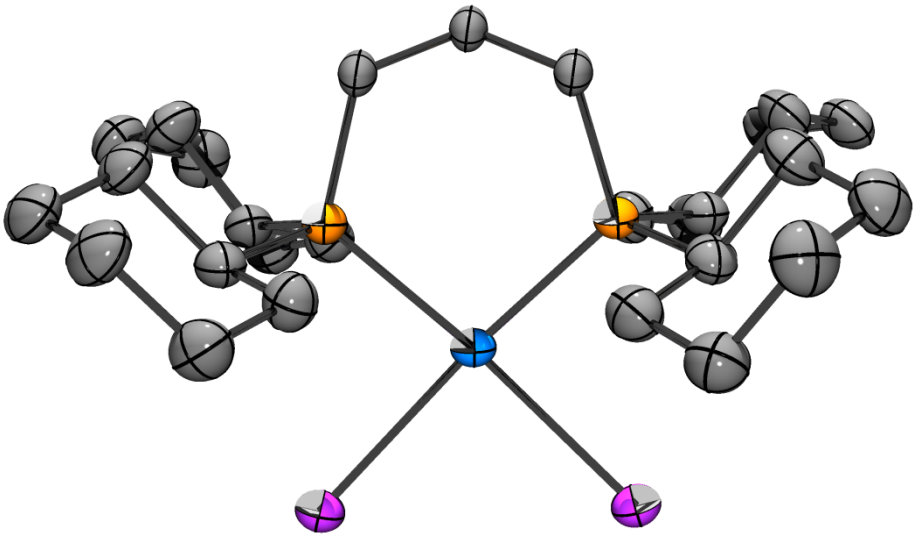


Table 1. Crystal data for $\mathbf{1_I}$

Compound	$\mathbf{1_I}$
Molecular formula	$C_{27}H_{50}I_2P_2Pt,2(CH_2Cl_2)$
Molecular weight	1055.35
Crystal habit	Colorless Plate
Crystal dimensions(mm)	0.18x0.16x0.12
Crystal system	monoclinic
Space group	C2/c
a(Å)	25.262(1)
b(Å)	9.278(1)
c(Å)	17.617(1)
α(°)	90.00
β(°)	117.018(1)
γ(°)	90.00
V(Å^3)	3678.5(5)
Z	4
d(g-cm^{-3})	1.906
F(000)	2040
μ(cm^{-1})	5.889
Absorption corrections	multi-scan ; 0.4170 min, 0.5384 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	27.45
HKL ranges	-32 25 ; -11 12 ; -16 22
Reflections measured	15410
Unique data	4176
Rint	0.0433

Reflections used	3500
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	constr
Parameters refined	174
Reflections / parameter	20
wR2	0.1069
R1	0.0387
Weights a, b	0.0622 ; 7.2716
GoF	1.101
difference peak / hole (e $Å^{-3}$)	2.268(0.179) / -1.643(0.179)

Table 2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1I

atom	x	y	z	U(eq)
Pt(1)	0	590(1)	2500	30(1)
I(1)	-14(1)	-1490(1)	1432(1)	37(1)
P(1)	3(1)	2213(2)	3467(1)	31(1)
C(1)	92(5)	4120(10)	3260(10)	30(2)
C(2)	-230(4)	4570(10)	2341(7)	30(2)
C(3)	120(5)	4080(10)	1870(10)	30(2)
C(4)	-660(2)	1938(6)	3646(4)	37(1)
C(5)	-1206(2)	1537(6)	2806(4)	42(1)
C(6)	-1745(3)	1200(7)	2948(4)	47(1)
C(7)	-1892(3)	2435(8)	3373(5)	55(2)
C(8)	-1357(3)	2852(8)	4206(4)	53(2)
C(9)	-812(3)	3217(7)	4071(4)	46(1)
C(10)	681(2)	1987(6)	4498(4)	37(1)
C(11)	804(3)	3228(6)	5139(4)	43(1)
C(12)	1370(3)	2906(7)	5972(4)	50(2)
C(13)	1904(3)	2645(7)	5811(4)	51(2)
C(14)	1787(3)	1458(7)	5164(4)	47(2)
C(15)	1223(2)	1751(7)	4333(4)	41(1)
Cl(1)	3227(1)	488(2)	1449(2)	104(1)
Cl(2)	3070(1)	3502(3)	971(2)	105(1)
C(16)	3534(4)	2190(10)	1593(7)	88(3)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table 3. Bond lengths (A) and angles (deg) for 1I

Pt(1)-P(1)#2	2.272(1)	Pt(1)-P(1)	2.272(1)
Pt(1)-I(1)#2	2.6843(4	Pt(1)-I(1)	2.6843(4)
P(1)-C(3)#2	1.81(1)	P(1)-C(1)	1.84(1)
P(1)-C(4)	1.857(6)	P(1)-C(10)	1.858(6)
C(1)-C(2)	1.51(2)	C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900	C(2)-C(3)	1.53(2)
C(2)-H(2A)	0.9900	C(2)-H(2B)	0.9900
C(3)-P(1)#2	1.81(1)	C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900	C(4)-C(5)	1.542(8)
C(4)-C(9)	1.542(8)	C(4)-H(4)	1.0000
C(5)-C(6)	1.52(1)	C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900	C(6)-C(7)	1.50(1)
C(6)-H(6A)	0.9900	C(6)-H(6B)	0.9900
C(7)-C(8)	1.53(1)	C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900	C(8)-C(9)	1.54(1)
C(8)-H(8A)	0.9900	C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900	C(9)-H(9B)	0.9900
C(10)-C(15)	1.539(8)	C(10)-C(11)	1.543(8)
C(10)-H(10)	1.0000	C(11)-C(12)	1.544(8)
C(11)-H(11A)	0.9900	C(11)-H(11B)	0.9900
C(12)-C(13)	1.52(1)	C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900	C(13)-C(14)	1.51(1)
C(13)-H(13A)	0.9900	C(13)-H(13B)	0.9900
C(14)-C(15)	1.533(8)	C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900	C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900	Cl(1)-C(16)	1.72(1)
Cl(2)-C(16)	1.70(1)	C(16)-H(15A)	0.9900
C(16)-H(15B)	0.9900		

P(1)#2-Pt(1)-P(1)	96.90(7)	P(1)#2-Pt(1)-I(1)#2	175.56(4)
P(1)-Pt(1)-I(1)#2	87.51(4)	P(1)#2-Pt(1)-I(1)	87.51(4)
P(1)-Pt(1)-I(1)	175.56(4)	I(1)#2-Pt(1)-I(1)	88.08(2)
C(3)#2-P(1)-C(1)	15.0(5)	C(3)#2-P(1)-C(4)	98.9(4)
C(1)-P(1)-C(4)	111.5(4)	C(3)#2-P(1)-C(10)	111.8(5)
C(1)-P(1)-C(10)	99.2(5)	C(4)-P(1)-C(10)	108.7(3)
C(3)#2-P(1)-Pt(1)	116.6(5)	C(1)-P(1)-Pt(1)	116.8(5)
C(4)-P(1)-Pt(1)	109.9(2)	C(10)-P(1)-Pt(1)	110.2(2)
C(2)-C(1)-P(1)	114.9(8)	C(2)-C(1)-H(1A)	108.6
P(1)-C(1)-H(1A)	108.6	C(2)-C(1)-H(1B)	108.6
P(1)-C(1)-H(1B)	108.6	H(1A)-C(1)-H(1B)	107.5
C(1)-C(2)-C(3)	110.0(8)	C(1)-C(2)-H(2A)	109.7
C(3)-C(2)-H(2A)	109.7	C(1)-C(2)-H(2B)	109.7
C(3)-C(2)-H(2B)	109.7	H(2A)-C(2)-H(2B)	108.2
C(2)-C(3)-P(1)#2	113.7(8)	C(2)-C(3)-H(3A)	108.8
P(1)#2-C(3)-H(3A)	108.8	C(2)-C(3)-H(3B)	108.8
P(1)#2-C(3)-H(3B)	108.8	H(3A)-C(3)-H(3B)	107.7
C(5)-C(4)-C(9)	109.8(5)	C(5)-C(4)-P(1)	110.7(4)
C(9)-C(4)-P(1)	114.8(4)	C(5)-C(4)-H(4)	107.0
C(9)-C(4)-H(4)	107.0	P(1)-C(4)-H(4)	107.0
C(6)-C(5)-C(4)	111.6(5)	C(6)-C(5)-H(5A)	109.3
C(4)-C(5)-H(5A)	109.3	C(6)-C(5)-H(5B)	109.3
C(4)-C(5)-H(5B)	109.3	H(5A)-C(5)-H(5B)	108.0
C(7)-C(6)-C(5)	111.5(5)	C(7)-C(6)-H(6A)	109.3
C(5)-C(6)-H(6A)	109.3	C(7)-C(6)-H(6B)	109.3
C(5)-C(6)-H(6B)	109.3	H(6A)-C(6)-H(6B)	108.0
C(6)-C(7)-C(8)	111.1(5)	C(6)-C(7)-H(7A)	109.4
C(8)-C(7)-H(7A)	109.4	C(6)-C(7)-H(7B)	109.4
C(8)-C(7)-H(7B)	109.4	H(7A)-C(7)-H(7B)	108.0
C(7)-C(8)-C(9)	111.7(6)	C(7)-C(8)-H(8A)	109.3
C(9)-C(8)-H(8A)	109.3	C(7)-C(8)-H(8B)	109.3
C(9)-C(8)-H(8B)	109.3	H(8A)-C(8)-H(8B)	107.9
C(8)-C(9)-C(4)	110.2(5)	C(8)-C(9)-H(9A)	109.6
C(4)-C(9)-H(9A)	109.6	C(8)-C(9)-H(9B)	109.6
C(4)-C(9)-H(9B)	109.6	H(9A)-C(9)-H(9B)	108.1
C(15)-C(10)-C(11)	110.1(5)	C(15)-C(10)-P(1)	109.7(4)
C(11)-C(10)-P(1)	114.9(4)	C(15)-C(10)-H(10)	107.3
C(11)-C(10)-H(10)	107.3	P(1)-C(10)-H(10)	107.3
C(10)-C(11)-C(12)	110.0(5)	C(10)-C(11)-H(11A)	109.7
C(12)-C(11)-H(11A)	109.7	C(10)-C(11)-H(11B)	109.7
C(12)-C(11)-H(11B)	109.7	H(11A)-C(11)-H(11B)	108.2
C(13)-C(12)-C(11)	111.8(5)	C(13)-C(12)-H(12A)	109.3
C(11)-C(12)-H(12A)	109.3	C(13)-C(12)-H(12B)	109.3
C(11)-C(12)-H(12B)	109.3	H(12A)-C(12)-H(12B)	107.9
C(14)-C(13)-C(12)	111.8(5)	C(14)-C(13)-H(13A)	109.3

C(12)-C(13)-H(13A)	109.3	C(14)-C(13)-H(13B)	109.3
C(12)-C(13)-H(13B)	109.3	H(13A)-C(13)-H(13B)	107.9
C(13)-C(14)-C(15)	111.6(5)	C(13)-C(14)-H(14A)	109.3
C(15)-C(14)-H(14A)	109.3	C(13)-C(14)-H(14B)	109.3
C(15)-C(14)-H(14B)	109.3	H(14A)-C(14)-H(14B)	108.0
C(14)-C(15)-C(10)	111.5(5)	C(14)-C(15)-H(15A)	109.3
C(10)-C(15)-H(15A)	109.3	C(14)-C(15)-H(15B)	109.3
C(10)-C(15)-H(15B)	109.3	H(15A)-C(15)-H(15B)	108.0
Cl(2)-C(16)-Cl(1)	115.4(5)	Cl(2)-C(16)-H(15A)	108.4
Cl(1)-C(16)-H(15A)	108.4	Cl(2)-C(16)-H(15B)	108.4
Cl(1)-C(16)-H(15B)	108.4	H(15A)-C(16)-H(15B)	107.5

Estimated standard deviations are given in the parenthesis.

Symmetry operators ::

1: x, y, z 2: -x, y, -z+1/2 3: x+1/2, y+1/2, z

4: -x+1/2, y+1/2, -z+1/ 5: -x, -y, -z 6: x, -y, z-1/2

7: -x+1/2, -y+1/2, -z 8: x+1/2, -y+1/2, z-1/2

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1I

atom	U11	U22	U33	U23	U13	U12
Pt(1)	37(1)	22(1)	31(1)	0	16(1)	0
I(1)	49(1)	26(1)	38(1)	-3(1)	22(1)	-1(1)
P(1)	40(1)	26(1)	30(1)	1(1)	17(1)	1(1)
C(1)	39(4)	30(3)	25(4)	-4(3)	19(4)	-6(2)
C(2)	39(4)	30(3)	25(4)	-4(3)	19(4)	-6(2)
C(3)	39(4)	30(3)	25(4)	-4(3)	19(4)	-6(2)
C(4)	44(3)	31(3)	36(3)	1(2)	18(2)	7(2)
C(5)	43(3)	39(3)	38(3)	1(2)	14(3)	5(2)
C(6)	44(3)	45(3)	47(4)	0(3)	18(3)	2(3)
C(7)	44(3)	63(4)	60(4)	1(3)	26(3)	7(3)
C(8)	58(4)	53(4)	55(4)	-3(3)	32(3)	10(3)
C(9)	48(3)	42(3)	50(4)	-7(3)	23(3)	7(3)
C(10)	44(3)	29(3)	36(3)	0(2)	17(2)	-1(2)
C(11)	48(3)	38(3)	38(3)	-11(3)	15(3)	-1(2)
C(12)	60(4)	43(3)	39(3)	-11(3)	15(3)	0(3)
C(13)	48(3)	51(4)	42(4)	-13(3)	10(3)	-3(3)
C(14)	39(3)	49(4)	45(4)	-2(3)	12(3)	4(2)
C(15)	38(3)	45(3)	39(3)	-2(3)	15(3)	0(2)
Cl(1)	69(1)	55(1)	169(3)	0(1)	37(2)	1(1)
Cl(2)	98(2)	72(2)	154(3)	27(2)	64(2)	-12(1)
C(16)	68(5)	82(6)	90(7)	12(5)	14(5)	-24(4)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table 5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1I

atom	x	y	z	U(eq)
H(1A)	-51	4724	3596	36
H(1B)	521	4322	3474	36
H(2A)	-279	5626	2303	36
H(2B)	-631	4125	2073	36
H(3A)	549	4231	2246	36
H(3B)	7.0000	4702	1361	36
H(4)	-573	1093	4037	44
H(5A)	-1303	2348	2399	51
H(5B)	-1111	687	2551	51
H(6A)	-2091	995	2393	56
H(6B)	-1663	328	3308	56
H(7A)	-2227	2158	3490	66
H(7B)	-2019	3276	2985	66
H(8A)	-1257	2044	4616	64
H(8B)	-1461	3697	4455	64
H(9A)	-469	3434	4626	55
H(9B)	-897	4082	3705	55
H(10)	628	1089	4770	44
H(11A)	461	3342	5263	52
H(11B)	855	4141	4889	52
H(12A)	1455	3730	6368	60
H(12B)	1302	2044	6247	60
H(13A)	2002	3545	5601	61
H(13B)	2251	2379	6353	61
H(14A)	1745	528	5406	57
H(14B)	2131	1377	5039	57
H(15A)	1146	925	3942	50
H(15B)	1285	2617	4054	50
H(15A)	3678	2461	2197	106
H(15B)	3883	2143	1480	106

4.4 X-Ray Structure of dcpp Platinum (II) Hydrido-Meta Toluene

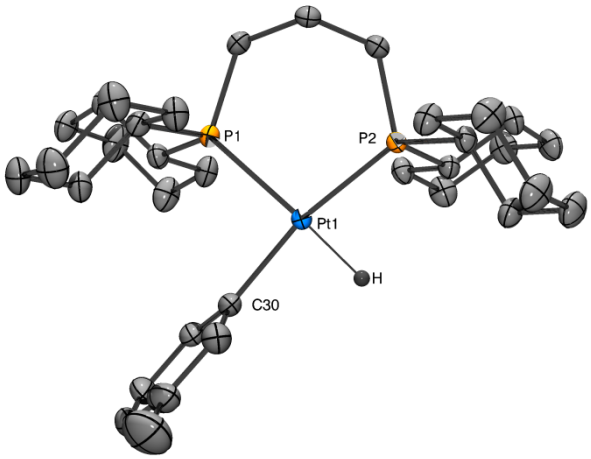


Table 1. Crystal data for en95

Compound	en95
Molecular formula	$C_{34}H_{58}P_2Pt,C_7H_8$
Molecular weight	815.97
Crystal habit	colorless plate
Crystal dimensions(mm)	0.22x0.22x0.15
Crystal system	monoclinic
Space group	$P2_1/n$
a(Å)	11.746(1)
b(Å)	13.520(1)
c(Å)	24.794(1)
α(°)	90.00
β(°)	102.577(1)
γ(°)	90.00
V(Å^3)	3843.0(5)
Z	4
d(g-cm^{-3})	1.410
F(000)	1680
μ(cm^{-1})	3.761
Absorption corrections	multi-scan ; 0.4917 min, 0.6023 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	30.07
HKL ranges	-16 16 ; -19 19 ; -34 34
Reflections measured	52601
Unique data	11214
Rint	0.0405
Reflections used	9852

Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	402
Reflections / parameter	24
wR2	0.0738
R1	0.0320
Weights a, b	0.0309 ; 10.692
GoF	1.016
difference peak / hole (e $Å^{-3}$)	1.585(0.110) / -1.504(0.110)

Table 2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for en95

atom	x	y	z	U(eq)
Pt(1)	3312(1)	2945(1)	3156(1)	20(1)
P(1)	2211(1)	2052(1)	2458(1)	18(1)
P(2)	3034(1)	1981(1)	3884(1)	20(1)
C(1)	1538(3)	899(2)	2633(1)	24(1)
C(2)	2218(3)	364(2)	3150(1)	25(1)
C(3)	2132(3)	865(2)	3696(1)	26(1)
C(4)	4359(3)	3939(2)	3668(1)	30(1)
C(5)	3916(4)	4648(3)	3992(1)	34(1)
C(6)	4647(4)	5297(3)	4343(2)	41(1)
C(7)	5831(4)	5264(3)	4381(2)	48(1)
C(8)	6309(4)	4604(3)	4070(2)	45(1)
C(9)	5563(3)	3955(3)	3710(2)	38(1)
C(10)	7565(5)	4537(5)	4110(3)	86(2)
C(11)	959(3)	2758(2)	2058(1)	22(1)
C(12)	230(3)	2189(2)	1565(1)	28(1)
C(13)	-757(3)	2827(3)	1244(1)	33(1)
C(14)	-1535(3)	3215(3)	1615(2)	35(1)
C(15)	-823(3)	3789(3)	2105(2)	34(1)
C(16)	190(3)	3166(3)	2430(1)	28(1)
C(17)	3009(3)	1633(2)	1932(1)	22(1)
C(18)	4108(3)	1049(3)	2207(1)	29(1)
C(19)	4780(3)	693(3)	1780(2)	35(1)
C(20)	5092(3)	1540(3)	1435(2)	35(1)
C(21)	3997(3)	2102(3)	1158(1)	35(1)
C(22)	3336(3)	2484(3)	1586(1)	28(1)
C(23)	2268(3)	2640(2)	4354(1)	25(1)
C(24)	1182(3)	3165(3)	4020(1)	32(1)
C(25)	621(4)	3810(3)	4400(2)	42(1)
C(26)	291(4)	3188(4)	4858(2)	43(1)
C(27)	1354(3)	2646(3)	5189(1)	36(1)
C(28)	1947(3)	2014(3)	4817(1)	29(1)
C(29)	4351(3)	1469(2)	4355(1)	24(1)
C(30)	5027(3)	2233(3)	4764(1)	29(1)
C(31)	6109(3)	1767(3)	5134(1)	37(1)
C(32)	6908(3)	1315(3)	4792(2)	41(1)
C(33)	6253(3)	550(3)	4389(2)	35(1)
C(34)	5159(3)	989(3)	4017(1)	30(1)
C(35)	-656(6)	85(6)	4222(3)	91(2)
C(36)	-1060(4)	288(5)	3609(2)	62(1)
C(37)	-765(5)	-398(5)	3262(3)	75(2)
C(38)	-1135(8)	-270(8)	2695(4)	114(3)
C(39)	-1818(7)	610(10)	2507(4)	117(4)
C(40)	-2068(7)	1260(10)	2894(5)	121(4)
C(41)	-1694(6)	1099(5)	3422(4)	93(2)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table 3. Bond lengths (A) and angles (deg) for en95

Pt(1)-C(4)	2.061(3)	Pt(1)-P(1)	2.2692(7)
Pt(1)-P(2)	2.3065(7	Pt(1)-H(1)	1.58(4)
P(1)-C(1)	1.841(3)	P(1)-C(11)	1.850(3)
P(1)-C(17)	1.854(3)	P(2)-C(3)	1.844(3)
P(2)-C(23)	1.848(3)	P(2)-C(29)	1.856(3)
C(1)-C(2)	1.537(4)	C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900	C(2)-C(3)	1.536(4)
C(2)-H(2A)	0.9900	C(2)-H(2B)	0.9900
C(3)-H(3A)	0.9900	C(3)-H(3B)	0.9900
C(4)-C(9)	1.395(5)	C(4)-C(5)	1.421(5)
C(5)-C(6)	1.393(5)	C(5)-H(5)	0.9500
C(6)-C(7)	1.374(7)	C(6)-H(6)	0.9500
C(7)-C(8)	1.377(7)	C(7)-H(7)	0.9500
C(8)-C(9)	1.412(5)	C(8)-C(10)	1.460(7)
C(9)-H(9)	0.9500	C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800	C(10)-H(10C)	0.9800
C(11)-C(16)	1.529(4)	C(11)-C(12)	1.537(4)
C(11)-H(11)	1.0000	C(12)-C(13)	1.523(5)
C(12)-H(12A)	0.9900	C(12)-H(12B)	0.9900
C(13)-C(14)	1.524(5)	C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900	C(14)-C(15)	1.529(5)
C(14)-H(14A)	0.9900	C(14)-H(14B)	0.9900
C(15)-C(16)	1.536(5)	C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900	C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900	C(17)-C(22)	1.533(4)
C(17)-C(18)	1.539(4)	C(17)-H(17)	1.0000
C(18)-C(19)	1.529(5)	C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900	C(19)-C(20)	1.522(5)
C(19)-H(19A)	0.9900	C(19)-H(19B)	0.9900
C(20)-C(21)	1.523(5)	C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900	C(21)-C(22)	1.536(5)
C(21)-H(21A)	0.9900	C(21)-H(21B)	0.9900
C(22)-H(22A)	0.9900	C(22)-H(22B)	0.9900
C(23)-C(24)	1.535(5)	C(23)-C(28)	1.537(4)
C(23)-H(23)	1.0000	C(24)-C(25)	1.534(5)
C(24)-H(24A)	0.9900	C(24)-H(24B)	0.9900
C(25)-C(26)	1.528(6)	C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900	C(26)-C(27)	1.524(5)
C(26)-H(26A)	0.9900	C(26)-H(26B)	0.9900
C(27)-C(28)	1.532(5)	C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900	C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900	C(29)-C(34)	1.539(4)
C(29)-C(30)	1.541(4)	C(29)-H(29)	1.0000
C(30)-C(31)	1.532(5)	C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900	C(31)-C(32)	1.525(5)
C(31)-H(31A)	0.9900	C(31)-H(31B)	0.9900
C(32)-C(33)	1.524(5)	C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900	C(33)-C(34)	1.530(5)
C(33)-H(33A)	0.9900	C(33)-H(33B)	0.9900
C(34)-H(34A)	0.9900	C(34)-H(34B)	0.9900
C(35)-C(36)	1.52(1)	C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800	C(35)-H(35C)	0.9800
C(36)-C(41)	1.35(1)	C(36)-C(37)	1.361(8)
C(37)-C(38)	1.39(1)	C(37)-H(37)	0.9500
C(38)-C(39)	1.45(1)	C(38)-H(38)	0.9500
C(39)-C(40)	1.38(1)	C(39)-H(39)	0.9500
C(40)-C(41)	1.31(1)	C(40)-H(40)	0.9500
C(41)-H(41)	0.9500		

C(4)-Pt(1)-P(1)	168.7(1)	C(4)-Pt(1)-P(2)	93.1(1)
P(1)-Pt(1)-P(2)	98.16(3)	C(4)-Pt(1)-H(1)	84(1)
P(1)-Pt(1)-H(1)	85(1)	P(2)-Pt(1)-H(1)	177(1)
C(1)-P(1)-C(11)	103.4(1)	C(1)-P(1)-C(17)	102.4(1)
C(11)-P(1)-C(17)	104.1(1)	C(1)-P(1)-Pt(1)	118.3(1)
C(11)-P(1)-Pt(1)	112.9(1)	C(17)-P(1)-Pt(1)	114.1(1)
C(3)-P(2)-C(23)	102.8(2)	C(3)-P(2)-C(29)	102.0(2)
C(23)-P(2)-C(29)	103.7(1)	C(3)-P(2)-Pt(1)	115.8(1)
C(23)-P(2)-Pt(1)	113.1(1)	C(29)-P(2)-Pt(1)	117.5(1)
C(2)-C(1)-P(1)	115.0(2)	C(2)-C(1)-H(1A)	108.5
P(1)-C(1)-H(1A)	108.5	C(2)-C(1)-H(1B)	108.5
P(1)-C(1)-H(1B)	108.5	H(1A)-C(1)-H(1B)	107.5
C(3)-C(2)-C(1)	114.0(3)	C(3)-C(2)-H(2A)	108.7
C(1)-C(2)-H(2A)	108.7	C(3)-C(2)-H(2B)	108.7
C(1)-C(2)-H(2B)	108.7	H(2A)-C(2)-H(2B)	107.6

C(2)-C(3)-P(2)	116.0(2)	C(2)-C(3)-H(3A)	108.3
P(2)-C(3)-H(3A)	108.3	C(2)-C(3)-H(3B)	108.3
P(2)-C(3)-H(3B)	108.3	H(3A)-C(3)-H(3B)	107.4
C(9)-C(4)-C(5)	115.9(3)	C(9)-C(4)-Pt(1)	121.1(3)
C(5)-C(4)-Pt(1)	123.0(3)	C(6)-C(5)-C(4)	121.8(4)
C(6)-C(5)-H(5)	119.1	C(4)-C(5)-H(5)	119.1
C(7)-C(6)-C(5)	119.9(4)	C(7)-C(6)-H(6)	120.0
C(5)-C(6)-H(6)	120.0	C(6)-C(7)-C(8)	120.9(4)
C(6)-C(7)-H(7)	119.6	C(8)-C(7)-H(7)	119.6
C(7)-C(8)-C(9)	119.0(4)	C(7)-C(8)-C(10)	122.1(5)
C(9)-C(8)-C(10)	118.9(5)	C(4)-C(9)-C(8)	122.5(4)
C(4)-C(9)-H(9)	118.8	C(8)-C(9)-H(9)	118.8
C(8)-C(10)-H(10A)	109.5	C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5	C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(10B)-C(10)-H(10C)	109.5
C(16)-C(11)-C(12)	111.1(3)	C(16)-C(11)-P(1)	111.5(2)
C(12)-C(11)-P(1)	114.1(2)	C(16)-C(11)-H(11)	106.5
C(12)-C(11)-H(11)	106.5	P(1)-C(11)-H(11)	106.5
C(13)-C(12)-C(11)	111.2(3)	C(13)-C(12)-H(12A)	109.4
C(11)-C(12)-H(12A)	109.4	C(13)-C(12)-H(12B)	109.4
C(11)-C(12)-H(12B)	109.4	H(12A)-C(12)-H(12B)	108.0
C(12)-C(13)-C(14)	111.6(3)	C(12)-C(13)-H(13A)	109.3
C(14)-C(13)-H(13A)	109.3	C(12)-C(13)-H(13B)	109.3
C(14)-C(13)-H(13B)	109.3	H(13A)-C(13)-H(13B)	108.0
C(13)-C(14)-C(15)	111.0(3)	C(13)-C(14)-H(14A)	109.4
C(15)-C(14)-H(14A)	109.4	C(13)-C(14)-H(14B)	109.4
C(15)-C(14)-H(14B)	109.4	H(14A)-C(14)-H(14B)	108.0
C(14)-C(15)-C(16)	111.5(3)	C(14)-C(15)-H(15A)	109.3
C(16)-C(15)-H(15A)	109.3	C(14)-C(15)-H(15B)	109.3
C(16)-C(15)-H(15B)	109.3	H(15A)-C(15)-H(15B)	108.0
C(11)-C(16)-C(15)	111.9(3)	C(11)-C(16)-H(16A)	109.2
C(15)-C(16)-H(16A)	109.2	C(11)-C(16)-H(16B)	109.2
C(15)-C(16)-H(16B)	109.2	H(16A)-C(16)-H(16B)	107.9
C(22)-C(17)-C(18)	110.1(3)	C(22)-C(17)-P(1)	113.0(2)
C(18)-C(17)-P(1)	110.4(2)	C(22)-C(17)-H(17)	107.7
C(18)-C(17)-H(17)	107.7	P(1)-C(17)-H(17)	107.7
C(19)-C(18)-C(17)	111.4(3)	C(19)-C(18)-H(18A)	109.3
C(17)-C(18)-H(18A)	109.3	C(19)-C(18)-H(18B)	109.3
C(17)-C(18)-H(18B)	109.3	H(18A)-C(18)-H(18B)	108.0
C(20)-C(19)-C(18)	112.1(3)	C(20)-C(19)-H(19A)	109.2
C(18)-C(19)-H(19A)	109.2	C(20)-C(19)-H(19B)	109.2
C(18)-C(19)-H(19B)	109.2	H(19A)-C(19)-H(19B)	107.9
C(19)-C(20)-C(21)	110.2(3)	C(19)-C(20)-H(20A)	109.6
C(21)-C(20)-H(20A)	109.6	C(19)-C(20)-H(20B)	109.6
C(21)-C(20)-H(20B)	109.6	H(20A)-C(20)-H(20B)	108.1
C(20)-C(21)-C(22)	111.2(3)	C(20)-C(21)-H(21A)	109.4
C(22)-C(21)-H(21A)	109.4	C(20)-C(21)-H(21B)	109.4
C(22)-C(21)-H(21B)	109.4	H(21A)-C(21)-H(21B)	108.0
C(17)-C(22)-C(21)	111.1(3)	C(17)-C(22)-H(22A)	109.4
C(21)-C(22)-H(22A)	109.4	C(17)-C(22)-H(22B)	109.4
C(21)-C(22)-H(22B)	109.4	H(22A)-C(22)-H(22B)	108.0
C(24)-C(23)-C(28)	110.3(3)	C(24)-C(23)-P(2)	110.2(2)
C(28)-C(23)-P(2)	115.9(2)	C(24)-C(23)-H(23)	106.7
C(28)-C(23)-H(23)	106.7	P(2)-C(23)-H(23)	106.7
C(25)-C(24)-C(23)	110.5(3)	C(25)-C(24)-H(24A)	109.6
C(23)-C(24)-H(24A)	109.6	C(25)-C(24)-H(24B)	109.6
C(23)-C(24)-H(24B)	109.6	H(24A)-C(24)-H(24B)	108.1
C(26)-C(25)-C(24)	110.9(3)	C(26)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25A)	109.5	C(26)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25B)	109.5	H(25A)-C(25)-H(25B)	108.1
C(27)-C(26)-C(25)	110.7(3)	C(27)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26A)	109.5	C(27)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26B)	109.5	H(26A)-C(26)-H(26B)	108.1
C(26)-C(27)-C(28)	111.8(3)	C(26)-C(27)-H(27A)	109.3
C(28)-C(27)-H(27A)	109.3	C(26)-C(27)-H(27B)	109.3
C(28)-C(27)-H(27B)	109.3	H(27A)-C(27)-H(27B)	107.9
C(27)-C(28)-C(23)	111.1(3)	C(27)-C(28)-H(28A)	109.4
C(23)-C(28)-H(28A)	109.4	C(27)-C(28)-H(28B)	109.4
C(23)-C(28)-H(28B)	109.4	H(28A)-C(28)-H(28B)	108.0
C(34)-C(29)-C(30)	110.5(3)	C(34)-C(29)-P(2)	110.1(2)
C(30)-C(29)-P(2)	113.8(2)	C(34)-C(29)-H(29)	107.4
C(30)-C(29)-H(29)	107.4	P(2)-C(29)-H(29)	107.4
C(31)-C(30)-C(29)	111.2(3)	C(31)-C(30)-H(30A)	109.4
C(29)-C(30)-H(30A)	109.4	C(31)-C(30)-H(30B)	109.4
C(29)-C(30)-H(30B)	109.4	H(30A)-C(30)-H(30B)	108.0
C(32)-C(31)-C(30)	111.2(3)	C(32)-C(31)-H(31A)	109.4
C(30)-C(31)-H(31A)	109.4	C(32)-C(31)-H(31B)	109.4

C(30)-C(31)-H(31B)	109.4	H(31A)-C(31)-H(31B)	108.0
C(33)-C(32)-C(31)	110.6(3)	C(33)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32A)	109.5	C(33)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32B)	109.5	H(32A)-C(32)-H(32B)	108.1
C(32)-C(33)-C(34)	111.7(3)	C(32)-C(33)-H(33A)	109.3
C(34)-C(33)-H(33A)	109.3	C(32)-C(33)-H(33B)	109.3
C(34)-C(33)-H(33B)	109.3	H(33A)-C(33)-H(33B)	107.9
C(33)-C(34)-C(29)	111.8(3)	C(33)-C(34)-H(34A)	109.3
C(29)-C(34)-H(34A)	109.3	C(33)-C(34)-H(34B)	109.3
C(29)-C(34)-H(34B)	109.3	H(34A)-C(34)-H(34B)	107.9
C(36)-C(35)-H(35A)	109.5	C(36)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5	C(36)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5	H(35B)-C(35)-H(35C)	109.5
C(41)-C(36)-C(37)	122.2(7)	C(41)-C(36)-C(35)	121.4(7)
C(37)-C(36)-C(35)	116.3(6)	C(36)-C(37)-C(38)	119.2(7)
C(36)-C(37)-H(37)	120.4	C(38)-C(37)-H(37)	120.4
C(37)-C(38)-C(39)	117.1(8)	C(37)-C(38)-H(38)	121.5
C(39)-C(38)-H(38)	121.5	C(40)-C(39)-C(38)	119.2(8)
C(40)-C(39)-H(39)	120.4	C(38)-C(39)-H(39)	120.4
C(41)-C(40)-C(39)	121(1)	C(41)-C(40)-H(40)	119.7
C(39)-C(40)-H(40)	119.7	C(40)-C(41)-C(36)	122(1)
C(40)-C(41)-H(41)	119.2	C(36)-C(41)-H(41)	119.2

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for en95

atom	U11	U22	U33	U23	U13	U12
Pt(1)	26(1)	18(1)	16(1)	0(1)	3(1)	-4(1)
P(1)	21(1)	18(1)	16(1)	-1(1)	3(1)	0(1)
P(2)	23(1)	21(1)	16(1)	1(1)	5(1)	-1(1)
C(1)	24(1)	21(1)	25(1)	1(1)	2(1)	-4(1)
C(2)	30(2)	18(1)	25(1)	1(1)	4(1)	-4(1)
C(3)	31(2)	25(2)	23(1)	3(1)	8(1)	-6(1)
C(4)	40(2)	24(2)	20(1)	3(1)	-4(1)	-11(1)
C(5)	45(2)	26(2)	25(2)	4(1)	-1(1)	-5(2)
C(6)	61(3)	30(2)	29(2)	-1(1)	3(2)	-5(2)
C(7)	66(3)	36(2)	32(2)	3(2)	-7(2)	-14(2)
C(8)	38(2)	47(2)	44(2)	7(2)	-4(2)	-15(2)
C(9)	39(2)	37(2)	35(2)	3(2)	1(2)	-7(2)
C(10)	57(4)	92(5)	98(5)	-3(4)	-8(3)	-22(3)
C(11)	25(1)	21(1)	20(1)	1(1)	2(1)	1(1)
C(12)	28(2)	31(2)	22(1)	-4(1)	1(1)	2(1)
C(13)	30(2)	41(2)	26(2)	-2(1)	-3(1)	7(1)
C(14)	25(2)	41(2)	35(2)	-2(2)	1(1)	8(1)
C(15)	31(2)	33(2)	36(2)	-4(1)	5(1)	12(1)
C(16)	32(2)	28(2)	23(1)	-4(1)	5(1)	4(1)
C(17)	23(1)	24(1)	18(1)	-4(1)	4(1)	1(1)
C(18)	31(2)	31(2)	28(2)	9(1)	10(1)	10(1)
C(19)	36(2)	34(2)	39(2)	2(2)	17(2)	9(2)
C(20)	33(2)	40(2)	35(2)	6(2)	17(1)	9(2)
C(21)	42(2)	43(2)	23(2)	8(1)	15(1)	9(2)
C(22)	31(2)	31(2)	23(1)	4(1)	10(1)	6(1)
C(23)	27(2)	27(2)	21(1)	1(1)	6(1)	1(1)
C(24)	32(2)	41(2)	24(2)	4(1)	9(1)	9(1)
C(25)	47(2)	50(2)	33(2)	9(2)	16(2)	22(2)
C(26)	39(2)	61(3)	34(2)	6(2)	17(2)	16(2)
C(27)	37(2)	49(2)	24(2)	4(2)	14(1)	9(2)
C(28)	31(2)	34(2)	22(1)	4(1)	9(1)	2(1)
C(29)	26(1)	28(2)	17(1)	3(1)	6(1)	-2(1)
C(30)	30(2)	34(2)	19(1)	-1(1)	1(1)	2(1)
C(31)	30(2)	51(2)	24(2)	0(2)	-4(1)	4(2)
C(32)	24(2)	58(3)	37(2)	-2(2)	1(1)	2(2)
C(33)	25(2)	43(2)	37(2)	-2(2)	7(1)	5(1)
C(34)	26(2)	37(2)	27(2)	-3(1)	5(1)	2(1)
C(35)	54(4)	94(5)	121(6)	3(5)	12(4)	-11(3)
C(36)	37(2)	76(4)	78(4)	-1(3)	21(2)	-19(2)
C(37)	46(3)	64(4)	126(6)	-9(4)	46(3)	-14(3)
C(38)	88(6)	160(10)	116(7)	-52(6)	62(5)	-78(6)
C(39)	70(5)	190(10)	83(5)	37(6)	8(4)	-73(6)
C(40)	66(5)	160(10)	137(8)	64(8)	30(5)	-35(5)
C(41)	61(4)	68(4)	164(8)	7(5)	54(5)	-8(3)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table 5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for en95

atom	x	y	z	U(eq)
H(1)	3560(30)	3630(30)	2680(20)	24
H(1A)	746	1053	2687	28
H(1B)	1449	441	2314	28
H(2A)	1922	-321	3151	30
H(2B)	3050	326	3130	30
H(3A)	2354	375	3998	31
H(3B)	1307	1046	3675	31
H(5)	3098	4681	3968	40
H(6)	4327	5763	4556	49
H(7)	6326	5701	4626	57
H(9)	5893	3513	3488	46
H(10A)	7798	5017	3858	129
H(10B)	7763	3868	4009	129
H(10C)	7975	4681	4490	129
H(11)	1293	3343	1900	27
H(12A)	738	1976	1317	33
H(12B)	-101.0000	1588	1701	33
H(13A)	-1233	2431	941	40
H(13B)	-423	3392	1077	40
H(14A)	-1932.9999	2654	1752	42
H(14B)	-2141	3653	1398	42
H(15A)	-1337	3987	2354	40
H(15B)	-509	4398	1970	40
H(16A)	671	3578	2724	34
H(16B)	-127	2608	2611	34
H(17)	2485	1173	1674	26
H(18A)	4620	1476	2481	35
H(18B)	3879	472	2405	35
H(19A)	5505	359	1974	42
H(19B)	4301	203	1534	42
H(20A)	5482	1274	1149	41
H(20B)	5641	1995	1674	41
H(21A)	3482	1659	893	42
H(21B)	4216	2667	948	42
H(22A)	3829	2966	1833	33
H(22B)	2619	2830	1394	33
H(23)	2809	3170	4539	30
H(24A)	1404	3583	3732	38
H(24B)	612	2667	3834	38
H(25A)	1174	4335	4567	50
H(25B)	-86	4133	4180	50
H(26A)	-38	3623	5107	52
H(26B)	-315	2702	4692	52
H(27A)	1110	2216	5467	43
H(27B)	1919	3134	5389	43
H(28A)	1416	1474	4651	34
H(28B)	2662	1712	5042	34
H(29)	4086	934	4577	28
H(30A)	5267	2791	4556	34
H(30B)	4511	2496	4997	34
H(31A)	6542	2279	5383	44
H(31B)	5865	1248	5367	44
H(32A)	7208	1843	4583	49
H(32B)	7583	996	5040	49
H(33A)	6028	-11	4600	42
H(33B)	6775	293	4157	42
H(34A)	4728	460	3781	36
H(34B)	5391	1493	3771	36
H(35A)	-1180	-397	4338	136
H(35B)	-666	702	4429	136
H(35C)	139	-182	4297	136
H(37)	-310	-958	3406	89
H(38)	-950	-738	2440	136
H(39)	-2089	734	2123	140
H(40)	-2515	1841	2773	145
H(41)	-1873	1561	3680	112

4.5 X-Ray Structure of [dcppPt-H]$_2$

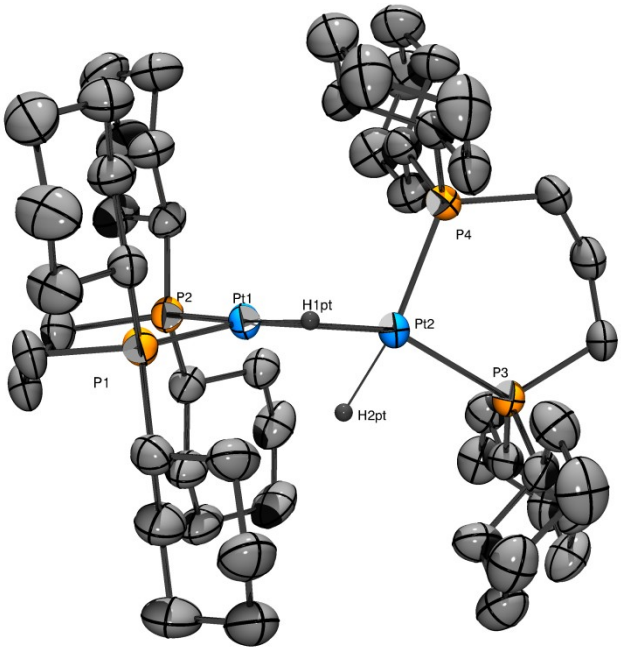


Table 1. Crystal data for en183bis

Compound	en183bis
Molecular formula	$C_{54}H_{102}P_4Pt_2$, C_7H_8
Molecular weight	1357.55
Crystal habit	Green Block
Crystal dimensions(mm)	0.20x0.18x0.10
Crystal system	triclinic
Space group	P-1
a(Å)	11.408(1)
b(Å)	17.246(1)
c(Å)	18.454(1)
α(°)	78.329(1)
β(°)	72.921(1)
γ(°)	85.186(1)
V(Å^3)	3397.7(4)
Z	2
d(g-cm^{-3})	1.327
F(000)	1384
μ(cm^{-1})	4.239
Absorption corrections	multi-scan ; 0.4844 min, 0.6765 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	293(2)
Scan mode	phi and omega scans
Maximum θ	27.48

HKL ranges	-14 14 ; -22 22 ; -20 23
Reflections measured	58812
Unique data	15501
Rint	0.0518
Reflections used	13088
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	555
Reflections / parameter	23
wR2	0.0719
R1	0.0339
Weights a, b	0.0202 ; 6.3036
GoF	1.073
difference peak / hole (e $Å^{-3}$)	1.337(0.099) / -1.124(0.099)

Table 2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for en183bis

atom	x	y	z	U(eq)
Pt(1)	2550(1)	7628(1)	1774(1)	34(1)
Pt(2)	2201(1)	7503(1)	3253(1)	36(1)
P(1)	3033(1)	7116(1)	692(1)	37(1)
P(2)	3092(1)	8892(1)	1235(1)	36(1)
P(3)	2750(1)	7031(1)	4338(1)	40(1)
P(4)	174(1)	7724(1)	3783(1)	42(1)
C(1A)	3688(4)	7768(3)	-249(2)	49(1)
C(2A)	4453(7)	8451(5)	-226(4)	50(2)
C(3A)	3734(4)	9087(3)	171(2)	49(1)
C(1B)	3688(4)	7768(3)	-249(2)	49(1)
C(2B)	3260(10)	8642(7)	-280(6)	50(2)
C(3B)	3734(4)	9087(3)	171(2)	49(1)
C(4)	4249(4)	6328(3)	678(3)	45(1)
C(5)	5382(4)	6645(3)	804(3)	64(1)
C(6)	6414(5)	6006(4)	807(4)	81(2)
C(7)	5945(5)	5273(4)	1400(4)	77(2)
C(8)	4842(5)	4953(3)	1286(4)	69(2)
C(9)	3811(4)	5589(3)	1281(3)	59(1)
C(10)	1780(4)	6637(2)	506(2)	41(1)
C(11)	2148(5)	6223(3)	-185(3)	63(1)
C(12)	1043(5)	5841(4)	-270(4)	74(2)
C(13)	26(5)	6441(4)	-335(3)	73(2)
C(14)	-360(5)	6859(3)	353(3)	64(1)
C(15)	724(4)	7239(3)	456(3)	53(1)
C(16)	4299(4)	9312(3)	1515(3)	44(1)
C(17)	3875(4)	9478(3)	2334(3)	50(1)
C(18)	4903(5)	9802(3)	2555(3)	65(1)
C(19)	6024(5)	9251(4)	2445(4)	77(2)
C(20)	6474(5)	9088(4)	1627(3)	67(2)
C(21)	5448(4)	8756(3)	1412(3)	55(1)
C(22)	1838(4)	9652(2)	1359(3)	43(1)
C(23)	2174(5)	10498(3)	957(3)	62(1)
C(24)	1101(6)	11082(3)	1114(4)	77(2)
C(25)	39(6)	10831(4)	891(4)	78(2)
C(26)	-344(5)	9993(4)	1306(4)	72(2)
C(27)	738(4)	9401(3)	1152(3)	57(1)
C(28A)	1542(4)	6919(3)	5268(2)	53(1)
C(29A)	490(10)	7566(7)	5304(5)	57(2)
C(30A)	-377(4)	7431(3)	4844(2)	54(1)
C(28B)	1542(4)	6919(3)	5268(2)	53(1)
C(29B)	291(8)	6702(6)	5206(5)	57(2)
C(30B)	-377(4)	7431(3)	4844(2)	54(1)
C(31)	3399(4)	6006(3)	4365(3)	47(1)
C(32)	4605(4)	5961(3)	3743(3)	56(1)
C(33)	5110(5)	5111(3)	3743(3)	64(1)
C(34)	4199(5)	4586(3)	3647(3)	67(1)
C(35)	3004(6)	4601(3)	4286(4)	76(2)
C(36)	2476(5)	5445(3)	4289(3)	64(1)
C(37)	3945(4)	7573(3)	4521(2)	43(1)
C(38)	4395(5)	7184(3)	5219(3)	61(1)
C(39)	5392(6)	7682(3)	5313(4)	73(2)
C(40)	4949(6)	8521(3)	5361(3)	71(2)
C(41)	4536(5)	8905(3)	4657(3)	65(1)
C(42)	3531(5)	8432(3)	4560(3)	58(1)
C(43)	-332(4)	8779(3)	3630(3)	47(1)
C(44)	475(5)	9288(3)	3870(3)	61(1)
C(45)	139(6)	10171(3)	3699(4)	75(2)
C(46)	-1215(6)	10325(4)	4070(4)	83(2)
C(47)	-2009(5)	9842(3)	3823(4)	74(2)
C(48)	-1685(4)	8964(3)	3996(3)	62(1)
C(49)	-956(4)	7207(3)	3514(3)	49(1)
C(50)	-673(5)	6324(3)	3614(3)	57(1)
C(51)	-1568(6)	5873(4)	3393(4)	78(2)
C(52)	-1608(6)	6199(4)	2568(3)	79(2)
C(53)	-1908(5)	7077(4)	2459(3)	71(2)
C(54)	-1020(4)	7535(3)	2687(3)	54(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table 3. Bond lengths (A) and angles (deg) for en183bis

Pt(1)-P(1)	2.249(1)	Pt(1)-P(2)	2.260(1)
Pt(1)-Pt(2)	2.6069(2	Pt(1)-H(1PT)	1.48(4)
Pt(2)-P(3)	2.249(1)	Pt(2)-P(4)	2.263(1)
Pt(2)-H(2PT)	1.59(4)	P(1)-C(1A)	1.851(4)
P(1)-C(4)	1.856(4)	P(1)-C(10)	1.857(4)
P(2)-C(16)	1.851(4)	P(2)-C(22)	1.852(4)
P(2)-C(3A)	1.854(4)	P(3)-C(28A)	1.844(4)
P(3)-C(31)	1.854(5)	P(3)-C(37)	1.860(4)
P(4)-C(30A)	1.848(4)	P(4)-C(43)	1.853(5)
P(4)-C(49)	1.859(5)	C(1A)-C(2A)	1.54(1)
C(1A)-H(1A1)	0.9700	C(1A)-H(1A2)	0.9700
C(2A)-C(3A)	1.50(1)	C(2A)-H(2A1)	0.9700
C(2A)-H(2A2)	0.9700	C(3A)-H(3A1)	0.9700
C(3A)-H(3A2)	0.9700	C(2B)-H(2B1)	0.9700
C(2B)-H(2B2)	0.9700	C(4)-C(9)	1.522(6)
C(4)-C(5)	1.539(6)	C(4)-H(4)	0.9800
C(5)-C(6)	1.544(7)	C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700	C(6)-C(7)	1.51(1)
C(6)-H(6A)	0.9700	C(6)-H(6B)	0.9700
C(7)-C(8)	1.501(8)	C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700	C(8)-C(9)	1.540(6)
C(8)-H(8A)	0.9700	C(8)-H(8B)	0.9700
C(9)-H(9A)	0.9700	C(9)-H(9B)	0.9700
C(10)-C(11)	1.520(6)	C(10)-C(15)	1.534(6)
C(10)-H(10)	0.9800	C(11)-C(12)	1.532(7)
C(11)-H(11A)	0.9700	C(11)-H(11B)	0.9700
C(12)-C(13)	1.505(8)	C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700	C(13)-C(14)	1.522(8)
C(13)-H(13A)	0.9700	C(13)-H(13B)	0.9700
C(14)-C(15)	1.523(7)	C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700	C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700	C(16)-C(17)	1.525(6)
C(16)-C(21)	1.546(6)	C(16)-H(16)	0.9800
C(17)-C(18)	1.529(6)	C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700	C(18)-C(19)	1.516(8)
C(18)-H(18A)	0.9700	C(18)-H(18B)	0.9700
C(19)-C(20)	1.521(8)	C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700	C(20)-C(21)	1.527(7)
C(20)-H(20A)	0.9700	C(20)-H(20B)	0.9700
C(21)-H(21A)	0.9700	C(21)-H(21B)	0.9700
C(22)-C(23)	1.522(6)	C(22)-C(27)	1.532(6)
C(22)-H(22)	0.9800	C(23)-C(24)	1.516(7)
C(23)-H(23A)	0.9700	C(23)-H(23B)	0.9700
C(24)-C(25)	1.510(8)	C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700	C(25)-C(26)	1.525(8)
C(25)-H(25A)	0.9700	C(25)-H(25B)	0.9700
C(26)-C(27)	1.532(7)	C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700	C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700	C(28A)-C(29A)	1.56(1)
C(28A)-H(28A)	0.9700	C(28A)-H(28B)	0.9700
C(29A)-C(30A)	1.54(1)	C(29A)-H(29A)	0.9700
C(29A)-H(29B)	0.9700	C(30A)-H(30A)	0.9700
C(30A)-H(30B)	0.9700	C(29B)-H(29C)	0.9700
C(29B)-H(29D)	0.9700	C(31)-C(32)	1.519(6)
C(31)-C(36)	1.542(7)	C(31)-H(31)	0.9800
C(32)-C(33)	1.530(6)	C(32)-H(32A)	0.9700
C(32)-H(32B)	0.9700	C(33)-C(34)	1.504(8)
C(33)-H(33A)	0.9700	C(33)-H(33B)	0.9700
C(34)-C(35)	1.521(8)	C(34)-H(34A)	0.9700
C(34)-H(34B)	0.9700	C(35)-C(36)	1.529(8)
C(35)-H(35A)	0.9700	C(35)-H(35B)	0.9700
C(36)-H(36A)	0.9700	C(36)-H(36B)	0.9700
C(37)-C(42)	1.526(6)	C(37)-C(38)	1.534(6)
C(37)-H(37)	0.9800	C(38)-C(39)	1.549(7)
C(38)-H(38A)	0.9700	C(38)-H(38B)	0.9700
C(39)-C(40)	1.504(8)	C(39)-H(39A)	0.9700
C(39)-H(39B)	0.9700	C(40)-C(41)	1.518(7)
C(40)-H(40A)	0.9700	C(40)-H(40B)	0.9700
C(41)-C(42)	1.532(7)	C(41)-H(41A)	0.9700
C(41)-H(41B)	0.9700	C(42)-H(42A)	0.9700
C(42)-H(42B)	0.9700	C(43)-C(48)	1.528(6)
C(43)-C(44)	1.532(7)	C(43)-H(43)	0.9800
C(44)-C(45)	1.530(7)	C(44)-H(44A)	0.9700
C(44)-H(44B)	0.9700	C(45)-C(46)	1.520(8)
C(45)-H(45A)	0.9700	C(45)-H(45B)	0.9700

C(46)-C(47)	1.499(8)	C(46)-H(46A)	0.9700
C(46)-H(46B)	0.9700	C(47)-C(48)	1.520(7)
C(47)-H(47A)	0.9700	C(47)-H(47B)	0.9700
C(48)-H(48A)	0.9700	C(48)-H(48B)	0.9700
C(49)-C(50)	1.515(7)	C(49)-C(54)	1.536(6)
C(49)-H(49)	0.9800	C(50)-C(51)	1.524(7)
C(50)-H(50A)	0.9700	C(50)-H(50B)	0.9700
C(51)-C(52)	1.525(8)	C(51)-H(51A)	0.9700
C(51)-H(51B)	0.9700	C(52)-C(53)	1.51(1)
C(52)-H(52A)	0.9700	C(52)-H(52B)	0.9700
C(53)-C(54)	1.534(7)	C(53)-H(53A)	0.9700
C(53)-H(53B)	0.9700	C(54)-H(54A)	0.9700
C(54)-H(54B)	0.9700		

P(1)-Pt(1)-P(2)	98.74(4)	P(1)-Pt(1)-Pt(2)	152.18(3)
P(2)-Pt(1)-Pt(2)	106.33(3)	P(1)-Pt(1)-H(1PT)	91(2)
P(2)-Pt(1)-H(1PT)	170(2)	Pt(2)-Pt(1)-H(1PT)	65(2)
P(3)-Pt(2)-P(4)	99.17(4)	P(3)-Pt(2)-Pt(1)	151.26(3)
P(4)-Pt(2)-Pt(1)	107.10(3)	P(3)-Pt(2)-H(2PT)	90(2)
P(4)-Pt(2)-H(2PT)	169(2)	Pt(1)-Pt(2)-H(2PT)	65(2)
C(1A)-P(1)-C(4)	100.8(2)	C(1A)-P(1)-C(10)	102.1(2)
C(4)-P(1)-C(10)	103.7(2)	C(1A)-P(1)-Pt(1)	119.0(2)
C(4)-P(1)-Pt(1)	112.3(1)	C(10)-P(1)-Pt(1)	116.7(1)
C(16)-P(2)-C(22)	103.4(2)	C(16)-P(2)-C(3A)	100.3(2)
C(22)-P(2)-C(3A)	100.9(2)	C(16)-P(2)-Pt(1)	118.2(1)
C(22)-P(2)-Pt(1)	116.2(1)	C(3A)-P(2)-Pt(1)	115.2(2)
C(28A)-P(3)-C(31)	101.2(2)	C(28A)-P(3)-C(37)	102.6(2)
C(31)-P(3)-C(37)	103.2(2)	C(28A)-P(3)-Pt(2)	118.1(2)
C(31)-P(3)-Pt(2)	112.2(2)	C(37)-P(3)-Pt(2)	117.2(1)
C(30A)-P(4)-C(43)	102.0(2)	C(30A)-P(4)-C(49)	99.4(2)
C(43)-P(4)-C(49)	104.0(2)	C(30A)-P(4)-Pt(2)	115.4(2)
C(43)-P(4)-Pt(2)	114.6(2)	C(49)-P(4)-Pt(2)	119.0(2)
C(2A)-C(1A)-P(1)	115.4(4)	C(2A)-C(1A)-H(1A1)	108.4
P(1)-C(1A)-H(1A1)	108.4	C(2A)-C(1A)-H(1A2)	108.4
P(1)-C(1A)-H(1A2)	108.4	H(1A1)-C(1A)-H(1A2)	107.5
C(3A)-C(2A)-C(1A)	114.9(6)	C(3A)-C(2A)-H(2A1)	108.5
C(1A)-C(2A)-H(2A1)	108.5	C(3A)-C(2A)-H(2A2)	108.5
C(1A)-C(2A)-H(2A2)	108.5	H(2A1)-C(2A)-H(2A2)	107.5
C(2A)-C(3A)-P(2)	120.0(4)	C(2A)-C(3A)-H(3A1)	107.3
P(2)-C(3A)-H(3A1)	107.3	C(2A)-C(3A)-H(3A2)	107.3
P(2)-C(3A)-H(3A2)	107.3	H(3A1)-C(3A)-H(3A2)	106.9
H(2B1)-C(2B)-H(2B2)	107.4	C(9)-C(4)-C(5)	109.8(4)
C(9)-C(4)-P(1)	112.4(3)	C(5)-C(4)-P(1)	110.0(3)
C(9)-C(4)-H(4)	108.1	C(5)-C(4)-H(4)	108.1
P(1)-C(4)-H(4)	108.1	C(4)-C(5)-C(6)	111.9(5)
C(4)-C(5)-H(5A)	109.2	C(6)-C(5)-H(5A)	109.2
C(4)-C(5)-H(5B)	109.2	C(6)-C(5)-H(5B)	109.2
H(5A)-C(5)-H(5B)	107.9	C(7)-C(6)-C(5)	110.7(5)
C(7)-C(6)-H(6A)	109.5	C(5)-C(6)-H(6A)	109.5
C(7)-C(6)-H(6B)	109.5	C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	108.1	C(8)-C(7)-C(6)	112.2(5)
C(8)-C(7)-H(7A)	109.2	C(6)-C(7)-H(7A)	109.2
C(8)-C(7)-H(7B)	109.2	C(6)-C(7)-H(7B)	109.2
H(7A)-C(7)-H(7B)	107.9	C(7)-C(8)-C(9)	111.5(5)
C(7)-C(8)-H(8A)	109.3	C(9)-C(8)-H(8A)	109.3
C(7)-C(8)-H(8B)	109.3	C(9)-C(8)-H(8B)	109.3
H(8A)-C(8)-H(8B)	108.0	C(4)-C(9)-C(8)	112.0(4)
C(4)-C(9)-H(9A)	109.2	C(8)-C(9)-H(9A)	109.2
C(4)-C(9)-H(9B)	109.2	C(8)-C(9)-H(9B)	109.2
H(9A)-C(9)-H(9B)	107.9	C(11)-C(10)-C(15)	111.0(4)
C(11)-C(10)-P(1)	116.0(3)	C(15)-C(10)-P(1)	109.6(3)
C(11)-C(10)-H(10)	106.5	C(15)-C(10)-H(10)	106.5
P(1)-C(10)-H(10)	106.5	C(10)-C(11)-C(12)	111.1(4)
C(10)-C(11)-H(11A)	109.4	C(12)-C(11)-H(11A)	109.4
C(10)-C(11)-H(11B)	109.4	C(12)-C(11)-H(11B)	109.4
H(11A)-C(11)-H(11B)	108.0	C(13)-C(12)-C(11)	111.2(5)
C(13)-C(12)-H(12A)	109.4	C(11)-C(12)-H(12A)	109.4
C(13)-C(12)-H(12B)	109.4	C(11)-C(12)-H(12B)	109.4
H(12A)-C(12)-H(12B)	108.0	C(12)-C(13)-C(14)	111.2(5)
C(12)-C(13)-H(13A)	109.4	C(14)-C(13)-H(13A)	109.4
C(12)-C(13)-H(13B)	109.4	C(14)-C(13)-H(13B)	109.4
H(13A)-C(13)-H(13B)	108.0	C(13)-C(14)-C(15)	111.6(4)
C(13)-C(14)-H(14A)	109.3	C(15)-C(14)-H(14A)	109.3
C(13)-C(14)-H(14B)	109.3	C(15)-C(14)-H(14B)	109.3
H(14A)-C(14)-H(14B)	108.0	C(14)-C(15)-C(10)	111.5(4)
C(14)-C(15)-H(15A)	109.3	C(10)-C(15)-H(15A)	109.3

C(14)-C(15)-H(15B)	109.3	C(10)-C(15)-H(15B)	109.3
H(15A)-C(15)-H(15B)	108.0	C(17)-C(16)-C(21)	110.4(4)
C(17)-C(16)-P(2)	113.3(3)	C(21)-C(16)-P(2)	110.0(3)
C(17)-C(16)-H(16)	107.7	C(21)-C(16)-H(16)	107.7
P(2)-C(16)-H(16)	107.7	C(16)-C(17)-C(18)	111.9(4)
C(16)-C(17)-H(17A)	109.2	C(18)-C(17)-H(17A)	109.2
C(16)-C(17)-H(17B)	109.2	C(18)-C(17)-H(17B)	109.2
H(17A)-C(17)-H(17B)	107.9	C(19)-C(18)-C(17)	111.1(4)
C(19)-C(18)-H(18A)	109.4	C(17)-C(18)-H(18A)	109.4
C(19)-C(18)-H(18B)	109.4	C(17)-C(18)-H(18B)	109.4
H(18A)-C(18)-H(18B)	108.0	C(18)-C(19)-C(20)	112.0(4)
C(18)-C(19)-H(19A)	109.2	C(20)-C(19)-H(19A)	109.2
C(18)-C(19)-H(19B)	109.2	C(20)-C(19)-H(19B)	109.2
H(19A)-C(19)-H(19B)	107.9	C(19)-C(20)-C(21)	110.7(4)
C(19)-C(20)-H(20A)	109.5	C(21)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5	C(21)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	108.1	C(20)-C(21)-C(16)	111.6(4)
C(20)-C(21)-H(21A)	109.3	C(16)-C(21)-H(21A)	109.3
C(20)-C(21)-H(21B)	109.3	C(16)-C(21)-H(21B)	109.3
H(21A)-C(21)-H(21B)	108.0	C(23)-C(22)-C(27)	110.4(4)
C(23)-C(22)-P(2)	116.8(3)	C(27)-C(22)-P(2)	110.8(3)
C(23)-C(22)-H(22)	106.0	C(27)-C(22)-H(22)	106.0
P(2)-C(22)-H(22)	106.0	C(24)-C(23)-C(22)	113.0(4)
C(24)-C(23)-H(23A)	109.0	C(22)-C(23)-H(23A)	109.0
C(24)-C(23)-H(23B)	109.0	C(22)-C(23)-H(23B)	109.0
H(23A)-C(23)-H(23B)	107.8	C(25)-C(24)-C(23)	110.6(5)
C(25)-C(24)-H(24A)	109.5	C(23)-C(24)-H(24A)	109.5
C(25)-C(24)-H(24B)	109.5	C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	108.1	C(24)-C(25)-C(26)	111.2(4)
C(24)-C(25)-H(25A)	109.4	C(26)-C(25)-H(25A)	109.4
C(24)-C(25)-H(25B)	109.4	C(26)-C(25)-H(25B)	109.4
H(25A)-C(25)-H(25B)	108.0	C(25)-C(26)-C(27)	111.2(5)
C(25)-C(26)-H(26A)	109.4	C(27)-C(26)-H(26A)	109.4
C(25)-C(26)-H(26B)	109.4	C(27)-C(26)-H(26B)	109.4
H(26A)-C(26)-H(26B)	108.0	C(26)-C(27)-C(22)	111.7(4)
C(26)-C(27)-H(27A)	109.3	C(22)-C(27)-H(27A)	109.3
C(26)-C(27)-H(27B)	109.3	C(22)-C(27)-H(27B)	109.3
H(27A)-C(27)-H(27B)	107.9	C(29A)-C(28A)-P(3)	114.5(4)
C(29A)-C(28A)-H(28A)	108.6	P(3)-C(28A)-H(28A)	108.6
C(29A)-C(28A)-H(28B)	108.6	P(3)-C(28A)-H(28B)	108.6
H(28A)-C(28A)-H(28B)	107.6	C(30A)-C(29A)-C(28A)	111.5(7)
C(30A)-C(29A)-H(29A)	109.3	C(28A)-C(29A)-H(29A)	109.3
C(30A)-C(29A)-H(29B)	109.3	C(28A)-C(29A)-H(29B)	109.3
H(29A)-C(29A)-H(29B)	108.0	C(29A)-C(30A)-P(4)	116.9(5)
C(29A)-C(30A)-H(30A)	108.1	P(4)-C(30A)-H(30A)	108.1
C(29A)-C(30A)-H(30B)	108.1	P(4)-C(30A)-H(30B)	108.1
H(30A)-C(30A)-H(30B)	107.3	H(29C)-C(29B)-H(29D)	107.9
C(32)-C(31)-C(36)	109.8(4)	C(32)-C(31)-P(3)	112.3(3)
C(36)-C(31)-P(3)	110.8(3)	C(32)-C(31)-H(31)	107.9
C(36)-C(31)-H(31)	107.9	P(3)-C(31)-H(31)	107.9
C(31)-C(32)-C(33)	112.3(4)	C(31)-C(32)-H(32A)	109.2
C(33)-C(32)-H(32A)	109.2	C(31)-C(32)-H(32B)	109.2
C(33)-C(32)-H(32B)	109.2	H(32A)-C(32)-H(32B)	107.9
C(34)-C(33)-C(32)	111.3(4)	C(34)-C(33)-H(33A)	109.4
C(32)-C(33)-H(33A)	109.4	C(34)-C(33)-H(33B)	109.4
C(32)-C(33)-H(33B)	109.4	H(33A)-C(33)-H(33B)	108.0
C(33)-C(34)-C(35)	110.0(5)	C(33)-C(34)-H(34A)	109.7
C(35)-C(34)-H(34A)	109.7	C(33)-C(34)-H(34B)	109.7
C(35)-C(34)-H(34B)	109.7	H(34A)-C(34)-H(34B)	108.2
C(34)-C(35)-C(36)	111.0(5)	C(34)-C(35)-H(35A)	109.4
C(36)-C(35)-H(35A)	109.4	C(34)-C(35)-H(35B)	109.4
C(36)-C(35)-H(35B)	109.4	H(35A)-C(35)-H(35B)	108.0
C(35)-C(36)-C(31)	111.8(5)	C(35)-C(36)-H(36A)	109.3
C(31)-C(36)-H(36A)	109.3	C(35)-C(36)-H(36B)	109.3
C(31)-C(36)-H(36B)	109.3	H(36A)-C(36)-H(36B)	107.9
C(42)-C(37)-C(38)	111.2(4)	C(42)-C(37)-P(3)	110.5(3)
C(38)-C(37)-P(3)	115.7(3)	C(42)-C(37)-H(37)	106.3
C(38)-C(37)-H(37)	106.3	P(3)-C(37)-H(37)	106.3
C(37)-C(38)-C(39)	111.2(4)	C(37)-C(38)-H(38A)	109.4
C(39)-C(38)-H(38A)	109.4	C(37)-C(38)-H(38B)	109.4
C(39)-C(38)-H(38B)	109.4	H(38A)-C(38)-H(38B)	108.0
C(40)-C(39)-C(38)	111.5(5)	C(40)-C(39)-H(39A)	109.3
C(38)-C(39)-H(39A)	109.3	C(40)-C(39)-H(39B)	109.3
C(38)-C(39)-H(39B)	109.3	H(39A)-C(39)-H(39B)	108.0
C(39)-C(40)-C(41)	110.7(5)	C(39)-C(40)-H(40A)	109.5
C(41)-C(40)-H(40A)	109.5	C(39)-C(40)-H(40B)	109.5
C(41)-C(40)-H(40B)	109.5	H(40A)-C(40)-H(40B)	108.1

C(40)-C(41)-C(42)	111.6(5)	C(40)-C(41)-H(41A)	109.3
C(42)-C(41)-H(41A)	109.3	C(40)-C(41)-H(41B)	109.3
C(42)-C(41)-H(41B)	109.3	H(41A)-C(41)-H(41B)	108.0
C(37)-C(42)-C(41)	111.4(4)	C(37)-C(42)-H(42A)	109.3
C(41)-C(42)-H(42A)	109.3	C(37)-C(42)-H(42B)	109.3
C(41)-C(42)-H(42B)	109.3	H(42A)-C(42)-H(42B)	108.0
C(48)-C(43)-C(44)	110.0(4)	C(48)-C(43)-P(4)	116.7(3)
C(44)-C(43)-P(4)	110.6(3)	C(48)-C(43)-H(43)	106.3
C(44)-C(43)-H(43)	106.3	P(4)-C(43)-H(43)	106.3
C(45)-C(44)-C(43)	112.0(4)	C(45)-C(44)-H(44A)	109.2
C(43)-C(44)-H(44A)	109.2	C(45)-C(44)-H(44B)	109.2
C(43)-C(44)-H(44B)	109.2	H(44A)-C(44)-H(44B)	107.9
C(46)-C(45)-C(44)	111.1(5)	C(46)-C(45)-H(45A)	109.4
C(44)-C(45)-H(45A)	109.4	C(46)-C(45)-H(45B)	109.4
C(44)-C(45)-H(45B)	109.4	H(45A)-C(45)-H(45B)	108.0
C(47)-C(46)-C(45)	111.6(5)	C(47)-C(46)-H(46A)	109.3
C(45)-C(46)-H(46A)	109.3	C(47)-C(46)-H(46B)	109.3
C(45)-C(46)-H(46B)	109.3	H(46A)-C(46)-H(46B)	108.0
C(46)-C(47)-C(48)	111.2(5)	C(46)-C(47)-H(47A)	109.4
C(48)-C(47)-H(47A)	109.4	C(46)-C(47)-H(47B)	109.4
C(48)-C(47)-H(47B)	109.4	H(47A)-C(47)-H(47B)	108.0
C(47)-C(48)-C(43)	112.5(5)	C(47)-C(48)-H(48A)	109.1
C(43)-C(48)-H(48A)	109.1	C(47)-C(48)-H(48B)	109.1
C(43)-C(48)-H(48B)	109.1	H(48A)-C(48)-H(48B)	107.8
C(50)-C(49)-C(54)	110.2(4)	C(50)-C(49)-P(4)	110.6(3)
C(54)-C(49)-P(4)	112.5(3)	C(50)-C(49)-H(49)	107.8
C(54)-C(49)-H(49)	107.8	P(4)-C(49)-H(49)	107.8
C(49)-C(50)-C(51)	112.7(5)	C(49)-C(50)-H(50A)	109.1
C(51)-C(50)-H(50A)	109.1	C(49)-C(50)-H(50B)	109.1
C(51)-C(50)-H(50B)	109.1	H(50A)-C(50)-H(50B)	107.8
C(50)-C(51)-C(52)	111.2(5)	C(50)-C(51)-H(51A)	109.4
C(52)-C(51)-H(51A)	109.4	C(50)-C(51)-H(51B)	109.4
C(52)-C(51)-H(51B)	109.4	H(51A)-C(51)-H(51B)	108.0
C(53)-C(52)-C(51)	110.8(5)	C(53)-C(52)-H(52A)	109.5
C(51)-C(52)-H(52A)	109.5	C(53)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52B)	109.5	H(52A)-C(52)-H(52B)	108.1
C(52)-C(53)-C(54)	112.0(5)	C(52)-C(53)-H(53A)	109.2
C(54)-C(53)-H(53A)	109.2	C(52)-C(53)-H(53B)	109.2
C(54)-C(53)-H(53B)	109.2	H(53A)-C(53)-H(53B)	107.9
C(53)-C(54)-C(49)	112.0(4)	C(53)-C(54)-H(54A)	109.2
C(49)-C(54)-H(54A)	109.2	C(53)-C(54)-H(54B)	109.2
C(49)-C(54)-H(54B)	109.2	H(54A)-C(54)-H(54B)	107.9

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for en183bis

atom	U11	U22	U33	U23	U13	U12
Pt(1)	33(1)	38(1)	28(1)	-2(1)	-7(1)	-4(1)
Pt(2)	35(1)	43(1)	28(1)	-3(1)	-7(1)	0(1)
P(1)	37(1)	41(1)	32(1)	-6(1)	-7(1)	-4(1)
P(2)	37(1)	40(1)	32(1)	-2(1)	-11(1)	-7(1)
P(3)	38(1)	50(1)	31(1)	-4(1)	-10(1)	1(1)
P(4)	34(1)	53(1)	35(1)	-8(1)	-7(1)	1(1)
C(1A)	54(3)	56(3)	29(2)	-9(2)	0(2)	-9(2)
C(2A)	55(4)	57(4)	31(3)	-5(3)	-2(3)	-8(3)
C(3A)	60(3)	47(2)	37(2)	1(2)	-11(2)	-15(2)
C(1B)	54(3)	56(3)	29(2)	-9(2)	0(2)	-9(2)
C(2B)	55(4)	57(4)	31(3)	-5(3)	-2(3)	-8(3)
C(3B)	60(3)	47(2)	37(2)	1(2)	-11(2)	-15(2)
C(4)	40(2)	53(3)	44(2)	-16(2)	-11(2)	0(2)
C(5)	44(3)	75(4)	71(3)	-8(3)	-17(2)	-6(2)
C(6)	41(3)	103(5)	93(5)	-13(4)	-19(3)	8(3)
C(7)	61(3)	102(5)	68(4)	-20(3)	-23(3)	28(3)
C(8)	68(3)	60(3)	80(4)	-12(3)	-26(3)	17(3)
C(9)	47(3)	51(3)	72(3)	-5(2)	-15(2)	6(2)
C(10)	42(2)	44(2)	36(2)	-7(2)	-10(2)	-5(2)
C(11)	54(3)	78(4)	66(3)	-35(3)	-17(2)	-4(3)
C(12)	61(3)	94(4)	86(4)	-49(4)	-26(3)	-9(3)
C(13)	60(3)	108(5)	62(3)	-23(3)	-26(3)	-19(3)
C(14)	47(3)	78(4)	71(4)	-14(3)	-21(2)	-4(2)
C(15)	47(3)	58(3)	57(3)	-12(2)	-19(2)	0(2)
C(16)	43(2)	45(2)	46(2)	-1(2)	-17(2)	-11(2)
C(17)	52(3)	54(3)	46(2)	-5(2)	-19(2)	-12(2)
C(18)	82(4)	59(3)	65(3)	-9(3)	-38(3)	-17(3)
C(19)	73(4)	94(4)	77(4)	1(3)	-49(3)	-18(3)
C(20)	48(3)	82(4)	72(4)	6(3)	-28(3)	-10(3)
C(21)	42(2)	65(3)	60(3)	-3(2)	-19(2)	-8(2)
C(22)	43(2)	42(2)	46(2)	-7(2)	-19(2)	-5(2)
C(23)	65(3)	44(3)	77(4)	0(2)	-28(3)	-6(2)
C(24)	86(4)	50(3)	100(5)	-7(3)	-45(4)	13(3)
C(25)	81(4)	79(4)	80(4)	-12(3)	-42(3)	26(3)
C(26)	53(3)	82(4)	85(4)	-13(3)	-28(3)	12(3)
C(27)	48(3)	60(3)	67(3)	-11(2)	-25(2)	0(2)
C(28A)	47(2)	73(3)	29(2)	4(2)	-6(2)	2(2)
C(29A)	53(4)	79(5)	35(3)	-8(3)	-6(3)	-3(4)
C(30A)	41(2)	81(3)	34(2)	-10(2)	-2(2)	4(2)
C(28B)	47(2)	73(3)	29(2)	4(2)	-6(2)	2(2)
C(29B)	53(4)	79(5)	35(3)	-8(3)	-6(3)	-3(4)
C(30B)	41(2)	81(3)	34(2)	-10(2)	-2(2)	4(2)
C(31)	50(3)	49(2)	41(2)	-1(2)	-19(2)	-2(2)
C(32)	46(3)	47(3)	73(3)	-11(2)	-17(2)	5(2)
C(33)	68(3)	59(3)	70(4)	-15(3)	-29(3)	14(3)
C(34)	90(4)	49(3)	64(3)	-12(3)	-26(3)	2(3)
C(35)	100(5)	51(3)	74(4)	-13(3)	-17(3)	-19(3)
C(36)	59(3)	65(3)	66(3)	-14(3)	-10(3)	-13(3)
C(37)	45(2)	48(2)	38(2)	-11(2)	-13(2)	-1(2)
C(38)	75(3)	59(3)	62(3)	-5(2)	-41(3)	-2(3)
C(39)	92(4)	74(4)	71(4)	-7(3)	-52(3)	-12(3)
C(40)	94(4)	68(3)	62(3)	-15(3)	-32(3)	-16(3)
C(41)	81(4)	54(3)	66(3)	-17(3)	-25(3)	-5(3)
C(42)	66(3)	51(3)	57(3)	-13(2)	-20(2)	7(2)
C(43)	42(2)	57(3)	42(2)	-13(2)	-10(2)	3(2)
C(44)	60(3)	62(3)	66(3)	-18(3)	-25(3)	4(2)
C(45)	87(4)	61(3)	85(4)	-26(3)	-30(3)	1(3)
C(46)	93(5)	76(4)	85(4)	-41(4)	-25(4)	22(3)
C(47)	65(3)	75(4)	87(4)	-32(3)	-22(3)	22(3)
C(48)	44(3)	69(3)	71(3)	-21(3)	-11(2)	10(2)
C(49)	38(2)	63(3)	44(2)	-12(2)	-8(2)	-2(2)
C(50)	62(3)	60(3)	48(3)	-4(2)	-12(2)	-13(2)
C(51)	93(4)	71(4)	74(4)	-8(3)	-24(3)	-36(3)
C(52)	91(4)	89(4)	63(4)	-14(3)	-24(3)	-33(4)
C(53)	62(3)	95(4)	65(3)	-14(3)	-28(3)	-15(3)
C(54)	52(3)	66(3)	49(3)	-10(2)	-19(2)	3(2)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table 5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for en183bis

atom	x	y	z	U(eq)
H(1PT)	2100(40)	6860(30)	2250(30)	51
H(2PT)	3590(40)	7480(30)	2750(30)	54
H(1A1)	4201	7446	-601	58
H(1A2)	3019	7991	-458	58
H(2A1)	5069	8234	31	60
H(2A2)	4880	8688	-752	60
H(3A1)	3055	9246	-48.0000	59
H(3A2)	4258	9540	34	59
H(1B1)	4575	7740	-366	58
H(1B2)	3468	7569	-646	58
H(2B1)	3493	8910	-815	60
H(2B2)	2369	8661	-99	60
H(3B1)	3610	9647	-14.0000	59
H(3B2)	4613	8985	54	59
H(4)	4491	6179	168	54
H(5A)	5146	6828	1292	77
H(5B)	5687	7094	397	77
H(6A)	6720	5868	299	97
H(6B)	7087	6215	923	97
H(7A)	6593	4868	1367	93
H(7B)	5734	5400	1912	93
H(8A)	4541	4507	1698	83
H(8B)	5076	4764	801	83
H(9A)	3134	5371	1175	70
H(9B)	3513	5732	1787	70
H(10)	1460	6228	961	49
H(11A)	2773	5819	-121	75
H(11B)	2493	6605	-650	75
H(12A)	1296	5601	-726	88
H(12B)	746	5425	174	88
H(13A)	-674	6178	-364	87
H(13B)	299	6829	-806	87
H(14A)	-719.9999	6480	817	77
H(14B)	-980	7264	280	77
H(15A)	460	7460	923	63
H(15B)	1013	7669	24	63
H(16)	4533	9817	1162	53
H(17A)	3586	8993	2692	60
H(17B)	3193	9859	2377	60
H(18A)	5125	10319	2238	77
H(18B)	4615	9864	3089	77
H(19A)	5824	8755	2806	92
H(19B)	6676	9487	2560	92
H(20A)	7160	8711	1588	81
H(20B)	6757	9574	1269	81
H(21A)	5230	8241	1734	66
H(21B)	5739	8687	879	66
H(22)	1556	9662	1913	51
H(23A)	2828	10659	1129	74
H(23B)	2482	10515	406	74
H(24A)	844	11111	1658	92
H(24B)	1353	11604	822	92
H(25A)	273	10852	337	94
H(25B)	-652	11196	1018	94
H(26A)	-999	9838	1132	87
H(26B)	-656	9984	1857	87
H(27A)	980	9361	611	68
H(27B)	483	8883	1454	68
H(28A)	1184	6403	5371	63
H(28B)	1917	6933	5674	63
H(29A)	26	7557	5838	69
H(29B)	847	8085	5097	69
H(30A)	-1142	7718	5023	65
H(30B)	-559	6872	4967	65
H(28C)	1798	6510	5639	63
H(28D)	1444	7411	5460	63
H(29C)	-223	6486	5717	69
H(29D)	420	6297	4893	69
H(30C)	-299	7878	5070	65
H(30D)	-1243	7320	4985	65
H(31)	3555	5823	4867	56

H(32A)	5202	6279	3824	67
H(32B)	4484	6183	3243	67
H(33A)	5861	5108	3325	77
H(33B)	5305	4904	4224	77
H(34A)	4530	4048	3665	80
H(34B)	4047	4768	3149	80
H(35A)	3150	4383	4781	91
H(35B)	2415	4272	4212	91
H(36A)	1736	5440	4716	77
H(36B)	2255	5642	3815	77
H(37)	4660	7589	4066	52
H(38A)	4729	6659	5154	74
H(38B)	3708	7130	5683	74
H(39A)	5616	7442	5778	88
H(39B)	6118	7682	4878	88
H(40A)	5605	8823	5394	85
H(40B)	4271	8526	5823	85
H(41A)	5233	8940	4200	78
H(41B)	4229	9438	4708	78
H(42A)	2801	8446	4990	69
H(42B)	3323	8677	4090	69
H(43)	-185	8951	3072	57
H(44A)	385	9124	4417	73
H(44B)	1328	9203	3595	73
H(45A)	626	10467	3895	90
H(45B)	328	10353	3146	90
H(46A)	-1384	10197	4627	99
H(46B)	-1412.9999	10883	3929	99
H(47A)	-1905	10008	3274	89
H(47B)	-2863	9932	4091	89
H(48A)	-2184	8671	3805	75
H(48B)	-1878	8787	4550	75
H(49)	-1767	7288	3865	58
H(50A)	-701	6118	4149	69
H(50B)	152	6233	3299	69
H(51A)	-2382	5914	3744	94
H(51B)	-1321	5317	3440	94
H(52A)	-819	6103	2211	94
H(52B)	-2223	5926	2454	94
H(53A)	-2737.9998	7165	2769	85
H(53B)	-1872	7277	1922	85
H(54A)	-1282	8088	2647	65
H(54B)	-207	7506	2331	65

5 Computational Details

5.1 Generalities

All calculations were performed using the Gaussian 09[8] series of programs. The ω-B97XD[9,10] functional was used in combination with the 6-31G*[11,12] basis set for all main group elements, except hydrogen atoms involved in the mechanism (i.e. hydrides, H_2, and one H of benzene) for which the 6-311+G** basis set[13,14] has been used, and the Def2-TZVP[15,16] basis set and electron core potential for Platinum. The stationary points and transition states were characterized by full vibration frequencies calculations, with no imaginary frequency for minima (stationary point), and one imaginary frequency for transition states.

5.2 Computed Structure of benzene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.061546	-1.391067	0.000000
2	6	0	-1.174623	-0.749330	0.000009
3	6	0	-1.236228	0.642350	-0.000012
4	6	0	-0.061512	1.391524	0.000001
5	6	0	1.174608	0.749155	0.000009
6	6	0	1.236202	-0.642622	-0.000007
7	1	0	0.110214	-2.476073	-0.000001
8	1	0	-2.090380	-1.333375	0.000014
9	1	0	-2.200174	1.143106	-0.000004
10	1	0	-0.110281	2.476706	0.000000
11	1	0	2.090624	1.332966	0.000009
12	1	0	2.200032	-1.143398	-0.000015

	1	2	3
	A	A	A
Frequencies --	415.8956	416.4576	624.4532
Red. masses --	2.9110	2.8959	6.0748
Frc consts --	0.2967	0.2959	1.3957
IR Inten --	0.0168	0.0001	0.0001

Sum of electronic and zero-point Energies= -232.061211
Sum of electronic and thermal Energies= -232.056854
Sum of electronic and thermal Enthalpies= -232.055910
Sum of electronic and thermal Free Energies= -232.088656

HF=-2 32.1629574

5.3 Computed Structure of biphenyl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.850211	-1.125669	0.424371
2	6	0	-3.551370	0.000002	-0.000005
3	6	0	-1.459148	-1.124657	0.425133
4	6	0	-2.850198	1.125678	-0.424377
5	1	0	-4.637372	0.000011	-0.000011
6	6	0	-0.742675	-0.000008	0.000004
7	1	0	-0.919927	-1.998057	0.781567
8	6	0	-1.459144	1.124657	-0.425129
9	1	0	-3.387420	2.006156	-0.764756
10	1	0	-0.919902	1.998049	-0.781551
11	6	0	0.742675	0.000000	0.000009
12	6	0	1.459143	1.124654	0.425133
13	6	0	1.459148	-1.124660	-0.425129
14	6	0	2.850208	1.125672	0.424372
15	1	0	0.919919	1.998054	0.781561
16	6	0	2.850201	-1.125674	-0.424377
17	1	0	0.919911	-1.998053	-0.781556
18	6	0	3.551370	0.000004	-0.000002
19	1	0	3.387420	2.006158	0.764748
20	1	0	4.637372	-0.000002	-0.000010
21	1	0	3.387429	-2.006151	-0.764757
22	1	0	-3.387430	-2.006151	0.764751

	1	2	3
	A	A	A
Frequencies --	72.0897	92.6400	124.6178
Red. masses --	3.7028	4.3194	4.0335
Frc consts --	0.0113	0.0218	0.0369
IR Inten --	0.0000	0.7708	0.0916

Sum of electronic and zero-point Energies= -462.953685
Sum of electronic and thermal Energies= -462.944877
Sum of electronic and thermal Enthalpies= -462.943933
Sum of electronic and thermal Free Energies= -462.988229

HF=-463.137661

5.4 Computed Structure of H_2

5.5 Computed Structure of A (dcppPt)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.938162	-0.141200	0.240989
2	78	0	-0.000010	-0.207761	-0.870445
3	6	0	-1.315795	-0.320988	1.999424
4	1	0	-2.101717	0.010566	2.690097
5	1	0	-1.182445	-1.395952	2.174804
6	6	0	0.000008	0.411859	2.347517
7	1	0	0.000009	0.562339	3.434670
8	1	0	-0.000012	1.417315	1.906841
9	6	0	1.315833	-0.320947	1.999415
10	1	0	1.182537	-1.395912	2.174832
11	1	0	2.101757	0.010663	2.690059
12	15	0	1.938158	-0.141196	0.240961
13	6	0	-3.175259	-1.537921	0.142355
14	6	0	-4.062521	-1.854978	1.357530
15	6	0	-4.019284	-1.450654	-1.138450
16	1	0	-2.493271	-2.393955	0.014442
17	6	0	-4.834229	-3.160710	1.126127
18	1	0	-4.782007	-1.046021	1.526636
19	1	0	-3.461728	-1.940140	2.269523
20	6	0	-4.804682	-2.746041	-1.368306
21	1	0	-4.728182	-0.614426	-1.054964
22	1	0	-3.372444	-1.236903	-1.997779
23	6	0	-5.670795	-3.097321	-0.154983
24	1	0	-5.476386	-3.373566	1.989234
25	1	0	-4.118335	-3.991699	1.051113
26	1	0	-5.426522	-2.654429	-2.266577
27	1	0	-4.094205	-3.563224	-1.556588
28	1	0	-6.186546	-4.050757	-0.318654
29	1	0	-6.450775	-2.331156	-0.036009
30	6	0	3.175220	-1.537947	0.142333
31	6	0	4.019488	-1.450507	-1.138300
32	6	0	4.062226	-1.855275	1.357624
33	1	0	2.493216	-2.393927	0.014151
34	6	0	4.804858	-2.745899	-1.368230
35	1	0	4.728415	-0.614330	-1.054543
36	1	0	3.372818	-1.236575	-1.997712
37	6	0	4.833886	-3.161019	1.126137
38	1	0	4.781736	-1.046401	1.527011
39	1	0	3.461248	-1.940555	2.269485
40	6	0	5.670708	-3.097453	-0.154799
41	1	0	5.426880	-2.654163	-2.266363
42	1	0	4.094369	-3.563005	-1.556801
43	1	0	5.475861	-3.374076	1.989330
44	1	0	4.117950	-3.991946	1.050831
45	1	0	6.186430	-4.050893	-0.318539
46	1	0	6.450714	-2.331361	-0.035532
47	6	0	2.835264	1.494947	0.330310
48	6	0	4.132821	1.544681	1.148248
49	6	0	3.053528	2.103581	-1.064854
50	1	0	2.093279	2.130550	0.841508
51	6	0	4.663004	2.978625	1.257194
52	1	0	4.895284	0.928901	0.653307
53	1	0	3.984803	1.122834	2.149400
54	6	0	3.598272	3.532273	-0.965452
55	1	0	3.761184	1.481588	-1.630419
56	1	0	2.109761	2.089498	-1.621205
57	6	0	4.878882	3.593038	-0.128323
58	1	0	5.599065	2.988435	1.828382
59	1	0	3.941887	3.589608	1.818668
60	1	0	3.779891	3.934407	-1.969056

61	1	0	2.834160	4.173445	-0.502690
62	1	0	5.225623	4.628933	-0.034881
63	1	0	5.674827	3.038250	-0.645994
64	6	0	-2.835262	1.494936	0.330392
65	6	0	-3.053170	2.103822	-1.064718
66	6	0	-4.133026	1.544532	1.148013
67	1	0	-2.093390	2.130440	0.841879
68	6	0	-3.597912	3.532504	-0.965191
69	1	0	-3.760699	1.481946	-1.630569
70	1	0	-2.109265	2.089824	-1.620839
71	6	0	-4.663228	2.978460	1.257081
72	1	0	-4.895367	0.928841	0.652770
73	1	0	-3.985265	1.122502	2.149125
74	6	0	-4.878736	3.593133	-0.128379
75	1	0	-3.779269	3.934826	-1.968767
76	1	0	-2.833908	4.173578	-0.502117
77	1	0	-5.599438	2.988174	1.828027
78	1	0	-3.942252	3.589333	1.818856
79	1	0	-5.225485	4.629016	-0.034835
80	1	0	-5.674558	3.038455	-0.646359

	1	2	3
	A	A	A
Frequencies --	14.8766	30.3521	49.4441
Red. masses --	5.0270	4.0165	3.9432
Frc consts --	0.0007	0.0022	0.0057
IR Inten --	0.1001	0.0028	0.0553

Sum of electronic and zero-point Energies= -1860.160616
Sum of electronic and thermal Energies= -1860.128645
Sum of electronic and thermal Enthalpies= -1860.127701
Sum of electronic and thermal Free Energies= -1860.224047

HF=-1860.9055876

5.6 Computed Structure of B (dcppPt-EtaBenzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.723200	0.199462	0.648183
2	78	0	-0.000247	-0.813297	-0.492956
3	6	0	-1.312230	0.411684	2.447312
4	1	0	-2.132189	0.931992	2.956188
5	1	0	-1.267793	-0.599618	2.872212
6	6	0	0.000571	1.151942	2.756303
7	1	0	0.001152	1.368498	3.832021
8	1	0	0.001014	2.134748	2.267752
9	6	0	1.312169	0.409901	2.446320
10	1	0	1.266147	-0.601739	2.870242
11	1	0	2.132859	0.928495	2.955718
12	15	0	1.723312	0.198675	0.647031
13	6	0	-3.299111	-0.796984	0.719515
14	6	0	-4.300996	-0.528522	1.853240
15	6	0	-4.006679	-0.803233	-0.644670
16	1	0	-2.895768	-1.811703	0.870069
17	6	0	-5.443036	-1.552729	1.819778
18	1	0	-4.722150	0.479656	1.756588
19	1	0	-3.804308	-0.574550	2.828368
20	6	0	-5.145107	-1.826978	-0.671159
21	1	0	-4.425316	0.193063	-0.844725
22	1	0	-3.280869	-1.013483	-1.438308
23	6	0	-6.145198	-1.572436	0.459599
24	1	0	-6.163001	-1.333726	2.617259
25	1	0	-5.032280	-2.550947	2.027401
26	1	0	-5.651001	-1.799852	-1.643258
27	1	0	-4.722574	-2.835662	-0.559989
28	1	0	-6.933791	-2.333613	0.450644
29	1	0	-6.637101	-0.602897	0.294061
30	6	0	3.298811	-0.798538	0.718099
31	6	0	4.007742	-0.802700	-0.645335
32	6	0	4.299930	-0.532480	1.853077
33	1	0	2.894901	-1.813348	0.866420
34	6	0	5.145182	-1.827514	-0.672648
35	1	0	4.427663	0.193565	-0.842892
36	1	0	3.282619	-1.010504	-1.440192
37	6	0	5.441460	-1.557249	1.818900
38	1	0	4.721610	0.475677	1.758402
39	1	0	3.802563	-0.579943	2.827778
40	6	0	6.144637	-1.575497	0.459231
41	1	0	5.651847	-1.799365	-1.644326
42	1	0	4.721594	-2.835960	-0.563310
43	1	0	6.160967	-1.339816	2.617227

44	1	0	5.029957	-2.555515	2.024813
45	1	0	6.932655	-2.337265	0.449758
46	1	0	6.637385	-0.606095	0.295450
47	6	0	2.101971	1.950506	0.130999
48	6	0	3.331375	2.628143	0.750042
49	6	0	2.098021	2.124447	-1.397345
50	1	0	1.211822	2.486318	0.498798
51	6	0	3.378483	4.114499	0.377090
52	1	0	4.241777	2.140700	0.376911
53	1	0	3.335321	2.515479	1.840702
54	6	0	2.149569	3.607916	-1.774612
55	1	0	2.963913	1.608442	-1.832097
56	1	0	1.206225	1.648581	-1.819976
57	6	0	3.356148	4.307623	-1.141977
58	1	0	4.272471	4.580927	0.807536
59	1	0	2.510421	4.622995	0.820823
60	1	0	2.174261	3.718088	-2.864952
61	1	0	1.226082	4.095646	-1.429203
62	1	0	3.350653	5.375965	-1.388051
63	1	0	4.278068	3.888589	-1.570082
64	6	0	-2.100853	1.951060	0.130530
65	6	0	-2.095028	2.123704	-1.397976
66	6	0	-3.330899	2.629434	0.747464
67	1	0	-1.211100	2.487046	0.499044
68	6	0	-2.145774	3.606845	-1.776581
69	1	0	-2.960514	1.607487	-1.833296
70	1	0	-1.202889	1.647174	-1.819176
71	6	0	-3.377166	4.115494	0.373239
72	1	0	-4.240925	2.141906	0.373542
73	1	0	-3.336247	2.517610	1.838214
74	6	0	-3.352931	4.307383	-1.145966
75	1	0	-2.169112	3.716092	-2.867042
76	1	0	-1.222571	4.094632	-1.430477
77	1	0	-4.271566	4.582468	0.802232
78	1	0	-2.509526	4.624144	0.817629
79	1	0	-3.346859	5.375527	-1.392893
80	1	0	-4.274441	3.888243	-1.574844
81	6	0	1.405457	-3.437048	-1.170852
82	6	0	0.718517	-4.409534	-0.514844
83	6	0	0.728944	-2.328431	-1.820475
84	6	0	-0.719714	-4.410146	-0.512976
85	1	0	1.250255	-5.222413	-0.027267
86	6	0	-0.734040	-2.328600	-1.816814
87	6	0	-1.408934	-3.437986	-1.166936
88	1	0	-1.249607	-5.224536	-0.025924
89	1	0	-1.259421	-1.866520	-2.651598
90	1	0	-2.494641	-3.484438	-1.228148
91	1	0	2.491092	-3.483279	-1.234828
92	1	0	1.250082	-1.871716	-2.662021

	1	2	3
	A	A	A
Frequencies --	26.1230	30.3581	37.6852
Red. masses --	4.9354	4.0783	4.8458
Frc consts --	0.0020	0.0022	0.0041
IR Inten --	0.1020	0.0194	0.1508

Sum of electronic and zero-point Energies= -2092.261495
Sum of electronic and thermal Energies= -2092.224333
Sum of electronic and thermal Enthalpies= -2092.223389
Sum of electronic and thermal Free Energies= -2092.329888

HF=-2093.1102801

5.7 Computed Structure of C (dcppPt-H-C_6H_5)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.003719	-0.118475	0.668833
2	78	0	-0.093092	-1.041891	-0.267704
3	6	0	-1.816038	0.373168	2.444576
4	1	0	-2.752458	0.812652	2.804761
5	1	0	-1.667748	-0.559204	3.004528
6	6	0	-0.665201	1.341133	2.756211
7	1	0	-0.789900	1.665936	3.796556
8	1	0	-0.765029	2.255232	2.157881
9	6	0	0.757333	0.776775	2.627635
10	1	0	0.823572	-0.168607	3.181534
11	1	0	1.450048	1.473629	3.110741
12	15	0	1.355544	0.413893	0.910028
13	6	0	-3.427646	-1.322310	0.727008
14	6	0	-4.520754	-1.089459	1.782739

15	6	0	-4.049578	-1.536634	-0.663215
16	1	0	-2.907031	-2.255906	0.988604
17	6	0	-5.526077	-2.248708	1.787178
18	1	0	-5.052341	-0.151590	1.577908
19	1	0	-4.083138	-0.995032	2.782129
20	6	0	-5.046846	-2.698434	-0.646940
21	1	0	-4.580785	-0.625886	-0.971930
22	1	0	-3.261059	-1.721178	-1.400461
23	6	0	-6.137500	-2.475648	0.403098
24	1	0	-6.311739	-2.052799	2.526467
25	1	0	-5.011009	-3.165170	2.108033
26	1	0	-5.492688	-2.818410	-1.641098
27	1	0	-4.509164	-3.630817	-0.426217
28	1	0	-6.826412	-3.327895	0.427758
29	1	0	-6.733511	-1.594701	0.122809
30	6	0	3.087390	-0.218213	1.205138
31	6	0	3.980896	-0.092194	-0.042396
32	6	0	3.822404	0.307227	2.450594
33	1	0	2.910772	-1.294075	1.351700
34	6	0	5.308146	-0.826897	0.158884
35	1	0	4.193948	0.968400	-0.233433
36	1	0	3.470916	-0.490046	-0.922418
37	6	0	5.166514	-0.408997	2.636576
38	1	0	3.998647	1.386912	2.355594
39	1	0	3.219440	0.161031	3.352716
40	6	0	6.048532	-0.304867	1.390862
41	1	0	5.925448	-0.718857	-0.740063
42	1	0	5.103165	-1.899456	0.271228
43	1	0	5.683371	0.003215	3.511437
44	1	0	4.975219	-1.469862	2.851656
45	1	0	6.984347	-0.855240	1.542948
46	1	0	6.322466	0.748251	1.229874
47	6	0	1.425662	2.109074	0.142159
48	6	0	2.388125	3.124586	0.774329
49	6	0	1.603505	2.046651	-1.385514
50	1	0	0.403093	2.482175	0.312246
51	6	0	2.213949	4.509162	0.139078
52	1	0	3.423102	2.793166	0.625453
53	1	0	2.229425	3.191315	1.857372
54	6	0	1.437316	3.434535	-2.009288
55	1	0	2.596087	1.652606	-1.631752
56	1	0	0.878760	1.343645	-1.810344
57	6	0	2.393838	4.451031	-1.380503
58	1	0	2.926741	5.214856	0.581699
59	1	0	1.207712	4.887798	0.370310
60	1	0	1.596982	3.376783	-3.091940
61	1	0	0.402045	3.774221	-1.860140
62	1	0	2.238985	5.443499	-1.819414
63	1	0	3.429556	4.161372	-1.608335
64	6	0	-2.550450	1.472320	-0.132083
65	6	0	-2.443607	1.423418	-1.666792
66	6	0	-3.904270	2.050548	0.305465
67	1	0	-1.774383	2.178101	0.204078
68	6	0	-2.674807	2.809888	-2.273384
69	1	0	-3.185943	0.723387	-2.069127
70	1	0	-1.462625	1.033471	-1.958177
71	6	0	-4.126796	3.438854	-0.306367
72	1	0	-4.710906	1.384796	-0.026867
73	1	0	-3.972024	2.111003	1.398211
74	6	0	-4.017611	3.398652	-1.832967
75	1	0	-2.620813	2.751413	-3.366371
76	1	0	-1.865375	3.481934	-1.952921
77	1	0	-5.106082	3.827048	-0.002778
78	1	0	-3.373549	4.133623	0.092684
79	1	0	-4.149747	4.403750	-2.249919
80	1	0	-4.831934	2.779179	-2.235167
81	1	0	-1.011030	-2.073816	-1.078777
82	6	0	1.444285	-2.042075	-1.207926
83	6	0	2.181656	-3.052484	-0.567155
84	6	0	1.847744	-1.709753	-2.513686
85	6	0	3.278413	-3.665766	-1.172429
86	1	0	1.897496	-3.368314	0.435361
87	6	0	2.946423	-2.312084	-3.124625
88	1	0	1.298611	-0.949281	-3.065575
89	6	0	3.676547	-3.289819	-2.452506
90	1	0	3.825298	-4.441067	-0.639637
91	1	0	4.535476	-3.759708	-2.923937
92	1	0	3.232528	-2.017341	-4.132006

	1	2	3
	A	A	A
Frequencies --	23.9113	33.7560	35.5246
Red. masses --	4.7278	4.2501	4.8189
Frc consts --	0.0016	0.0029	0.0036
IR Inten --	0.1043	0.1142	0.0501

Sum of electronic and zero-point Energies= -2092.271234

```
 Sum of electronic and thermal Energies=             -2092.234278
 Sum of electronic and thermal Enthalpies=           -2092.233333
 Sum of electronic and thermal Free Energies=        -2092.338714

HF=-2093.1190831
```

5.8 Computed Structure of D (dcppPt-bisBenzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.710152	0.683617	-0.864037
2	78	0	-0.000015	-0.752403	-0.089706
3	6	0	1.301172	1.526832	-2.462842
4	1	0	2.127956	2.186762	-2.743891
5	1	0	1.254158	0.737985	-3.224455
6	6	0	-0.000043	2.338053	-2.493290
7	1	0	-0.000053	2.913040	-3.427583
8	1	0	-0.000056	3.089610	-1.694363
9	6	0	-1.301230	1.526783	-2.462850
10	1	0	-1.254150	0.737914	-3.224440
11	1	0	-2.128041	2.186654	-2.743951
12	15	0	-1.710210	0.683617	-0.864009
13	6	0	3.344643	-0.136957	-1.252969
14	6	0	4.213840	0.520411	-2.340065
15	6	0	4.192673	-0.419835	0.000555
16	1	0	3.018152	-1.115373	-1.634572
17	6	0	5.430945	-0.354354	-2.668910
18	1	0	4.556723	1.507359	-2.000903
19	1	0	3.643105	0.679788	-3.260171
20	6	0	5.387101	-1.313233	-0.342546
21	1	0	4.569368	0.527644	0.409226
22	1	0	3.590205	-0.895661	0.775736
23	6	0	6.260927	-0.679492	-1.425372
24	1	0	6.048526	0.146404	-3.424117
25	1	0	5.078090	-1.292668	-3.119772
26	1	0	5.971059	-1.506462	0.564412
27	1	0	5.009841	-2.285462	-0.685158
28	1	0	7.091607	-1.344177	-1.690056
29	1	0	6.707228	0.247089	-1.035415
30	6	0	-3.344729	-0.136935	-1.252892
31	6	0	-4.192755	-0.419806	0.000632
32	6	0	-4.213919	0.520404	-2.340021
33	1	0	-3.018259	-1.115364	-1.634477
34	6	0	-5.387199	-1.313184	-0.342461
35	1	0	-4.569430	0.527675	0.409310
36	1	0	-3.590289	-0.895647	0.775814
37	6	0	-5.431009	-0.354382	-2.668858
38	1	0	-4.556821	1.507355	-2.000889
39	1	0	-3.643156	0.679772	-3.260110
40	6	0	-6.261005	-0.679469	-1.425318
41	1	0	-5.971180	-1.506372	0.564491
42	1	0	-5.009956	-2.285430	-0.685037
43	1	0	-6.048585	0.146334	-3.424096
44	1	0	-5.078135	-1.292713	-3.119675
45	1	0	-7.091684	-1.344163	-1.689984
46	1	0	-6.707303	0.247127	-1.035398
47	6	0	-1.993964	2.124398	0.279709
48	6	0	-3.132124	3.088857	-0.084856
49	6	0	-2.071714	1.697645	1.756263
50	1	0	-1.052498	2.686135	0.178553
51	6	0	-3.126428	4.309979	0.842171
52	1	0	-4.097191	2.576183	0.009047
53	1	0	-3.047075	3.415472	-1.127996
54	6	0	-2.082057	2.923026	2.674455
55	1	0	-2.976944	1.104583	1.929842
56	1	0	-1.223593	1.046596	1.995453
57	6	0	-3.211711	3.890716	2.312061
58	1	0	-3.956460	4.977871	0.584152
59	1	0	-2.199235	4.878800	0.680597
60	1	0	-2.171709	2.604673	3.719237
61	1	0	-1.118916	3.445784	2.584877
62	1	0	-3.180987	4.773516	2.961190
63	1	0	-4.178935	3.399448	2.489691
64	6	0	1.993985	2.124322	0.279731
65	6	0	2.071864	1.697457	1.756248
66	6	0	3.132145	3.088760	-0.084868
67	1	0	1.052515	2.686080	0.178686
68	6	0	2.082337	2.922767	2.674534
69	1	0	2.977098	1.104361	1.929695
70	1	0	1.223752	1.046407	1.995465
71	6	0	3.126604	4.309812	0.842258
72	1	0	4.097195	2.576023	0.008890
73	1	0	3.047006	3.415461	-1.127975

74	6	0	3.212000	3.890433	2.312106
75	1	0	2.172082	2.604323	3.719280
76	1	0	1.119210	3.445571	2.585095
77	1	0	3.956644	4.977684	0.584215
78	1	0	2.199423	4.878689	0.680810
79	1	0	3.181384	4.773187	2.961305
80	1	0	4.179216	3.399102	2.489609
81	6	0	-1.360059	-2.112584	0.639857
82	6	0	-1.944452	-3.087294	-0.183292
83	6	0	-1.745808	-2.116499	1.990204
84	6	0	-2.890241	-3.990037	0.301593
85	1	0	-1.654344	-3.149043	-1.230833
86	6	0	-2.694727	-3.010294	2.483015
87	1	0	-1.302495	-1.398313	2.677457
88	6	0	-3.281581	-3.948444	1.637005
89	1	0	-3.321403	-4.730781	-0.368362
90	1	0	-4.021874	-4.647395	2.016424
91	1	0	-2.974497	-2.974809	3.533459
92	6	0	1.360034	-2.112594	0.639795
93	6	0	1.745846	-2.116530	1.990124
94	6	0	1.944376	-3.087296	-0.183397
95	6	0	2.694748	-3.010376	2.482886
96	1	0	1.302615	-1.398308	2.677393
97	6	0	2.890167	-3.990066	0.301437
98	1	0	1.654245	-3.149002	-1.230933
99	6	0	3.281546	-3.948524	1.636838
100	1	0	2.974561	-2.974900	3.533319
101	1	0	3.321297	-4.730791	-0.368559
102	1	0	4.021838	-4.647498	2.016213

	1	2	3
	A	A	A
Frequencies --	17.8286	31.6480	34.4448
Red. masses --	4.9682	4.7358	4.2163
Frc consts --	0.0009	0.0028	0.0029
IR Inten --	0.0028	0.0696	0.0002

Sum of electronic and zero-point Energies= -2323.163056
Sum of electronic and thermal Energies= -2323.121078
Sum of electronic and thermal Enthalpies= -2323.120134
Sum of electronic and thermal Free Energies= -2323.235962

HF=-2324.0936195

5.9 Computed Structure of E (dcppPt-H_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.703334	-0.335327	0.469170
2	78	0	-0.000075	-1.123941	-0.908761
3	6	0	-1.308560	-0.498700	2.273834
4	1	0	-2.134539	-0.093553	2.868835
5	1	0	-1.268260	-1.575973	2.481130
6	6	0	-0.000027	0.157700	2.742487
7	1	0	-0.000031	0.129527	3.839184
8	1	0	0.000021	1.223991	2.483888
9	6	0	1.308453	-0.498806	2.273842
10	1	0	1.268060	-1.576076	2.481135
11	1	0	2.134471	-0.093735	2.868841
12	15	0	1.703232	-0.335459	0.469182
13	6	0	-3.287593	-1.303036	0.311511
14	6	0	-4.273898	-1.291686	1.490535
15	6	0	-4.011719	-0.987438	-1.007135
16	1	0	-2.895137	-2.327356	0.219334
17	6	0	-5.420428	-2.280038	1.237789
18	1	0	-4.689794	-0.285903	1.629818
19	1	0	-3.769502	-1.560133	2.424893
20	6	0	-5.151702	-1.978891	-1.254984
21	1	0	-4.432188	0.026755	-0.959056
22	1	0	-3.297884	-1.009642	-1.837497
23	6	0	-6.137365	-1.992927	-0.083754
24	1	0	-6.130850	-2.246130	2.072268
25	1	0	-5.010502	-3.299564	1.211398
26	1	0	-5.669748	-1.725861	-2.187257
27	1	0	-4.727344	-2.983243	-1.390652
28	1	0	-6.925226	-2.735787	-0.254933
29	1	0	-6.633563	-1.013664	-0.018134
30	6	0	3.287441	-1.303214	0.311552
31	6	0	4.011587	-0.987577	-1.007069
32	6	0	4.273723	-1.291740	1.490584
33	1	0	2.894987	-2.327538	0.219400
34	6	0	5.151644	-1.978952	-1.254879

35	1	0	4.431980	0.026650	-0.958972
36	1	0	3.297776	-1.009831	-1.837449
37	6	0	5.420329	-2.280021	1.237904
38	1	0	4.689536	-0.285912	1.629814
39	1	0	3.769320	-1.560165	2.424945
40	6	0	6.137283	-1.992902	-0.083627
41	1	0	5.669691	-1.725896	-2.187144
42	1	0	4.727359	-2.983335	-1.390543
43	1	0	6.130724	-2.246035	2.072404
44	1	0	5.010474	-3.299575	1.211534
45	1	0	6.925197	-2.735714	-0.254769
46	1	0	6.633414	-1.013605	-0.018016
47	6	0	2.046549	1.487686	0.300302
48	6	0	3.258958	2.045639	1.058493
49	6	0	2.061463	1.947440	-1.168441
50	1	0	1.144246	1.933388	0.749717
51	6	0	3.303062	3.575481	0.966916
52	1	0	4.179565	1.638445	0.620737
53	1	0	3.242346	1.735003	2.110027
54	6	0	2.111831	3.475098	-1.258807
55	1	0	2.935007	1.525281	-1.680236
56	1	0	1.180237	1.557941	-1.689001
57	6	0	3.307601	4.044966	-0.490797
58	1	0	4.186131	3.956135	1.493326
59	1	0	2.423873	3.992092	1.479245
60	1	0	2.149642	3.785036	-2.309368
61	1	0	1.183328	3.890673	-0.840387
62	1	0	3.304899	5.140182	-0.537148
63	1	0	4.237144	3.709410	-0.972365
64	6	0	-2.046424	1.487880	0.300311
65	6	0	-2.061813	1.947584	-1.168444
66	6	0	-3.258376	2.046171	1.058984
67	1	0	-1.143858	1.933438	0.749340
68	6	0	-2.111847	3.475253	-1.258844
69	1	0	-2.935662	1.525615	-1.679876
70	1	0	-1.180890	1.557855	-1.689345
71	6	0	-3.302105	3.576019	0.967382
72	1	0	-4.179271	1.639245	0.621603
73	1	0	-3.241425	1.735558	2.110519
74	6	0	-3.307149	4.045449	-0.490346
75	1	0	-2.150023	3.785168	-2.309399
76	1	0	-1.183066	3.890612	-0.840829
77	1	0	-4.184845	3.956929	1.494157
78	1	0	-2.422582	3.992410	1.479318
79	1	0	-3.304193	5.140663	-0.536737
80	1	0	-4.236982	3.710109	-0.971505
81	1	0	-1.051184	-1.786644	-1.929937
82	1	0	1.050995	-1.786720	-1.929936

	1	2	3
	A	A	A
Frequencies --	23.3846	24.4850	44.8973
Red. masses --	5.3643	3.8269	4.0051
Frc consts --	0.0017	0.0014	0.0048
IR Inten --	0.7015	0.0186	0.8009

Sum of electronic and zero-point Energies= -1861.383320
Sum of electronic and thermal Energies= -1861.350770
Sum of electronic and thermal Enthalpies= -1861.349826
Sum of electronic and thermal Free Energies= -1861.446707

HF=-1862.14491

5.10 Computed Structure of F (dcppPt(C_6H_5)$_2$)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.710152	0.683617	-0.864037
2	78	0	-0.000015	-0.752403	-0.089706
3	6	0	1.301172	1.526832	-2.462842
4	1	0	2.127956	2.186762	-2.743891
5	1	0	1.254158	0.737985	-3.224455
6	6	0	-0.000043	2.338053	-2.493290
7	1	0	-0.000053	2.913040	-3.427583
8	1	0	-0.000056	3.089610	-1.694363
9	6	0	-1.301230	1.526783	-2.462850
10	1	0	-1.254150	0.737914	-3.224440
11	1	0	-2.128041	2.186654	-2.743951
12	15	0	-1.710210	0.683617	-0.864009
13	6	0	3.344643	-0.136957	-1.252969
14	6	0	4.213840	0.520411	-2.340065
15	6	0	4.192673	-0.419835	0.000555

16	1	0	3.018152	-1.115373	-1.634572
17	6	0	5.430945	-0.354354	-2.668910
18	1	0	4.556723	1.507359	-2.000903
19	1	0	3.643105	0.679788	-3.260171
20	6	0	5.387101	-1.313233	-0.342546
21	1	0	4.569368	0.527644	0.409226
22	1	0	3.590205	-0.895661	0.775736
23	6	0	6.260927	-0.679492	-1.425372
24	1	0	6.048526	0.146404	-3.424117
25	1	0	5.078090	-1.292668	-3.119772
26	1	0	5.971059	-1.506462	0.564412
27	1	0	5.009841	-2.285462	-0.685158
28	1	0	7.091607	-1.344177	-1.690056
29	1	0	6.707228	0.247089	-1.035415
30	6	0	-3.344729	-0.136935	-1.252892
31	6	0	-4.192755	-0.419806	0.000632
32	6	0	-4.213919	0.520404	-2.340021
33	1	0	-3.018259	-1.115364	-1.634477
34	6	0	-5.387199	-1.313184	-0.342461
35	1	0	-4.569430	0.527675	0.409310
36	1	0	-3.590289	-0.895647	0.775814
37	6	0	-5.431009	-0.354382	-2.668858
38	1	0	-4.556821	1.507355	-2.000889
39	1	0	-3.643156	0.679772	-3.260110
40	6	0	-6.261005	-0.679469	-1.425318
41	1	0	-5.971180	-1.506372	0.564491
42	1	0	-5.009956	-2.285430	-0.685037
43	1	0	-6.048585	0.146334	-3.424096
44	1	0	-5.078135	-1.292713	-3.119675
45	1	0	-7.091684	-1.344163	-1.689984
46	1	0	-6.707303	0.247127	-1.035398
47	6	0	-1.993964	2.124398	0.279709
48	6	0	-3.132124	3.088857	-0.084856
49	6	0	-2.071714	1.697645	1.756263
50	1	0	-1.052498	2.686135	0.178553
51	6	0	-3.126428	4.309979	0.842171
52	1	0	-4.097191	2.576183	0.009047
53	1	0	-3.047075	3.415472	-1.127996
54	6	0	-2.082057	2.923026	2.674455
55	1	0	-2.976944	1.104583	1.929842
56	1	0	-1.223593	1.046596	1.995453
57	6	0	-3.211711	3.890716	2.312061
58	1	0	-3.956460	4.977871	0.584152
59	1	0	-2.199235	4.878800	0.680597
60	1	0	-2.171709	2.604673	3.719237
61	1	0	-1.118916	3.445784	2.584877
62	1	0	-3.180987	4.773516	2.961190
63	1	0	-4.178935	3.399448	2.489691
64	6	0	1.993985	2.124322	0.279731
65	6	0	2.071864	1.697457	1.756248
66	6	0	3.132145	3.088760	-0.084868
67	1	0	1.052515	2.686080	0.178686
68	6	0	2.082337	2.922767	2.674534
69	1	0	2.977098	1.104361	1.929695
70	1	0	1.223752	1.046407	1.995465
71	6	0	3.126604	4.309812	0.842258
72	1	0	4.097195	2.576023	0.008890
73	1	0	3.047006	3.415461	-1.127975
74	6	0	3.212000	3.890433	2.312106
75	1	0	2.172082	2.604323	3.719280
76	1	0	1.119210	3.445571	2.585095
77	1	0	3.956644	4.977684	0.584215
78	1	0	2.199423	4.878689	0.680810
79	1	0	3.181384	4.773187	2.961305
80	1	0	4.179216	3.399102	2.489609
81	6	0	-1.360059	-2.112584	0.639857
82	6	0	-1.944452	-3.087294	-0.183292
83	6	0	-1.745808	-2.116499	1.990204
84	6	0	-2.890241	-3.990037	0.301593
85	1	0	-1.654344	-3.149043	-1.230833
86	6	0	-2.694727	-3.010294	2.483015
87	1	0	-1.302495	-1.398313	2.677457
88	6	0	-3.281581	-3.948444	1.637005
89	1	0	-3.321403	-4.730781	-0.368362
90	1	0	-4.021874	-4.647395	2.016424
91	1	0	-2.974497	-2.974809	3.533459
92	6	0	1.360034	-2.112594	0.639795
93	6	0	1.745846	-2.116530	1.990124
94	6	0	1.944376	-3.087296	-0.183397
95	6	0	2.694748	-3.010376	2.482886
96	1	0	1.302615	-1.398308	2.677393
97	6	0	2.890167	-3.990066	0.301437
98	1	0	1.654245	-3.149002	-1.230933
99	6	0	3.281546	-3.948524	1.636838
100	1	0	2.974561	-2.974900	3.533319
101	1	0	3.321297	-4.730791	-0.368559
102	1	0	4.021838	-4.647498	2.016213

	1	2	3
	A	A	A
Frequencies --	17.8286	31.6480	34.4448
Red. masses --	4.9682	4.7358	4.2163
Frc consts --	0.0009	0.0028	0.0029
IR Inten --	0.0028	0.0696	0.0002

Sum of electronic and zero-point Energies= -2323.163056
Sum of electronic and thermal Energies= -2323.121078
Sum of electronic and thermal Enthalpies= -2323.120134
Sum of electronic and thermal Free Energies= -2323.235962

HF=-2324.0936195

5.11 Computed Structure of TS_{BC}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.417799	0.412090	0.905240
2	78	0	0.093375	-0.937520	-0.207916
3	6	0	-0.779254	0.775624	2.612739
4	1	0	-1.452624	1.472954	3.125460
5	1	0	-0.826393	-0.171535	3.165950
6	6	0	0.651231	1.339802	2.688873
7	1	0	0.792254	1.711212	3.711857
8	1	0	0.735537	2.229080	2.051551
9	6	0	1.819245	0.378522	2.401974
10	1	0	1.680698	-0.545009	2.979323
11	1	0	2.740487	0.844158	2.771003
12	15	0	2.052552	-0.149917	0.631349
13	6	0	-3.114967	-0.288143	1.243278
14	6	0	-3.911591	0.257639	2.438865
15	6	0	-3.969823	-0.290311	-0.034735
16	1	0	-2.877542	-1.342648	1.459238
17	6	0	-5.219489	-0.522264	2.627622
18	1	0	-4.146042	1.317949	2.282247
19	1	0	-3.319790	0.196869	3.358939
20	6	0	-5.269679	-1.071829	0.168687
21	1	0	-4.222985	0.744402	-0.304774
22	1	0	-3.402720	-0.714152	-0.869387
23	6	0	-6.067216	-0.521442	1.353021
24	1	0	-5.785786	-0.099938	3.466395
25	1	0	-4.980257	-1.560960	2.897456
26	1	0	-5.867421	-1.041267	-0.749981
27	1	0	-5.024918	-2.127429	0.348023
28	1	0	-6.982765	-1.104966	1.505901
29	1	0	-6.381638	0.508854	1.130650
30	6	0	3.541294	-1.278289	0.770129
31	6	0	4.137897	-1.565003	-0.616658
32	6	0	4.646362	-0.936379	1.782622
33	1	0	3.066166	-2.211152	1.111555
34	6	0	5.191524	-2.674537	-0.553274
35	1	0	4.613656	-0.653805	-1.005359
36	1	0	3.335897	-1.833366	-1.314803
37	6	0	5.700539	-2.050391	1.836812
38	1	0	5.136520	0.005567	1.509115
39	1	0	4.222953	-0.795231	2.782861
40	6	0	6.292435	-2.334708	0.454510
41	1	0	5.622750	-2.837379	-1.548117
42	1	0	4.705904	-3.615709	-0.259720
43	1	0	6.492701	-1.776774	2.543930
44	1	0	5.233009	-2.966901	2.224046
45	1	0	7.023464	-3.149557	0.513389
46	1	0	6.836955	-1.445016	0.105962
47	6	0	2.564604	1.452230	-0.182955
48	6	0	3.900352	2.081774	0.234716
49	6	0	2.453389	1.384015	-1.715837
50	1	0	1.766700	2.136276	0.147521
51	6	0	4.062571	3.475135	-0.385425
52	1	0	4.727510	1.445734	-0.107001
53	1	0	3.979980	2.148624	1.326310
54	6	0	2.621061	2.772474	-2.338111
55	1	0	3.223015	0.710269	-2.114261
56	1	0	1.486277	0.949370	-1.992859
57	6	0	3.939388	3.423938	-1.910926
58	1	0	5.028896	3.904152	-0.094985
59	1	0	3.286356	4.141065	0.018610
60	1	0	2.565299	2.702855	-3.430718
61	1	0	1.782993	3.409921	-2.019538
62	1	0	4.023062	4.432203	-2.333269
63	1	0	4.777254	2.840072	-2.318330
64	6	0	-1.581659	2.123816	0.177787

65	6	0	-1.709464	2.082232	-1.354943
66	6	0	-2.617741	3.075313	0.791548
67	1	0	-0.586792	2.550533	0.384237
68	6	0	-1.595478	3.487164	-1.952272
69	1	0	-2.673470	1.641470	-1.638596
70	1	0	-0.934375	1.424879	-1.765396
71	6	0	-2.492967	4.480375	0.189581
72	1	0	-3.628158	2.694003	0.595693
73	1	0	-2.502863	3.125737	1.881019
74	6	0	-2.618870	4.445257	-1.336184
75	1	0	-1.721045	3.442552	-3.040398
76	1	0	-0.582807	3.874568	-1.766724
77	1	0	-3.254451	5.141613	0.620055
78	1	0	-1.515412	4.903221	0.462676
79	1	0	-2.497160	5.452558	-1.751465
80	1	0	-3.631561	4.111363	-1.604151
81	6	0	-1.156345	-2.355056	-1.422358
82	6	0	-1.925829	-3.307615	-0.730095
83	6	0	-1.625035	-1.904329	-2.669751
84	6	0	-3.160525	-3.716627	-1.220171
85	1	0	-1.551359	-3.711403	0.206324
86	6	0	-2.863132	-2.310821	-3.153736
87	1	0	-1.015536	-1.214159	-3.246687
88	6	0	-3.641980	-3.212018	-2.427965
89	1	0	-3.751672	-4.435936	-0.659237
90	1	0	-3.221497	-1.928749	-4.106025
91	1	0	-4.606513	-3.533393	-2.809976
92	1	0	0.049641	-2.376977	-1.271165

	1	2	3
	A	A	A
Frequencies --	-111.2012	19.8848	28.2665
Red. masses --	6.8945	4.7998	5.0532
Frc consts --	0.0502	0.0011	0.0024
IR Inten --	53.8722	0.0611	0.1666

Sum of electronic and zero-point Energies= -2092.238235
Sum of electronic and thermal Energies= -2092.200935
Sum of electronic and thermal Enthalpies= -2092.199991
Sum of electronic and thermal Free Energies= -2092.308290

HF=-2093.0830231

5.12 Computed Structure of TS_{CD}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.025516	0.562633	-0.568791
2	78	0	0.064330	-0.022556	0.572229
3	6	0	1.718126	0.830629	-2.375934
4	1	0	2.593865	1.316122	-2.819860
5	1	0	1.656404	-0.168345	-2.825816
6	6	0	0.451690	1.632006	-2.727621
7	1	0	0.597642	2.065684	-3.723851
8	1	0	0.338264	2.485784	-2.046038
9	6	0	-0.845555	0.803552	-2.764373
10	1	0	-0.639434	-0.167344	-3.227925
11	1	0	-1.580484	1.297489	-3.409746
12	15	0	-1.598391	0.501693	-1.094296
13	6	0	3.332435	-0.756918	-0.588765
14	6	0	4.440545	-0.688071	-1.651984
15	6	0	3.929605	-0.993697	0.805649
16	1	0	2.728030	-1.642133	-0.825672
17	6	0	5.248450	-1.992875	-1.636447
18	1	0	5.115275	0.153953	-1.457767
19	1	0	4.017266	-0.535627	-2.650804
20	6	0	4.747318	-2.287936	0.823377
21	1	0	4.582693	-0.151192	1.074649
22	1	0	3.130426	-1.039135	1.553983
23	6	0	5.838331	-2.271326	-0.251059
24	1	0	6.044949	-1.946826	-2.388682
25	1	0	4.585508	-2.822163	-1.920643
26	1	0	5.192299	-2.436641	1.814390
27	1	0	4.067033	-3.131563	0.644865
28	1	0	6.381008	-3.223855	-0.256429
29	1	0	6.572819	-1.489233	-0.009202
30	6	0	-2.807469	-0.883804	-1.366138
31	6	0	-3.852855	-0.957491	-0.240759
32	6	0	-3.480351	-1.017368	-2.740681
33	1	0	-2.158430	-1.761769	-1.239171
34	6	0	-4.615009	-2.283141	-0.310784
35	1	0	-4.570524	-0.132738	-0.345735

36	1	0	-3.374148	-0.848841	0.736930
37	6	0	-4.253012	-2.341092	-2.815506
38	1	0	-4.171315	-0.182043	-2.911179
39	1	0	-2.737868	-0.985133	-3.545747
40	6	0	-5.274367	-2.468257	-1.680897
41	1	0	-5.368613	-2.321538	0.484165
42	1	0	-3.912519	-3.107201	-0.123554
43	1	0	-4.752177	-2.428284	-3.787947
44	1	0	-3.535447	-3.171183	-2.750865
45	1	0	-5.778437	-3.440152	-1.735683
46	1	0	-6.051172	-1.700414	-1.810155
47	6	0	-2.531392	2.096492	-0.834161
48	6	0	-3.690878	2.367545	-1.806442
49	6	0	-2.991682	2.297571	0.618997
50	1	0	-1.750135	2.851372	-1.022988
51	6	0	-4.261473	3.776025	-1.603295
52	1	0	-4.489830	1.636650	-1.628731
53	1	0	-3.377734	2.242767	-2.849349
54	6	0	-3.572476	3.700169	0.821638
55	1	0	-3.752004	1.551880	0.879042
56	1	0	-2.152126	2.132278	1.296941
57	6	0	-4.714436	3.986414	-0.156631
58	1	0	-5.095882	3.941373	-2.295112
59	1	0	-3.489787	4.517752	-1.854547
60	1	0	-3.920050	3.809336	1.855504
61	1	0	-2.776207	4.444728	0.675892
62	1	0	-5.091448	5.006734	-0.020021
63	1	0	-5.551406	3.306959	0.059314
64	6	0	2.752569	2.189289	-0.024519
65	6	0	2.850363	2.334468	1.503784
66	6	0	4.088386	2.592225	-0.667228
67	1	0	1.982516	2.902467	-0.361690
68	6	0	3.219918	3.770705	1.887575
69	1	0	3.614977	1.648080	1.889964
70	1	0	1.902855	2.048385	1.967504
71	6	0	4.454079	4.035393	-0.300436
72	1	0	4.877542	1.924825	-0.297415
73	1	0	4.062650	2.479709	-1.757048
74	6	0	4.521118	4.220940	1.217690
75	1	0	3.306897	3.853474	2.977155
76	1	0	2.403919	4.442299	1.584172
77	1	0	5.411840	4.304599	-0.761046
78	1	0	3.698370	4.715991	-0.718049
79	1	0	4.735663	5.267735	1.462608
80	1	0	5.355055	3.624487	1.614294
81	6	0	-1.075343	-0.548247	2.352236
82	6	0	-1.716905	-1.795278	2.446626
83	6	0	-1.440411	0.436835	3.286919
84	6	0	-2.724627	-2.017276	3.381362
85	1	0	-1.448183	-2.589414	1.758834
86	6	0	-2.448183	0.215808	4.218976
87	1	0	-0.925358	1.392605	3.271519
88	6	0	-3.103311	-1.012285	4.267165
89	1	0	-3.219832	-2.984413	3.410547
90	1	0	-3.889203	-1.188238	4.996081
91	1	0	0.344502	-0.485060	2.134794
92	1	0	-0.052469	1.519709	1.042726
93	6	0	0.410280	-2.048188	-0.018802
94	6	0	0.945517	-2.975177	0.898404
95	6	0	0.304005	-2.521974	-1.340124
96	6	0	1.346135	-4.258486	0.531561
97	1	0	1.064908	-2.685489	1.940965
98	6	0	0.704986	-3.801256	-1.728235
99	1	0	-0.081495	-1.865357	-2.117367
100	6	0	1.235444	-4.681080	-0.791415
101	1	0	1.753739	-4.930103	1.283881
102	1	0	1.552960	-5.678236	-1.083362
103	1	0	-2.717060	1.004851	4.916355
104	1	0	0.603725	-4.105501	-2.767719

	1	2	3
	A	A	A
Frequencies --	-705.8325	13.5046	30.9180
Red. masses --	1.2646	4.6993	4.3487
Frc consts --	0.3712	0.0005	0.0024
IR Inten --	438.3951	0.0418	0.0625

Sum of electronic and zero-point Energies= -2324.288020
Sum of electronic and thermal Energies= -2324.245603
Sum of electronic and thermal Enthalpies= -2324.244659
Sum of electronic and thermal Free Energies= -2324.362468

HF=-2325.234612 9

5.13 Computed Structure of TS_{DE}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.868587	0.484215	0.489358
2	78	0	-0.087024	-0.692665	-0.534759
3	6	0	-1.635583	0.663757	2.310691
4	1	0	-2.519763	1.149309	2.736599
5	1	0	-1.615516	-0.359054	2.703543
6	6	0	-0.385406	1.426794	2.773629
7	1	0	-0.492640	1.593620	3.852438
8	1	0	-0.367860	2.428714	2.327355
9	6	0	0.970488	0.739000	2.555619
10	1	0	0.942958	-0.270647	2.981675
11	1	0	1.727765	1.294333	3.119797
12	15	0	1.528279	0.560654	0.793536
13	6	0	-3.496436	-0.402720	0.400818
14	6	0	-4.715390	0.302517	1.012765
15	6	0	-3.840401	-0.908098	-1.010041
16	1	0	-3.276029	-1.296965	1.004399
17	6	0	-5.905220	-0.663719	1.083433
18	1	0	-4.990731	1.164020	0.387914
19	1	0	-4.499046	0.691225	2.014220
20	6	0	-5.011772	-1.890897	-0.942139
21	1	0	-4.114193	-0.063032	-1.654389
22	1	0	-2.968334	-1.386970	-1.460632
23	6	0	-6.240262	-1.247473	-0.292111
24	1	0	-6.778643	-0.150037	1.502261
25	1	0	-5.655235	-1.480953	1.774079
26	1	0	-5.258508	-2.246886	-1.949166
27	1	0	-4.697251	-2.769284	-0.361564
28	1	0	-7.052112	-1.978626	-0.203055
29	1	0	-6.609470	-0.441715	-0.943140
30	6	0	3.184803	-0.275834	0.959050
31	6	0	4.052926	-0.060177	-0.293433
32	6	0	3.996790	-0.013800	2.238142
33	1	0	2.902298	-1.338259	0.960402
34	6	0	5.298808	-0.948591	-0.253206
35	1	0	4.370459	0.990276	-0.345852
36	1	0	3.476802	-0.275052	-1.197468
37	6	0	5.253404	-0.893762	2.266665
38	1	0	4.293631	1.041247	2.293320
39	1	0	3.397679	-0.223676	3.130696
40	6	0	6.115018	-0.699743	1.016584
41	1	0	5.908401	-0.766277	-1.145673
42	1	0	4.982991	-1.998502	-0.297423
43	1	0	5.833836	-0.676178	3.171392
44	1	0	4.947540	-1.947389	2.332153
45	1	0	6.984401	-1.366902	1.050854
46	1	0	6.505187	0.328760	1.002932
47	6	0	1.794844	2.359926	0.346101
48	6	0	2.898640	3.114199	1.103391
49	6	0	1.904671	2.607545	-1.165185
50	1	0	0.840927	2.813704	0.657245
51	6	0	2.845351	4.614499	0.789968
52	1	0	3.880648	2.723401	0.810294
53	1	0	2.806370	2.961289	2.184633
54	6	0	1.851526	4.106338	-1.474474
55	1	0	2.842908	2.186153	-1.547114
56	1	0	1.095305	2.082512	-1.683750
57	6	0	2.935843	4.875641	-0.715524
58	1	0	3.654717	5.133561	1.316834
59	1	0	1.901165	5.028286	1.173739
60	1	0	1.952282	4.269290	-2.553683
61	1	0	0.863256	4.496966	-1.186487
62	1	0	2.855937	5.949729	-0.919080
63	1	0	3.922955	4.555675	-1.078299
64	6	0	-2.044284	2.230810	-0.131061
65	6	0	-2.620927	2.295724	-1.554201
66	6	0	-2.755478	3.253564	0.769006
67	1	0	-0.993430	2.543643	-0.211593
68	6	0	-2.444926	3.699234	-2.140775
69	1	0	-3.691706	2.054522	-1.520248
70	1	0	-2.143138	1.552221	-2.200968
71	6	0	-2.581176	4.665501	0.194176
72	1	0	-3.824261	3.015423	0.837268
73	1	0	-2.361737	3.227613	1.790184
74	6	0	-3.094145	4.758078	-1.245261
75	1	0	-2.874573	3.740083	-3.148152
76	1	0	-1.370981	3.910470	-2.244827
77	1	0	-3.097900	5.393777	0.829900
78	1	0	-1.512499	4.926363	0.217438
79	1	0	-2.914120	5.761108	-1.648606
80	1	0	-4.183131	4.607246	-1.246447
81	6	0	1.365902	-1.893473	-1.412476
82	6	0	1.955600	-2.993376	-0.767619

83	6	0	1.850731	-1.599364	-2.700150
84	6	0	2.981434	-3.732878	-1.355741
85	1	0	1.603505	-3.288976	0.216455
86	6	0	2.872006	-2.335533	-3.296728
87	1	0	1.437646	-0.757944	-3.251555
88	6	0	3.451953	-3.407080	-2.623979
89	1	0	3.410427	-4.574341	-0.816390
90	1	0	4.251526	-3.981680	-3.083199
91	1	0	-0.739831	-0.483190	-2.118739
92	1	0	-0.178148	0.260989	-2.021901
93	6	0	-0.851995	-2.443426	0.373102
94	6	0	-1.580927	-3.397774	-0.360011
95	6	0	-0.687427	-2.721965	1.740180
96	6	0	-2.143706	-4.524050	0.236853
97	1	0	-1.707743	-3.263328	-1.430802
98	6	0	-1.242633	-3.848084	2.351192
99	1	0	-0.093876	-2.048765	2.355342
100	6	0	-1.987727	-4.751995	1.602455
101	1	0	-2.703636	-5.230402	-0.371871
102	1	0	-2.427939	-5.628141	2.070499
103	1	0	3.216196	-2.066431	-4.292692
104	1	0	-1.086747	-4.017251	3.414367

	1	2	3
	A	A	A
Frequencies --	-145.2426	22.5225	36.0676
Red. masses --	3.8781	4.5050	4.4337
Frc consts --	0.0482	0.0013	0.0034
IR Inten --	4.6817	0.0239	0.2563

Sum of electronic and zero-point Energies= -2324.284712
Sum of electronic and thermal Energies= -2324.242381
Sum of electronic and thermal Enthalpies= -2324.241437
Sum of electronic and thermal Free Energies= -2324.358186

HF=-2325.2294505

5.14 Computed Structure of TS_{DF}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.782213	0.722985	0.795227
2	78	0	-0.000001	-0.613395	0.020892
3	6	0	-1.307093	1.520995	2.398669
4	1	0	-2.119926	2.172051	2.737728
5	1	0	-1.229768	0.703415	3.125862
6	6	0	-0.000007	2.329814	2.401149
7	1	0	0.000000	2.933231	3.317511
8	1	0	-0.000033	3.058485	1.580442
9	6	0	1.307110	1.521052	2.398616
10	1	0	1.229877	0.703508	3.125859
11	1	0	2.119932	2.172167	2.737587
12	15	0	1.782194	0.722997	0.795183
13	6	0	-3.327671	-0.209308	1.253374
14	6	0	-4.243816	0.407606	2.323149
15	6	0	-4.136601	-0.594944	0.005824
16	1	0	-2.908748	-1.141359	1.663625
17	6	0	-5.397761	-0.543321	2.667440
18	1	0	-4.657483	1.357478	1.960291
19	1	0	-3.682729	0.632662	3.236212
20	6	0	-5.276791	-1.550792	0.363179
21	1	0	-4.569326	0.312505	-0.437637
22	1	0	-3.484054	-1.048566	-0.746067
23	6	0	-6.196164	-0.942714	1.423924
24	1	0	-6.053543	-0.074709	3.411043
25	1	0	-4.984488	-1.448430	3.134593
26	1	0	-5.841399	-1.806209	-0.541201
27	1	0	-4.847579	-2.488057	0.740034
28	1	0	-6.990265	-1.648189	1.695115
29	1	0	-6.689671	-0.051462	1.009663
30	6	0	3.327639	-0.209294	1.253372
31	6	0	4.136659	-0.594926	0.005878
32	6	0	4.243705	0.407621	2.323213
33	1	0	2.908689	-1.141353	1.663579
34	6	0	5.276825	-1.550776	0.363322
35	1	0	4.569411	0.312518	-0.437567
36	1	0	3.484164	-1.048558	-0.746050
37	6	0	5.397623	-0.543305	2.667589
38	1	0	4.657390	1.357496	1.960381
39	1	0	3.682553	0.632671	3.236238
40	6	0	6.196121	-0.942700	1.424134
41	1	0	5.841500	-1.806188	-0.541018

42	1	0	4.847578	-2.488041	0.740138
43	1	0	6.053349	-0.074704	3.411247
44	1	0	4.984306	-1.448414	3.134701
45	1	0	6.990203	-1.648174	1.695386
46	1	0	6.689659	-0.051449	1.009906
47	6	0	2.204732	2.196478	-0.266990
48	6	0	3.323142	3.124346	0.230890
49	6	0	2.416884	1.862994	-1.753325
50	1	0	1.259258	2.762035	-0.218294
51	6	0	3.361659	4.413206	-0.599923
52	1	0	4.288940	2.609783	0.138221
53	1	0	3.194983	3.372541	1.290393
54	6	0	2.447492	3.147090	-2.588181
55	1	0	3.364988	1.327656	-1.885096
56	1	0	1.622244	1.196667	-2.100290
57	6	0	3.527305	4.113117	-2.092062
58	1	0	4.172785	5.061901	-0.248568
59	1	0	2.423584	4.964832	-0.442515
60	1	0	2.613148	2.903084	-3.643893
61	1	0	1.464203	3.636571	-2.527722
62	1	0	3.504976	5.044487	-2.670022
63	1	0	4.515423	3.660461	-2.257943
64	6	0	-2.204733	2.196497	-0.266905
65	6	0	-2.416938	1.863078	-1.753247
66	6	0	-3.323083	3.124405	0.231029
67	1	0	-1.259227	2.761999	-0.218245
68	6	0	-2.447447	3.147220	-2.588039
69	1	0	-3.365089	1.327831	-1.885039
70	1	0	-1.622358	1.196699	-2.100253
71	6	0	-3.361525	4.413309	-0.599716
72	1	0	-4.288908	2.609896	0.138325
73	1	0	-3.194916	3.372534	1.290546
74	6	0	-3.527188	4.113307	-2.091872
75	1	0	-2.613121	2.903279	-3.643763
76	1	0	-1.464123	3.636628	-2.527555
77	1	0	-4.172610	5.062036	-0.248327
78	1	0	-2.423417	4.964870	-0.442280
79	1	0	-3.504780	5.044704	-2.669784
80	1	0	-4.515340	3.660736	-2.257786
81	6	0	0.885448	-2.423772	-0.846079
82	6	0	1.517388	-3.301220	0.067778
83	6	0	1.506576	-2.297099	-2.112665
84	6	0	2.677879	-3.988747	-0.256626
85	1	0	1.081182	-3.442304	1.050932
86	6	0	2.666539	-2.985543	-2.433979
87	1	0	1.069505	-1.635192	-2.852353
88	6	0	3.266256	-3.841906	-1.511220
89	1	0	3.125857	-4.650172	0.480782
90	1	0	4.171450	-4.384838	-1.765359
91	1	0	-0.000018	0.082948	-1.451025
92	1	0	3.109844	-2.848530	-3.416856
93	1	0	0.000017	-1.283502	1.531903
94	6	0	-0.885463	-2.423744	-0.846100
95	6	0	-1.506540	-2.297098	-2.112714
96	6	0	-1.517455	-3.301154	0.067758
97	6	0	-2.666494	-2.985545	-2.434055
98	1	0	-1.069436	-1.635215	-2.852403
99	6	0	-2.677935	-3.988685	-0.256673
100	1	0	-1.081293	-3.442208	1.050937
101	6	0	-3.266254	-3.841881	-1.511298
102	1	0	-3.109757	-2.848558	-3.416954
103	1	0	-3.125951	-4.650081	0.480739
104	1	0	-4.171442	-4.384814	-1.765461

	1	2	3
	A	A	A
Frequencies --	-323.9611	17.2978	37.6724
Red. masses --	8.0520	4.7127	5.0311
Frc consts --	0.4979	0.0008	0.0042
IR Inten --	84.5480	0.0224	0.0041

Sum of electronic and zero-point Energies= -2324.266705
Sum of electronic and thermal Energies= -2324.224895
Sum of electronic and thermal Enthalpies= -2324.223950
Sum of electronic and thermal Free Energies= -2324.338826

HF=-2325.2129177

5.15 Computed Structure of TS_{FA}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	15	0	1.714534	0.607961	-0.926592
2	78	0	-0.014587	-0.667907	-0.038382
3	6	0	1.248639	1.310697	-2.580970
4	1	0	2.061911	1.941285	-2.958514
5	1	0	1.169666	0.456236	-3.265683
6	6	0	-0.055908	2.124502	-2.627574
7	1	0	-0.091430	2.613700	-3.609098
8	1	0	-0.008931	2.946401	-1.902175
9	6	0	-1.377370	1.353879	-2.464453
10	1	0	-1.375150	0.483191	-3.133469
11	1	0	-2.196640	2.001840	-2.796396
12	15	0	-1.752142	0.697383	-0.765987
13	6	0	3.308046	-0.289214	-1.294328
14	6	0	4.248735	0.281307	-2.367482
15	6	0	4.082636	-0.591769	-0.001648
16	1	0	2.929968	-1.256009	-1.664471
17	6	0	5.420360	-0.676074	-2.625977
18	1	0	4.643005	1.253202	-2.044799
19	1	0	3.712999	0.451925	-3.307771
20	6	0	5.235121	-1.560656	-0.271801
21	1	0	4.499444	0.342131	0.400386
22	1	0	3.412677	-1.001665	0.759667
23	6	0	6.181746	-1.007286	-1.339256
24	1	0	6.098101	-0.241714	-3.370819
25	1	0	5.028224	-1.606910	-3.060119
26	1	0	5.774809	-1.763618	0.660508
27	1	0	4.818689	-2.519114	-0.609101
28	1	0	6.984633	-1.723660	-1.549742
29	1	0	6.662348	-0.094383	-0.958371
30	6	0	-3.397720	-0.146338	-1.016348
31	6	0	-4.105688	-0.369839	0.329877
32	6	0	-4.370965	0.428113	-2.058443
33	1	0	-3.082126	-1.140835	-1.370174
34	6	0	-5.328137	-1.275414	0.167101
35	1	0	-4.436994	0.595892	0.736027
36	1	0	-3.406542	-0.807301	1.049744
37	6	0	-5.602971	-0.474760	-2.207149
38	1	0	-4.695288	1.433472	-1.760702
39	1	0	-3.881302	0.528990	-3.033215
40	6	0	-6.302979	-0.706649	-0.866012
41	1	0	-5.826281	-1.404646	1.135485
42	1	0	-4.989827	-2.270370	-0.149402
43	1	0	-6.299285	-0.036638	-2.932492
44	1	0	-5.285058	-1.443500	-2.618118
45	1	0	-7.157384	-1.381016	-0.997727
46	1	0	-6.706511	0.248485	-0.498610
47	6	0	-1.997464	2.270786	0.207725
48	6	0	-3.179131	3.168690	-0.185370
49	6	0	-1.969708	2.025289	1.726271
50	1	0	-1.075297	2.826997	-0.023858
51	6	0	-3.147441	4.490223	0.591500
52	1	0	-4.122235	2.652435	0.034572
53	1	0	-3.173194	3.369628	-1.263328
54	6	0	-1.949728	3.348398	2.497216
55	1	0	-2.851318	1.445980	2.026770
56	1	0	-1.094576	1.417171	1.983040
57	6	0	-3.125272	4.246243	2.102595
58	1	0	-4.011564	5.106360	0.315773
59	1	0	-2.249548	5.056091	0.303250
60	1	0	-1.962520	3.153273	3.575806
61	1	0	-1.008018	3.874653	2.283459
62	1	0	-3.074371	5.200424	2.639862
63	1	0	-4.065737	3.762307	2.402761
64	6	0	2.085679	2.145917	0.062976
65	6	0	2.149080	1.859395	1.573427
66	6	0	3.270185	3.013928	-0.381825
67	1	0	1.171031	2.740304	-0.091813
68	6	0	2.208323	3.163743	2.373308
69	1	0	3.031580	1.250117	1.803266
70	1	0	1.278023	1.264618	1.869482
71	6	0	3.318939	4.319863	0.420757
72	1	0	4.207360	2.465795	-0.222032
73	1	0	3.210867	3.235983	-1.454008
74	6	0	3.377516	4.045274	1.926054
75	1	0	2.284692	2.943940	3.444483
76	1	0	1.266667	3.713397	2.230275
77	1	0	4.181873	4.919799	0.108099
78	1	0	2.421112	4.913410	0.194897
79	1	0	3.379641	4.989310	2.483389
80	1	0	4.323090	3.535988	2.160876
81	6	0	-0.842492	-2.539275	0.649713
82	6	0	-1.210424	-3.281223	-0.505717
83	6	0	-1.690517	-2.691954	1.777464
84	6	0	-2.360612	-4.059022	-0.542909
85	1	0	-0.580703	-3.235199	-1.390735
86	6	0	-2.824926	-3.483792	1.740417
87	1	0	-1.436172	-2.183297	2.702744
88	6	0	-3.178532	-4.175102	0.578679

```
    89          1           0       -2.611538   -4.592113   -1.456701
    90          1           0       -4.064290   -4.802771    0.557067
    91          1           0       -3.445169   -3.565766    2.629517
    92          6           0        0.830462   -2.355778    0.991464
    93          6           0        1.189648   -1.929139    2.299387
    94          6           0        1.700214   -3.302762    0.389418
    95          6           0        2.348928   -2.370366    2.922293
    96          1           0        0.548086   -1.226251    2.825213
    97          6           0        2.839881   -3.760445    1.028471
    98          1           0        1.452378   -3.698791   -0.591092
    99          6           0        3.185394   -3.295385    2.299571
   100          1           0        2.594466   -1.995559    3.912796
   101          1           0        3.471547   -4.491548    0.529901
   102          1           0        4.078747   -3.659485    2.797308
 -------------------------------------------------------------------

                     1                      2                      3
                     A                      A                      A
 Frequencies --  -240.1951               15.9831                17.4080
 Red. masses --     6.6542                4.6413                 5.0267
 Frc consts  --     0.2262                0.0007                 0.0009
 IR Inten    --    80.1081                0.0311                 0.1520

 Sum of electronic and zero-point Energies=          -2323.110002
 Sum of electronic and thermal Energies=             -2323.068200
 Sum of electronic and thermal Enthalpies=           -2323.067255
 Sum of electronic and thermal Free Energies=        -2323.183701

HF=-2324.0379955
```

5.16 Details of computation of TS_{EA}

The search for the transition state of the addition of H_2 to the Pt(0) species was performed through the usual distance scan, starting from the PtH_2 species, and reducing the H-H distance of 0.01 Å at every step.

The input file is as follows:

```
%chk=TS-dcppPt-H2-Scan-631.chk
%mem=150MW
%nproc=4
#wB97XD genecp opt=(modredundant,maxcycle=20)

Scan Elim H2 6-31G*/Def2-TZVP/6-311+G** (P C H/Pt/Pt-H)

     0     1
  P                                          -1.697899000000     -0.376403000000      0.488380000000
  Pt                                          0.000012000000     -1.242043000000     -0.952302000000
  C                                          -1.305242000000     -0.507900000000      2.337711000000
  H                                          -2.139594000000     -0.083184000000      2.904916000000
  H                                          -1.249369000000     -1.577318000000      2.570238000000
  C                                          -0.000001000000      0.187331000000      2.773474000000
  H                                          -0.000004000000      0.218716000000      3.870617000000
  H                                          -0.000008000000      1.231945000000      2.443964000000
  C                                           1.305252000000     -0.507883000000      2.337714000000
  H                                           1.249392000000     -1.577301000000      2.570246000000
  H                                           2.139596000000     -0.083156000000      2.904921000000
  P                                           1.697913000000     -0.376386000000      0.488382000000
  C                                          -3.351162000000     -1.305692000000      0.353101000000
  C                                          -4.323274000000     -1.181329000000      1.537404000000
  C                                          -4.048380000000     -0.954039000000     -0.973037000000
  H                                          -3.021048000000     -2.351325000000      0.283334000000
  C                                          -5.544774000000     -2.096765000000      1.308773000000
  H                                          -4.667837000000     -0.146638000000      1.636010000000
  H                                          -3.830397000000     -1.465452000000      2.473027000000
  C                                          -5.266612000000     -1.868631000000     -1.194999000000
  H                                          -4.391816000000      0.086887000000     -0.937565000000
  H                                          -3.335615000000     -1.056503000000     -1.798916000000
  C                                          -6.249222000000     -1.752505000000     -0.015798000000
  H                                          -6.243515000000     -1.997931000000      2.147270000000
  H                                          -5.206457000000     -3.140497000000      1.274621000000
  H                                          -5.765561000000     -1.601572000000     -2.133188000000
  H                                          -4.922160000000     -2.906872000000     -1.282056000000
  H                                          -7.106214000000     -2.417716000000     -0.169251000000
  H                                          -6.628827000000     -0.723281000000      0.036019000000
  C                                           3.351183000000     -1.305668000000      0.353096000000
  C                                           4.048429000000     -0.953954000000     -0.973012000000
  C                                           4.323272000000     -1.181379000000      1.537427000000
  H                                           3.021069000000     -2.351296000000      0.283269000000
  C                                           5.266662000000     -1.868541000000     -1.194994000000
  H                                           4.391868000000      0.086968000000     -0.937483000000
```

H	3.335679000000	-1.056375000000	-1.798909000000
C	5.544772000000	-2.096807000000	1.308770000000
H	4.667840000000	-0.146697000000	1.636101000000
H	3.830376000000	-1.465554000000	2.473025000000
C	6.249248000000	-1.752477000000	-0.015768000000
H	5.765631000000	-1.601436000000	-2.133160000000
H	4.922208000000	-2.906776000000	-1.282110000000
H	6.243498000000	-1.998022000000	2.147286000000
H	5.206452000000	-3.140535000000	1.274555000000
H	7.106242000000	-2.417682000000	-0.169239000000
H	6.628854000000	-0.723257000000	0.036111000000
C	1.987187000000	1.491314000000	0.295728000000
C	3.197799000000	2.071908000000	1.039965000000
C	2.008170000000	1.903520000000	-1.188614000000
H	1.078503000000	1.929963000000	0.730840000000
C	3.196764000000	3.609555000000	0.924882000000
H	4.117912000000	1.684380000000	0.588385000000
H	3.188125000000	1.776257000000	2.095169000000
C	2.013856000000	3.437961000000	-1.308153000000
H	2.902439000000	1.497664000000	-1.673282000000
H	1.138354000000	1.478052000000	-1.699162000000
C	3.211951000000	4.042201000000	-0.553198000000
H	4.064741000000	4.023816000000	1.450026000000
H	2.292350000000	4.003703000000	1.407056000000
H	2.043258000000	3.729341000000	-2.363722000000
H	1.082353000000	3.830892000000	-0.880479000000
H	3.194046000000	5.135257000000	-0.626196000000
H	4.142067000000	3.690541000000	-1.018642000000
C	-1.987199000000	1.491291000000	0.295738000000
C	-2.008208000000	1.903499000000	-1.188604000000
C	-3.197817000000	2.071850000000	1.039989000000
H	-1.078518000000	1.929952000000	0.730845000000
C	-2.013935000000	3.437939000000	-1.308140000000
H	-2.902472000000	1.497623000000	-1.673264000000
H	-1.138388000000	1.478053000000	-1.699164000000
C	-3.196826000000	3.609498000000	0.924908000000
H	-4.117926000000	1.684297000000	0.588420000000
H	-3.188123000000	1.776196000000	2.095193000000
C	-3.212038000000	4.042147000000	-0.553171000000
H	-2.043356000000	3.729320000000	-2.363709000000
H	-1.082438000000	3.830893000000	-0.880476000000
H	-4.064809000000	4.023734000000	1.450062000000
H	-2.292418000000	4.003669000000	1.407074000000
H	-3.194163000000	5.135204000000	-0.626167000000
H	-4.142150000000	3.690464000000	-1.018606000000
H	-0.880057000000	-1.937462000000	-2.061449000000
H	0.880089000000	-1.937451000000	-2.061452000000

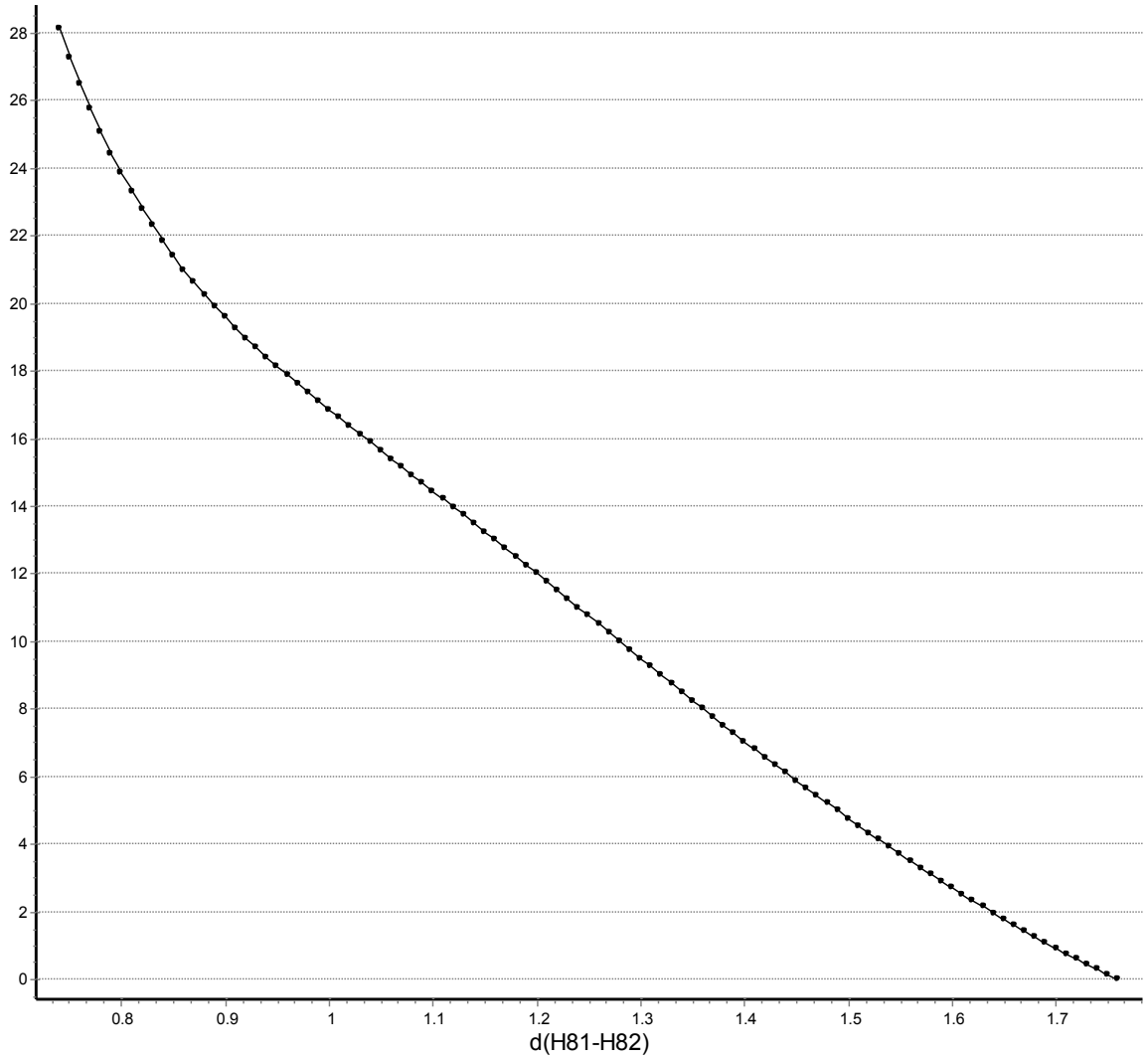
```
B 81 82 S 100 -0.01

P C H 0
3-21G
****
81 82 0
6-311+G**
****
Pt     0
S   3   1.00
     30.000000000           0.27148263900
     27.000000000          -0.42226758774
     14.408318564           0.44361581995
S   1   1.00
      5.5335788010          1.0000000
S   1   1.00
      1.2986438223          1.0000000
S   1   1.00
      0.58759393108         1.0000000
S   1   1.00
      0.13845587261         1.0000000
S   1   1.00
      0.49204459888E-01           1.0000000
P   4   1.00
     15.500000000          -0.15672718629
     14.000000000           0.23853412989
      6.1161212339         -0.31041379733
      1.5715586385          0.56473525089
P   1   1.00
      0.75132510781         1.0000000
P   1   1.00
      0.33306466812         1.0000000
P   1   1.00
      0.57000000000E-01           1.0000000
D   4   1.00
      8.3207937611          0.62945798646E-01
      7.4207226520         -0.90271847072E-01
      1.6570410639          0.16812526416
      0.73943569960         0.25045416970
D   1   1.00
```

```
      0.30510856008          1.0000000
D   1   1.00
      0.11350405268          1.0000000
F   1   1.00
      0.6681300              1.0000000
****

PT     0
PT-ECP     3     60
f-ul potential
  1
2       3.30956857            24.31437573
s-ul potential
  3
2      13.42865130           579.22386092
2       6.71432560            29.66949062
2       3.30956857           -24.31437573
p-ul potential
  3
2      10.36594420           280.86077422
2       5.18297210            26.74538204
2       3.30956857           -24.31437573
d-ul potential
  3
2       7.60047949           120.39644429
2       3.80023974            15.81092058
2       3.30956857           -24.31437573
```

The results of the scan is as follows: (image obtained with Chemcraft



It can be clearly seen that no TS could be optimized from any part of the geometry, and that the addition of H_2 proceeds downhill from the Pt(0) species.

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