# $Ir^{I}(\eta^4$-diene) precatalyst activation by strong bases: formation of anionic $Ir^{III}H_4$

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SUPPORTING INFORMATION

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## X-ray diffraction results

### Experimental details for the structural analysis of compounds 1 and [IrH(dppe)$_2$]

Single crystals of compound **1** ($C_{34}H_{36}P_2ClIr$) and [IrH(dppe)$_2$] ($C_{52}H_{49}IrP_4$) were obtained by crystallisation from dichloromethane/toluene. Diffraction data were collected at 110 K on an Oxford Diffraction SuperNova diffractometer with Cu-Ka radiation (l = 1.54184 Å) using an EOS CCD camera. The crystal was cooled with an Oxford Instruments Cryojet. Diffractometer control, data collection, initial unit cell determination, frame integration and unit-cell refinement were carried out with CrysAlisPro (Oxford Diffraction Ltd.). Face-indexed absorption corrections were applied using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm within CrysAlisPro. OLEX2[1] was used for overall structure solution, refinement and preparation of publication data. Within OLEX2, the algorithm used for structure solution was SHELXT[2] dual-spaced. Refinement by full-matrix least-squares used the SHELXL[3] algorithm within OLEX2. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using a “riding model” and included in the refinement at calculated positions.

**sbd21004**

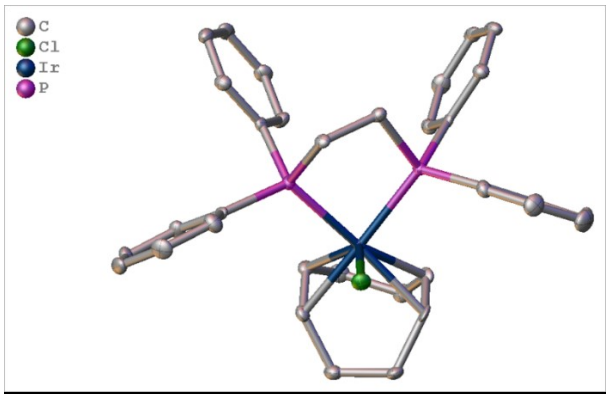



Table S 1. Crystal data and structure refinement for compound **1**.

| | |
|---|---|
| Identification code | sbd21004 |
| Empirical formula | $C_{34}H_{36}P_2ClIr$ |
| Formula weight | 734.22 |
| Temperature/K | 110.00(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 14.0891(2) |
| b/Å | 10.14941(14) |
| c/Å | 20.5215(3) |
| α/° | 90 |
| β/° | 90.8366(15) |
| γ/° | 90 |
| Volume/Å$^3$ | 2934.17(8) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.662 |
| μ/mm$^{-1}$ | 4.773 |
| F(000) | 1456.0 |
| Crystal size/mm$^3$ | 0.263 × 0.196 × 0.05 |
| Radiation | Mo Kα (λ = 0.71073) |
| 2Θ range for data collection/° | 6.968 to 52.736 |
| Index ranges | $-17 \le h \le 9$, $-12 \le k \le 12$, $-23 \le l \le 25$ |
| Reflections collected | 12585 |
| Independent reflections | 5993 [$R_{int}$ = 0.0286, $R_{sigma}$ = 0.0456] |
| Data/restraints/parameters | 5993/0/343 |
| Goodness-of-fit on $F^2$ | 1.054 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0271, $wR_2$ = 0.0518 |
| Final R indexes [all data] | $R_1$ = 0.0367, $wR_2$ = 0.0569 |
| Largest diff. peak/hole / e Å$^{-3}$ | 1.18/-0.77 |

**sbd21001**

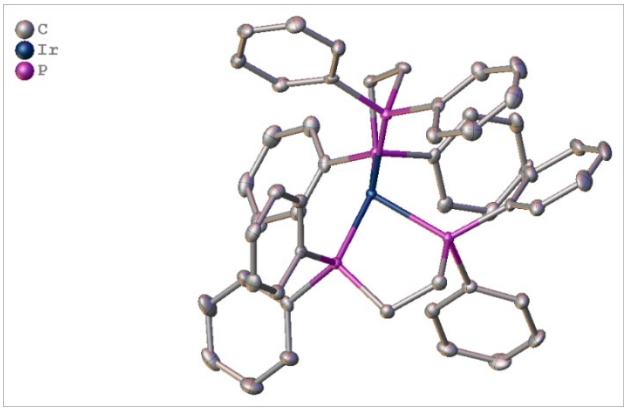



Table S 2. Crystal data and structure refinement for compound [IrH(dppe)$_2$].

| | |
|---|---|
| Identification code | sbd21001 |
| Empirical formula | $C_{52}H_{49}IrP_4$ |
| Formula weight | 989.99 |
| Temperature/K | 110.00(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 10.09632(17) |
| b/Å | 20.7085(4) |
| c/Å | 20.9765(3) |
| α/° | 90 |
| β/° | 90.7143(16) |
| γ/° | 90 |
| Volume/Å$^3$ | 4385.44(13) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.499 |
| μ/mm$^{-1}$ | 7.536 |
| F(000) | 1992.0 |
| Crystal size/mm$^3$ | 0.155 × 0.119 × 0.045 |
| Radiation | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 8.432 to 134.134 |
| Index ranges | $-11 \leq h \leq 12$, $-24 \leq k \leq 19$, $-24 \leq l \leq 25$ |
| Reflections collected | 15880 |
| Independent reflections | 7820 [$R_{int}$ = 0.0281, $R_{sigma}$ = 0.0397] |
| Data/restraints/parameters | 7820/0/518 |
| Goodness-of-fit on F$^2$ | 1.032 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0238, $wR_2$ = 0.0499 |
| Final R indexes [all data] | $R_1$ = 0.0336, $wR_2$ = 0.0540 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.71/-0.45 |

## Characterization of hydrides 2 and 3

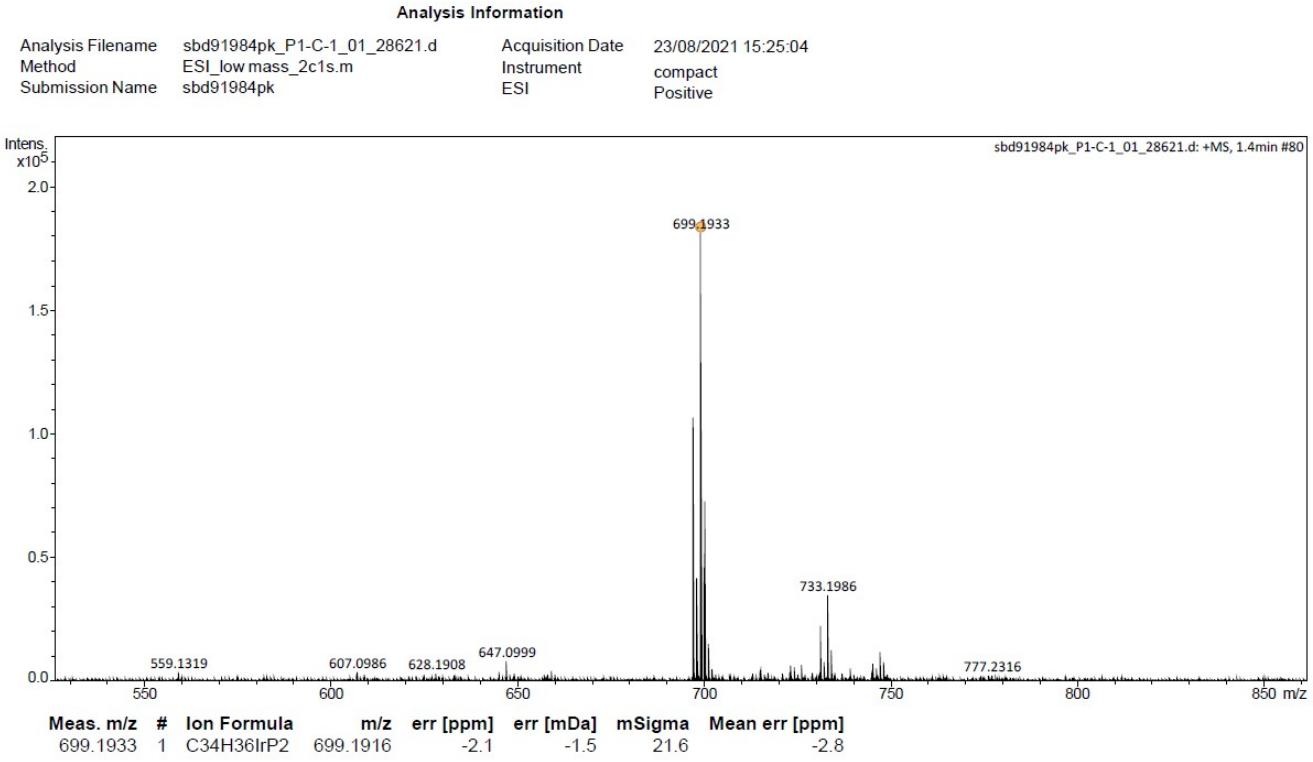



Figure S 1. ESI-HRMS (positive mode, in $CH_2Cl_2$ solution) of the mixture of compounds **2** and **3**.

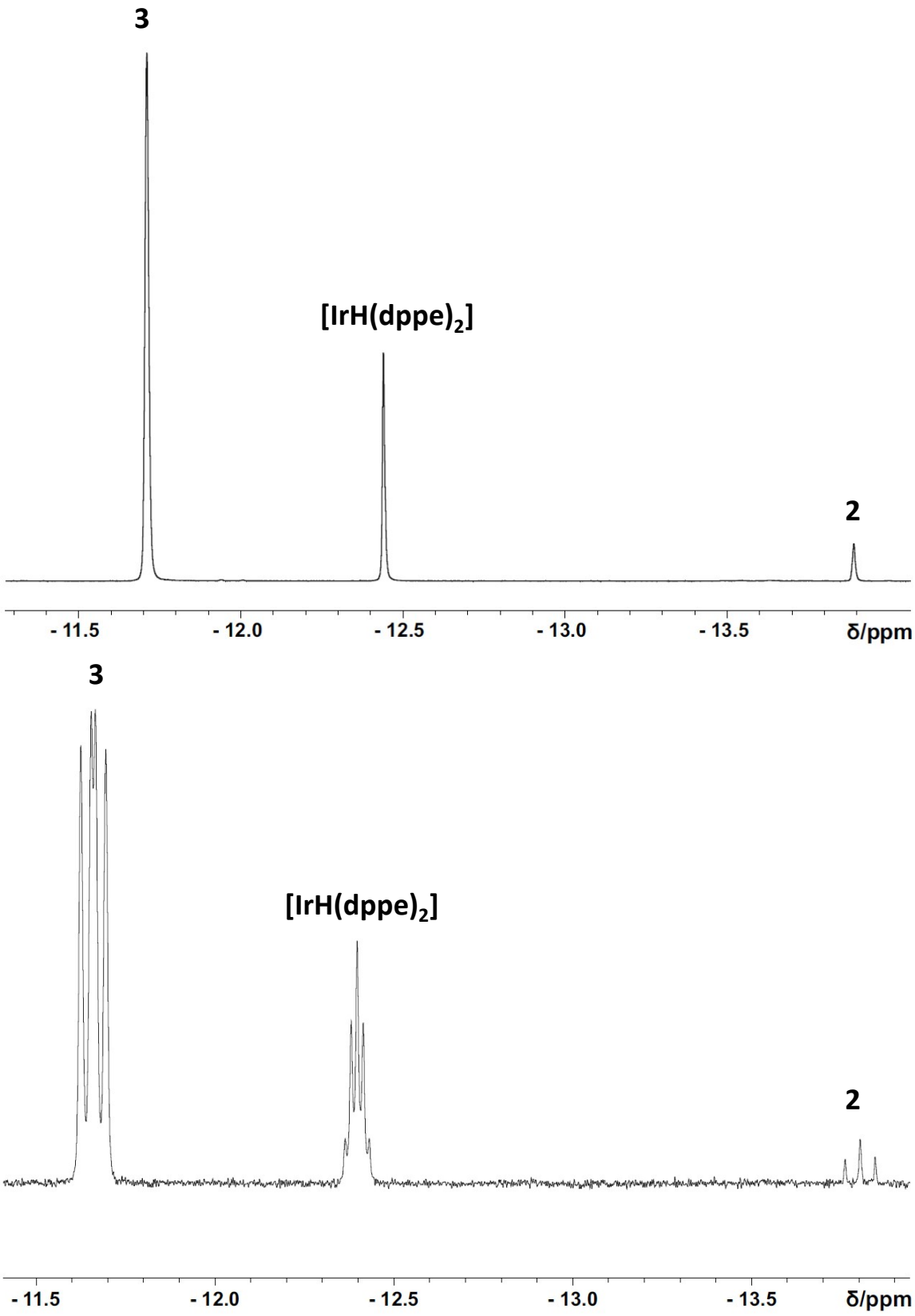



Figure S 2. $^{1}H\{^{31}P\}$ (above) and $^{1}H$ (below) NMR spectra in the hydride region of the product obtained by addition of KO$^{t}$Bu to $[IrCl(COD)]_2$/dppe (with dppe/Ir slightly > 1) in $^{i}$PrOH at 298 K. Solvent = $C_6D_6$.

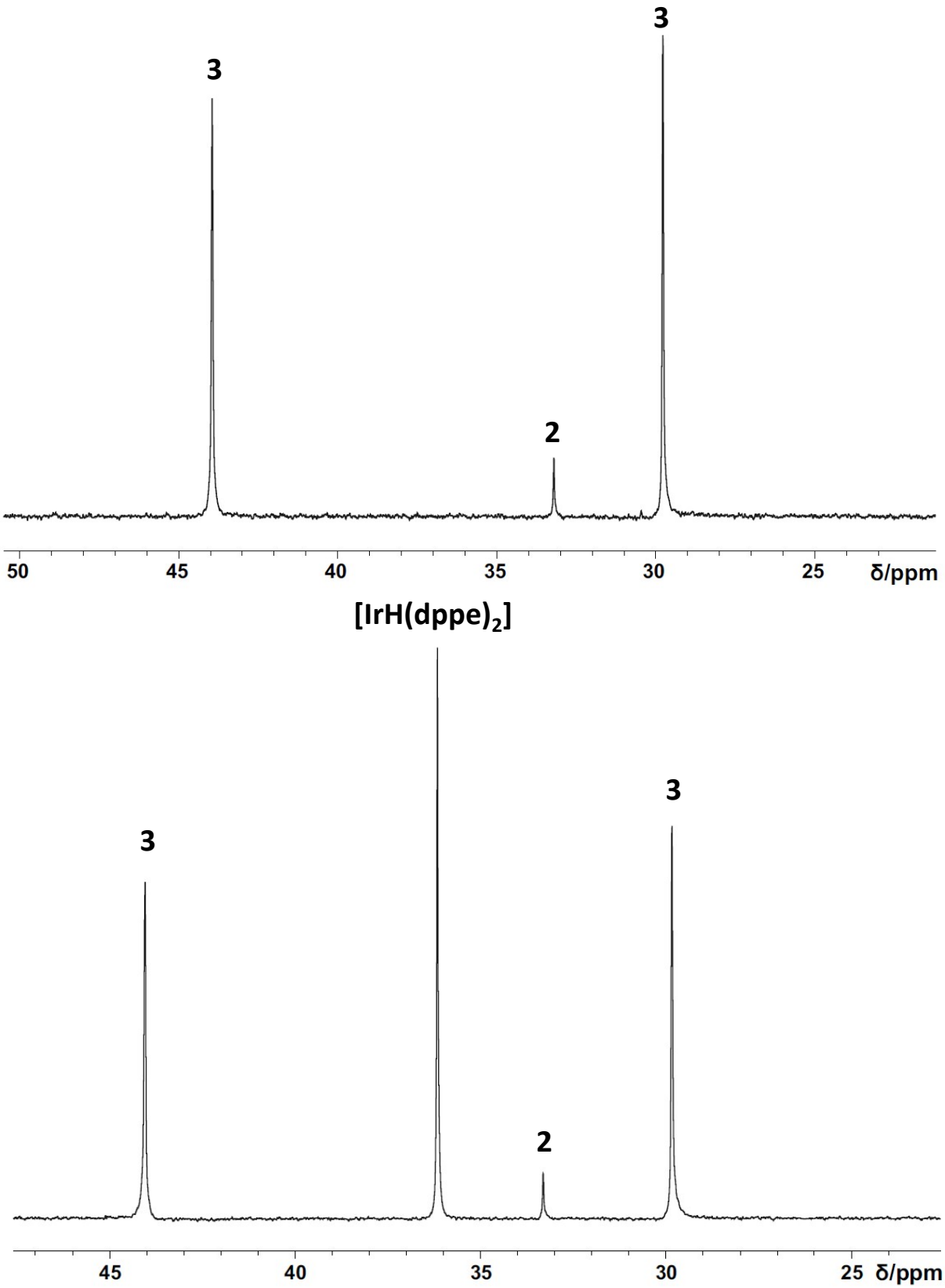



Figure S 3. $^{31}P\{^{1}H\}$ NMR spectrum of the product obtained by addition of $KO^{t}Bu$ to $[IrCl(COD)]_2$/dppe in $^{i}PrOH$ at 298 K. Solvent = $C_6D_6$. The dppe/Ir ratio is 1:1 (above) and slightly > 1 (below).

Table S 3. NMR properties of isomeric [IrH(1,2,5,6-$\eta^2$:$\eta^2$-COD)(dppe)] (**2**) and [Ir(1-$\kappa$-4,5,6-$\eta^3$-$C_8H_{12}$)H(dppe)] (**3**) in $C_6D_6$.

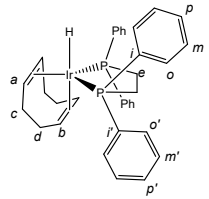
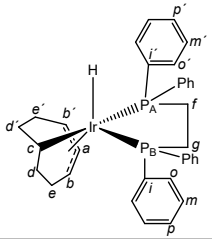
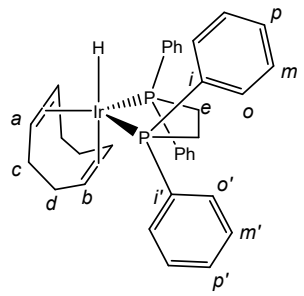
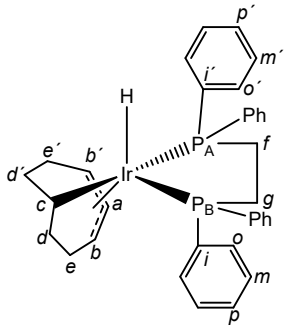
| Compound **2** | | | | Compound **3** | | | |
|---|---|---|---|---|---|---|---|
|  | | | |  | | | |
| | lit.[4] ($CDCl_3$) | this work ($C_6D_6$) | this work (DFT) | | lit.,[5] ($C_6D_6$) | this work ($C_6D_6$) | this work (DFT) |
| **$^1$H** | | | | | | | |
| Ph | 7.3 (m) | 8.01 – 7.0 | | Ph | 8.2-7.0 (m) | 8.05 ($o_{B,down}$), 8.00 ($o_{A,up}$), 7.60 ($o_{B,up}$), 7.23 ($m_{B,down}$), 7.18 ($p_{B,down}$), 7.15 ($m_{A,up}$), 7.10 ($p_{A,up}$), 7.05 ($m_{B,up}$), 6.99 ($p_{B,up}$), 6.92 ($m_{A,down}$), 6.85 ($p_{A,down}$), 6.83 ($o_{A,down}$) | |
| COD CH | [a] | 3.81 (bs) | 3.6 (*a*)<br>2.7 (*b*) | $C_8H_{12}$ allyl | 5.15 (bm) (*b,b'*)<br>5.07 (bm) (*b,b'*)<br>4.01 (m) (*a*) | 5.06 (bm) (*b*)<br>4.97 (bm) (*b'*)<br>3.91 (dt, $J_{HH}$ = 7.5; $J_{PH}$ = 14.3) (*a*) | 4.5 (*b*)<br>4.7 (*b´*)<br>3.2 (*a*) |
| COD $CH_2$ | [a] | 2.45, 2.36 | 2.52 ($c_{exo}$)[b], 2.50 ($c_{endo}$)[b]<br>1.78 ($d_{exo}$)[b], 1.91 ($d_{endo}$)[b] | | | | |
| dppe $CH_2$ | 2.05 | 2.21, 1.81 | 2.2, 2.7 | $C_8H_{12}$ Ir-CH | 2.2-1.8 (multiplets) | 2.34 (bm) (*c*) | 0.9 |
| | | | | $C_8H_{12}$ $CH_2$ | | 2.47, 2.17 (*d'*)<br>2.50, 2.26 (*d*)<br>2.23, 1.88 (*e'*)<br>2.10, 1.78 (*e*) | 1.3, 2.1 (*d*)<br>1.4, 1.8 (*d´*)<br>1.9, 2.0 (*e*)<br>1.8, 1.9 (*e´*) |
| | | | | dppe $CH_2$ | 2.5 (bm), 2.0 (bm) | $2.07_{(up)}$, $1.47_{(down)}$ (*f*)<br>$2.46_{(down)}$, $1.94_{(up)}$ (*g*) | |
| Ir-H | -14 (t, $J_{PH}$ = 21.5 Hz) | -14.0 (t, $J_{PH}$ = 21.6) | -7.66 | Ir-H | -11.55 (dd, $J_{HP}$ = 14.7, $J_{HP}$ 20.6 Hz) | -11.66 (dd, $J_{PH}$ = 14.9 ($P_A$), 22.2($P_B$)) | -4.0 |

Table S 3(contd).

| Compound **2** | Compound **3** |
|---|---|

|  | | |  | | |
|---|---|---|---|---|---|
| | lit.[6] ($CDCl_3$) | this work ($C_6D_6$) | | lit.,[5] ($C_6D_6$) | this work ($C_6D_6$) |
| **$^{13}$C** | | | | | |
| Ph | Not reported | [c] 134.5 (*o*) 127.9 (*m*) 128.9 (*p*) | Ph | 138-128 | 137.07 (d, $J_{PC}$ = 30 Hz, $i_{A,down}$), 136.97 (d, $J_{PC}$ = 53 Hz, $i_{B,up}$), 135.46 ($o_{A,up}$), 135.36 (d, $J_{PC}$ = 38 Hz, $i_{A,up}$), 134.77 ($o_{B,down}$), 134.32 (d, $J_{PC}$ = 34 Hz, $i_{A,up}$), 130.82 ($o_{A,down}$), 132.00 ($o_{B,up}$), 128.92 ($p_{B,up}$), 129.94 ($p_{B,down}$), 129.82 ($p_{A,up}$), 128.23 ($p_{A,down}$), 127.91 ($m_{A,up}$), 127.71 ($m_{A,down}$), 127.62 ($m_{B(up)}$), 127.94 ($m_{B,down}$) |
| COD CH | | 63.2 (*a*, *b*) | $C_8H_{12}$ allyl | 91.3 (s), 63.2 (d, $J_{CP}$ = 37.2 Hz) | 91.00 (s) (*a*)<br>62.80 (s) (*b'*)<br>72.00 (s) (*b*) |
| COD $CH_2$ | | 35.5 (*c*, *d*) | | | |
| dppe $CH_2$ | | 29.3 (e) | $C_8H_{12}$ $CH_2$ | 56.5 (s), 55.3 (d, $J_{CP}$ = 13.9 Hz), 29.4 (s), 27.0 (d, $J_{PC}$ = 29.3, 13.9 Hz) | 29.13 (*e'*)<br>56.22 (d')<br>26.72 (e)<br>54.95 (*d*) |
| | | | $C_8H_{12}$ Ir-CH | 33.0 (dd, $J_{PC}$ = 72.6, 4.6 Hz) | 32.72 (d, $J_{PC}$ = 30 Hz) |
| | | | dppe $CH_2$ | 35.7 (m), 29.6 (m) | 29.42 (*f*)<br>35.09 (*g*) |
| **$^{31}$P** | | | | | |
| | Not reported | 33.2 (s) | | 43.8 (d), 29.7 (d), $J_{PP}$ = 2.0 Hz | 43.9 (d, $P_B$), 29.1 (d, $P_A$) $J_{PP}$ = 2.8 |

[a] Assignment prevented by decomposition in $CDCl_3$. [b]The static optimized structure ($C_1$ symmetry) gave two different values for two pseudo-symmetric $CH_{exo}$ and for the two pseudo-symmetric $CH_{endo}$ on each C atom (*c* and *d*); the reported numbers are the averages of each pair. [c]The assignment of the Ph *ipso* $^{13}$C resonances of compound **2** was prevented by large overlap with other major resonances.

**Comments on the NMR characterisation of 2 and 3.**

The COD allyl region shown in Figure S 4, establishes the peak positions for each of the $\kappa^3$ CH resonances seen in product **3**, and a minor COD-CH peak at 3.8 ppm for **2**. The previous work by Oro *et al*.[6] did not mention the observation of an allylic peak due to the decomposition in solvent, however, in $C_6D_6$ this compound appeared to be perfectly stable. A signal is seen for the □²:□² CH groups. A single broad peak is observed for the allylic CH of **2** (*a* and *b*) rather than two. The DFT calculated NMR resonances give two separate resonance values, as one of the alkene groups is *trans* to the hydride whereas the other is *syn*. Two $^1$H signals are observed for the ethylene backbone of the dppe, in both the experimental and calculated chemical shifts, this can easily be assigned due to the stability of **2**. The major difference between the experimental and calculated chemical shifts arise from the COD $CH_2$. Two signals are observed experimentally, whereas, there are four calculated chemical shifts for both the *exo* and *endo* hydrogens on each carbon 2*c*, and 2*d*. The large overlap of the signals makes it difficult to extract each resonance for 2*c*, and 2*d*

The two closely placed multiplets observed for **3** around 5 ppm do not change in shape upon $^{31}$P decoupling, whereas the doublet of triplet signals at 3.91 ppm collapses to a triplet (Figure S 4). This difference in shape upon decoupling aids the distinction of the positions for the η-bound portion of the ligand, specifically $3H_a$. The chemical shifts for each of the $sp^2$-hybridised protons are not significantly different from those previously reported. In this case the calculated DFT results show a similar trend to the experimentally determined chemical shifts.

The phenyl region of the $^1$H (and $^1$H{$^{31}$P}) spectra shows several multiplets arising from HP and HH coupling of the protons on the phenyl rings (Figure S 5). When the HP coupling is removed, the region is easier to interpret and allows assignment of each resonance to the proton at the corresponding position on the phenyl ring. Given the minor amount of **2** (~5%), $^{31}$P-$^1$H HMQC methods were deployed to resolve minor peak positions (Figure S 6). More importantly through the HMQC experiments the specific phenyl and $CH_2$ groups both on the COD ligand and ethylene bridge of the dppe (Figure S 9) could be assigned. Through this process of elimination, we could easily assign the rest of the peaks based on what would not couple to the P atoms from long range. The $sp^3$ CH region of the $^1$H spectrum shows a complex region of multiplets, even when decoupled from $^{31}$P, as protons for both COD $CH_2$ (8H) groups on **2** and **3** are observed. This is further complicated by the $CH_2$ resonances on the $C_2H_4$ fragment on the dppe ligand. Notably, no H-P couplings could be clearly discerned. The spectrum can be resolved by using 2D NMR methods (Figure S 8). These experiments allow the $CH_2$ peaks to be easily assigned based on their coupling to the known resonances of protons in the other regions of the spectrum.

The excerpt of the HMQC spectrum in Figure S 10 highlights the correlation between the proton and carbon resonances of the allyl protons. The relative peak position of the $^{13}$C resonance correspond to those seen for allyl-type bonding (for **3**).

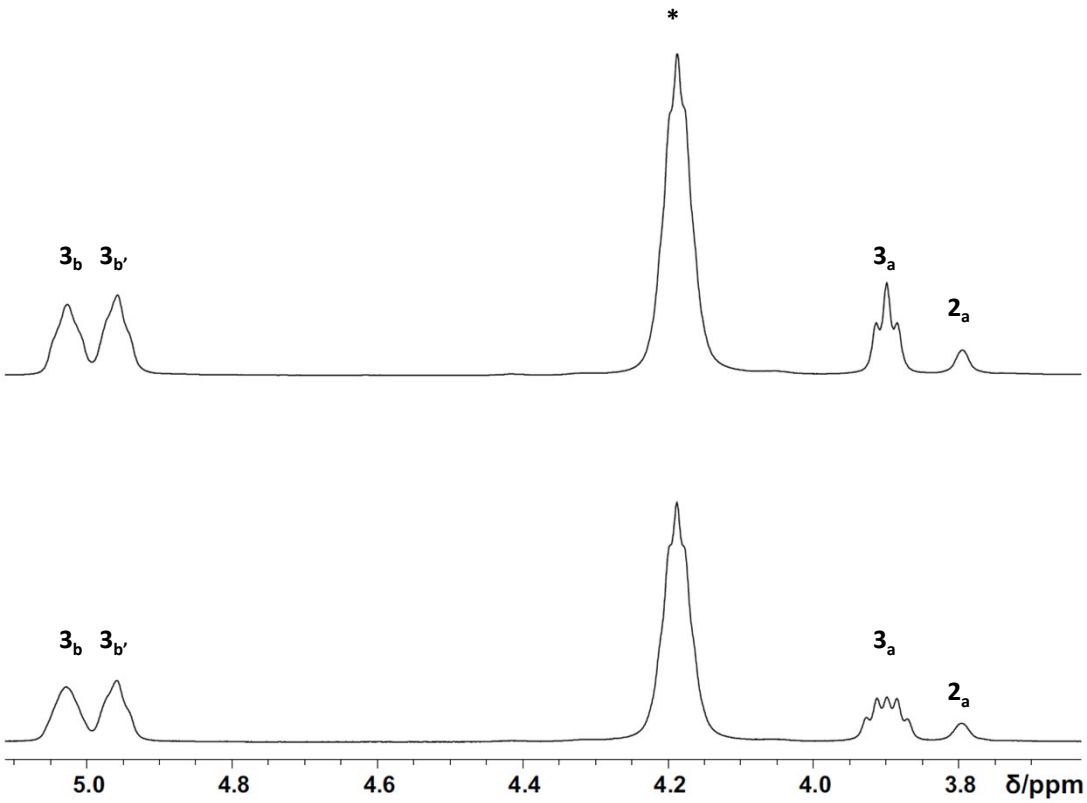



Figure S 4. $^{1}H$ (below) and $^{1}H\{^{31}P\}$ (above) NMR spectra of the COD CH proton resonances for the mixture of **2** and **3** in $C_6D_6$ at 298 K. The large starred resonance at 4.2 ppm presumably belongs to CH protons of residual isopropanol.

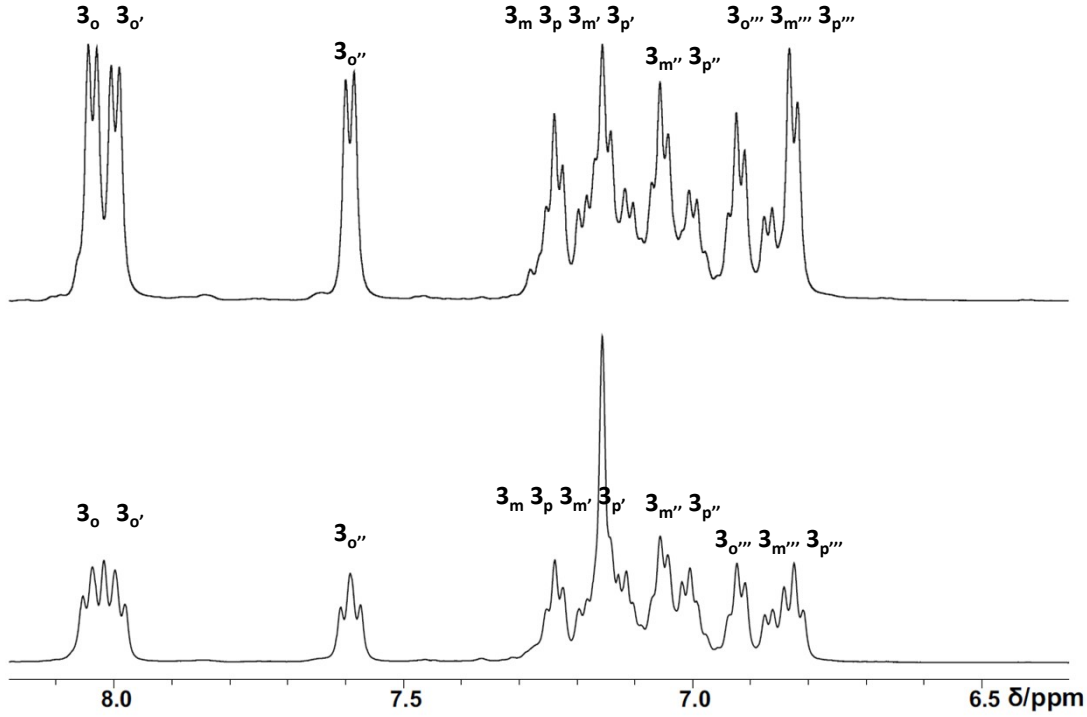



Figure S 5. $^{1}H$ (below) and $^{1}H\{^{31}P\}$ (above) NMR spectra of the phenyl proton resonance region for **2** and **3** in $C_6D_6$ at 298 K.

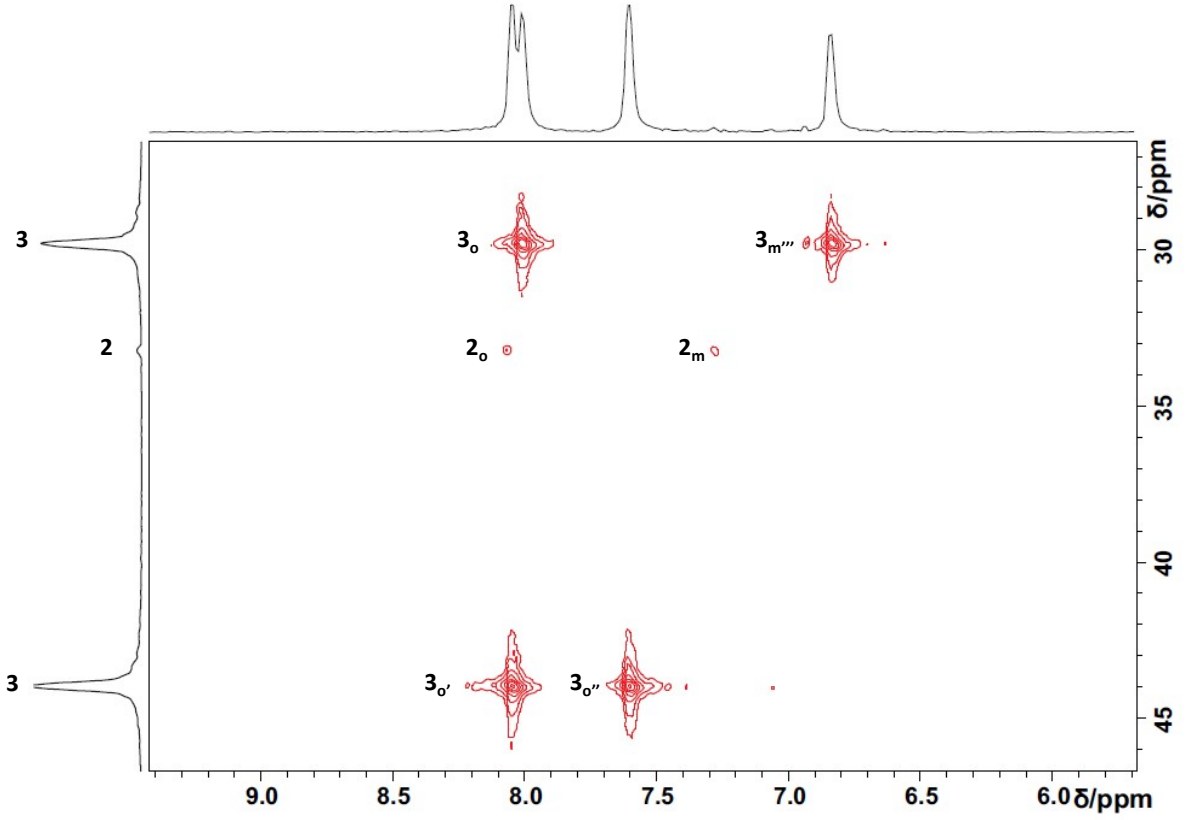



Figure S 6. Excerpt of the $^{31}P$-$^{1}H$ HMQC spectrum of **2** and **3** in the aromatic CH resonance region, in $C_6D_6$ at 298 K.

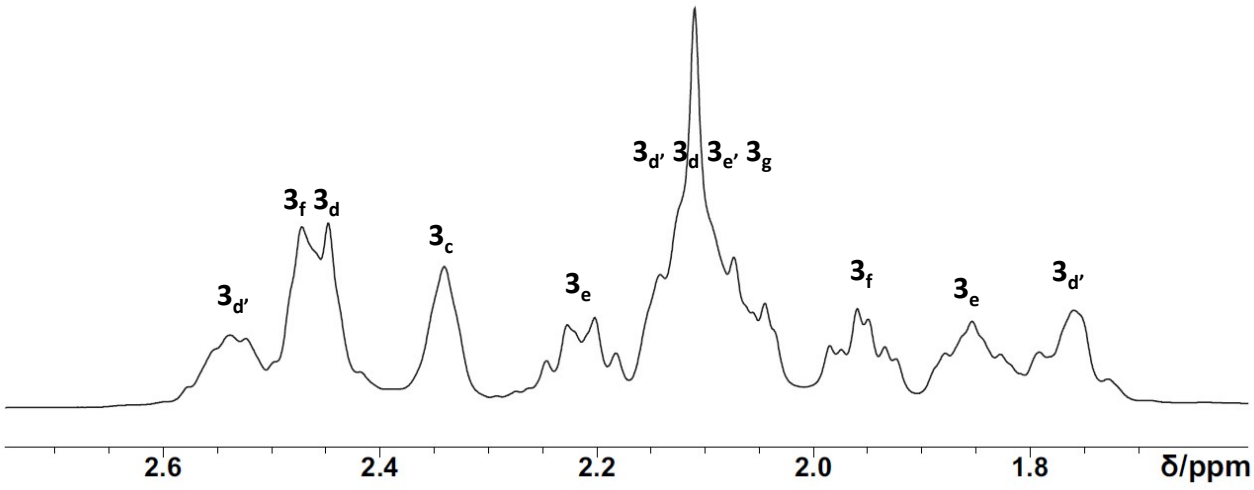



Figure S 7. $^{1}H\{^{31}P\}$ NMR spectrum of the $sp^3$ CH proton resonance region for **2** and **3**, in $C_6D_6$ at 298 K.

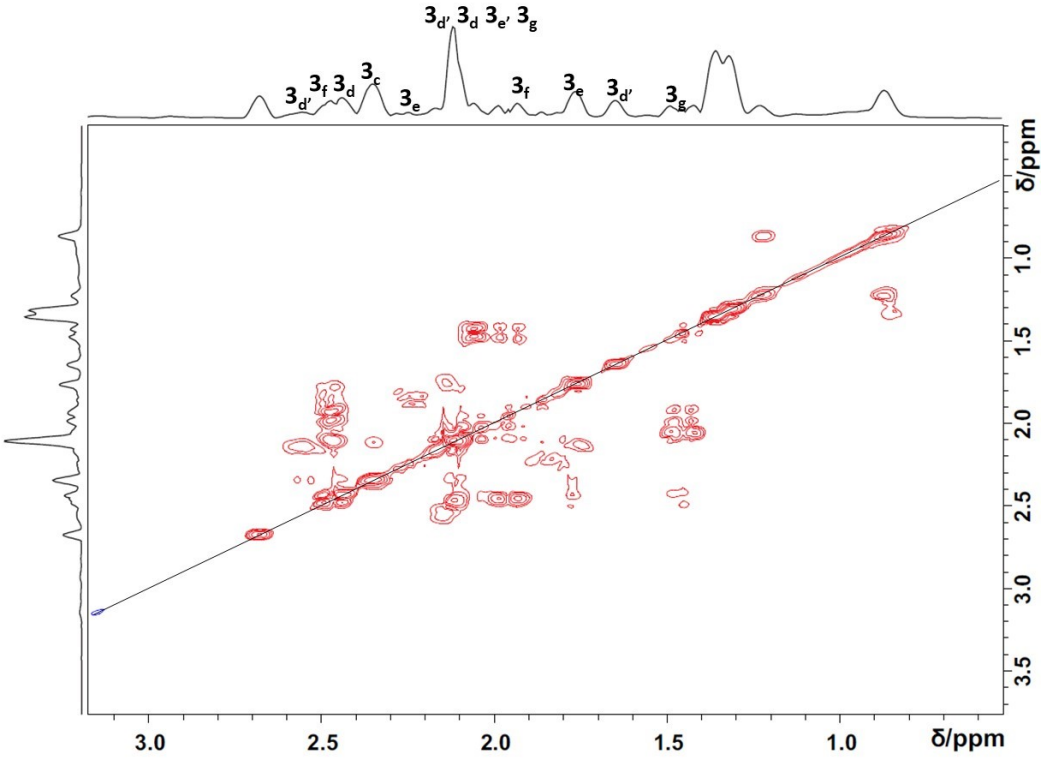



Figure S 8. Excerpt of the $^{1}$H-$^{1}$H COSY spectrum of **2** and **3** in the COD and dppe sp$^{3}$ CH region, in $C_6D_6$ at 298 K.

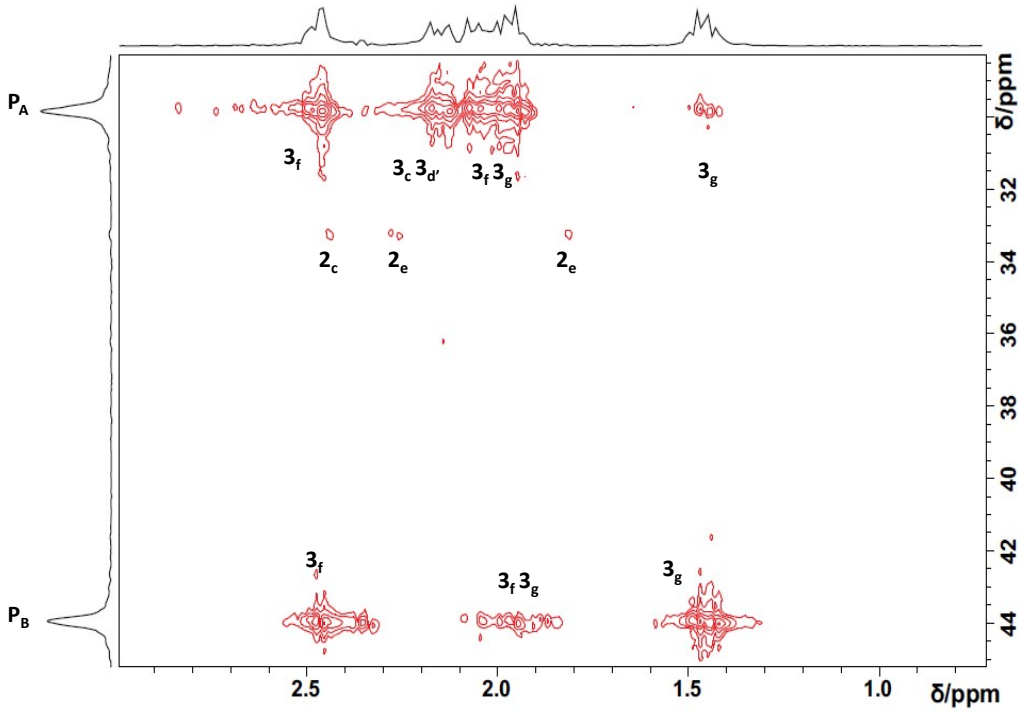



Figure S 9. Excerpt of the $^{31}$P-$^{1}$H HMQC spectrum of **2** and **3** in the COD and dppe sp$^{3}$ CH region, in $C_6D_6$ at 298 K.

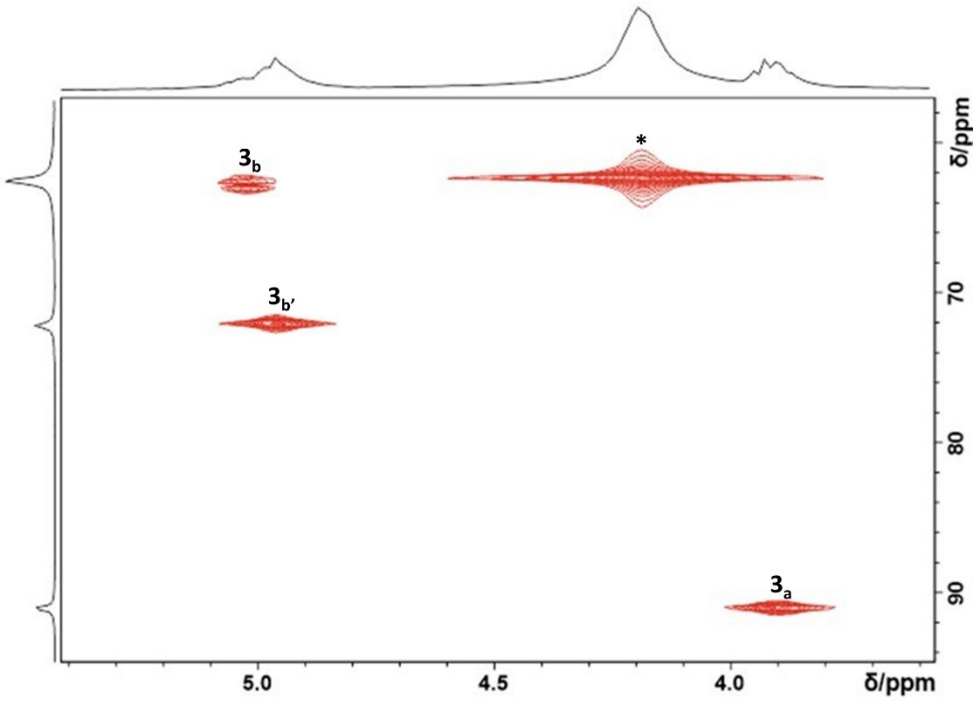
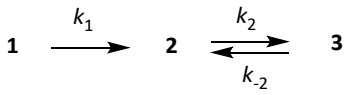



Figure S 10. Excerpt of the $^{13}C\{^{31}P\}$-$^{1}H$ HMQC spectrum for **2** and **3** in $C_6D_6$ in the COD $sp^2$ CH region. The starred resonance belongs to isopropanol, in $C_6D_6$ at 298 K.

**Kinetic analysis of the generation of 2 from 1 followed by its equilibrated transformation to 3**

The transformation follows the general kinetic scheme




With the boundary conditions

Time zero: [**1**] = [**1**]$_0$; [**2**]$_0$ = [**3**]$_0$ = 0

Time infinity (equilibrium): [**1**] = 0; [**2**] = [**2**]$_{eq}$; [**3**] = [**3**]$_{eq}$; [**3**]$_{eq}$/[**3**]$_{eq}$ = $k_2/k_{-2}$

Mass conservation: [**1**] + [**2**] + [**3**] = [**1**]$_0$

1. Data:

| Time/s | x(**1**) | x(**2**) | x(**3**) |
|---|---|---|---|
| 30 | 0.9124 | 0.0584 | 0.0292 |
| 2280 | 0.7752 | 0.1256 | 0.0992 |
| 4500 | 0.6207 | 0.1769 | 0.2024 |
| 6780 | 0.4919 | 0.1736 | 0.3345 |
| 9060 | 0.3648 | 0.1755 | 0.4597 |
| 11340 | 0.2814 | 0.1559 | 0.5627 |
| 13560 | 0.2147 | 0.1239 | 0.6614 |
| 15780 | 0.1586 | 0.1026 | 0.7389 |
| 18120 | 0.1186 | 0.0842 | 0.7972 |
| 20400 | 0.1045 | 0.0711 | 0.8245 |
| 26520 | 0.0701 | 0.0561 | 0.8738 |
| 29100 | 0.0313 | 0.0466 | 0.9221 |
| 32340 | 0.0168 | 0.0476 | 0.9356 |
| 35040 | 0.0036 | 0.0402 | 0.9562 |

2. Decay of **1**

This is a first-order decay ($-\frac{d[1]}{dt} = k_1[1]$), easily integrated to yield the well-known solution $[1] = [1]_0 e^{-k_1 t}$ or $ln\frac{[1]_0}{[1]} = k_1 t$.

Analysis of the first-order decay of **1** yields $k_1$ = (6.09±0.16)·10$^{-3}$ min$^{-1}$ = (1.13±0.03)·10$^{-4}$ s$^{-1}$.

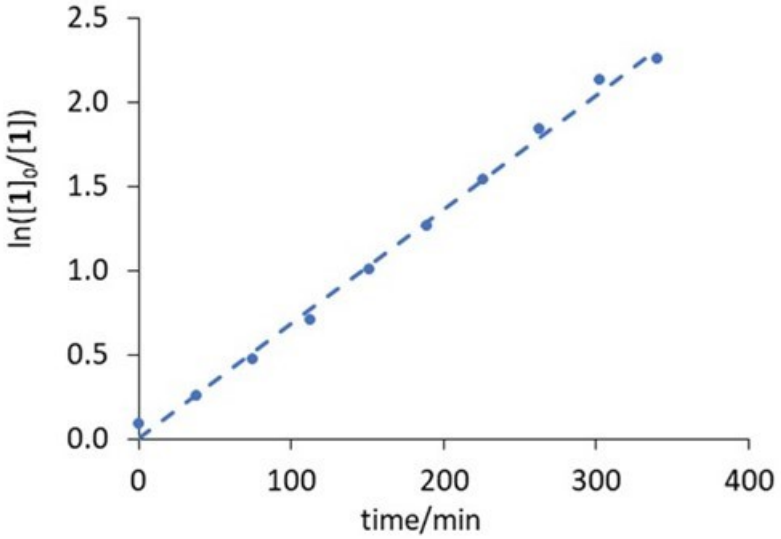



Figure S 11. Plot of the first-order decay analysis for the conversion of **1** to **2** and **3** in Figure 3.

3. Global fit

The three rate constants $k_1$, $k_2$ and $k_{-2}$ were obtained by numerical integration of the differential equations

$$-\frac{d[1]}{dt} = k_1[1]; \quad -d[1] = k_1[1]dt$$

$$\frac{d[2]}{dt} = k_1[1] - k_2[2] + k_{-2}[3]; \quad d[2] = \left(k_1[1] - k_2[2] + k_{-2}[3]\right)dt$$

$$\frac{d[3]}{dt} = k_2[2] - k_{-2}[3]; \quad d[3] = \left(k_2[2] - k_{-2}[3]\right)dt$$

to yield the concentration variations during each short time interval Δt, which was set to 1 s for the analysis, as follows:

$$[1]_{t+\Delta t} = [1]_t - k_1[1]_t\Delta t$$

$$[2]_{t+\Delta t} = [2]_t + \left(k_1[1]_t - k_2[2]_t + k_{-2}[3]_t\right)\Delta t$$

$$[3]_{t+\Delta t} = [3]_t + \left(k_2[2]_t - k_{-2}[3]_t\right)\Delta t$$

Since all elementary steps are first order processes, the analysis was more conveniently carried out on the molar fractions ($x_1 = \frac{[1]}{([1]+[2]+[3])}$; $x_B = \frac{[2]}{([1]+[2]+[3])}$; $x_C = \frac{[3]}{([1]+[2]+[3])}$):

$$x_{1,t+\Delta t} = x_{1,t} - k_1 x_{1,t}\Delta t$$

$$x_{2,t+\Delta t} = x_{2,t} + \left(k_1 x_{1,t} - k_2 x_{2,t} + k_{-2} x_{3,t}\right)\Delta t$$

$$x_{3,t+\Delta t} = x_{3,t} + \left(k_2 x_{2,t} - k_{-2} x_{3,t}\right)\Delta t$$

By imposing the initial condition at time zero ($x_{1,0}$ = 1; $x_{2,0}$= $x_{3,0}$ = 0), the calculated **1**, **2** and **3** fractions at the times $t_i$ of the experimental observations ($x_{1,i,calc}$, $x_{2,i,calc}$, $x_{3,i,calc}$) were derived by numerical integration on the basis of initial guess values of the rate constants $k_1$, $k_2$ and $k_{-2}$, which were treated as adjustable parameters during the fit. A non-linear least-squares fit was then performed to minimize the function

$$SUM = \sum_i \left[\left(x_{1,i} - x_{1,i}\right)^2 + \left(x_{2,i} - x_{2,i}\right)^2 + \left(x_{3,i} - x_{3,i}\right)^2\right]$$

By using the Solver tool of Excel. The resulting fits of the time evolutions of **1**, **2** and **3** are shown in Figure 3. The standard deviations on the optimized parameters were obtained with the Excel Macro Solver Aid.

**NMR characterization of hydrides 4 and 5**

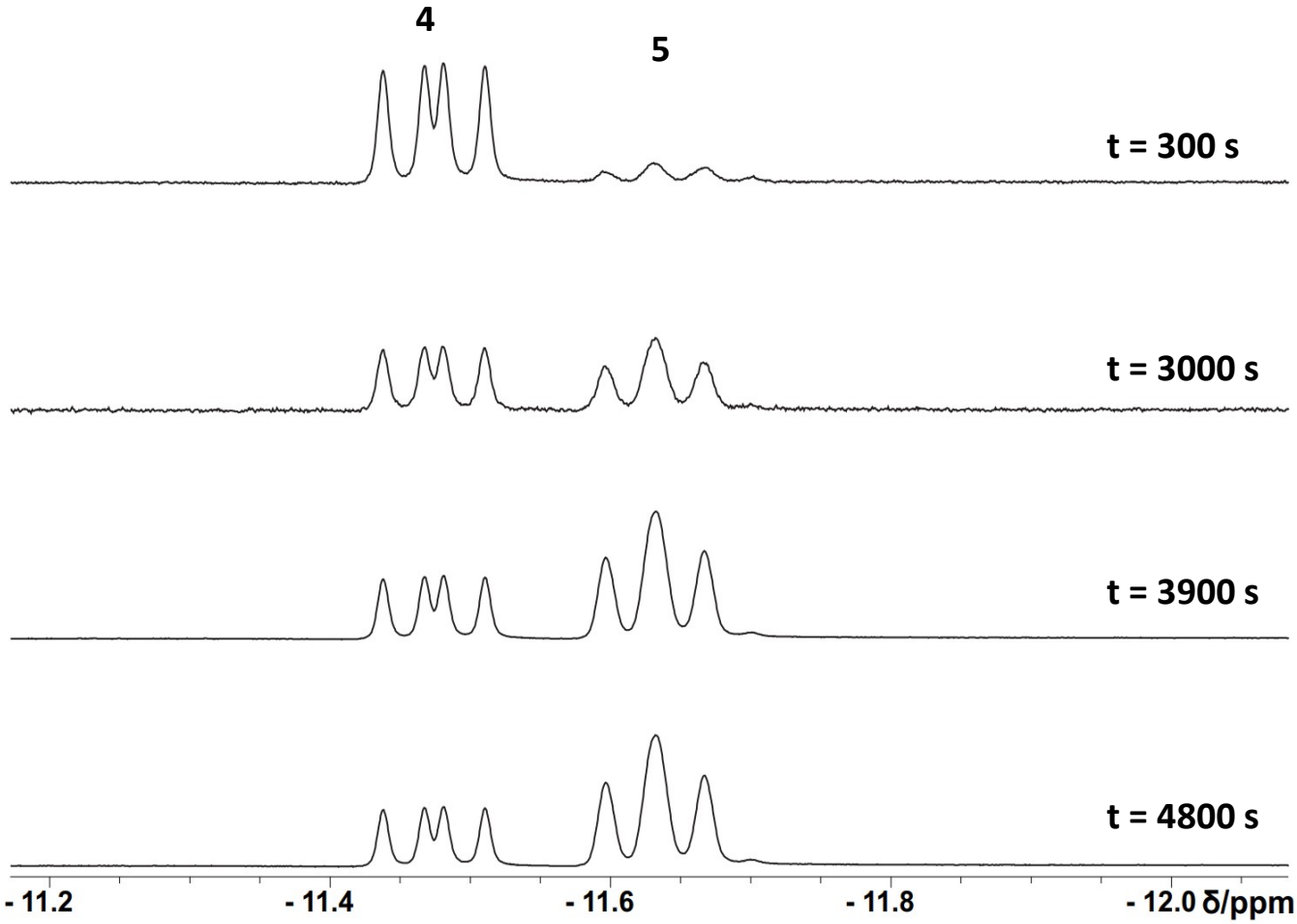



Figure S 12. $^{1}H$ NMR monitoring in the hydride resonance region of the solution obtained after addition of KO$^{t}$Bu to **1** in $C_6D_6$ at 298 K with generation of **4** and its isomerization to **5.**

Table S 4. NMR properties of isomeric [IrH($C_8H_{10}$)(dppe)] complexes **4** and **5** in $C_6D_6$ ($^1$H peak multiplicities for $^{31}$P-decoupled spectra).

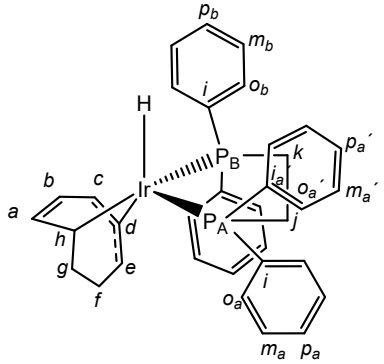
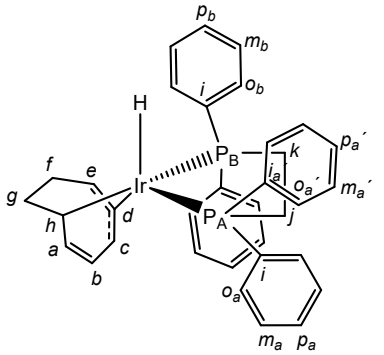
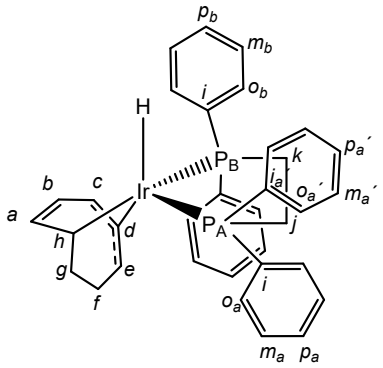
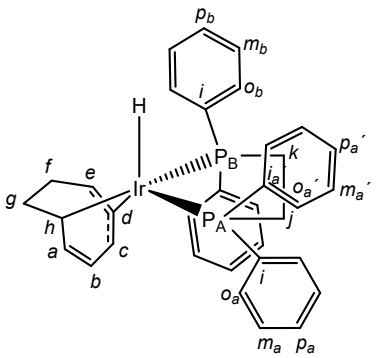
| Compound **4** | | Compound **5** | |
|---|---|---|---|
|  | |  | |
| **$^1$H** | | | |
| Ph | 8.11 ($o_{B,up}$), 8.09 ($o_{A,down}$), 7.55 ($o_{A,up}$), 7.25 ($m_{A,down}$), 7.21 ($p_{A,down}$), 7.15 ($m_{B,up}$), 7.12 ($p_{B,up}$), 7.05 ($m_{A,up}$), 7.02 ($p_{A,up}$), 6.92 ($m_{B,down}$), 6.85 ($o_{B,down}$), 6.85 ($p_{B,down}$) | Ph | 7.96 ($o_{A,up}$), 7.91 ($o_{B,up}$), 7.84 ($o_{B,down}$), 7.19 ($m_{B,down}$), 7.12 ($p_{B,down}$), 7.11 ($m_{A,up}$), 7.08 ($m_{B,up}$), 7.07 ($p_{A,up}$), 7.01 ($p_{B,up}$), 6.90 ($m_{A,down}$), 6.88 ($o_{A,down}$), 6.86 ($p_{A,down}$) |
| $C_8H_{10}$ C-H (olefin) | 5.47 (dd, $J_{HH}$ = 4, 6.4 Hz) (*a*)<br>5.94 (dd, $J_{HH}$ = 4, 6.4 with $J_{PH}$ = 4 Hz) (*b*) | $C_8H_{10}$ C-H (olefin) | 5.61 (dd, $J_{HH}$ = 4, 7 Hz) (*a*)<br>5.52 (dd, $J_{HH}$ = 4, 8Hz) (*b*) |
| $C_8H_{10}$ C-H (allyl) | 4.98 (dd, $J_{HH}$ = 4, 7 with $J_{PH}$ = 4 Hz) (*c*)<br>3.79 (t, $J_{HH}$ = 7 with $J_{PH}$ = 7 Hz) (*d*)<br>5.02 (m) (*e*) | $C_8H_{10}$ C-H (allyl) | 4.31 (dd, $J_{HH}$ = 4, 8 Hz) (*c*)<br>3.83 (t, $J_{HH}$ = 8 with $J_{PH}$ = 8 Hz) (*d*)<br>5.11 (dd, $J_{HH}$ = 8, 4 Hz) (*e*) |
| $C_8H_{10}$ $CH_2$ | 2.14 $_{(up)}$, 1.98 $_{(down)}$ (*f*)<br>1.96 $_{(up)}$, 2.41 $_{(down)}$ (*g*) | $C_8H_{10}$ $CH_2$ (f) | 2.43, 2.12 (*f*)<br>2.82, 2.12 (*g*) |
| $C_8H_{10}$ Ir-C-H | 2.59 br | $C_8H_{10}$ Ir-C-H | 2.78 br |
| dppe $CH_2$ | 2.48 $_{(down)}$, 1.80 $_{(up)}$ (*j*)<br>2.15, 1.26 (*k*) | dppe $CH_2$ | 2.51 $_{(down)}$, 1.89 $_{(up)}$ (*j*)<br>1.89, 1.85 (*k*) |
| Ir-H | -11.43 (dd, $J_{HPB}$ = 14.1, $J_{HPA}$ 21.8 Hz) | Ir-H | -11.57 (t, $J_{HP}$ = 19.5 Hz) |

Table S 4 (contd)

| Compound **4** | Compound **5** |
|---|---|

|  | |  | |
|---|---|---|---|
| **$^{13}$C** | | | |
| Ph | [a]<br>136.07 ($o_{B,up}$), 135.36 ($o_{A,down}$), 132.04 ($o_{A,up}$), 130.29 ($p_{A,down}$),<br>130.78 ($o_{B,down}$), 130.04 ($p_{B,up}$), 128.97 ($p_{A,up}$), 128.27 ($p_{B,down}$),<br>128.06 ($m_{B(up)}$), 128.06 ($m_{A,down}$), 127.73 ($m_{B,down}$), 127.62 ($m_{A,up}$) | Ph | 135.0, 133.0, 135.1, 130.9 (*i*,*i*',*i*'',*i*''')<br>134.98 ($o_{A,up}$), 133.28 ($o_{B,up}$), 132.72 ($o_{B,down}$), 130.78 ($o_{A(down)}$),<br>129.80 ($p_{A,up}$), 129.38 ($p_{B,up}$), 129.25 ($p_{B,down}$), 128.40 ($p_{A(down)}$),<br>127.98 ($m_{B,up}$), 127.90 ($m_{A,up}$), 127.78 ($m_{A,down}$), 126.67 ($m_{B,down}$) |
| $C_8H_{10}$ C-H (olefin) | 146.42 (*a*)<br>129.90 (*b*) | $C_8H_{10}$ C-H (olefin) | 127.5 (*a*)<br>148.1 (*b*) |
| $C_8H_{10}$ C-H (allyl) | 62.5 ($J_{PC}$ = 50 Hz) (*c*)<br>93.1 (*d*)<br>72.4 (*e*) | $C_8H_{10}$ C-H (allyl) | 73.3 (*c*)<br>94.1 (*d*)<br>62.88 d ($J_{PC}$ = 50 Hz) (*e*) |
| $C_8H_{10}$ $CH_2$ | 22.9 (*f*)<br>54.3 (*g*) | $C_8H_{10}$ $CH_2$ | 25.40 (*f*)<br>52.06 (*g*) |
| $C_8H_{10}$ Ir-C-H | 35.5 ($J_{PC}$ = 70 Hz) (h) | $C_8H_{10}$ Ir-C-H | 34.47 ($J_{PC}$ = 70 Hz) (h) |
| dppe $CH_2$ | 35.10 (j)<br>28.9 (*k*) | dppe $CH_2$ | 30.6 (*j*)<br>33.79 (*k*) |
| **$^{31}$P** | | | |
| $P_A$ | 30.6 (d, $J_{PP}$ = 2.4) | | 32.4 (d, $J_{PP}$ = 2.7) |
| $P_B$ | 46.7 (d, $J_{PP}$ = 2.4) | | 39.4 (d, $J_{PP}$ = 2.7) |

[a]The assignment of the Ph *ipso* $^{13}$C resonances of compound **4** was prevented by overlap with other major resonances.

**Comments on the NMR characterisation of 4 and 5.**

The *ortho*- phenyl protons on product **4** and **5** are readily identified as the downfield signals because they show a large difference in splitting when decoupled from $^{31}P$, resulting in doublet signals (Figure S 13 and Figure S 14). The phenyl region of the spectrum is quite crowded due to significant overlap for each isomer, possessing in total 20 H (and 24 C) signals for each isomer. Hence, the upfield phenyl region is much more difficult to distinguish the individual proton resonances, as many of the minor signals for **4** and, major signals for **5**, overlap. To identify the couplings, and indeed assign each proton, which is difficult on the sole basis of these $^{1}H$ spectra, $^{13}C$-$^{1}H$ (Figure S 15) and $^{31}P$-$^{1}H$ (Figure S 17) HMQC, COSY (Figure S 16), and NOESY (Figure S 18) methods were used to support the analysis of each structure.

The 1-D NOESY experiments were used to probe the signals within the allyl region of the $^{1}H$ NMR spectra, because the significant overlap between signals for **4** and **5** in the $^{1}H$ NMR makes these signals difficult to distinguish with a single experiment. They were used to confirm the structure and binding of the $C_8H_{10}$ ligands with $\kappa^1,\eta^3$ binding. The through-space interactions between the olefinic protons and the CH groups provided insight into the $C_8H_{10}$ ligand arrangement. The COSY spectrum (Figure S 16) allowed full characterization and assignment of the $sp^2$ hybridised protons.

In the $^{13}C$-$^{1}H$ HMQC spectrum, four proton resonances in the 5 – 6 ppm region correlate with downfield shifted carbon signals. These signals arise from the two unbound alkene moieties of **4** and **5**. The combination of the HMQC spectra (Figure S 15, Figure S 17) alongside selective 1D-NOESY (Figure S 18) and COSY (Figure S 16) experiments aided the assignment of all resonances, as reported in Table S 4.

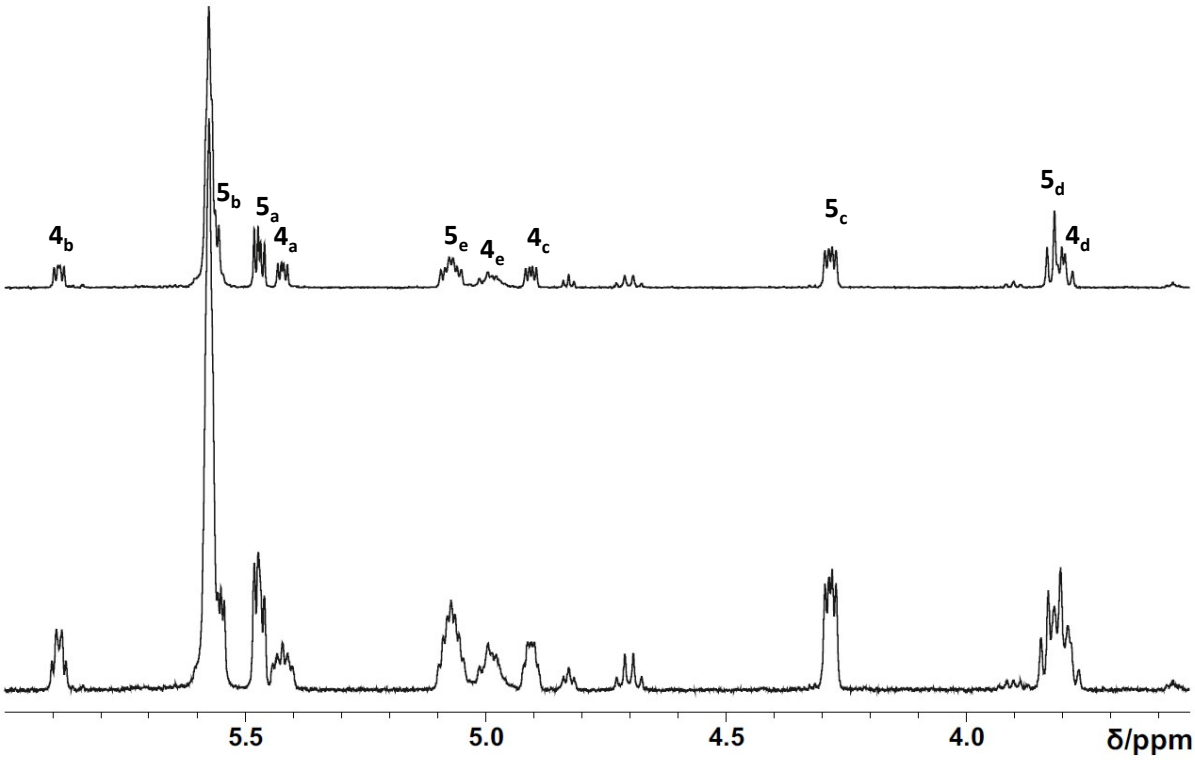



Figure S 13. $^{1}H\{^{31}P\}$ (above) and $^{1}H$ (below) spectra of the alkene region for the mixture of product **4** and **5** in $C_7D_8$.

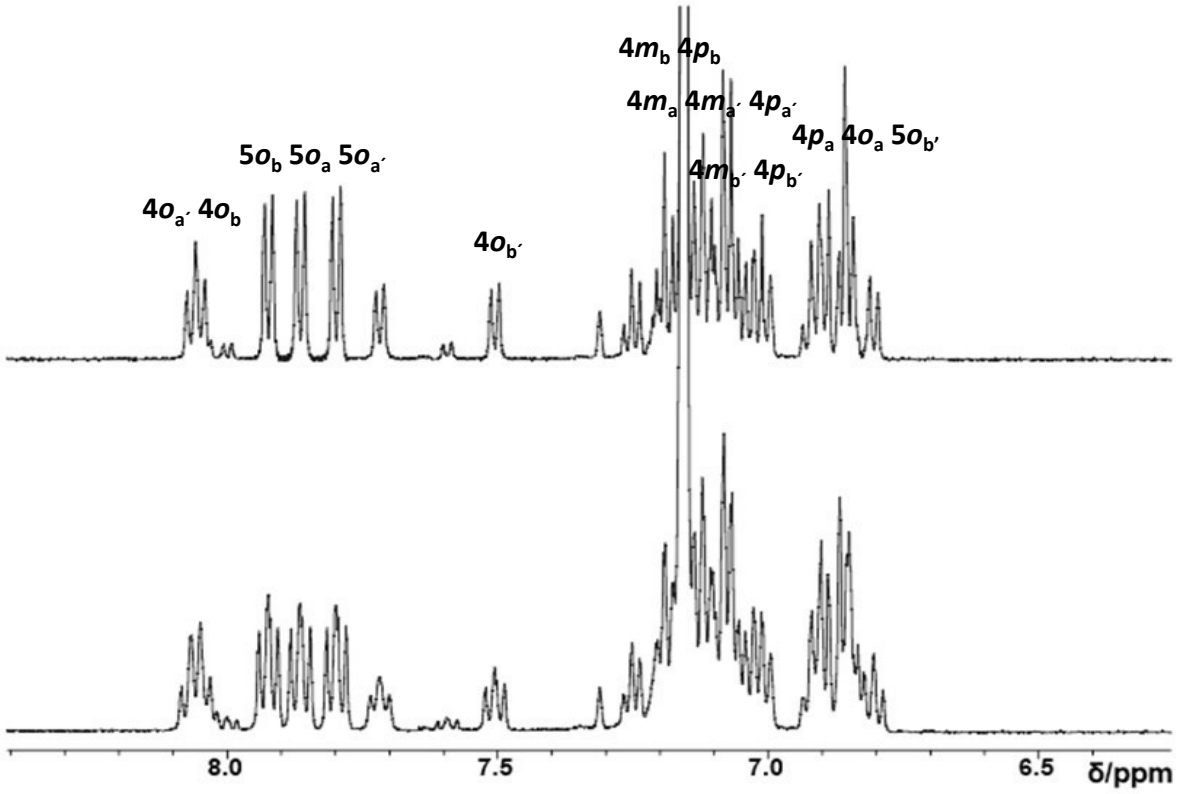



Figure S 14.$^{1}H\{^{31}P\}$ (above) and $^{1}H$ (below) spectra of the phenyl region for the mixture of products **4** and **5** in $C_6D_6$.

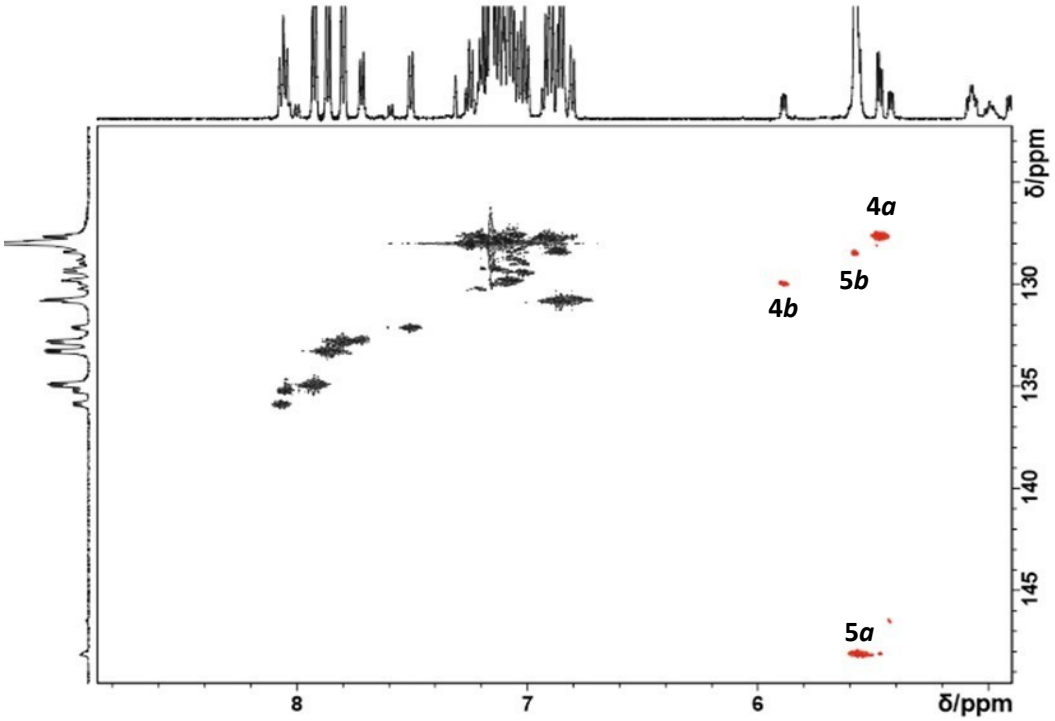



Figure S 15. Excerpt of the $^{13}C$-$^{1}H$ HMQC NMR spectrum of the mixture of products **4** and **5** in $C_6D_6$ in the $sp^2$ CH resonance region. The unbound alkene groups are highlighted in red.

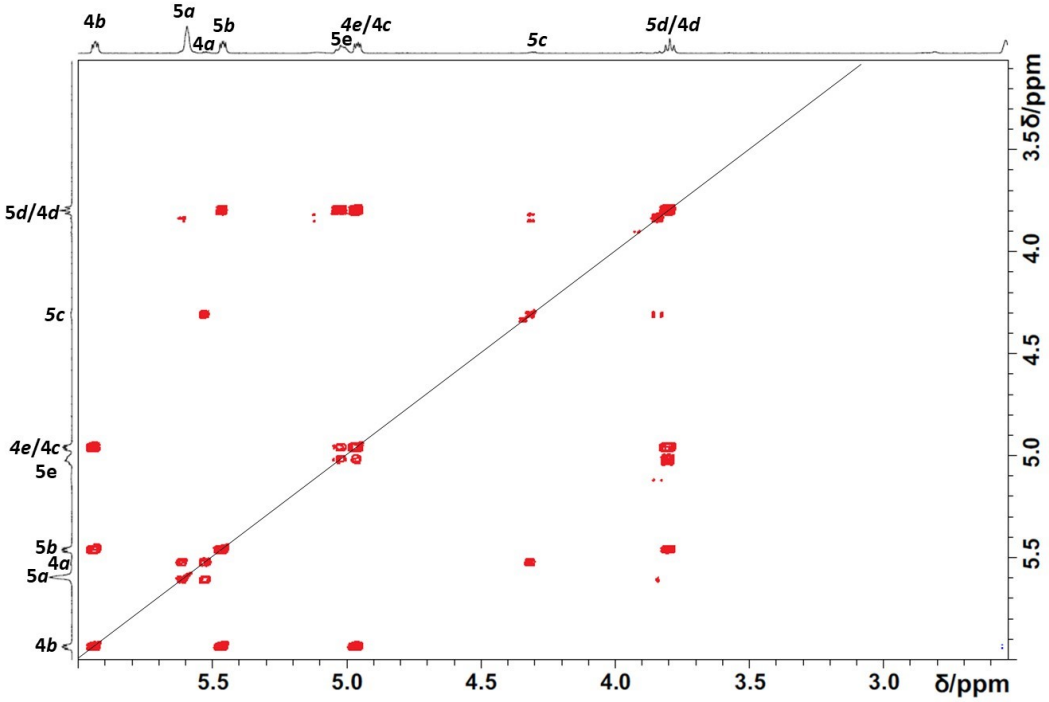



Figure S 16. $^{31}P$-decoupled H-H COSY spectrum of the mixture of products **4** and **5** in $C_6D_6$ in the $sp^2$-CH region.

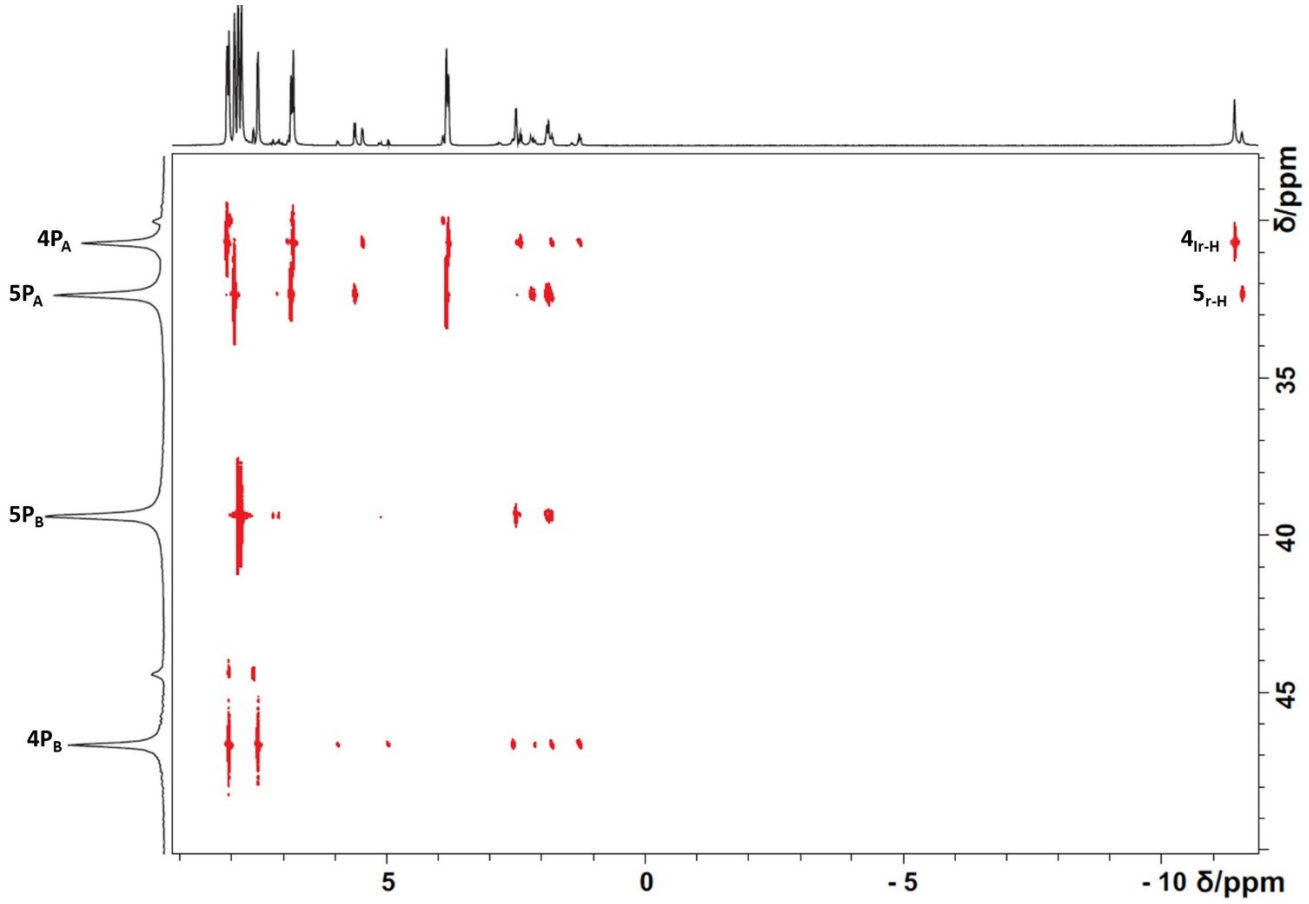



Figure S 17. $^{31}P$-$^{1}H$ HMQC spectrum of **4** and **5** in $C_6D_6$ at 298 K.

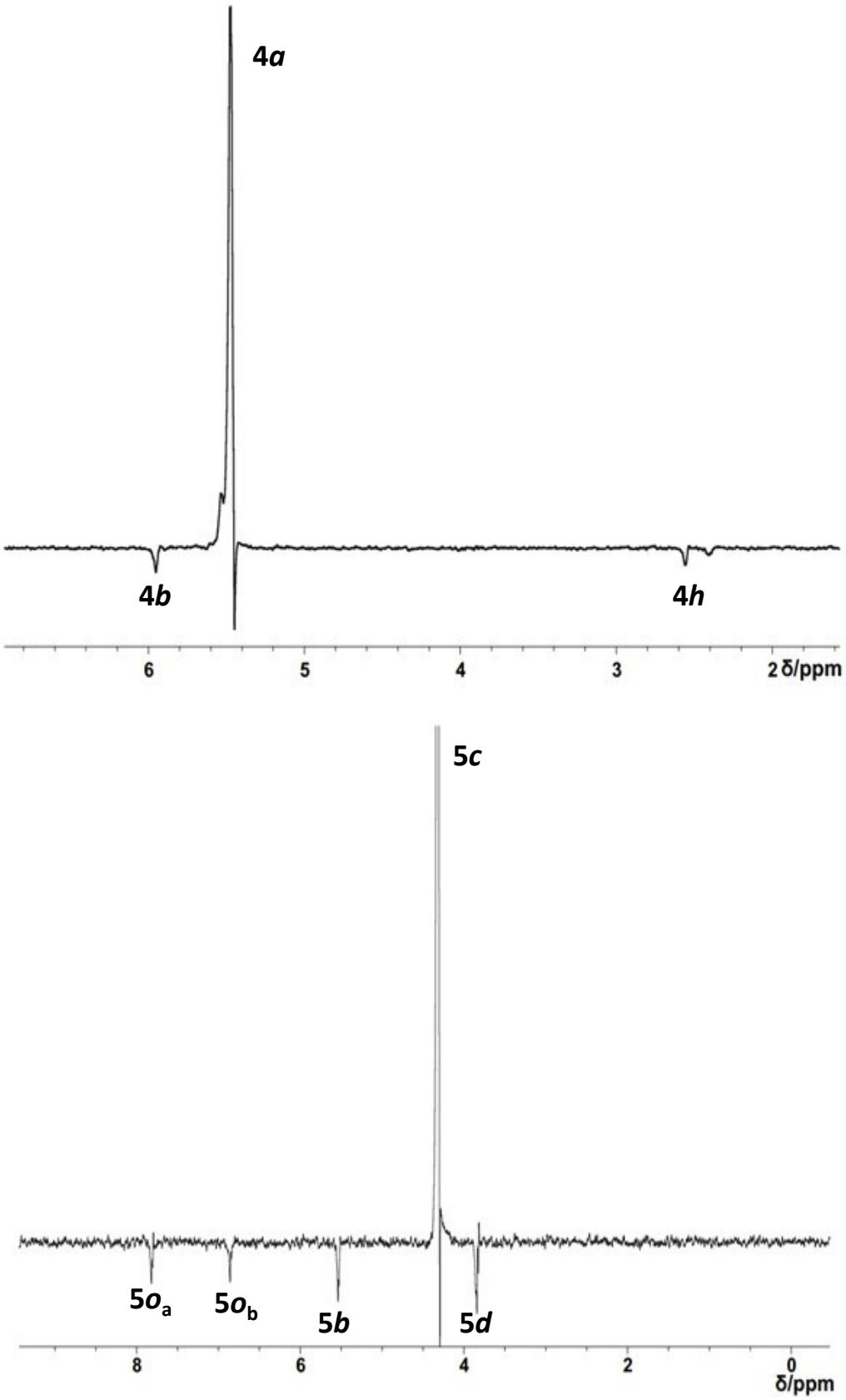



Figure S 18. NOE spectra highlighting the interaction between the alkene and allylic protons for **4** and **5**.

**Kinetic analysis of the equilibrated transformation of 4 to 5**

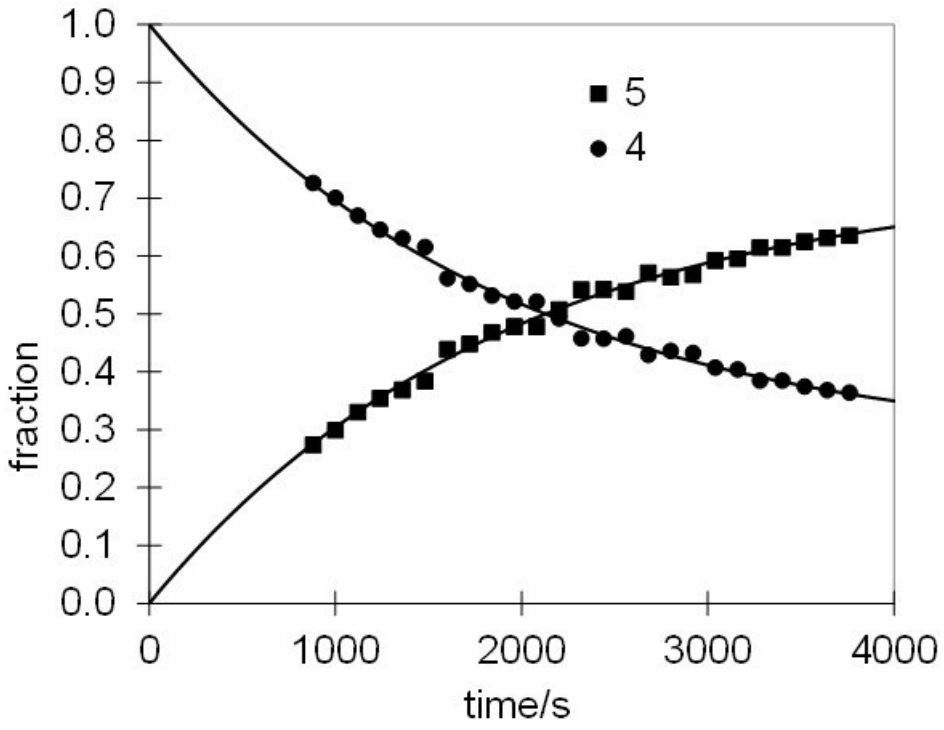



Figure S 19. First-order kinetic analysis of the $^{1}$H data for the **4**-**5** isomerisation in toluene-$d_8$ at 298 K.

**Energy profile for the isomerisation of II'**

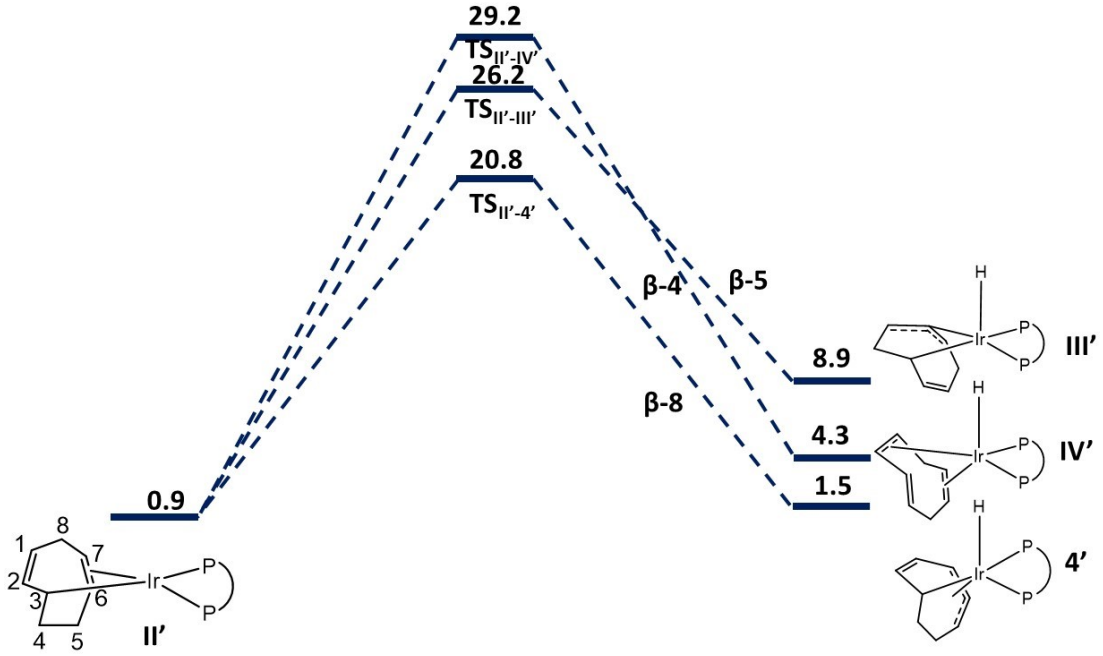



Figure S 20. Gibbs-energy profile (in kcal mol$^{-1}$) for the β-H elimination reactions from intermediate **II'**.

**Analysis of the NMR spectra of the $[IrH_4(dppe)]^-$ anion.**

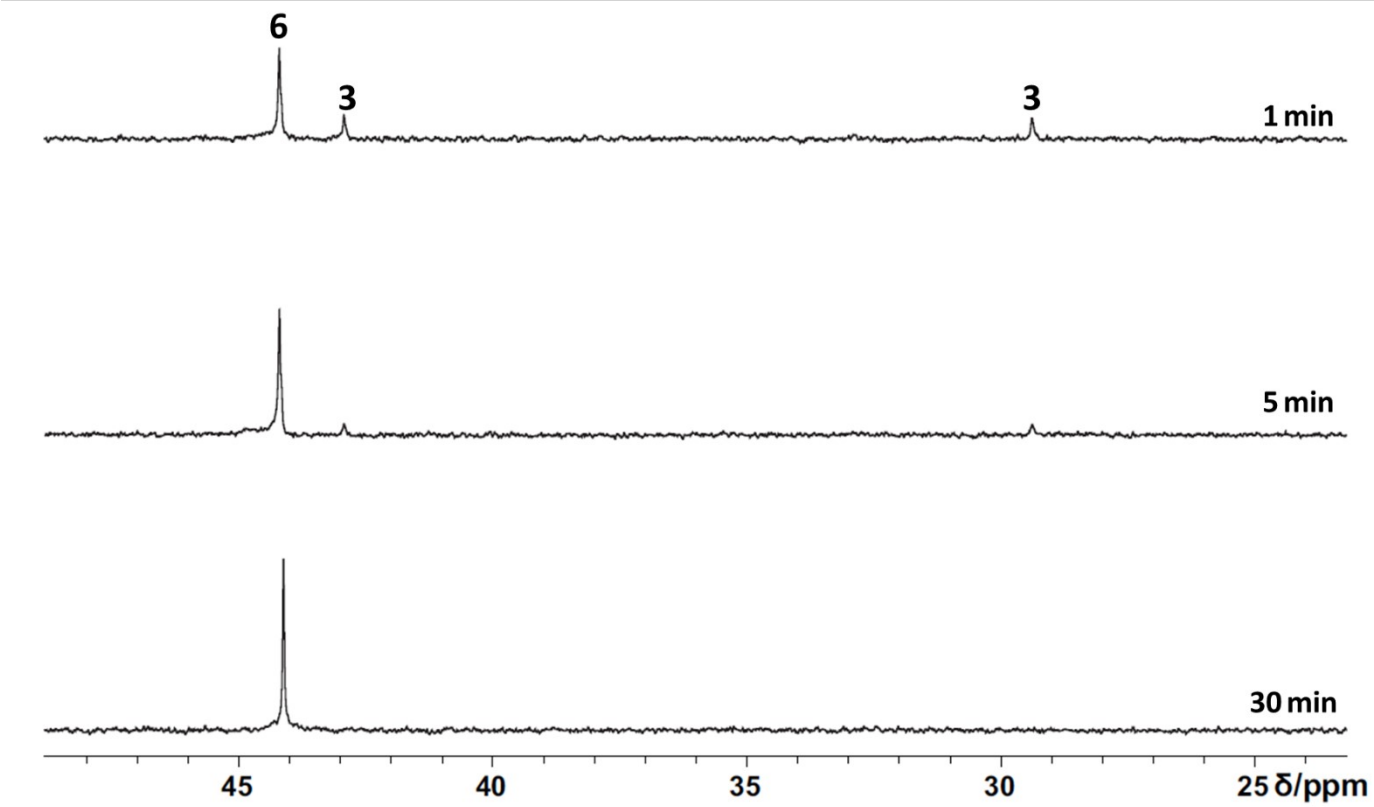



Figure S 21. $^{31}P\{^1H\}$ NMR monitoring of the formation of **6** from a solution of **2**/**3** in $C_7D_8$ at 353 K. The resonance of **2** is not visible because of the low concentration.

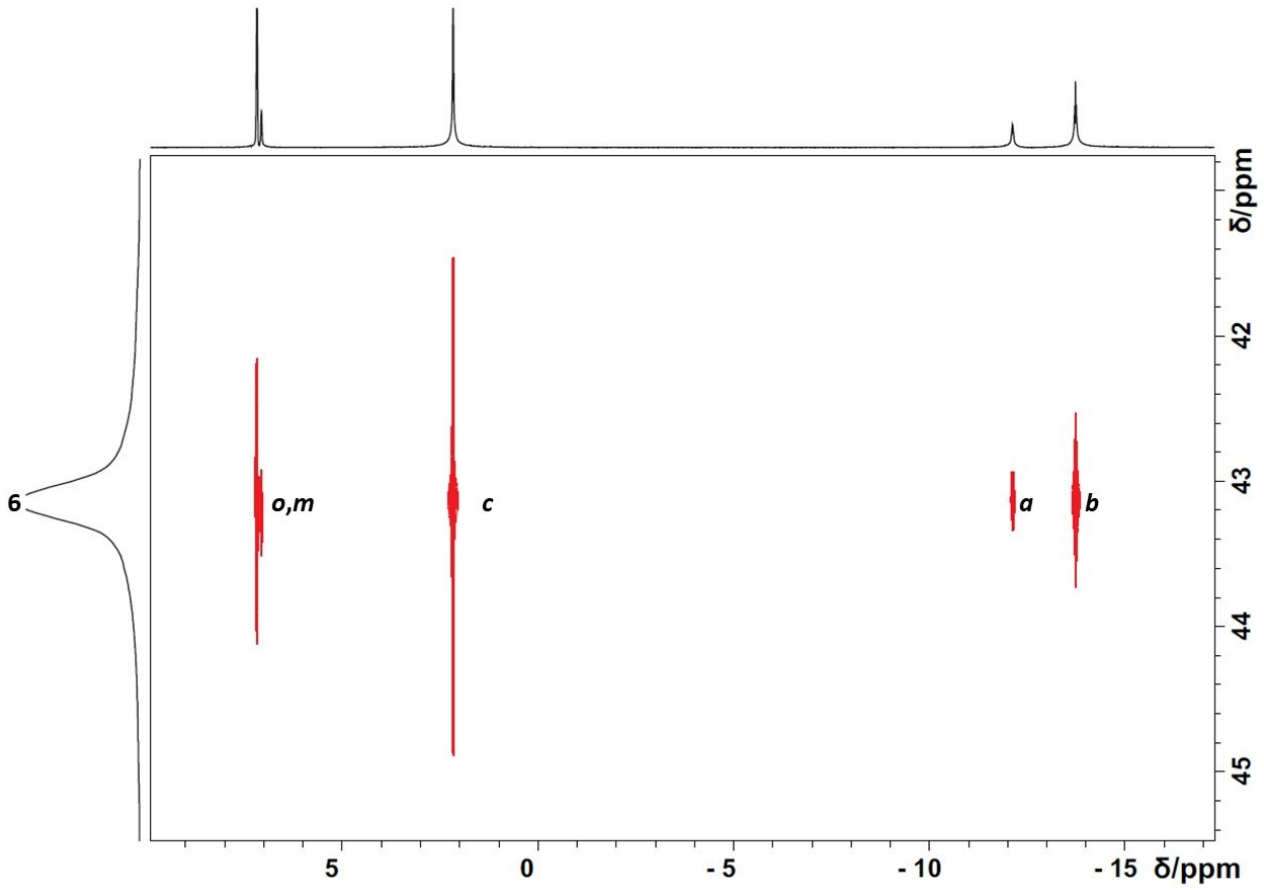



Figure S 22. $^{31}P$-$^{1}H$ HMQC spectrum of **6** in $C_7D_8$ at 298 K, highlighting the proton phosphorus interactions.

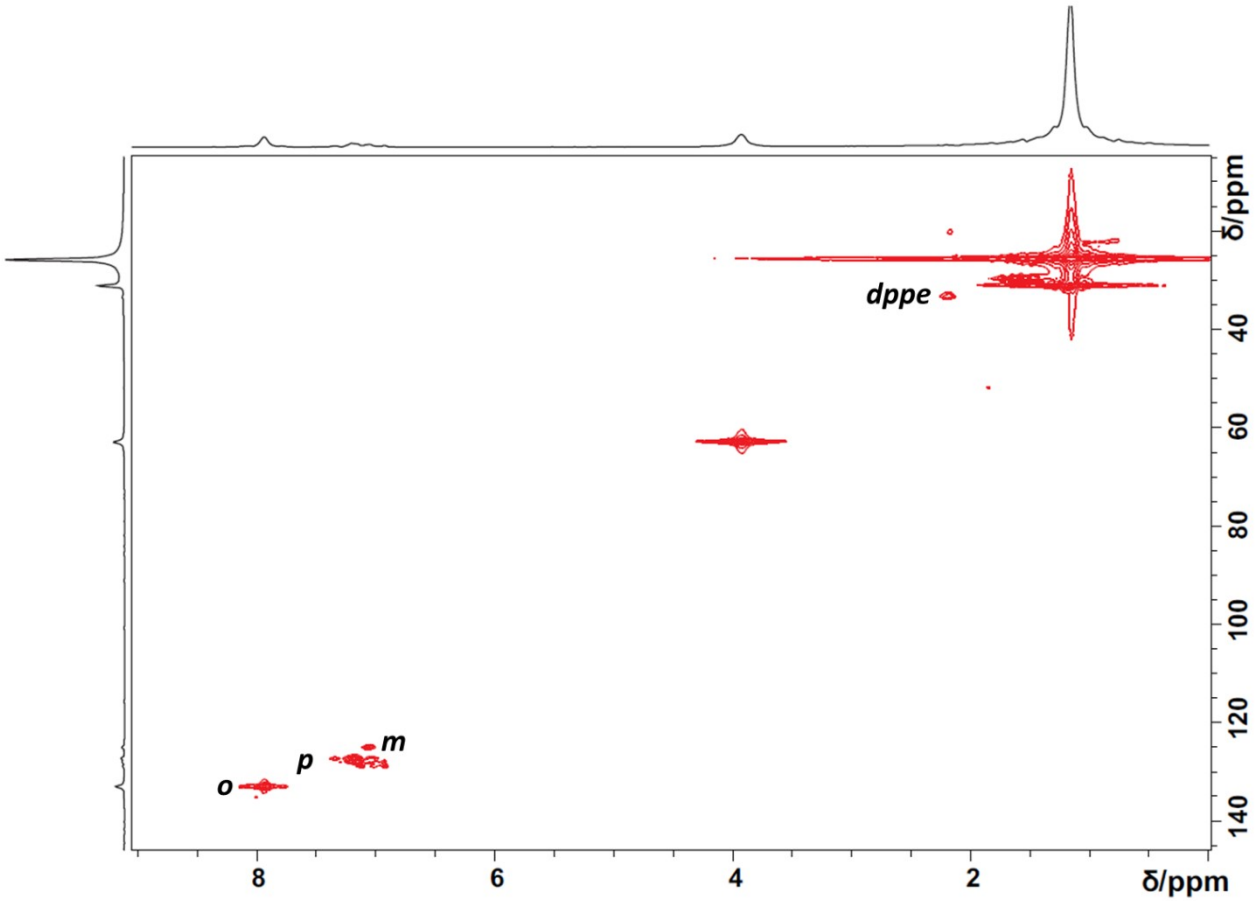



Figure S 23. $^{13}C$-$^{1}H$ HMQC spectrum of **6** in $C_7D_8$ at 298 K.

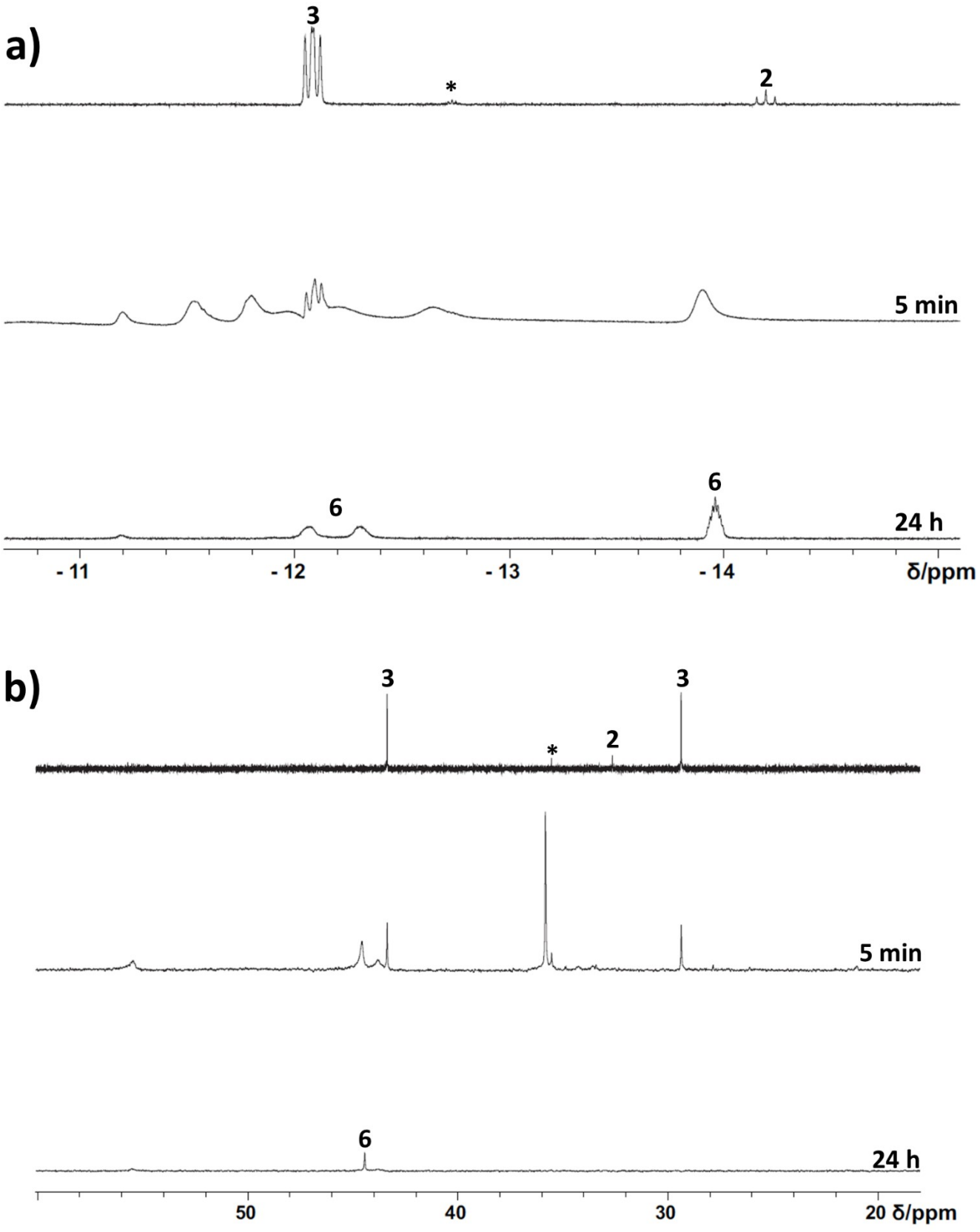



Figure S 24. $^{1}H$ (a) and $^{31}P\{^{1}H\}$ (b) NMR study of the interaction of **2/3** with $H_2$ in THF-$d_8$ at room temperature. Three bars of $H_2$ were first added, followed by 5 equivalents of KO$^{t}$Bu.

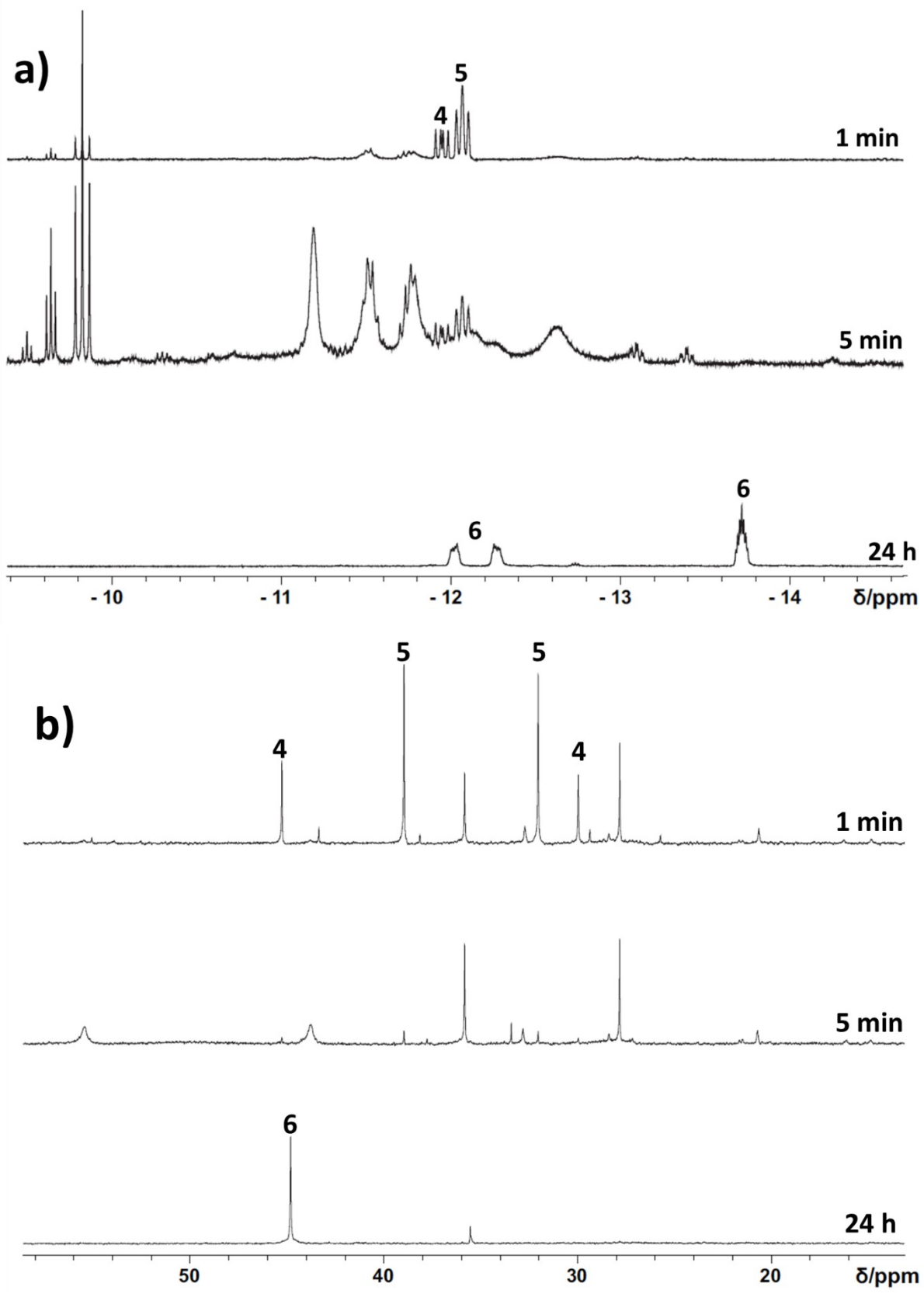



Figure S 25. $^{1}H$ (a) and $^{31}P\{^{1}H\}$ (b) NMR study of the interaction of **4/5** with $H_2$ in THF-$d_8$ at room temperature. Three bars of $H_2$ were first added, followed by 5 equivalents of KO$^{t}$Bu.

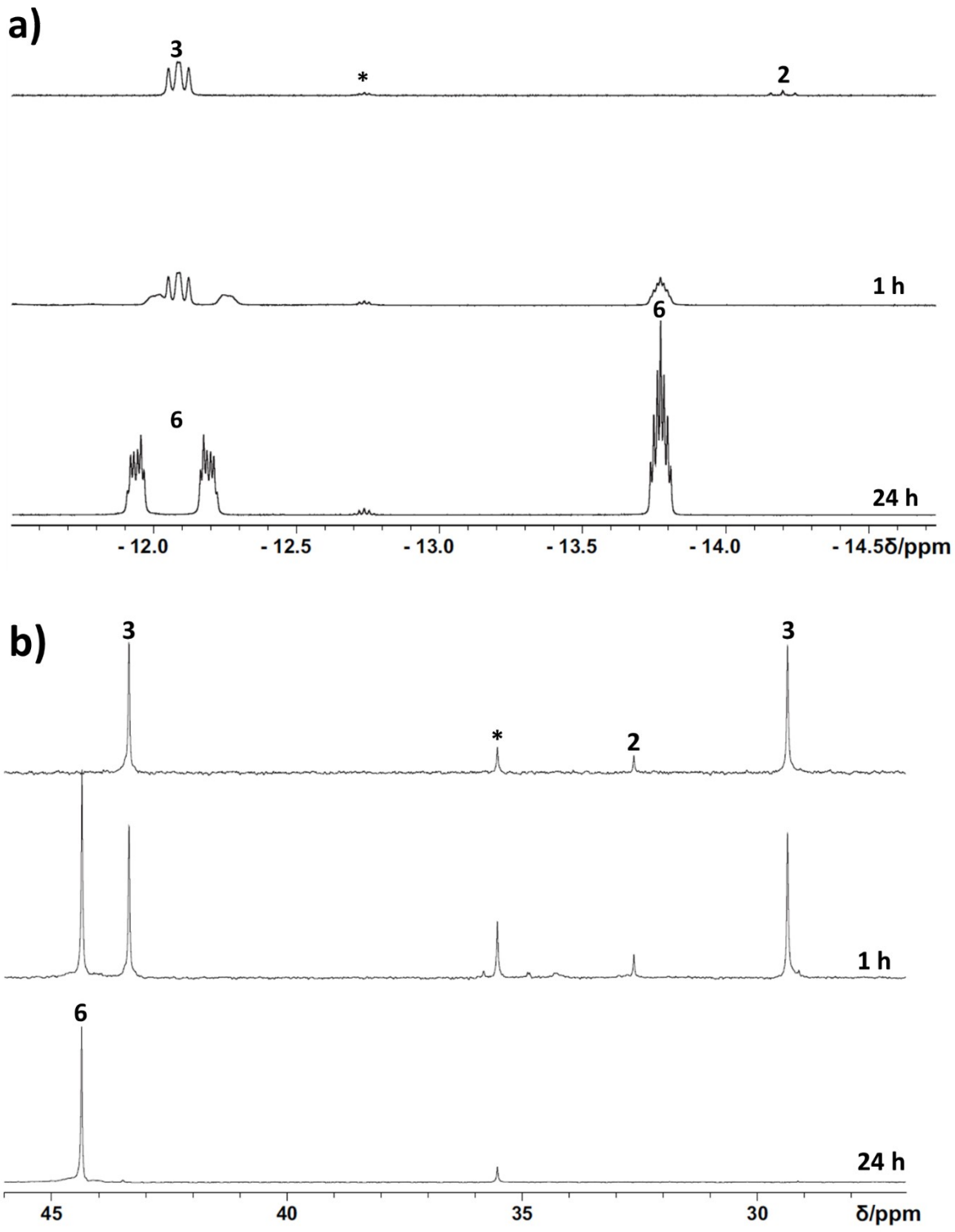



Figure S 26. $^{1}H$ (a) and $^{31}P\{^{1}H\}$ (b) NMR study of the interaction of **2/3** with $H_2$ in THF-$d_8$ at room temperature. Five equivalents of KO$^{t}$Bu were first added, followed by 3 bars of $H_2$.

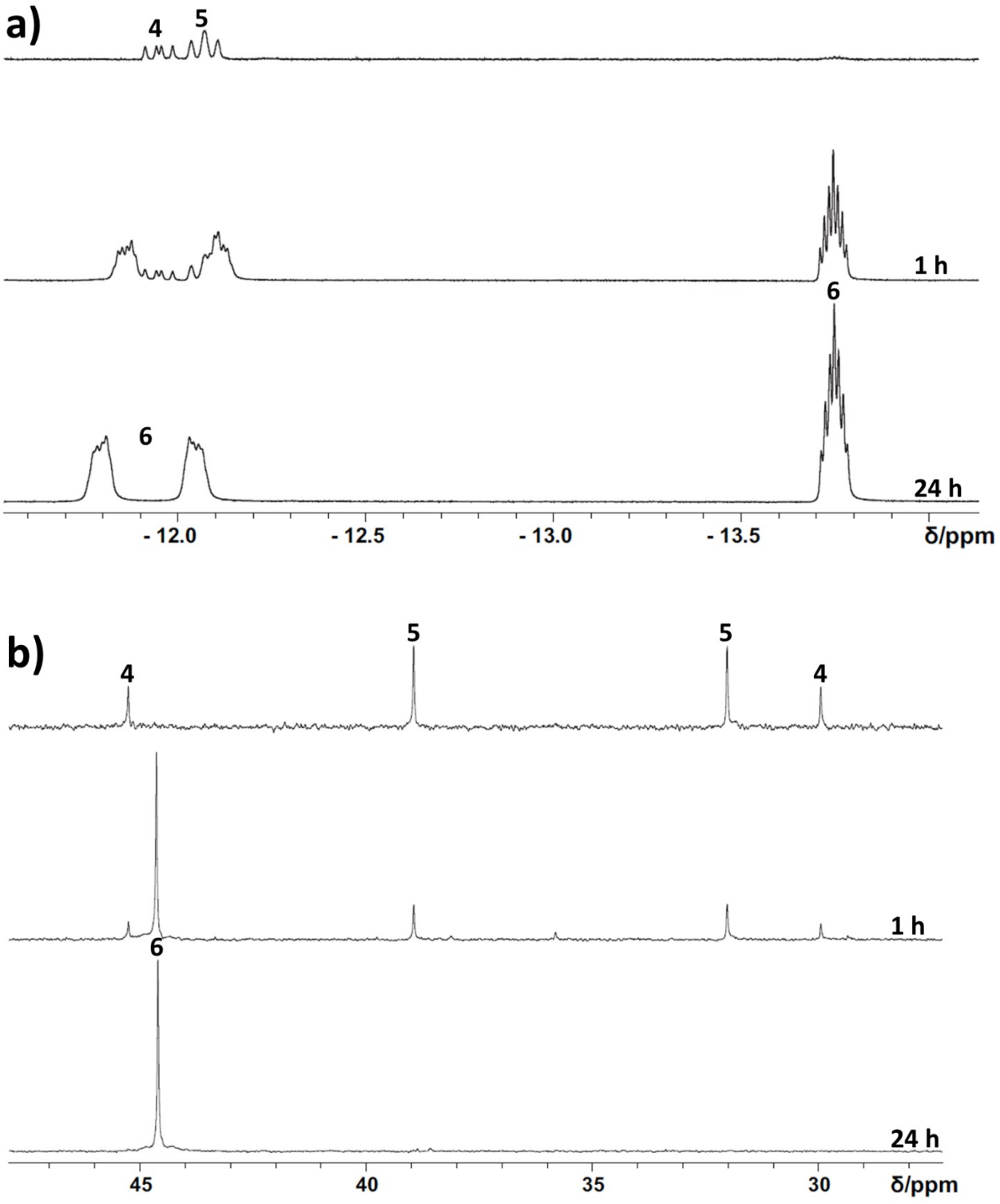
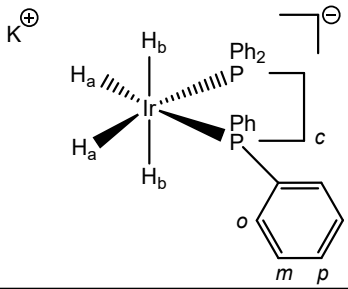



Figure S 27. $^{1}H$ (a) and $^{31}P\{^{1}H\}$ (b) NMR study of the interaction of **4/5** with $H_2$ in THF-$d_8$ at room temperature. Five equivalents of KO$^{t}$Bu were first added, followed by 3 bars of $H_2$.

Table S 5. NMR properties of $K^+[IrH_4(dppe)]^-$ (**6**) in $C_6D_6$.




| | |
|---|---|
| **$^1$H** | |
| Ph | 7.98 (dd, $J_{HH}$ = 7.6) (*o*)<br>7.26 (t, $J_{HH}$ = 7.4) (*m*)<br>7.17 (dd, $J_{HH}$ = 7.6) (*p*) |
| dppe $CH_2$ | 2.20 ($J_{HH}$ = 5.5) |
| Ir-H | -12.12 ($J_{HH'}$ = 6.0, $J_{HHb}$ = 5.7, $J_{HPcis}$ = -15.2, $J_{HPtrans}$ = 121.6) (*a*)<br>-13.80 ($J_{HHa}$ = 5.7, $J_{HPcis}$ = 17.8) (*b*) |
| **$^{13}$C** | |
| Ph | 133.1 (*o*)<br>126.8 (*m*)<br>127.8 (*p*) |
| dppe $CH_2$ | 32.9 |
| **$^{31}$P** | |
| | 44.4 (s) |

**DFT-optimized geometries.**

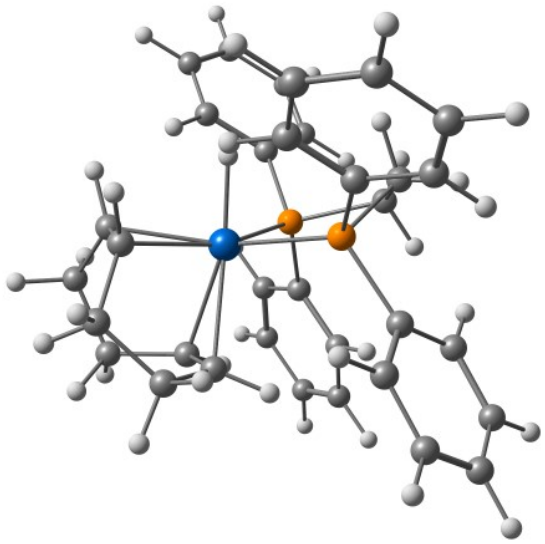
Table S 6. Energies (hartrees), views and Cartesian coordinates (Å) of all optimized geometries.

**[IrH(1,2,5,6-$\eta^2$:$\eta^2$-COD)(dppe)] (Compound 2)**

E (BS1) = -2105.218792

E (BS2) = -2105.73709

$G_{298.15,1M}$ (BS2) = -2105.18585



| | | | |
|---|---|---|---|
| 15 | -1.602863000 | -0.075212000 | -0.830449000 |
| 77 | 0.008518000 | -0.557697000 | 0.801472000 |
| 6 | -0.745710000 | -0.296408000 | -2.483969000 |
| 1 | -1.352123000 | 0.115075000 | -3.297695000 |
| 6 | -0.660698000 | 1.216948000 | 2.077136000 |
| 6 | 0.728084000 | 1.123089000 | 2.211042000 |
| 6 | 1.424139000 | 0.575160000 | 3.454834000 |
| 6 | 1.750994000 | -0.927907000 | 3.349879000 |
| 6 | 0.765816000 | -1.686156000 | 2.470347000 |
| 6 | -0.681282000 | -1.586493000 | 2.577085000 |
| 6 | -1.379295000 | -0.704354000 | 3.622595000 |
| 6 | -1.667788000 | 0.719748000 | 3.101798000 |
| 1 | 0.798025000 | 0.768829000 | 4.332114000 |
| 1 | 2.348085000 | 1.142029000 | 3.614295000 |
| 1 | -2.327899000 | -1.170649000 | 3.913201000 |
| 1 | -0.779978000 | -0.663242000 | 4.540345000 |
| 1 | -1.736009000 | 1.436324000 | 3.936540000 |
| 1 | -2.648800000 | 0.724128000 | 2.615676000 |
| 1 | 1.819136000 | -1.374559000 | 4.356121000 |
| 1 | 2.743316000 | -1.039153000 | 2.896263000 |
| 1 | 1.321924000 | 1.808230000 | 1.615250000 |
| 1 | -1.042533000 | 1.989474000 | 1.413417000 |
| 1 | -1.220705000 | -2.510188000 | 2.368194000 |
| 1 | 1.140716000 | -2.674668000 | 2.197644000 |
| 6 | -3.061499000 | -1.186781000 | -1.044865000 |
| 6 | -3.155105000 | -2.353603000 | -0.275068000 |
| 6 | -4.065464000 | -0.907890000 | -1.987383000 |
| 6 | -4.229304000 | -3.230627000 | -0.446821000 |
| 6 | -5.137345000 | -1.783569000 | -2.157493000 |
| 6 | -5.220709000 | -2.947791000 | -1.387362000 |
| 1 | -2.382684000 | -2.561653000 | 0.457238000 |
| 1 | -4.016064000 | 0.000466000 | -2.581392000 |
| 1 | -4.291224000 | -4.131245000 | 0.157793000 |
| 1 | -5.908943000 | -1.558056000 | -2.888595000 |
| 1 | -6.057702000 | -3.627962000 | -1.518800000 |
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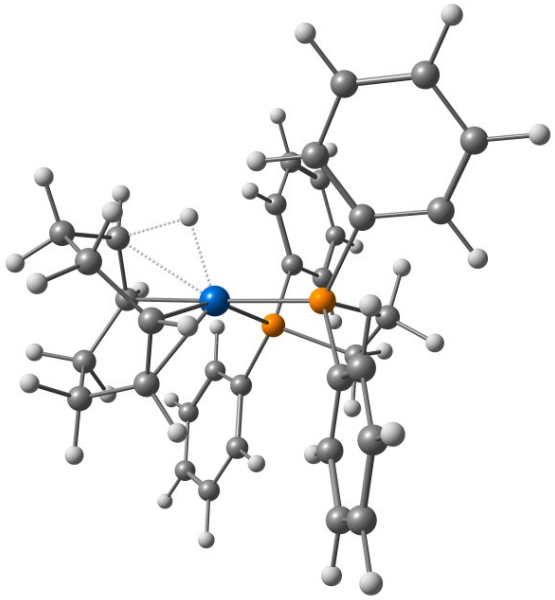
| 6 | -1.935945000 | 2.604748000 | -1.770852000 |
| 6 | -4.009459000 | 3.152847000 | 0.011475000 |
| 6 | -2.500718000 | 3.882352000 | -1.724860000 |
| 6 | -3.535617000 | 4.161951000 | -0.831926000 |
| 1 | -3.828150000 | 1.100358000 | 0.620443000 |
| 1 | -1.141784000 | 2.410852000 | -2.483273000 |
| 1 | -4.821061000 | 3.357616000 | 0.704169000 |
| 1 | -2.132945000 | 4.655771000 | -2.393720000 |
| 1 | -3.974085000 | 5.155065000 | -0.796277000 |
| 1 | -0.710384000 | -1.382604000 | -2.618719000 |
| 6 | 0.677489000 | 0.279501000 | -2.498055000 |
| 1 | 1.258154000 | -0.162699000 | -3.312445000 |
| 1 | 0.661338000 | 1.358349000 | -2.670692000 |
| 15 | 1.568891000 | -0.010428000 | -0.853999000 |
| 6 | 2.851904000 | -1.257587000 | -1.316219000 |
| 6 | 2.977351000 | -2.428826000 | -0.558970000 |
| 6 | 3.713897000 | -1.058030000 | -2.408752000 |
| 6 | 3.940585000 | -3.386730000 | -0.888374000 |
| 6 | 4.674924000 | -2.013156000 | -2.737139000 |
| 6 | 4.788784000 | -3.181606000 | -1.976900000 |
| 1 | 2.312343000 | -2.580849000 | 0.284321000 |
| 1 | 3.645776000 | -0.145437000 | -2.995001000 |
| 1 | 4.025417000 | -4.291911000 | -0.293379000 |
| 1 | 5.335887000 | -1.846576000 | -3.583336000 |
| 1 | 5.537290000 | -3.926213000 | -2.233480000 |
| 6 | 2.559827000 | 1.535934000 | -0.666488000 |
| 6 | 1.905700000 | 2.778528000 | -0.743513000 |
| 6 | 3.911878000 | 1.513808000 | -0.290830000 |
| 6 | 2.592032000 | 3.964699000 | -0.483982000 |
| 6 | 4.596266000 | 2.702020000 | -0.025041000 |
| 6 | 3.942002000 | 3.931012000 | -0.125316000 |
| 1 | 0.847301000 | 2.823495000 | -0.984884000 |
| 1 | 4.436299000 | 0.567414000 | -0.206787000 |
| 1 | 2.068449000 | 4.914366000 | -0.552867000 |
| 1 | 5.644154000 | 2.664064000 | 0.260030000 |
| 1 | 4.476558000 | 4.853922000 | 0.080763000 |
| 1 | -0.037671000 | -1.985882000 | 0.059331000 |

**$TS_{2\text{-}I}$**

E (BS1) = -2105.183724

E (BS2) = -2105.702271

$G_{298.15,1M}$ (BS2) = -2105.156042



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| 6 | 0.792015000 | 1.199535000 | -2.176229000 |
| 1 | 1.410318000 | 1.072684000 | -3.070307000 |
| 6 | 1.324371000 | -1.788232000 | 1.720054000 |
| 6 | 0.307874000 | -2.529974000 | 1.046956000 |
| 6 | -0.820545000 | -3.213756000 | 1.827394000 |
| 6 | -2.028607000 | -2.292001000 | 2.067812000 |
| 6 | -1.682736000 | -0.806033000 | 2.090173000 |
| 6 | -0.727650000 | -0.175636000 | 2.985167000 |
| 6 | 0.148610000 | -1.032982000 | 3.908637000 |
| 6 | 1.419590000 | -1.589445000 | 3.230847000 |
| 1 | -0.424286000 | -3.584988000 | 2.781630000 |
| 1 | -1.151118000 | -4.103665000 | 1.279940000 |
| 1 | 0.439509000 | -0.436985000 | 4.780211000 |
| 1 | -0.473861000 | -1.849456000 | 4.293005000 |
| 1 | 1.724462000 | -2.525041000 | 3.726442000 |
| 1 | 2.233459000 | -0.875289000 | 3.401287000 |
| 1 | -2.579767000 | -2.585446000 | 2.977950000 |
| 1 | -2.726193000 | -2.416366000 | 1.232841000 |
| 1 | 0.601213000 | -3.024565000 | 0.123925000 |
| 1 | 2.306321000 | -1.792846000 | 1.247216000 |
| 1 | -1.066121000 | 0.757519000 | 3.434504000 |
| 1 | -2.566701000 | -0.193799000 | 1.901182000 |
| 6 | 2.908158000 | 1.552450000 | -0.244554000 |
| 6 | 3.074626000 | 1.899404000 | 1.101506000 |
| 6 | 3.739179000 | 2.148439000 | -1.208452000 |
| 6 | 4.052983000 | 2.821128000 | 1.482628000 |
| 6 | 4.710940000 | 3.074934000 | -0.829713000 |
| 6 | 4.870417000 | 3.411950000 | 0.517903000 |
| 1 | 2.419499000 | 1.447114000 | 1.841488000 |
| 1 | 3.635520000 | 1.883541000 | -2.257209000 |
| 1 | 4.171512000 | 3.080146000 | 2.531318000 |
| 1 | 5.344434000 | 3.533070000 | -1.584396000 |
| 1 | 5.628459000 | 4.132629000 | 0.812074000 |
| 6 | 2.558828000 | -1.040354000 | -1.465950000 |
| 6 | 3.943118000 | -1.198933000 | -1.307560000 |
| 6 | 1.845438000 | -2.027632000 | -2.168223000 |
| 6 | 4.598347000 | -2.308177000 | -1.850720000 |
| 6 | 2.501211000 | -3.126041000 | -2.721879000 |
| 6 | 3.882652000 | -3.270306000 | -2.563526000 |
| 1 | 4.516937000 | -0.458308000 | -0.760448000 |
| 1 | 0.766744000 | -1.944949000 | -2.256071000 |
| 1 | 5.670956000 | -2.416546000 | -1.714398000 |
| 1 | 1.933144000 | -3.875381000 | -3.266600000 |
| 1 | 4.393807000 | -4.130347000 | -2.986894000 |
| 1 | 0.781627000 | 2.265906000 | -1.926022000 |
| 6 | -0.637837000 | 0.700773000 | -2.408875000 |
| 1 | -1.192318000 | 1.388145000 | -3.055807000 |
| 1 | -0.636054000 | -0.280097000 | -2.891725000 |
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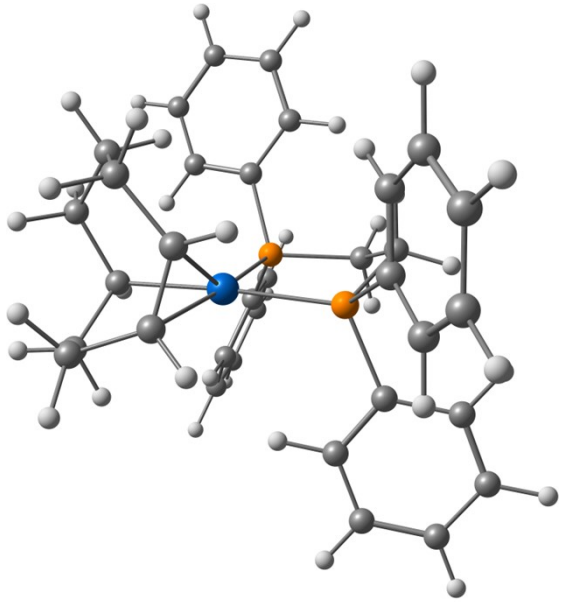
| 6 | -2.231075000 | 2.205255000 | -0.541181000 |
| 6 | -1.831926000 | 2.975105000 | 0.558206000 |
| 6 | -3.118616000 | 2.766943000 | -1.475276000 |
| 6 | -2.311938000 | 4.276774000 | 0.729556000 |
| 6 | -3.596488000 | 4.066393000 | -1.307704000 |
| 6 | -3.194132000 | 4.824057000 | -0.202910000 |
| 1 | -1.128495000 | 2.543608000 | 1.266493000 |
| 1 | -3.447807000 | 2.182128000 | -2.330212000 |
| 1 | -1.993215000 | 4.862146000 | 1.587877000 |
| 1 | -4.282348000 | 4.488807000 | -2.037183000 |
| 1 | -3.566527000 | 5.836637000 | -0.073884000 |
| 6 | -2.974706000 | -0.533147000 | -1.132306000 |
| 6 | -2.765401000 | -1.786203000 | -1.734302000 |
| 6 | -4.266728000 | -0.211525000 | -0.690759000 |
| 6 | -3.821080000 | -2.675713000 | -1.921047000 |
| 6 | -5.322900000 | -1.112306000 | -0.860538000 |
| 6 | -5.106772000 | -2.341955000 | -1.481815000 |
| 1 | -1.762031000 | -2.080679000 | -2.028537000 |
| 1 | -4.455347000 | 0.743065000 | -0.210636000 |
| 1 | -3.639630000 | -3.635560000 | -2.397197000 |
| 1 | -6.315563000 | -0.846738000 | -0.506892000 |
| 1 | -5.928247000 | -3.040020000 | -1.616141000 |
| 1 | 0.257858000 | 0.678431000 | 2.125161000 |

**[Ir(1-$\kappa$-4,5-$\eta^2$-$C_8H_{13}$)(dppe)] (Intermediate I)**

E (BS1) = -2105.215951

E (BS2) = -2105.736259

$G_{298.15,1M}$ (BS2) = -2105.183709



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| 77 | -0.001595000 | -0.358534000 | 0.761686000 |
| 6 | 0.406386000 | 1.213455000 | -2.266862000 |
| 1 | 0.973893000 | 1.153090000 | -3.201038000 |
| 6 | 1.594278000 | -0.825456000 | 2.135846000 |
| 6 | 2.148579000 | -2.275696000 | 2.058829000 |
| 6 | 1.379831000 | -3.257624000 | 1.159749000 |
| 6 | -0.099067000 | -3.446927000 | 1.537315000 |
| 6 | -1.003465000 | -2.219876000 | 1.434394000 |
| 6 | -1.164895000 | -1.254036000 | 2.449380000 |
| 6 | -0.334219000 | -1.251857000 | 3.726924000 |
| 6 | 0.994180000 | -0.499735000 | 3.518499000 |
| 1 | 1.872273000 | -4.240814000 | 1.196249000 |
| 1 | 1.436917000 | -2.908277000 | 0.122701000 |
| 1 | -0.910021000 | -0.807219000 | 4.546898000 |
| 1 | -0.118032000 | -2.286404000 | 4.027323000 |
| 1 | 1.692636000 | -0.738578000 | 4.340313000 |
| 1 | 0.801888000 | 0.580771000 | 3.582777000 |
| 1 | -0.149213000 | -3.844418000 | 2.562524000 |
| 1 | 2.202376000 | -2.709624000 | 3.072013000 |
| 1 | 2.445085000 | -0.143886000 | 1.993423000 |
| 1 | -2.121395000 | -0.733727000 | 2.496829000 |
| 1 | -1.849567000 | -2.364538000 | 0.767004000 |
| 6 | 2.499722000 | 1.895318000 | -0.384929000 |
| 6 | 2.271866000 | 2.571840000 | 0.822749000 |
| 6 | 3.526306000 | 2.336497000 | -1.234332000 |
| 6 | 3.052109000 | 3.676238000 | 1.172403000 |
| 6 | 4.306635000 | 3.437893000 | -0.882408000 |
| 6 | 4.069407000 | 4.110041000 | 0.320376000 |
| 1 | 1.486247000 | 2.221571000 | 1.486999000 |
| 1 | 3.724236000 | 1.811067000 | -2.164462000 |
| 1 | 2.868860000 | 4.191659000 | 2.111056000 |
| 1 | 5.100772000 | 3.771335000 | -1.544787000 |
| 1 | 4.679588000 | 4.966554000 | 0.593201000 |
| 6 | 2.527134000 | -0.733923000 | -1.577798000 |
| 6 | 3.727173000 | -1.047379000 | -0.917889000 |
| 6 | 2.178119000 | -1.456229000 | -2.728634000 |
| 6 | 4.557467000 | -2.058094000 | -1.400009000 |
| 6 | 3.010879000 | -2.469186000 | -3.208927000 |
| 6 | 4.201020000 | -2.774189000 | -2.545766000 |
| 1 | 4.010963000 | -0.498074000 | -0.025767000 |
| 1 | 1.254063000 | -1.238005000 | -3.255101000 |
| 1 | 5.482172000 | -2.287356000 | -0.877843000 |
| 1 | 2.729155000 | -3.019152000 | -4.102634000 |
| 1 | 4.847224000 | -3.563583000 | -2.918817000 |
| 1 | 0.281326000 | 2.275311000 | -2.028099000 |
| 6 | -0.966732000 | 0.540534000 | -2.381485000 |
| 1 | -1.637556000 | 1.121550000 | -3.021884000 |
| 1 | -0.876083000 | -0.459542000 | -2.815717000 |
| 15 | -1.694543000 | 0.312961000 | -0.661363000 |
| 6 | -2.425297000 | 1.984177000 | -0.352327000 |
| 6 | -2.037420000 | 2.675464000 | 0.805135000 |
| 6 | -3.312669000 | 2.605203000 | -1.247096000 |
| 6 | -2.521213000 | 3.960782000 | 1.062606000 |
| 6 | -3.797693000 | 3.887403000 | -0.989822000 |
| 6 | -3.400695000 | 4.568449000 | 0.165169000 |
| 1 | -1.349499000 | 2.193855000 | 1.496406000 |
| 1 | -3.637180000 | 2.080157000 | -2.141596000 |
| 1 | -2.211065000 | 4.485046000 | 1.962272000 |
| 1 | -4.484952000 | 4.355743000 | -1.689083000 |
| 1 | -3.777293000 | 5.568163000 | 0.362997000 |
| 6 | -3.160239000 | -0.758185000 | -0.988156000 |
| 6 | -2.953366000 | -1.997959000 | -1.620524000 |
| 6 | -4.442667000 | -0.459368000 | -0.502920000 |
| 6 | -4.005799000 | -2.896979000 | -1.790241000 |
| 6 | -5.494271000 | -1.364535000 | -0.666536000 |
| 6 | -5.281801000 | -2.581684000 | -1.315414000 |
| 1 | -1.959294000 | -2.272964000 | -1.963248000 |
| 1 | -4.625504000 | 0.483576000 | 0.002420000 |
| 1 | -3.827537000 | -3.847134000 | -2.286320000 |
| 1 | -6.481236000 | -1.114181000 | -0.287018000 |
| 1 | -6.100710000 | -3.283914000 | -1.443125000 |
| 1 | 3.183913000 | -2.252783000 | 1.695350000 |
| 1 | -0.523361000 | -4.222154000 | 0.888004000 |

**$TS_{I-3}$**

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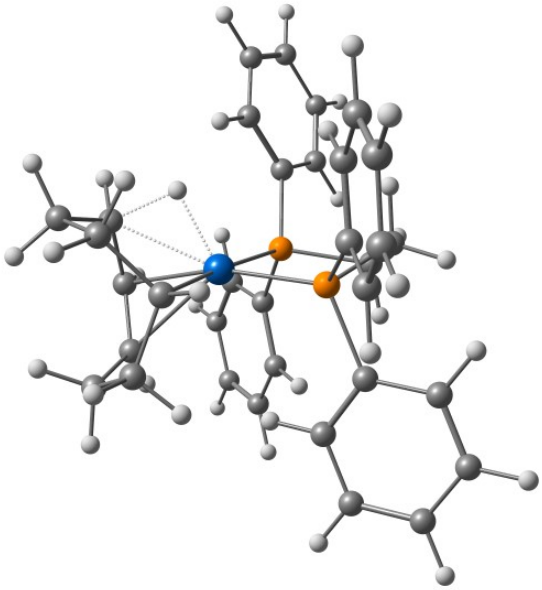
E (BS2) = -2105.702657

$G_{298.15,1M}$ (BS2) = -2105.154267



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| 6 | -0.529265000 | -0.262647000 | -2.506812000 |
| 1 | -1.108547000 | 0.110753000 | -3.356895000 |
| 6 | -2.926530000 | -1.068923000 | -1.042045000 |
| 6 | -2.696459000 | -2.446915000 | -1.190980000 |
| 6 | -4.245123000 | -0.616855000 | -0.895932000 |
| 6 | -3.760834000 | -3.345182000 | -1.231082000 |
| 6 | -5.311794000 | -1.520481000 | -0.921175000 |
| 6 | -5.074152000 | -2.883707000 | -1.095742000 |
| 1 | -1.676241000 | -2.816830000 | -1.247252000 |
| 1 | -4.446543000 | 0.439996000 | -0.756725000 |
| 1 | -3.565976000 | -4.407085000 | -1.354221000 |
| 1 | -6.327788000 | -1.154657000 | -0.800461000 |
| 1 | -5.903373000 | -3.585351000 | -1.116539000 |
| 6 | -2.116985000 | 1.732441000 | -1.219576000 |
| 6 | -1.711013000 | 2.780614000 | -0.383071000 |
| 6 | -2.931185000 | 2.027522000 | -2.326421000 |
| 6 | -2.114610000 | 4.094339000 | -0.637566000 |
| 6 | -3.334252000 | 3.338419000 | -2.582401000 |
| 6 | -2.926231000 | 4.375370000 | -1.737512000 |
| 1 | -1.065655000 | 2.549910000 | 0.460661000 |
| 1 | -3.261083000 | 1.229907000 | -2.986788000 |
| 1 | -1.792380000 | 4.895479000 | 0.022276000 |
| 1 | -3.964342000 | 3.552054000 | -3.441604000 |
| 1 | -3.239600000 | 5.396000000 | -1.939129000 |
| 1 | -0.409768000 | -1.344133000 | -2.625548000 |
| 6 | 0.835034000 | 0.426617000 | -2.410306000 |
| 1 | 1.489533000 | 0.150997000 | -3.242517000 |
| 1 | 0.709998000 | 1.513701000 | -2.430103000 |
| 15 | 1.629619000 | -0.033156000 | -0.773782000 |
| 6 | 2.723653000 | -1.441526000 | -1.266835000 |
| 6 | 2.520742000 | -2.701582000 | -0.689266000 |
| 6 | 3.724016000 | -1.297137000 | -2.244472000 |
| 6 | 3.303306000 | -3.794853000 | -1.071968000 |
| 6 | 4.504424000 | -2.387334000 | -2.627398000 |
| 6 | 4.295787000 | -3.639359000 | -2.040010000 |
| 1 | 1.736253000 | -2.820932000 | 0.051784000 |
| 1 | 3.902625000 | -0.325793000 | -2.697853000 |
| 1 | 3.134065000 | -4.765553000 | -0.613999000 |
| 1 | 5.275300000 | -2.261828000 | -3.382748000 |
| 1 | 4.904598000 | -4.488118000 | -2.338913000 |
| 6 | 2.810796000 | 1.348171000 | -0.451481000 |
| 6 | 2.299537000 | 2.658343000 | -0.421044000 |
| 6 | 4.145947000 | 1.139881000 | -0.074068000 |
| 6 | 3.111425000 | 3.731393000 | -0.057712000 |
| 6 | 4.955329000 | 2.216137000 | 0.301880000 |
| 6 | 4.444091000 | 3.513889000 | 0.305600000 |
| 1 | 1.255919000 | 2.839390000 | -0.662237000 |
| 1 | 4.562098000 | 0.137590000 | -0.075521000 |
| 1 | 2.700976000 | 4.737442000 | -0.049735000 |
| 1 | 5.987237000 | 2.035447000 | 0.590276000 |
| 1 | 5.074722000 | 4.349753000 | 0.594792000 |
| 1 | 0.302507000 | -1.880461000 | 1.315488000 |
| 6 | -1.752754000 | -0.482761000 | 2.163079000 |
| 6 | -1.933217000 | 0.831723000 | 2.937518000 |
| 6 | -0.627869000 | 1.316050000 | 3.587349000 |
| 6 | 0.600205000 | 1.146274000 | 2.694825000 |
| 6 | 1.368792000 | -0.016941000 | 2.525234000 |
| 6 | 0.927065000 | -1.413408000 | 2.612608000 |
| 6 | -0.134937000 | -1.862844000 | 3.629061000 |
| 6 | -1.560979000 | -1.719191000 | 3.066624000 |
| 1 | -0.467377000 | 0.786680000 | 4.533384000 |
| 1 | -0.715809000 | 2.375858000 | 3.854512000 |
| 1 | 0.058445000 | -2.907785000 | 3.897729000 |
| 1 | -0.013658000 | -1.283173000 | 4.549620000 |
| 1 | -2.291081000 | -1.724861000 | 3.893689000 |
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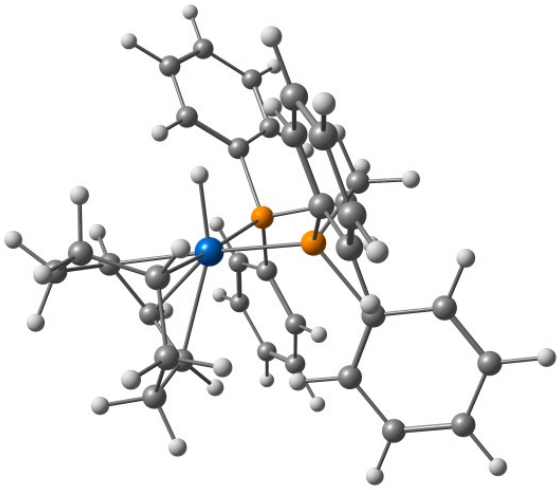
| 1 | 1.141666000 | 2.062625000 | 2.466342000 |
| 1 | -2.723805000 | 0.741139000 | 3.704826000 |
| 1 | -2.684402000 | -0.656373000 | 1.611054000 |
| 1 | 1.770818000 | -2.096868000 | 2.517049000 |
| 1 | 2.388024000 | 0.129029000 | 2.170606000 |
| 1 | -2.270263000 | 1.601480000 | 2.23309900 |

**[IrH(1-$\kappa$-4,5,6-$\eta^3$-$C_8H_{12}$)(dppe)] (Compound 3)**

E (BS1) = -2105.224667

E (BS2) = -2105.743037

$G_{298.15,1M}$ (BS2) = -2105.743037



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| 77 | -0.027936000 | -0.562780000 | 0.768259000 |
| 6 | -0.498885000 | -0.023772000 | -2.512351000 |
| 1 | -1.060287000 | 0.411244000 | -3.344278000 |
| 6 | -2.940770000 | -0.923685000 | -1.189194000 |
| 6 | -2.756103000 | -2.275369000 | -1.525859000 |
| 6 | -4.243342000 | -0.449932000 | -0.978043000 |
| 6 | -3.851167000 | -3.124865000 | -1.673144000 |
| 6 | -5.338759000 | -1.306310000 | -1.115726000 |
| 6 | -5.147003000 | -2.642348000 | -1.468303000 |
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| 6 | -2.088672000 | 1.848442000 | -1.006977000 |
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| 6 | -2.268057000 | 4.066193000 | -0.027952000 |
| 6 | -3.221979000 | 3.634294000 | -2.206208000 |
| 6 | -2.959107000 | 4.516253000 | -1.153274000 |
| 1 | -1.295485000 | 2.379396000 | 0.911324000 |
| 1 | -3.017449000 | 1.631626000 | -2.951936000 |
| 1 | -2.063535000 | 4.744440000 | 0.795803000 |
| 1 | -3.764510000 | 3.978143000 | -3.082485000 |
| 1 | -3.294096000 | 5.548021000 | -1.212156000 |
| 1 | -0.373955000 | -1.092490000 | -2.711470000 |
| 6 | 0.863705000 | 0.656298000 | -2.342336000 |
| 1 | 1.516798000 | 0.455791000 | -3.196342000 |
| 1 | 0.736946000 | 1.741228000 | -2.271802000 |
| 15 | 1.675174000 | 0.075005000 | -0.748437000 |
| 6 | 2.887409000 | -1.183997000 | -1.334764000 |
| 6 | 2.870484000 | -2.464821000 | -0.766080000 |
| 6 | 3.821709000 | -0.898794000 | -2.345997000 |
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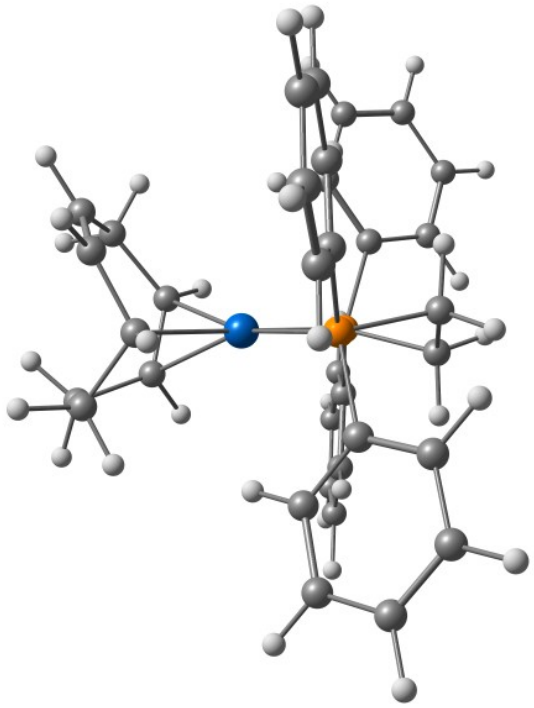
| 1 | 3.861169000 | 0.094408000 | -2.785376000 |
| 1 | 3.744601000 | -4.432940000 | -0.752224000 |
| 1 | 5.433144000 | -1.644445000 | -3.562383000 |
| 1 | 5.387124000 | -3.913717000 | -2.545899000 |
| 6 | 2.720864000 | 1.515868000 | -0.267505000 |
| 6 | 2.071738000 | 2.744947000 | -0.048745000 |
| 6 | 4.085686000 | 1.411805000 | 0.037994000 |
| 6 | 2.777617000 | 3.847058000 | 0.429756000 |
| 6 | 4.789473000 | 2.516346000 | 0.527007000 |
| 6 | 4.141031000 | 3.736413000 | 0.719465000 |
| 1 | 1.005679000 | 2.835732000 | -0.237573000 |
| 1 | 4.605789000 | 0.470211000 | -0.105106000 |
| 1 | 2.261052000 | 4.790382000 | 0.584815000 |
| 1 | 5.846800000 | 2.418743000 | 0.757492000 |
| 1 | 4.690030000 | 4.593614000 | 1.098664000 |
| 1 | -0.098479000 | -2.004729000 | 0.046126000 |
| 6 | -1.653023000 | -1.281376000 | 1.977390000 |
| 6 | -2.273298000 | -0.098304000 | 2.736204000 |
| 6 | -1.215108000 | 0.801761000 | 3.399652000 |
| 6 | 0.030948000 | 1.010654000 | 2.534384000 |
| 6 | 1.158249000 | 0.158276000 | 2.485651000 |
| 6 | 1.119449000 | -1.275293000 | 2.550353000 |
| 6 | 0.221968000 | -2.067729000 | 3.512025000 |
| 6 | -1.129971000 | -2.417165000 | 2.872607000 |
| 1 | -0.923236000 | 0.381229000 | 4.368305000 |
| 1 | -1.651025000 | 1.783050000 | 3.622833000 |
| 1 | 0.747100000 | -2.982221000 | 3.813038000 |
| 1 | 0.071452000 | -1.494962000 | 4.434077000 |
| 1 | -1.865195000 | -2.695727000 | 3.648198000 |
| 1 | -0.986972000 | -3.300778000 | 2.238021000 |
| 1 | 0.267359000 | 2.049994000 | 2.309893000 |
| 1 | -3.005118000 | -0.439069000 | 3.489995000 |
| 1 | -2.437528000 | -1.707595000 | 1.340894000 |
| 1 | 2.083829000 | -1.742305000 | 2.353461000 |
| 1 | 2.095831000 | 0.615559000 | 2.174152000 |
| 1 | -2.831943000 | 0.513239000 | 2.015418000 |

**[Ir(1-$\kappa$-3,4-$\eta^2$-$C_8H_{11}$)(dppe)] (Intermediate II)**

E (BS1) = -2103.986413

E (BS2) = -2104.51041

$G_{298.15,1M}$ (BS2) = -2103.985559



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| 1 | -1.216250000 | 0.262978000 | -3.356389000 |
| 6 | -1.533444000 | -0.089419000 | 2.351128000 |
| 6 | -1.250931000 | 1.045514000 | 3.364125000 |
| 6 | 0.223290000 | 1.020985000 | 3.795460000 |
| 6 | 1.138087000 | 0.660959000 | 2.628482000 |
| 6 | 1.488265000 | -0.664851000 | 2.330736000 |
| 6 | 1.060022000 | -1.880254000 | 3.142720000 |
| 6 | -0.408578000 | -2.178583000 | 3.340721000 |
| 6 | -1.484662000 | -1.455365000 | 2.978901000 |
| 1 | 0.352056000 | 0.275389000 | 4.590373000 |
| 1 | 0.524049000 | 1.986937000 | 4.217466000 |
| 1 | -0.587772000 | -3.137443000 | 3.829942000 |
| 1 | -2.452093000 | -1.922674000 | 3.186167000 |
| 1 | 1.801662000 | 1.448227000 | 2.273017000 |
| 1 | -1.904828000 | 0.987088000 | 4.250538000 |
| 1 | -2.554631000 | 0.057561000 | 1.974620000 |
| 1 | 1.544797000 | -1.813688000 | 4.133157000 |
| 1 | 2.436159000 | -0.821473000 | 1.817578000 |
| 6 | -2.846323000 | -1.152726000 | -0.937732000 |
| 6 | -2.434978000 | -2.497249000 | -0.955331000 |
| 6 | -4.213817000 | -0.861772000 | -0.842115000 |
| 6 | -3.373630000 | -3.525685000 | -0.907325000 |
| 6 | -5.152453000 | -1.895827000 | -0.784158000 |
| 6 | -4.737086000 | -3.226882000 | -0.821790000 |
| 1 | -1.375247000 | -2.737717000 | -0.982680000 |
| 1 | -4.551700000 | 0.168501000 | -0.807094000 |
| 1 | -3.041548000 | -4.559989000 | -0.924257000 |
| 1 | -6.209527000 | -1.656172000 | -0.708072000 |
| 1 | -5.469243000 | -4.028229000 | -0.776846000 |
| 6 | -2.369661000 | 1.739681000 | -1.133695000 |
| 6 | -3.186937000 | 1.992009000 | -2.248402000 |
| 6 | -2.154807000 | 2.762594000 | -0.198571000 |
| 6 | -2.751581000 | 4.013753000 | -0.370488000 |
| 6 | -3.781325000 | 3.242364000 | -2.418738000 |
| 6 | -3.564998000 | 4.254828000 | -1.478980000 |
| 1 | -3.369656000 | 1.208608000 | -2.978827000 |
| 1 | -1.507957000 | 2.564124000 | 0.651387000 |
| 1 | -2.578874000 | 4.797917000 | 0.361279000 |
| 1 | -4.412371000 | 3.427343000 | -3.283525000 |
| 1 | -4.029201000 | 5.227910000 | -1.613023000 |
| 1 | -0.469813000 | -1.180640000 | -2.661214000 |
| 6 | 0.737646000 | 0.613707000 | -2.430214000 |
| 1 | 1.367705000 | 0.388721000 | -3.296113000 |
| 1 | 0.591614000 | 1.698634000 | -2.393116000 |
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| 6 | 2.083554000 | -2.640485000 | -0.652871000 |
| 6 | 3.297852000 | -1.536469000 | -2.428490000 |
| 6 | 2.636295000 | -3.865351000 | -1.036234000 |
| 6 | 3.850365000 | -2.758980000 | -2.811037000 |
| 6 | 3.520878000 | -3.925796000 | -2.114162000 |
| 1 | 1.383806000 | -2.584009000 | 0.176999000 |
| 1 | 3.566884000 | -0.634391000 | -2.971818000 |
| 1 | 2.375136000 | -4.769339000 | -0.492800000 |
| 1 | 4.537739000 | -2.802662000 | -3.651511000 |
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| 6 | 2.943183000 | 1.325036000 | -0.640065000 |
| 6 | 2.583919000 | 2.678904000 | -0.504984000 |
| 6 | 4.291357000 | 0.968507000 | -0.489435000 |
| 6 | 3.552400000 | 3.651745000 | -0.264393000 |
| 6 | 5.259744000 | 1.944476000 | -0.236370000 |
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| 1 | 4.592735000 | -0.070660000 | -0.571379000 |
| 1 | 3.258415000 | 4.693730000 | -0.171371000 |
| 1 | 6.299925000 | 1.651022000 | -0.123263000 |
| 1 | 5.650244000 | 4.044258000 | 0.063501000 |
| 1 | 1.512702000 | -2.766208000 | 2.674995000 |
| 1 | -1.467314000 | 2.005300000 | 2.878720000 |

**$TS_{II-4}$**

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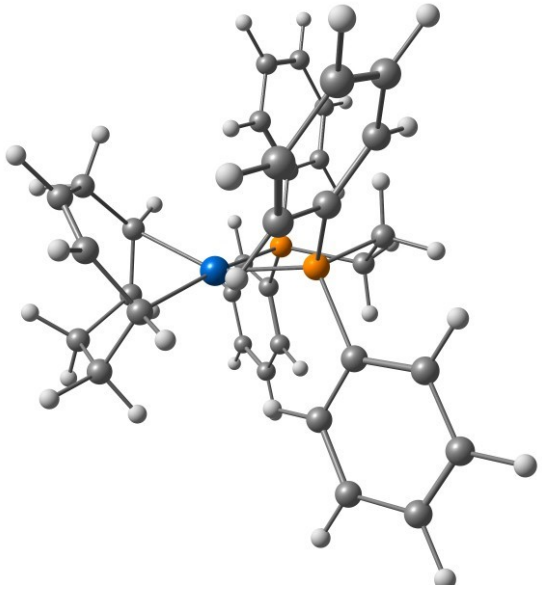
E (BS2) = -2104.509184

$G_{298.15,1M}$ (BS2) = -2103.980745



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| 1 | 1.234341000 | 0.513938000 | -3.304477000 |
| 6 | 1.378180000 | -0.917099000 | 2.292261000 |
| 6 | 0.773410000 | -2.191031000 | 2.934576000 |
| 6 | -0.665543000 | -1.916677000 | 3.396922000 |
| 6 | -1.406979000 | -1.055237000 | 2.380665000 |
| 6 | -1.395051000 | 0.351365000 | 2.417862000 |
| 6 | -0.733960000 | 1.201586000 | 3.493227000 |
| 6 | 0.724763000 | 1.013411000 | 3.839349000 |
| 6 | 1.619824000 | 0.161675000 | 3.310499000 |
| 1 | -0.640276000 | -1.396172000 | 4.362777000 |
| 1 | -1.210099000 | -2.854325000 | 3.557376000 |
| 1 | 1.073383000 | 1.704165000 | 4.608705000 |
| 1 | 2.639393000 | 0.247420000 | 3.699561000 |
| 1 | -2.238302000 | -1.532668000 | 1.863395000 |
| 1 | 1.380376000 | -2.560916000 | 3.778495000 |
| 1 | 2.352040000 | -1.209614000 | 1.877799000 |
| 1 | -1.329210000 | 1.082913000 | 4.416114000 |
| 1 | -2.248028000 | 0.859972000 | 1.968897000 |
| 6 | 2.871554000 | 1.302747000 | -0.603237000 |
| 6 | 2.995433000 | 2.503681000 | -1.316773000 |
| 6 | 3.813332000 | 1.010964000 | 0.399494000 |
| 6 | 4.034395000 | 3.394059000 | -1.030717000 |
| 6 | 4.850230000 | 1.897909000 | 0.679110000 |
| 6 | 4.962738000 | 3.095256000 | -0.033767000 |
| 1 | 2.290950000 | 2.758538000 | -2.100849000 |
| 1 | 3.731263000 | 0.087239000 | 0.961675000 |
| 1 | 4.115824000 | 4.320537000 | -1.592444000 |
| 1 | 5.568186000 | 1.656478000 | 1.457850000 |
| 1 | 5.768844000 | 3.788942000 | 0.187692000 |
| 6 | 2.384607000 | -1.405081000 | -1.477941000 |
| 6 | 3.455152000 | -1.323270000 | -2.381942000 |
| 6 | 1.936769000 | -2.666386000 | -1.056999000 |
| 6 | 2.542405000 | -3.828222000 | -1.542082000 |
| 6 | 4.060188000 | -2.484416000 | -2.862457000 |
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| 1 | 1.116960000 | -2.723278000 | -0.344462000 |
| 1 | 2.189835000 | -4.800028000 | -1.207966000 |
| 1 | 4.889495000 | -2.412112000 | -3.560711000 |
| 1 | 4.078487000 | -4.641114000 | -2.818554000 |
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| 6 | -2.305237000 | 1.865314000 | -1.006424000 |
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| 6 | -3.274777000 | 2.193451000 | -1.969117000 |
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| 6 | -3.222699000 | 4.507717000 | -1.263364000 |
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| 1 | -3.680710000 | 1.419045000 | -2.614599000 |
| 1 | -1.855586000 | 4.969546000 | 0.339961000 |
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| 1 | -3.579377000 | 5.529187000 | -1.363158000 |
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| 6 | -4.311118000 | -0.571240000 | -0.484343000 |
| 6 | -3.862411000 | -3.229265000 | -1.204462000 |
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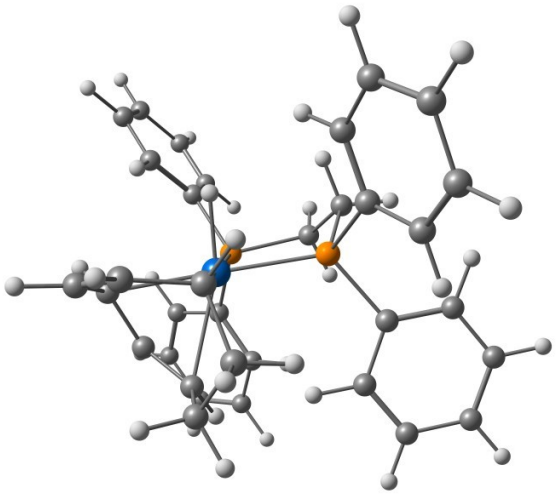
| 1 | -5.941345000 | -3.553603000 | -0.722237000 |
| 1 | -0.869442000 | 2.255920000 | 3.210873000 |
| 1 | 0.762575000 | -2.989464000 | 2.181007000 |

**[IrH(1-$\kappa$-3,4-$\eta^2$-$C_8H_{10}$)(dppe)] (4)**

E (BS1) = -2103.99503

E (BS2) = -2104.5165

$G_{298.15,1M}$ (BS2) = -2103.988472



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| 6 | -1.645822000 | -1.234155000 | 2.046026000 |
| 6 | -2.352851000 | 0.005558000 | 2.635270000 |
| 6 | -1.311442000 | 0.904469000 | 3.328374000 |
| 6 | -0.023032000 | 1.072940000 | 2.518032000 |
| 6 | 1.114963000 | 0.231182000 | 2.523791000 |
| 6 | 1.121124000 | -1.211287000 | 2.585734000 |
| 6 | 0.210054000 | -2.023712000 | 3.447567000 |
| 6 | -1.097842000 | -2.060891000 | 3.181818000 |
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| 1 | -1.737862000 | 1.896758000 | 3.517382000 |
| 1 | 0.644866000 | -2.551858000 | 4.297388000 |
| 1 | -1.790762000 | -2.581781000 | 3.848954000 |
| 1 | 0.224730000 | 2.104257000 | 2.268718000 |
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| 1 | 2.113353000 | -1.641841000 | 2.445227000 |
| 1 | 2.052548000 | 0.701454000 | 2.229375000 |
| 6 | -2.929339000 | -1.000457000 | -1.129475000 |
| 6 | -2.740889000 | -2.362280000 | -1.419635000 |
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| 6 | -2.272384000 | 4.040495000 | -0.191220000 |
| 6 | -3.254908000 | 3.502766000 | -2.333014000 |
| 6 | -2.983136000 | 4.433812000 | -1.325546000 |
| 1 | -3.047396000 | 1.468826000 | -2.988447000 |
| 1 | -1.276462000 | 2.404988000 | 0.811165000 |
| 1 | -2.060621000 | 4.757212000 | 0.597334000 |
| 1 | -3.812267000 | 3.802170000 | -3.216208000 |
| 1 | -3.325891000 | 5.459764000 | -1.426614000 |
| 1 | -0.352430000 | -1.207486000 | -2.658465000 |
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| 1 | 0.733783000 | 1.649543000 | -2.310262000 |
| 15 | 1.677589000 | 0.042853000 | -0.726022000 |
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| 6 | 2.881782000 | -2.494298000 | -0.660280000 |
| 6 | 3.836819000 | -0.968349000 | -2.277243000 |
| 6 | 3.785099000 | -3.481488000 | -1.064394000 |
| 6 | 4.736124000 | -1.954522000 | -2.680305000 |
| 6 | 4.710849000 | -3.214455000 | -2.073553000 |
| 1 | 2.151731000 | -2.698383000 | 0.116329000 |
| 1 | 3.875189000 | 0.012807000 | -2.743084000 |
| 1 | 3.761144000 | -4.458499000 | -0.589897000 |
| 1 | 5.456818000 | -1.741405000 | -3.464976000 |
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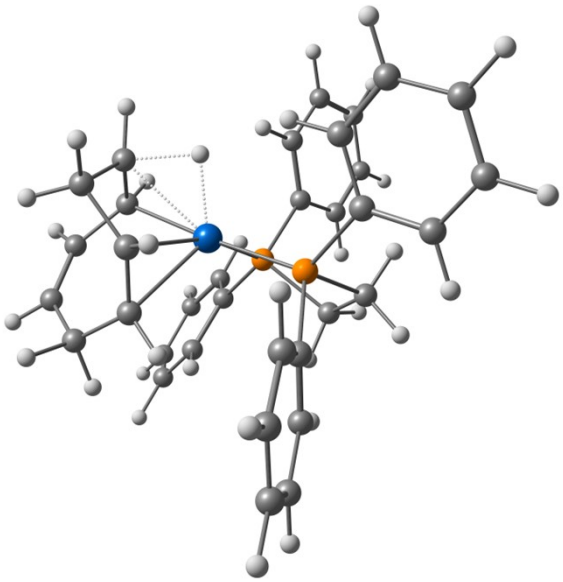
| 6 | 2.714150000 | 1.501366000 | -0.281579000 |
| 6 | 2.061338000 | 2.735758000 | -0.109407000 |
| 6 | 4.076029000 | 1.409163000 | 0.040577000 |
| 6 | 2.761511000 | 3.854082000 | 0.339092000 |
| 6 | 4.773784000 | 2.530071000 | 0.499889000 |
| 6 | 4.122170000 | 3.754921000 | 0.645424000 |
| 1 | 0.997163000 | 2.818686000 | -0.311359000 |
| 1 | 4.598627000 | 0.464218000 | -0.066434000 |
| 1 | 2.242672000 | 4.801360000 | 0.458202000 |
| 1 | 5.828866000 | 2.441466000 | 0.743873000 |
| 1 | 4.666627000 | 4.624902000 | 1.001343000 |
| 1 | -0.076746000 | -2.011734000 | 0.118105000 |
| 1 | -2.837796000 | 0.568979000 | 1.829017000 |

**$TS_{II-III}$**

E (BS1) = -2103.93930388

E (BS2) = -2104.46483112

$G_{298.15,1M}$ (BS2) = -2103.943577



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| 1 | 1.494763000 | 1.034159000 | -2.991813000 |
| 6 | 1.129057000 | -1.852590000 | 1.965146000 |
| 6 | 0.504694000 | -2.557764000 | 0.899764000 |
| 6 | -0.570393000 | -3.616801000 | 1.027642000 |
| 6 | -1.858259000 | -3.329794000 | 1.744569000 |
| 6 | -2.313966000 | -2.154471000 | 2.197748000 |
| 6 | -1.663996000 | -0.825254000 | 2.206353000 |
| 6 | -0.524106000 | -0.489840000 | 3.052714000 |
| 6 | 0.485497000 | -1.601673000 | 3.333156000 |
| 1 | -0.646586000 | 0.287947000 | 3.805708000 |
| 1 | -0.001823000 | -2.484665000 | 3.769050000 |
| 1 | 1.244398000 | -1.253421000 | 4.039274000 |
| 1 | 0.268497000 | 0.589898000 | 2.214933000 |
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| 1 | 2.202054000 | -1.686042000 | 1.911656000 |
| 1 | -2.410365000 | -0.028651000 | 2.187042000 |
| 1 | -3.324156000 | -2.152206000 | 2.612154000 |
| 6 | 2.923530000 | 1.555795000 | -0.119767000 |
| 6 | 3.940468000 | 1.939826000 | -1.010044000 |
| 6 | 2.876193000 | 2.139611000 | 1.151002000 |
| 6 | 4.886169000 | 2.893015000 | -0.633979000 |
| 6 | 3.825905000 | 3.092452000 | 1.529851000 |
| 6 | 4.830453000 | 3.471182000 | 0.638388000 |
| 1 | 3.999605000 | 1.485082000 | -1.995403000 |
| 1 | 2.086608000 | 1.839075000 | 1.835016000 |
| 1 | 5.668232000 | 3.183645000 | -1.330247000 |
| 1 | 3.779900000 | 3.536675000 | 2.520533000 |
| 1 | 5.569556000 | 4.211529000 | 0.932030000 |
| 6 | 2.657807000 | -1.025456000 | -1.324189000 |
| 6 | 2.220310000 | -1.745961000 | -2.446561000 |
| 6 | 3.817544000 | -1.453055000 | -0.658541000 |
| 6 | 2.931816000 | -2.857961000 | -2.899812000 |
| 6 | 4.525489000 | -2.569036000 | -1.108517000 |
| 6 | 4.085496000 | -3.274072000 | -2.230733000 |
| 1 | 1.317203000 | -1.445693000 | -2.968751000 |
| 1 | 4.175361000 | -0.905685000 | 0.208566000 |
| 1 | 2.584008000 | -3.400331000 | -3.774763000 |
| 1 | 5.421600000 | -2.885377000 | -0.581934000 |
| 1 | 4.637303000 | -4.141459000 | -2.581594000 |
| 1 | 0.891329000 | 2.259901000 | -1.873957000 |
| 6 | -0.574726000 | 0.734239000 | -2.336925000 |
| 1 | -1.099091000 | 1.417674000 | -3.012138000 |
| 1 | -0.612126000 | -0.266162000 | -2.778281000 |
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| 6 | -2.058691000 | 2.336154000 | -0.441201000 |
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| 6 | -2.160481000 | 4.306853000 | 0.981757000 |
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| 1 | -1.197057000 | 2.446619000 | 1.520957000 |
| 1 | -3.007667000 | 2.560605000 | -2.374102000 |
| 1 | -1.922749000 | 4.795355000 | 1.922869000 |
| 1 | -3.687258000 | 4.902260000 | -2.000246000 |
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| 6 | -2.973436000 | -0.358853000 | -1.101423000 |
| 6 | -2.787862000 | -1.714469000 | -1.423540000 |
| 6 | -4.279775000 | 0.144558000 | -1.034012000 |
| 6 | -3.876478000 | -2.532360000 | -1.717743000 |
| 6 | -5.373126000 | -0.682679000 | -1.308998000 |
| 6 | -5.175628000 | -2.018062000 | -1.660559000 |
| 1 | -1.782365000 | -2.126382000 | -1.406938000 |
| 1 | -4.454507000 | 1.179988000 | -0.762228000 |
| 1 | -3.713671000 | -3.576762000 | -1.970021000 |
| 1 | -6.379866000 | -0.277999000 | -1.247913000 |
| 1 | -6.026903000 | -2.657919000 | -1.875933000 |
| 1 | -0.837097000 | -3.957710000 | 0.015219000 |
| 1 | 1.173594000 | -2.775120000 | 0.069990000 |
| 1 | -0.114557000 | -4.503106000 | 1.501934000 |

**[IrH($\eta^2$:$\eta^2$-1,3,6-COT)(dppe)] (III)**

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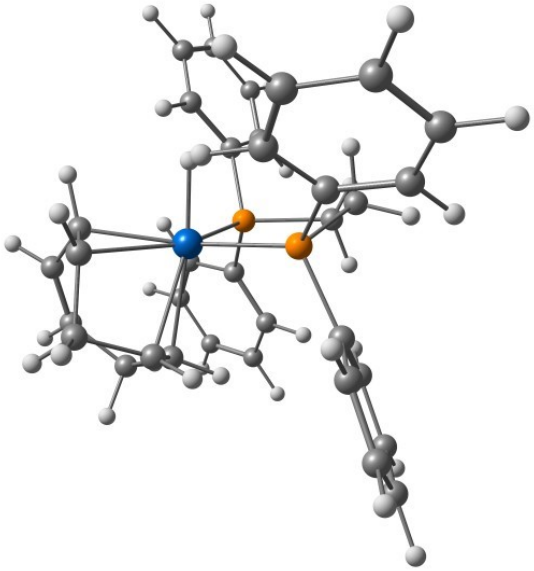
E (BS2) = -2104.50157745

$G_{298.15,1M}$ (BS2) = -2103.974424



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| 6 | 1.023999000 | 0.992813000 | -2.200866000 |
| 1 | 1.657041000 | 0.776628000 | -3.067249000 |
| 6 | 0.795320000 | -1.838122000 | 1.825385000 |
| 6 | -0.350299000 | -2.162192000 | 1.098245000 |
| 6 | -1.685595000 | -2.603652000 | 1.669397000 |
| 6 | -2.423753000 | -1.770682000 | 2.683936000 |
| 6 | -2.166895000 | -0.528178000 | 3.118578000 |
| 6 | -1.030410000 | 0.370680000 | 2.806147000 |
| 6 | 0.357741000 | 0.068018000 | 3.111642000 |
| 6 | 0.781014000 | -1.382869000 | 3.278498000 |
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| 1 | 0.100231000 | -1.971942000 | 3.908242000 |
| 1 | 1.785736000 | -1.452337000 | 3.703837000 |
| 1 | 0.236481000 | 1.754610000 | 0.983911000 |
| 1 | -3.318458000 | -2.260105000 | 3.069794000 |
| 1 | 1.767067000 | -2.046910000 | 1.388857000 |
| 1 | -1.290726000 | 1.415540000 | 2.978689000 |
| 1 | -2.895944000 | -0.102660000 | 3.812462000 |
| 6 | 3.223232000 | 1.362249000 | -0.388845000 |
| 6 | 4.181417000 | 1.545101000 | -1.400355000 |
| 6 | 3.373932000 | 2.043819000 | 0.825463000 |
| 6 | 5.264744000 | 2.399915000 | -1.200402000 |
| 6 | 4.460640000 | 2.899707000 | 1.025158000 |
| 6 | 5.405674000 | 3.079054000 | 0.014014000 |
| 1 | 4.087792000 | 1.010677000 | -2.341837000 |
| 1 | 2.629549000 | 1.896438000 | 1.602593000 |
| 1 | 6.000293000 | 2.534856000 | -1.988749000 |
| 1 | 4.567466000 | 3.423683000 | 1.971006000 |
| 1 | 6.250985000 | 3.743714000 | 0.169654000 |
| 6 | 2.541606000 | -1.327262000 | -1.148397000 |
| 6 | 1.829922000 | -2.234296000 | -1.951542000 |
| 6 | 3.780937000 | -1.730960000 | -0.623414000 |
| 6 | 2.348170000 | -3.497511000 | -2.238382000 |
| 6 | 4.296400000 | -2.997329000 | -0.905730000 |
| 6 | 3.583997000 | -3.884372000 | -1.715536000 |
| 1 | 0.861880000 | -1.958999000 | -2.353603000 |
| 1 | 4.348729000 | -1.051533000 | 0.004848000 |
| 1 | 1.784223000 | -4.180070000 | -2.868417000 |
| 1 | 5.258089000 | -3.289231000 | -0.492839000 |
| 1 | 3.986489000 | -4.869060000 | -1.935116000 |
| 1 | 1.056073000 | 2.074484000 | -2.030077000 |
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| 15 | -1.394437000 | 0.453191000 | -0.830412000 |
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| 6 | -3.299812000 | 2.223609000 | -1.965932000 |
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| 6 | -4.057629000 | 3.391971000 | -2.022719000 |
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| 1 | -4.526534000 | 5.265576000 | -1.059220000 |
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| 6 | -3.912549000 | -0.740542000 | -0.483690000 |
| 6 | -3.324157000 | -3.044003000 | -1.940416000 |
| 6 | -4.845187000 | -1.774364000 | -0.563734000 |
| 6 | -4.556107000 | -2.930331000 | -1.292643000 |
| 1 | -1.430335000 | -2.137515000 | -2.349613000 |
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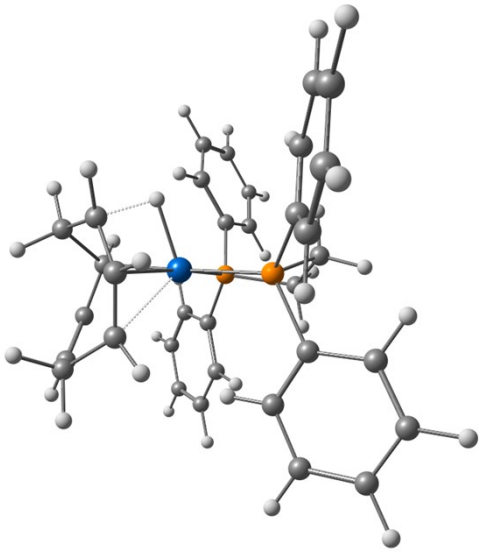
| 1 | -5.797641000 | -1.677450000 | -0.050151000 |
| 1 | -5.282471000 | -3.735759000 | -1.352674000 |
| 1 | -2.374260000 | -2.772027000 | 0.832072000 |
| 1 | -0.165419000 | -2.568920000 | 0.105482000 |
| 1 | -1.535156000 | -3.605733000 | 2.105691000 |

**$TS_{II-IV}$**

E (BS1) = -2103.93361962

E (BS2) = -2104.46016537

$G_{298.15,1M}$ (BS2) = -2103.936954



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| 1 | 1.577130000 | 0.485457000 | -3.187700000 |
| 6 | 1.356411000 | -0.107345000 | 2.631738000 |
| 6 | 0.855961000 | -1.423401000 | 2.437040000 |
| 6 | -0.123324000 | -2.208266000 | 3.324119000 |
| 6 | -1.609566000 | -2.142738000 | 3.069210000 |
| 6 | -2.252630000 | -1.060786000 | 2.608428000 |
| 6 | -1.624619000 | 0.254526000 | 2.321413000 |
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| 6 | 0.599060000 | 1.079071000 | 2.966777000 |
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| 1 | 1.185937000 | 1.940928000 | 3.283163000 |
| 1 | 0.259600000 | 1.694186000 | 1.579455000 |
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| 1 | -2.171528000 | -3.050322000 | 3.284066000 |
| 1 | 2.396977000 | 0.073381000 | 2.362760000 |
| 1 | -2.389622000 | 0.950564000 | 1.969180000 |
| 1 | -3.319025000 | -1.154644000 | 2.401563000 |
| 6 | 3.157339000 | 1.206555000 | -0.467630000 |
| 6 | 3.006898000 | 2.601876000 | -0.546210000 |
| 6 | 4.380639000 | 0.686574000 | -0.014581000 |
| 6 | 4.061349000 | 3.450857000 | -0.211807000 |
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| 6 | 5.278461000 | 2.922446000 | 0.227756000 |
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| 1 | 3.930144000 | 4.526765000 | -0.287960000 |
| 1 | 6.371469000 | 1.118684000 | 0.678896000 |
| 1 | 6.097413000 | 3.584829000 | 0.493319000 |
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| 6 | 1.815271000 | -2.673878000 | -0.844795000 |
| 6 | 3.451338000 | -1.551117000 | -2.226474000 |
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| 6 | 3.908125000 | -2.784892000 | -2.689588000 |
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| 1 | 3.918600000 | -0.638238000 | -2.585721000 |
| 1 | 1.808239000 | -4.825136000 | -0.953178000 |
| 1 | 4.721534000 | -2.824355000 | -3.409025000 |
| 1 | 3.677286000 | -4.928198000 | -2.591933000 |
| 1 | 0.820746000 | 1.812433000 | -2.286257000 |
| 6 | -0.450496000 | 0.062469000 | -2.484254000 |
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| 1 | -0.337155000 | -1.007719000 | -2.683984000 |
| 15 | -1.390976000 | 0.246572000 | -0.870884000 |
| 6 | -2.360076000 | 1.801858000 | -1.179950000 |
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| 6 | -3.750953000 | 4.199085000 | -1.650059000 |
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| 1 | -3.358155000 | 1.086869000 | -2.962175000 |
| 1 | -2.778546000 | 4.922476000 | 0.133948000 |
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| 1 | -4.289587000 | 5.125089000 | -1.831760000 |
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| 6 | -2.266468000 | -2.398397000 | -1.118331000 |
| 6 | -4.040212000 | -0.818544000 | -0.682263000 |
| 6 | -3.182408000 | -3.446650000 | -1.061883000 |
| 6 | -4.955871000 | -1.872029000 | -0.609902000 |
| 6 | -4.532108000 | -3.186595000 | -0.804999000 |
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| 1 | 0.177124000 | -3.261081000 | 3.262574000 |
| 1 | 1.622352000 | -2.077697000 | 2.025997000 |
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**IV**

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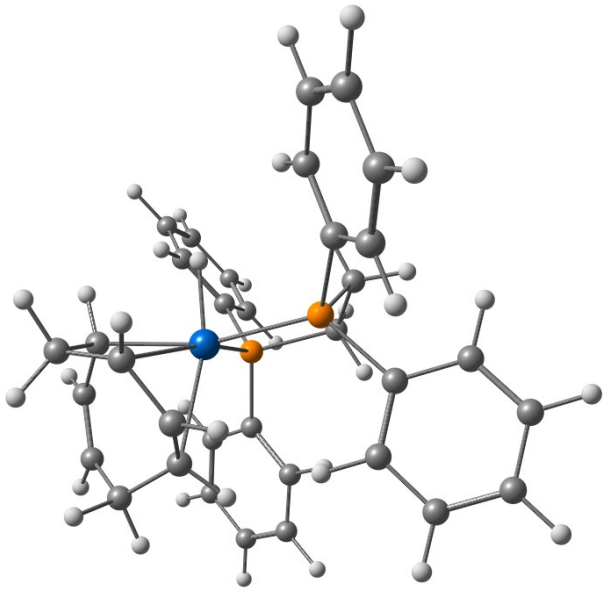
E (BS2) = -2104.49844470

$G_{298.15,1M}$ (BS2) = -2103.971557



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| 1 | -1.785938000 | -0.084923000 | -3.088930000 |
| 6 | -0.818621000 | 0.560547000 | 2.629828000 |
| 6 | 0.348139000 | 1.299371000 | 2.268590000 |
| 6 | 1.652734000 | 1.407933000 | 3.083302000 |
| 6 | 2.815069000 | 0.499789000 | 2.764147000 |
| 6 | 2.686390000 | -0.770443000 | 2.358294000 |
| 6 | 1.395190000 | -1.486205000 | 2.200311000 |
| 6 | 0.447646000 | -1.532055000 | 3.428270000 |
| 6 | -0.817800000 | -0.818020000 | 2.967943000 |
| 1 | 0.883209000 | -1.086343000 | 4.333171000 |
| 1 | -1.782724000 | -1.283662000 | 3.153871000 |
| 1 | -0.300957000 | -2.022624000 | 0.322987000 |
| 1 | 0.199603000 | -2.569993000 | 3.673666000 |
| 1 | 3.807254000 | 0.933859000 | 2.870440000 |
| 1 | -1.792025000 | 1.010207000 | 2.432891000 |
| 1 | 1.581015000 | -2.502675000 | 1.852269000 |
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| 6 | -3.149878000 | -2.484012000 | -0.731933000 |
| 6 | -4.510771000 | -0.625577000 | -0.001829000 |
| 6 | -4.232665000 | -3.344852000 | -0.560410000 |
| 6 | -5.590473000 | -1.492728000 | 0.183227000 |
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| 1 | -3.877770000 | 5.240283000 | -1.566820000 |
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| 1 | 0.784868000 | 0.027053000 | -3.337834000 |
| 1 | 0.100418000 | 1.405425000 | -2.474498000 |
| 15 | 1.319397000 | -0.057892000 | -0.921641000 |
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| 6 | 3.220373000 | -3.657608000 | -1.593353000 |
| 6 | 4.150289000 | -2.075681000 | -3.166468000 |
| 6 | 4.096666000 | -3.370190000 | -2.640086000 |
| 1 | 1.713085000 | -2.875689000 | -0.259673000 |
| 1 | 3.389831000 | -0.069833000 | -3.052360000 |
| 1 | 3.171907000 | -4.661950000 | -1.181881000 |
| 1 | 4.828863000 | -1.846255000 | -3.983424000 |
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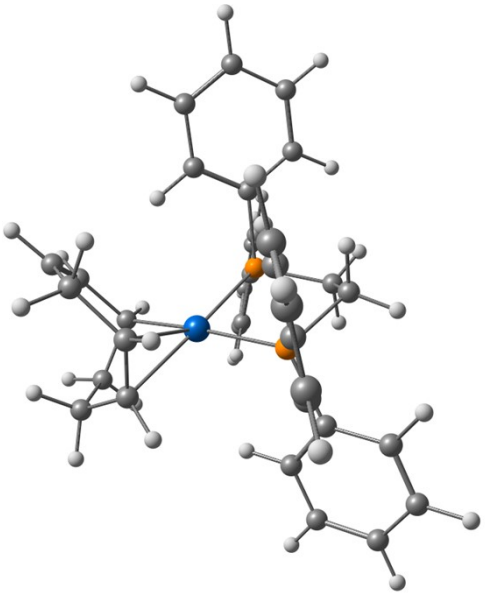
| 6 | 1.782257000 | 2.700435000 | -0.714229000 |
| 6 | 3.761114000 | 1.337136000 | -0.472620000 |
| 6 | 2.534648000 | 3.843860000 | -0.452804000 |
| 6 | 4.513781000 | 2.483975000 | -0.208169000 |
| 6 | 3.905394000 | 3.739271000 | -0.198725000 |
| 1 | 0.712996000 | 2.798363000 | -0.874259000 |
| 1 | 4.247308000 | 0.367896000 | -0.463835000 |
| 1 | 2.049688000 | 4.816205000 | -0.442613000 |
| 1 | 5.576639000 | 2.391172000 | -0.002803000 |
| 1 | 4.491796000 | 4.629902000 | 0.008859000 |
| 1 | 2.002829000 | 2.441122000 | 2.975600000 |
| 1 | 0.118979000 | 2.258847000 | 1.810310000 |
| 1 | 1.396034000 | 1.305919000 | 4.148628000 |

**II'**

E (BS1) = -2103.98805492

E (BS2) = -2104.51145700

$G_{298.15,1M}$ (BS2) = -2103.984063



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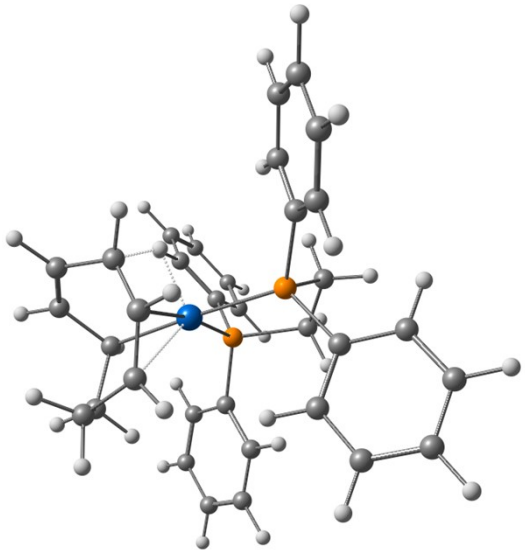
| 77 | 0.024655000 | 0.115654000 | 0.853667000 |
| 6 | 0.562227000 | 0.743307000 | -2.446815000 |
| 1 | 1.135678000 | 0.584958000 | -3.364973000 |
| 6 | 1.519709000 | 0.273223000 | 2.389155000 |
| 6 | 1.908214000 | -1.040402000 | 3.006060000 |
| 6 | 1.118160000 | -2.101317000 | 3.237741000 |
| 6 | -0.324276000 | -2.300949000 | 2.840775000 |
| 6 | -1.122095000 | -1.178795000 | 2.195853000 |
| 6 | -1.254358000 | 0.138096000 | 2.684597000 |
| 6 | -0.479827000 | 0.673002000 | 3.885714000 |
| 6 | 0.893677000 | 1.213684000 | 3.452038000 |
| 1 | -1.063382000 | 1.453141000 | 4.388426000 |
| 1 | -0.336498000 | -0.133138000 | 4.616593000 |
| 1 | 1.547048000 | 1.342148000 | 4.331606000 |
| 1 | 0.765147000 | 2.210830000 | 3.009644000 |
| 1 | -0.888081000 | -2.626093000 | 3.732808000 |
| 1 | 2.437802000 | 0.753669000 | 2.024875000 |
| 1 | -2.182417000 | 0.658035000 | 2.448141000 |
| 1 | -1.969585000 | -1.571782000 | 1.636440000 |
| 6 | 2.918573000 | 1.349755000 | -0.857315000 |
| 6 | 2.707404000 | 2.574712000 | -0.201550000 |
| 6 | 4.177796000 | 1.080286000 | -1.410054000 |
| 6 | 3.730465000 | 3.518542000 | -0.117621000 |
| 6 | 5.204152000 | 2.023392000 | -1.316276000 |
| 6 | 4.982495000 | 3.243124000 | -0.674248000 |
| 1 | 1.742425000 | 2.773281000 | 0.259578000 |
| 1 | 4.364811000 | 0.132961000 | -1.905852000 |
| 1 | 3.555272000 | 4.460681000 | 0.394278000 |
| 1 | 6.178294000 | 1.801781000 | -1.743599000 |
| 1 | 5.783517000 | 3.973325000 | -0.600364000 |
| 6 | 2.197497000 | -1.447674000 | -1.386962000 |
| 6 | 2.326831000 | -2.424123000 | -0.385640000 |
| 6 | 2.593600000 | -1.759796000 | -2.697671000 |
| 6 | 2.846451000 | -3.682737000 | -0.690757000 |
| 6 | 3.105895000 | -3.023137000 | -3.000744000 |
| 6 | 3.234164000 | -3.986519000 | -1.997895000 |
| 1 | 2.011349000 | -2.193411000 | 0.627372000 |
| 1 | 2.508257000 | -1.023341000 | -3.490470000 |
| 1 | 2.941732000 | -4.427460000 | 0.094657000 |
| 1 | 3.403905000 | -3.252946000 | -4.019993000 |
| 1 | 3.631312000 | -4.969424000 | -2.235940000 |
| 1 | 0.426831000 | 1.825047000 | -2.331548000 |
| 6 | -0.793743000 | 0.030356000 | -2.486048000 |
| 1 | -1.442293000 | 0.446185000 | -3.262738000 |
| 1 | -0.656886000 | -1.034581000 | -2.701379000 |
| 15 | -1.602719000 | 0.161351000 | -0.790589000 |
| 6 | -2.569614000 | 1.728212000 | -0.957090000 |
| 6 | -2.367118000 | 2.737550000 | -0.003687000 |
| 6 | -3.465779000 | 1.963212000 | -2.013473000 |
| 6 | -3.045619000 | 3.955192000 | -0.101746000 |
| 6 | -4.145551000 | 3.177393000 | -2.109968000 |
| 6 | -3.936542000 | 4.175667000 | -1.153262000 |
| 1 | -1.666233000 | 2.556027000 | 0.807529000 |
| 1 | -3.644422000 | 1.190295000 | -2.756262000 |
| 1 | -2.878231000 | 4.728339000 | 0.643081000 |
| 1 | -4.838743000 | 3.345483000 | -2.929632000 |
| 1 | -4.465784000 | 5.121402000 | -1.230407000 |
| 6 | -2.872996000 | -1.175542000 | -0.849834000 |
| 6 | -2.405222000 | -2.496259000 | -0.982998000 |
| 6 | -4.241528000 | -0.966011000 | -0.627452000 |
| 6 | -3.288739000 | -3.573028000 | -0.932884000 |
| 6 | -5.124795000 | -2.047888000 | -0.567719000 |
| 6 | -4.653988000 | -3.351537000 | -0.726761000 |
| 1 | -1.340672000 | -2.680532000 | -1.104946000 |
| 1 | -4.624189000 | 0.041521000 | -0.501379000 |
| 1 | -2.910858000 | -4.585683000 | -1.044068000 |
| 1 | -6.182574000 | -1.867562000 | -0.396493000 |
| 1 | -5.342742000 | -4.190419000 | -0.681520000 |
| 1 | -0.364047000 | -3.163787000 | 2.158815000 |
| 1 | 2.945068000 | -1.132531000 | 3.345224000 |
| 1 | 1.553772000 | -2.966232000 | 3.740727000 |

**$TS_{II'-4'}$**

E (BS1) = -2103.951725

E (BS2) = -2104.476139

$G_{298.15,1M}$ (BS2) = -2103.952333



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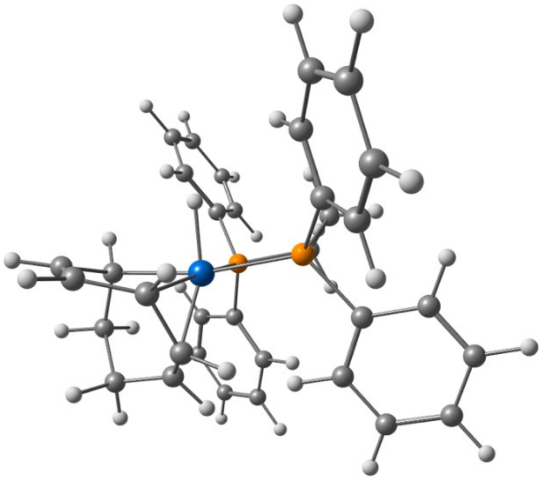
| 6 | 0.439872000 | 0.612665000 | -2.431891000 |
| 1 | 1.017559000 | 0.392605000 | -3.334293000 |
| 6 | 1.720079000 | -0.666202000 | 2.070878000 |
| 6 | 1.473520000 | -1.825381000 | 3.007135000 |
| 6 | 0.241230000 | -2.304521000 | 3.204686000 |
| 6 | -0.908944000 | -1.761215000 | 2.413345000 |
| 6 | -1.374720000 | -0.374984000 | 2.569412000 |
| 6 | -0.635175000 | 0.784408000 | 2.877302000 |
| 6 | 0.636260000 | 0.913723000 | 3.713140000 |
| 6 | 1.918339000 | 0.611390000 | 2.920284000 |
| 1 | 0.680432000 | 1.930877000 | 4.119571000 |
| 1 | 0.573195000 | 0.240641000 | 4.576010000 |
| 1 | 2.775687000 | 0.514647000 | 3.610437000 |
| 1 | 2.139345000 | 1.452408000 | 2.254260000 |
| 1 | -1.740083000 | -2.453432000 | 2.276623000 |
| 1 | 2.650722000 | -0.851296000 | 1.516420000 |
| 1 | -1.233154000 | 1.692132000 | 2.821590000 |
| 1 | -2.414966000 | -0.215685000 | 2.285578000 |
| 6 | 2.624468000 | 1.428563000 | -0.643332000 |
| 6 | 2.154531000 | 2.749133000 | -0.533760000 |
| 6 | 3.978499000 | 1.172823000 | -0.384108000 |
| 6 | 3.021972000 | 3.788412000 | -0.204072000 |
| 6 | 4.844405000 | 2.213741000 | -0.035919000 |
| 6 | 4.371933000 | 3.523047000 | 0.049040000 |
| 1 | 1.099861000 | 2.963756000 | -0.683368000 |
| 1 | 4.362732000 | 0.160330000 | -0.449636000 |
| 1 | 2.643682000 | 4.804672000 | -0.133982000 |
| 1 | 5.889148000 | 1.996004000 | 0.168466000 |
| 1 | 5.045998000 | 4.331788000 | 0.316975000 |
| 6 | 2.431362000 | -1.311581000 | -1.554105000 |
| 6 | 2.338121000 | -2.576916000 | -0.961523000 |
| 6 | 3.293181000 | -1.135114000 | -2.649823000 |
| 6 | 3.092700000 | -3.646665000 | -1.450654000 |
| 6 | 4.043004000 | -2.203448000 | -3.141488000 |
| 6 | 3.944389000 | -3.462470000 | -2.540838000 |
| 1 | 1.667615000 | -2.710365000 | -0.117010000 |
| 1 | 3.392169000 | -0.155777000 | -3.111061000 |
| 1 | 3.014097000 | -4.621838000 | -0.977791000 |
| 1 | 4.705422000 | -2.054433000 | -3.989870000 |
| 1 | 4.530636000 | -4.294006000 | -2.922314000 |
| 1 | 0.305772000 | 1.697486000 | -2.379453000 |
| 6 | -0.924628000 | -0.087253000 | -2.452133000 |
| 1 | -1.580746000 | 0.332993000 | -3.220863000 |
| 1 | -0.803563000 | -1.156403000 | -2.652331000 |
| 15 | -1.686927000 | 0.089508000 | -0.752788000 |
| 6 | -2.410557000 | 1.786845000 | -0.873996000 |
| 6 | -1.887912000 | 2.798755000 | -0.056260000 |
| 6 | -3.399117000 | 2.117129000 | -1.816945000 |
| 6 | -2.345195000 | 4.114422000 | -0.173998000 |
| 6 | -3.855251000 | 3.429974000 | -1.933938000 |
| 6 | -3.328630000 | 4.431464000 | -1.111875000 |
| 1 | -1.113060000 | 2.542137000 | 0.660481000 |
| 1 | -3.820214000 | 1.344782000 | -2.454917000 |
| 1 | -1.931328000 | 4.888365000 | 0.466604000 |
| 1 | -4.620710000 | 3.673059000 | -2.665817000 |
| 1 | -3.684273000 | 5.453841000 | -1.205334000 |
| 6 | -3.146908000 | -1.032010000 | -0.763470000 |
| 6 | -2.949404000 | -2.382393000 | -1.102334000 |
| 6 | -4.408097000 | -0.632843000 | -0.294495000 |
| 6 | -3.993917000 | -3.300170000 | -1.003626000 |
| 6 | -5.450645000 | -1.557121000 | -0.185382000 |
| 6 | -5.249428000 | -2.890056000 | -0.544754000 |
| 1 | -1.969541000 | -2.722387000 | -1.425490000 |
| 1 | -4.582375000 | 0.401603000 | -0.015980000 |
| 1 | -3.826118000 | -4.338083000 | -1.277818000 |
| 1 | -6.420539000 | -1.230697000 | 0.179747000 |
| 1 | -6.061146000 | -3.607295000 | -0.462704000 |
| 1 | -0.396772000 | -1.959417000 | 1.000209000 |
| 1 | 2.302033000 | -2.185492000 | 3.623793000 |
| 1 | 0.026652000 | -3.083020000 | 3.935077000 |

**4’**

E (BS1) = -2103.990169

E (BS2) = -2104.511906

$G_{298.15,1M}$ (BS2) = -2103.983184



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| 1 | 1.021693000 | 0.491211000 | -3.251127000 |
| 6 | 1.448606000 | -1.462445000 | 2.090897000 |
| 6 | 0.756516000 | -2.212532000 | 3.203528000 |
| 6 | -0.527581000 | -1.957681000 | 3.466033000 |
| 6 | -1.284883000 | -0.998763000 | 2.605832000 |
| 6 | -1.042799000 | 0.429020000 | 2.559010000 |
| 6 | 0.225184000 | 1.060747000 | 2.569415000 |
| 6 | 1.439923000 | 0.671651000 | 3.414257000 |
| 6 | 2.335678000 | -0.370900000 | 2.725938000 |
| 1 | 2.017185000 | 1.577321000 | 3.632742000 |
| 1 | 1.098318000 | 0.278882000 | 4.378193000 |
| 1 | 3.051555000 | -0.792414000 | 3.453186000 |
| 1 | 2.927707000 | 0.122361000 | 1.949622000 |
| 1 | -2.330238000 | -1.264007000 | 2.443233000 |
| 1 | 2.088157000 | -2.146354000 | 1.518969000 |
| 1 | 0.194646000 | 2.117057000 | 2.306145000 |
| 1 | -1.890863000 | 1.046156000 | 2.262382000 |
| 6 | 2.610732000 | 1.431086000 | -0.524536000 |
| 6 | 2.116876000 | 2.740450000 | -0.395957000 |
| 6 | 3.968935000 | 1.196950000 | -0.260018000 |
| 6 | 2.961695000 | 3.787888000 | -0.032285000 |
| 6 | 4.812562000 | 2.246379000 | 0.112189000 |
| 6 | 4.313964000 | 3.544443000 | 0.224135000 |
| 1 | 1.063755000 | 2.946438000 | -0.560506000 |
| 1 | 4.372870000 | 0.193127000 | -0.338674000 |
| 1 | 2.562355000 | 4.794575000 | 0.055412000 |
| 1 | 5.860183000 | 2.043943000 | 0.316465000 |
| 1 | 4.970568000 | 4.360069000 | 0.513173000 |
| 6 | 2.465910000 | -1.259387000 | -1.620148000 |
| 6 | 2.295966000 | -2.603158000 | -1.260966000 |
| 6 | 3.390273000 | -0.939140000 | -2.631086000 |
| 6 | 3.040373000 | -3.604630000 | -1.891293000 |
| 6 | 4.132172000 | -1.938606000 | -3.258347000 |
| 6 | 3.959600000 | -3.275721000 | -2.887330000 |
| 1 | 1.572789000 | -2.861026000 | -0.495804000 |
| 1 | 3.539512000 | 0.096939000 | -2.922026000 |
| 1 | 2.898583000 | -4.641583000 | -1.599818000 |
| 1 | 4.843954000 | -1.674861000 | -4.035691000 |
| 1 | 4.538341000 | -4.054833000 | -3.375582000 |
| 1 | 0.295380000 | 1.737196000 | -2.231197000 |
| 6 | -0.911794000 | -0.053713000 | -2.386823000 |
| 1 | -1.555246000 | 0.367550000 | -3.165414000 |
| 1 | -0.780439000 | -1.121004000 | -2.588662000 |
| 15 | -1.704339000 | 0.118841000 | -0.703202000 |
| 6 | -2.338641000 | 1.851365000 | -0.823329000 |
| 6 | -1.745630000 | 2.844026000 | -0.031432000 |
| 6 | -3.324803000 | 2.226031000 | -1.752424000 |
| 6 | -2.129853000 | 4.182037000 | -0.157654000 |
| 6 | -3.709928000 | 3.560520000 | -1.877770000 |
| 6 | -3.113323000 | 4.541610000 | -1.079376000 |
| 1 | -0.971329000 | 2.564474000 | 0.673215000 |
| 1 | -3.798420000 | 1.471051000 | -2.373606000 |
| 1 | -1.659835000 | 4.938621000 | 0.464470000 |
| 1 | -4.474389000 | 3.836356000 | -2.598823000 |
| 1 | -3.414415000 | 5.580716000 | -1.178459000 |
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| 6 | -3.103039000 | -2.258872000 | -1.187773000 |
| 6 | -4.456576000 | -0.468213000 | -0.291067000 |
| 6 | -4.208340000 | -3.107642000 | -1.161184000 |
| 6 | -5.560087000 | -1.324274000 | -0.254850000 |
| 6 | -5.441413000 | -2.642858000 | -0.694912000 |
| 1 | -2.142518000 | -2.645194000 | -1.514871000 |
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| 1 | -4.104057000 | -4.136412000 | -1.494407000 |
| 1 | -6.511982000 | -0.956604000 | 0.118143000 |
| 1 | -6.300270000 | -3.307395000 | -0.668759000 |
| 1 | -0.235181000 | -1.973362000 | 0.163525000 |
| 1 | 1.347767000 | -2.851399000 | 3.866135000 |
| 1 | -1.049229000 | -2.417483000 | 4.306507000 |

**$TS_{II'-III'}$**

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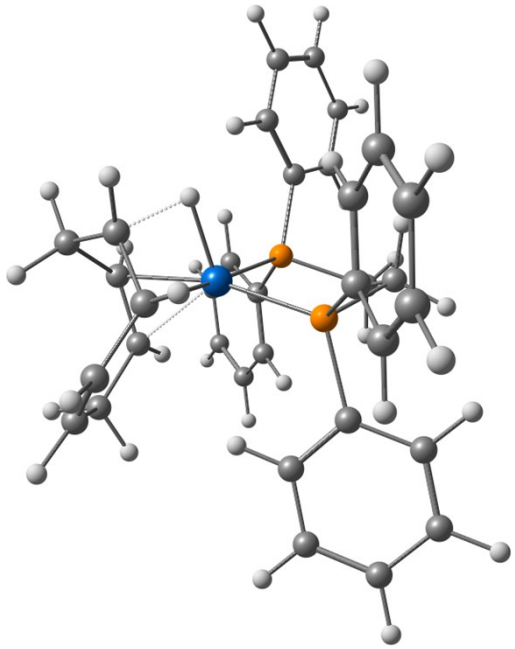
E (BS2) = -2104.466884

$G_{298.15,1M}$ (BS2) = -2103.943826



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| 6 | 0.522396000 | 1.052204000 | -2.290155000 |
| 1 | 1.097884000 | 0.960794000 | -3.216043000 |
| 6 | 1.626983000 | -0.009925000 | 2.381989000 |
| 6 | 2.159644000 | -1.282860000 | 2.919062000 |
| 6 | 1.597460000 | -2.498279000 | 2.966384000 |
| 6 | 0.274488000 | -2.935766000 | 2.404499000 |
| 6 | -0.703970000 | -1.927417000 | 1.837586000 |
| 6 | -1.246489000 | -0.804645000 | 2.520438000 |
| 6 | -0.561040000 | -0.088050000 | 3.689612000 |
| 6 | 0.537279000 | 0.728478000 | 3.009918000 |
| 1 | -1.274643000 | 0.576780000 | 4.184401000 |
| 1 | -0.147193000 | -0.764313000 | 4.450196000 |
| 1 | 0.741429000 | 1.728901000 | 3.389678000 |
| 1 | -0.178410000 | 1.450004000 | 1.802875000 |
| 1 | -0.247362000 | -3.506177000 | 3.192323000 |
| 1 | 2.434987000 | 0.648347000 | 2.059308000 |
| 1 | -2.302265000 | -0.581710000 | 2.385918000 |
| 1 | -1.401948000 | -2.400890000 | 1.151557000 |
| 6 | 2.809278000 | 1.599475000 | -0.578072000 |
| 6 | 2.417190000 | 2.883183000 | -0.158723000 |
| 6 | 4.177413000 | 1.320931000 | -0.701192000 |
| 6 | 3.366654000 | 3.870955000 | 0.097058000 |
| 6 | 5.130010000 | 2.308069000 | -0.430150000 |
| 6 | 4.729102000 | 3.585191000 | -0.037465000 |
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| 1 | 5.470777000 | 4.351549000 | 0.169877000 |
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| 6 | 3.043453000 | -1.018382000 | -2.793447000 |
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| 6 | 3.544633000 | -3.383464000 | -2.679923000 |
| 1 | 1.703514000 | -2.383305000 | 0.010425000 |
| 1 | 3.139074000 | -0.067338000 | -3.310479000 |
| 1 | 2.785535000 | -4.417946000 | -0.945424000 |
| 1 | 4.171474000 | -2.084749000 | -4.286131000 |
| 1 | 4.006318000 | -4.268600000 | -3.109043000 |
| 1 | 0.376567000 | 2.118862000 | -2.090138000 |
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| 1 | -1.490363000 | 0.828179000 | -3.112694000 |
| 1 | -0.675027000 | -0.694797000 | -2.739787000 |
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| 6 | -2.726586000 | 1.753414000 | -0.739491000 |
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| 6 | -3.685644000 | 1.934085000 | -1.751744000 |
| 6 | -3.380155000 | 3.892206000 | 0.212083000 |
| 6 | -4.480254000 | 3.079536000 | -1.780674000 |
| 6 | -4.327556000 | 4.062880000 | -0.797850000 |
| 1 | -1.838424000 | 2.604270000 | 1.017511000 |
| 1 | -3.824524000 | 1.169118000 | -2.511153000 |
| 1 | -3.258168000 | 4.651417000 | 0.979933000 |
| 1 | -5.218978000 | 3.205496000 | -2.567522000 |
| 1 | -4.946435000 | 4.955627000 | -0.820666000 |
| 6 | -2.827578000 | -1.134225000 | -0.851600000 |
| 6 | -2.364362000 | -2.379228000 | -1.312314000 |
| 6 | -4.147808000 | -1.038354000 | -0.387072000 |
| 6 | -3.209199000 | -3.488273000 | -1.337152000 |
| 6 | -4.990411000 | -2.153069000 | -0.402988000 |
| 6 | -4.526717000 | -3.378218000 | -0.883581000 |
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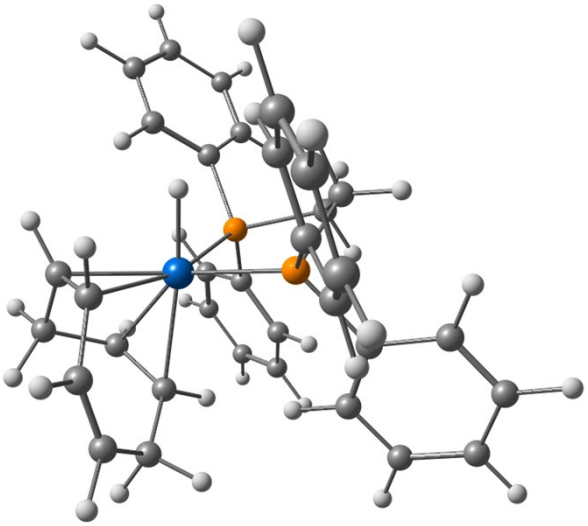
| 1 | -4.525043000 | -0.091036000 | -0.015444000 |
| 1 | -2.835925000 | -4.440907000 | -1.702831000 |
| 1 | -6.010523000 | -2.060013000 | -0.040625000 |
| 1 | -5.183596000 | -4.243311000 | -0.898865000 |
| 1 | 0.484509000 | -3.685158000 | 1.625044000 |
| 1 | 3.169684000 | -1.197858000 | 3.326176000 |
| 1 | 2.172261000 | -3.301382000 | 3.428307000 |

**III'**

E (BS1) = -2103.97501012

E (BS2) = -2104.49800014

$G_{298.15,1M}$ (BS2) = -2103.971391



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| 1 | -1.093044000 | 0.074893000 | -3.335954000 |
| 6 | -1.172618000 | -1.646285000 | 2.303339000 |
| 6 | -2.121759000 | -0.903996000 | 3.165594000 |
| 6 | -2.116215000 | 0.383141000 | 3.542337000 |
| 6 | -1.198034000 | 1.500018000 | 3.120386000 |
| 6 | 0.038463000 | 1.232995000 | 2.280549000 |
| 6 | 1.077553000 | 0.348809000 | 2.592859000 |
| 6 | 0.930837000 | -0.838486000 | 3.532801000 |
| 6 | 0.234760000 | -1.820128000 | 2.606829000 |
| 1 | 1.915517000 | -1.208755000 | 3.829982000 |
| 1 | 0.361751000 | -0.606226000 | 4.443056000 |
| 1 | 0.684682000 | -2.801426000 | 2.479450000 |
| 1 | -0.068207000 | -1.973943000 | -0.036151000 |
| 1 | -0.873148000 | 2.028370000 | 4.032888000 |
| 1 | -1.636859000 | -2.526408000 | 1.858143000 |
| 1 | 2.086426000 | 0.605497000 | 2.283677000 |
| 1 | 0.360883000 | 2.106913000 | 1.717905000 |
| 6 | -2.976576000 | -1.076868000 | -1.040322000 |
| 6 | -2.813709000 | -2.436012000 | -1.358342000 |
| 6 | -4.262563000 | -0.606873000 | -0.731723000 |
| 6 | -3.912430000 | -3.293686000 | -1.395113000 |
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| 1 | -1.822968000 | -2.833464000 | -1.556358000 |
| 1 | -4.411659000 | 0.435012000 | -0.467482000 |
| 1 | -3.768735000 | -4.340074000 | -1.650260000 |
| 1 | -6.348013000 | -1.088741000 | -0.517008000 |
| 1 | -6.045351000 | -3.483639000 | -1.122530000 |
| 6 | -2.148589000 | 1.694779000 | -1.206771000 |
| 6 | -1.769795000 | 2.753720000 | -0.373942000 |
| 6 | -2.960687000 | 1.968863000 | -2.321524000 |
| 6 | -2.186522000 | 4.060679000 | -0.642785000 |
| 6 | -3.379174000 | 3.271457000 | -2.590408000 |
| 6 | -2.990765000 | 4.321685000 | -1.752055000 |
| 1 | -1.141428000 | 2.543282000 | 0.480830000 |
| 1 | -3.277337000 | 1.160263000 | -2.974433000 |
| 1 | -1.881872000 | 4.869832000 | 0.015315000 |
| 1 | -4.007281000 | 3.468886000 | -3.454748000 |
| 1 | -3.316293000 | 5.336121000 | -1.964660000 |
| 1 | -0.407324000 | -1.373584000 | -2.581152000 |
| 6 | 0.832914000 | 0.397921000 | -2.362777000 |
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| 1 | 0.703822000 | 1.484197000 | -2.397910000 |
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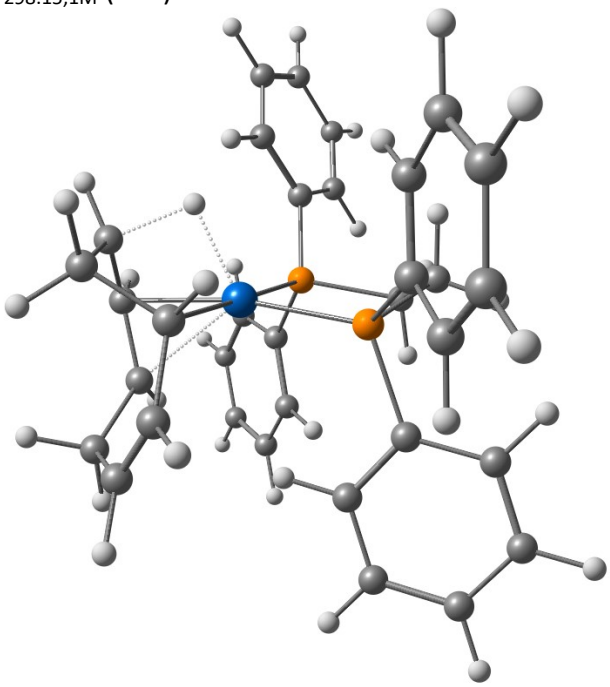
| 6 | 2.938579000 | -2.527302000 | -0.584687000 |
| 6 | 3.857720000 | -1.018576000 | -2.236310000 |
| 6 | 3.871177000 | -3.499528000 | -0.957734000 |
| 6 | 4.788655000 | -1.987939000 | -2.607214000 |
| 6 | 4.795075000 | -3.232449000 | -1.968721000 |
| 1 | 2.212709000 | -2.723341000 | 0.199255000 |
| 1 | 3.870624000 | -0.048987000 | -2.727322000 |
| 1 | 3.873626000 | -4.463986000 | -0.457319000 |
| 1 | 5.509227000 | -1.774139000 | -3.391933000 |
| 1 | 5.519441000 | -3.988253000 | -2.259572000 |
| 6 | 2.674320000 | 1.465859000 | -0.345459000 |
| 6 | 2.065344000 | 2.733229000 | -0.367403000 |
| 6 | 3.996140000 | 1.365079000 | 0.117437000 |
| 6 | 2.767966000 | 3.868948000 | 0.034755000 |
| 6 | 4.696159000 | 2.503004000 | 0.524863000 |
| 6 | 4.087033000 | 3.758284000 | 0.481945000 |
| 1 | 1.034126000 | 2.836720000 | -0.691118000 |
| 1 | 4.485890000 | 0.397104000 | 0.154275000 |
| 1 | 2.282182000 | 4.840432000 | 0.002426000 |
| 1 | 5.720205000 | 2.405512000 | 0.874805000 |
| 1 | 4.633614000 | 4.642553000 | 0.797035000 |
| 1 | -1.818722000 | 2.236521000 | 2.588681000 |
| 1 | -2.941938000 | -1.513105000 | 3.552611000 |
| 1 | -2.907885000 | 0.709655000 | 4.217538000 |

**$TS_{II'-IV'}$**

E (BS1) = -2103.93553307

E (BS2) = -2104.46162337

$G_{298.15,1M}$ (BS2) = -2103.938989



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| 6 | -1.693519000 | -0.386630000 | 2.303209000 |
| 6 | -2.410666000 | 0.888751000 | 2.554711000 |
| 6 | -1.835467000 | 2.029687000 | 2.959044000 |
| 6 | -0.352780000 | 2.226208000 | 3.164795000 |
| 6 | 0.679766000 | 1.427077000 | 2.352498000 |
| 6 | 1.250554000 | 0.154362000 | 2.634806000 |
| 6 | 0.548037000 | -1.067710000 | 2.990131000 |
| 6 | -0.885061000 | -0.965930000 | 3.500700000 |
| 1 | 0.229075000 | -1.768382000 | 1.680634000 |
| 1 | 1.179732000 | -1.877052000 | 3.357251000 |
| 1 | -0.941907000 | -0.348766000 | 4.405459000 |
| 1 | -1.250231000 | -1.964650000 | 3.764325000 |
| 1 | -0.120116000 | 2.082739000 | 4.232131000 |
| 1 | -2.396077000 | -1.142806000 | 1.947248000 |
| 1 | 2.307456000 | 0.029272000 | 2.400907000 |
| 1 | 1.420596000 | 2.093508000 | 1.913702000 |
| 6 | -2.862769000 | -1.412056000 | -0.855594000 |
| 6 | -2.598850000 | -2.786907000 | -0.736539000 |
| 6 | -4.193641000 | -0.974284000 | -0.823724000 |
| 6 | -3.641566000 | -3.704264000 | -0.624428000 |
| 6 | -5.238964000 | -1.894195000 | -0.696226000 |
| 6 | -4.967365000 | -3.259199000 | -0.603859000 |
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| 1 | -4.420594000 | 0.084498000 | -0.891940000 |
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| 1 | -6.265620000 | -1.539312000 | -0.667860000 |
| 1 | -5.780571000 | -3.973145000 | -0.507097000 |
| 6 | -2.128599000 | 1.343273000 | -1.463002000 |
| 6 | -1.855269000 | 2.497577000 | -0.716755000 |
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| 6 | -2.312348000 | 3.745723000 | -1.147823000 |
| 6 | -3.323078000 | 2.707443000 | -3.083303000 |
| 6 | -3.042469000 | 3.853351000 | -2.332628000 |
| 1 | -1.280773000 | 2.399041000 | 0.199504000 |
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| 1 | -2.096227000 | 4.632069000 | -0.557367000 |
| 1 | -3.892763000 | 2.786004000 | -4.005324000 |
| 1 | -3.394045000 | 4.824131000 | -2.671315000 |
| 1 | -0.317121000 | -1.882959000 | -2.344478000 |
| 6 | 0.890161000 | -0.073447000 | -2.413985000 |
| 1 | 1.571112000 | -0.486562000 | -3.163792000 |
| 1 | 0.747624000 | 0.987082000 | -2.644208000 |
| 15 | 1.662737000 | -0.182198000 | -0.704605000 |
| 6 | 2.850725000 | -1.587846000 | -0.889125000 |
| 6 | 2.763389000 | -2.676214000 | -0.011503000 |
| 6 | 3.825275000 | -1.609937000 | -1.902128000 |
| 6 | 3.634287000 | -3.762343000 | -0.135650000 |
| 6 | 4.691736000 | -2.695061000 | -2.029482000 |
| 6 | 4.597713000 | -3.774129000 | -1.144807000 |
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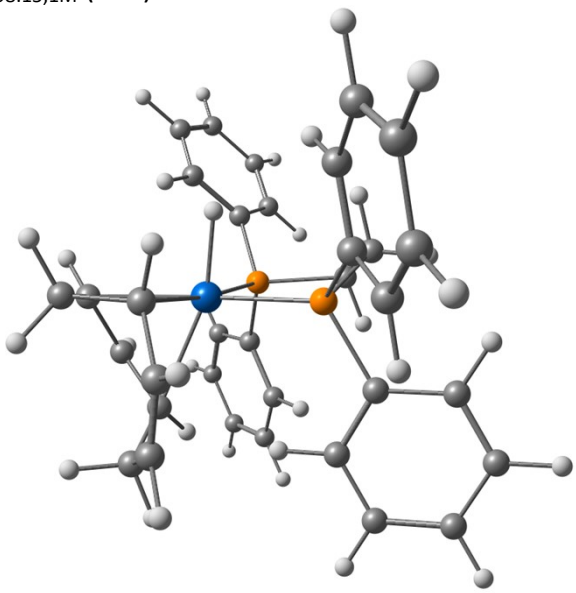
| 1 | 3.918186000 | -0.768506000 | -2.583659000 |
| 1 | 3.555182000 | -4.598631000 | 0.553561000 |
| 1 | 5.441062000 | -2.699174000 | -2.816405000 |
| 1 | 5.273817000 | -4.618747000 | -1.244353000 |
| 6 | 2.756555000 | 1.304441000 | -0.641129000 |
| 6 | 2.155384000 | 2.562736000 | -0.827646000 |
| 6 | 4.109528000 | 1.253583000 | -0.275372000 |
| 6 | 2.896706000 | 3.734015000 | -0.684931000 |
| 6 | 4.848065000 | 2.430452000 | -0.119104000 |
| 6 | 4.247723000 | 3.671974000 | -0.328933000 |
| 1 | 1.096728000 | 2.626256000 | -1.063303000 |
| 1 | 4.594838000 | 0.296512000 | -0.113045000 |
| 1 | 2.416449000 | 4.696337000 | -0.840251000 |
| 1 | 5.895292000 | 2.371925000 | 0.164944000 |
| 1 | 4.823514000 | 4.585380000 | -0.209304000 |
| 1 | -0.136584000 | 3.285654000 | 2.977770000 |
| 1 | -3.489111000 | 0.894502000 | 2.385314000 |
| 1 | -2.456877000 | 2.900551000 | 3.163395000 |

**IV'**

E (BS1) = -2103.98125896

E (BS2) = -2104.50470226

$G_{298.15,1M}$ (BS2) = -2103.978708



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| 1 | -0.942722000 | -0.152492000 | -3.380493000 |
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| 6 | -2.621303000 | -0.185445000 | 2.452832000 |
| 6 | -2.414940000 | 1.062031000 | 2.899835000 |
| 6 | -1.054488000 | 1.661109000 | 3.175513000 |
| 6 | 0.145396000 | 1.274657000 | 2.287142000 |
| 6 | 1.098832000 | 0.249218000 | 2.577320000 |
| 6 | 0.776940000 | -1.094662000 | 2.880797000 |
| 6 | -0.601491000 | -1.521837000 | 3.372978000 |
| 1 | -0.049586000 | -2.058495000 | 0.263733000 |
| 1 | 1.610578000 | -1.783410000 | 3.000095000 |
| 1 | -0.883710000 | -1.033076000 | 4.315504000 |
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| 1 | -2.009900000 | -2.114591000 | 1.813794000 |
| 1 | 2.144461000 | 0.455225000 | 2.348144000 |
| 1 | 0.624996000 | 2.156705000 | 1.864549000 |
| 6 | -2.873716000 | -1.195989000 | -1.065633000 |
| 6 | -2.688174000 | -2.579220000 | -1.224873000 |
| 6 | -4.175042000 | -0.700129000 | -0.901664000 |
| 6 | -3.782990000 | -3.442102000 | -1.247815000 |
| 6 | -5.269447000 | -1.568133000 | -0.914817000 |
| 6 | -5.077590000 | -2.938779000 | -1.092566000 |
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| 1 | -6.271489000 | -1.169497000 | -0.783345000 |
| 1 | -5.929365000 | -3.612936000 | -1.103127000 |
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| 6 | -1.794608000 | 2.604482000 | -0.346874000 |
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| 6 | -3.167471000 | 3.176078000 | -2.710108000 |
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| 1 | -2.044155000 | 4.690981000 | 0.124394000 |
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| 6 | 3.951956000 | -1.223732000 | -2.023811000 |
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| 6 | 4.905050000 | -3.370235000 | -1.443429000 |
| 1 | 2.249769000 | -2.630945000 | 0.560536000 |
| 1 | 3.969798000 | -0.326062000 | -2.636091000 |
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| 6 | 2.057477000 | 2.699187000 | -0.433068000 |
| 6 | 4.066597000 | 1.426458000 | -0.005037000 |
| 6 | 2.736272000 | 3.877164000 | -0.125409000 |
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| 6 | 4.082635000 | 3.835829000 | 0.248671000 |
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| 1 | 5.787000000 | 2.564741000 | 0.607437000 |
| 1 | 4.610627000 | 4.753424000 | 0.492071000 |
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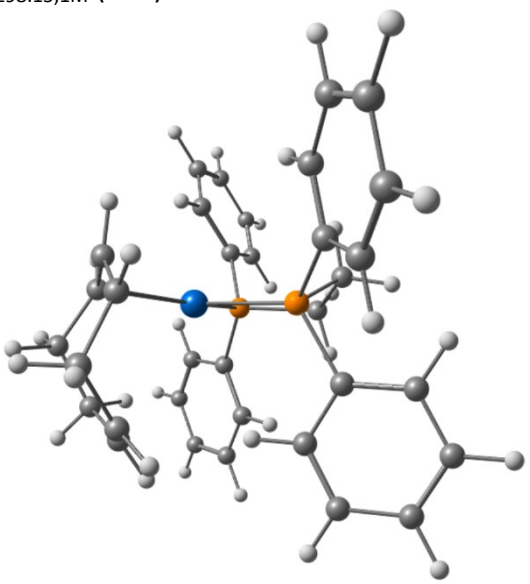
| 1 | -3.648413000 | -0.487047000 | 2.242403000 |
| 1 | -3.270171000 | 1.708128000 | 3.093191000 |

**II''**

E (BS1) = -2103.98194491

E (BS2) = -2104.50831575

$G_{298.15,1M}$ (BS2) = -2103.979656



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| 1 | -1.544757000 | -0.673331000 | -3.173388000 |
| 6 | 0.467335000 | 2.561649000 | 2.369953000 |
| 6 | 1.809881000 | 1.945229000 | 2.669205000 |
| 6 | 1.867483000 | 0.576207000 | 3.364056000 |
| 6 | 1.311767000 | -0.646311000 | 2.609737000 |
| 6 | -0.003153000 | -1.185372000 | 2.793986000 |
| 6 | -1.167696000 | -0.365803000 | 2.814629000 |
| 6 | -1.246615000 | 0.999327000 | 3.522225000 |
| 6 | -0.777318000 | 2.199041000 | 2.716301000 |
| 1 | 1.396683000 | 0.649780000 | 4.350148000 |
| 1 | 2.926664000 | 0.374776000 | 3.564456000 |
| 1 | -0.713102000 | 0.950680000 | 4.478137000 |
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| 1 | 2.072897000 | -1.407551000 | 2.442139000 |
| 1 | 2.379620000 | 2.664223000 | 3.279925000 |
| 1 | 0.548168000 | 3.457331000 | 1.750825000 |
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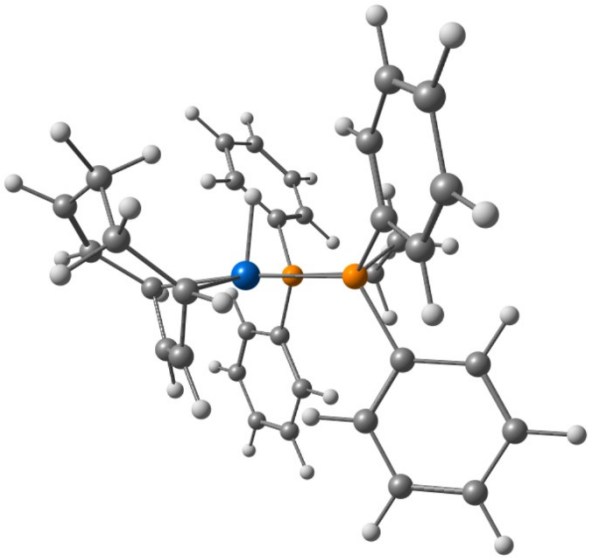
| 1 | -0.802501000 | -1.954947000 | -2.200249000 |
| 6 | 0.488386000 | -0.229496000 | -2.501048000 |
| 1 | 1.059395000 | -0.716536000 | -3.296887000 |
| 1 | 0.379054000 | 0.826663000 | -2.768173000 |
| 15 | 1.419314000 | -0.319028000 | -0.865213000 |
| 6 | 2.450941000 | -1.832760000 | -1.099474000 |
| 6 | 2.271070000 | -2.923033000 | -0.237892000 |
| 6 | 3.374097000 | -1.941038000 | -2.152999000 |
| 6 | 3.002279000 | -4.099662000 | -0.421659000 |
| 6 | 4.103437000 | -3.115614000 | -2.336438000 |
| 6 | 3.919244000 | -4.197191000 | -1.469370000 |
| 1 | 1.542655000 | -2.837192000 | 0.563401000 |
| 1 | 3.532734000 | -1.101015000 | -2.824280000 |
| 1 | 2.853236000 | -4.938241000 | 0.253081000 |
| 1 | 4.816938000 | -3.187212000 | -3.152835000 |
| 1 | 4.487668000 | -5.111904000 | -1.613542000 |
| 6 | 2.632148000 | 1.071001000 | -0.962685000 |
| 6 | 2.152211000 | 2.362829000 | -1.241037000 |
| 6 | 3.974416000 | 0.920280000 | -0.582971000 |
| 6 | 2.997600000 | 3.468602000 | -1.162868000 |
| 6 | 4.818968000 | 2.030176000 | -0.498811000 |
| 6 | 4.335154000 | 3.306303000 | -0.789882000 |
| 1 | 1.106563000 | 2.512359000 | -1.494981000 |
| 1 | 4.363772000 | -0.064822000 | -0.346232000 |
| 1 | 2.610122000 | 4.459122000 | -1.385509000 |
| 1 | 5.855505000 | 1.894739000 | -0.202177000 |
| 1 | 4.992156000 | 4.168764000 | -0.722667000 |
| 1 | 2.354640000 | 1.878846000 | 1.719020000 |
| 1 | -2.296220000 | 1.170172000 | 3.781799000 |

**V**

E (BS1) = -2103.97728329

E (BS2) = -2104.50155895

$G_{298.15,1M}$ (BS2) = -2103.976381



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| 1 | -1.155295000 | 1.492249000 | 3.004197000 |
| 6 | -0.904861000 | -3.797302000 | -2.465871000 |
| 6 | 0.480982000 | -3.870312000 | -1.888788000 |
| 6 | 1.492153000 | -2.892325000 | -2.508243000 |
| 6 | 1.419094000 | -1.413771000 | -2.090024000 |
| 6 | 0.650395000 | -0.347684000 | -2.744381000 |
| 6 | -0.751336000 | -0.288087000 | -2.663584000 |
| 6 | -1.522240000 | -1.342158000 | -1.980057000 |
| 6 | -1.714546000 | -2.729320000 | -2.489237000 |
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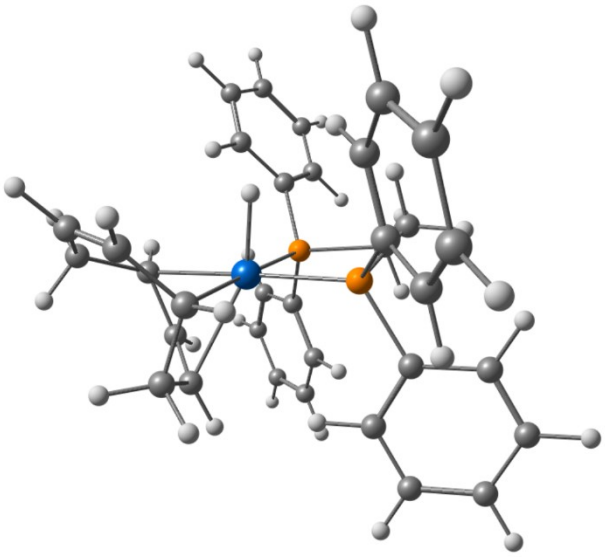
| 1 | 2.493444000 | -3.241836000 | -2.224776000 |
| 1 | -2.508424000 | -0.942756000 | -1.725019000 |
| 1 | -2.702626000 | -2.887846000 | -2.931583000 |
| 1 | 2.442976000 | -1.063027000 | -1.931868000 |
| 1 | 0.861561000 | -4.891087000 | -2.017605000 |
| 1 | -1.290282000 | -4.714265000 | -2.912094000 |
| 1 | -1.245511000 | 0.631484000 | -2.977607000 |
| 1 | 1.164064000 | 0.531597000 | -3.134737000 |
| 6 | -2.582527000 | 1.726554000 | -0.025510000 |
| 6 | -2.006039000 | 2.906151000 | -0.529302000 |
| 6 | -3.943515000 | 1.486146000 | -0.266834000 |
| 6 | -2.776673000 | 3.831035000 | -1.231216000 |
| 6 | -4.711583000 | 2.409565000 | -0.981881000 |
| 6 | -4.133962000 | 3.585122000 | -1.461352000 |
| 1 | -0.946729000 | 3.098828000 | -0.386713000 |
| 1 | -4.410580000 | 0.580326000 | 0.105530000 |
| 1 | -2.316214000 | 4.741747000 | -1.604594000 |
| 1 | -5.763792000 | 2.206084000 | -1.160530000 |
| 1 | -4.733188000 | 4.303576000 | -2.013415000 |
| 6 | -2.671273000 | -0.570522000 | 1.721945000 |
| 6 | -3.491129000 | -0.015935000 | 2.719775000 |
| 6 | -2.777033000 | -1.938700000 | 1.435586000 |
| 6 | -3.681290000 | -2.738727000 | 2.139539000 |
| 6 | -4.389083000 | -0.816886000 | 3.424402000 |
| 6 | -4.484616000 | -2.181717000 | 3.135217000 |
| 1 | -3.442644000 | 1.047928000 | 2.936804000 |
| 1 | -2.147692000 | -2.368108000 | 0.663440000 |
| 1 | -3.754111000 | -3.797488000 | 1.906935000 |
| 1 | -5.016401000 | -0.377139000 | 4.194871000 |
| 1 | -5.185590000 | -2.805212000 | 3.683307000 |
| 1 | -0.423829000 | 2.453028000 | 1.718861000 |
| 6 | 0.802304000 | 0.778882000 | 2.348204000 |
| 1 | 1.432979000 | 1.413378000 | 2.978368000 |
| 1 | 0.679461000 | -0.186151000 | 2.849137000 |
| 15 | 1.623537000 | 0.438544000 | 0.703708000 |
| 6 | 2.241047000 | 2.124326000 | 0.263054000 |
| 6 | 1.772906000 | 2.735053000 | -0.907778000 |
| 6 | 3.099574000 | 2.847373000 | 1.109291000 |
| 6 | 2.154170000 | 4.040199000 | -1.231680000 |
| 6 | 3.480556000 | 4.149675000 | 0.786694000 |
| 6 | 3.007360000 | 4.748775000 | -0.384957000 |
| 1 | 1.097383000 | 2.182693000 | -1.553250000 |
| 1 | 3.480884000 | 2.388208000 | 2.017219000 |
| 1 | 1.781437000 | 4.500412000 | -2.142526000 |
| 1 | 4.145217000 | 4.697716000 | 1.448782000 |
| 1 | 3.303301000 | 5.763951000 | -0.634039000 |
| 6 | 3.135179000 | -0.517391000 | 1.129692000 |
| 6 | 2.973696000 | -1.730207000 | 1.821974000 |
| 6 | 4.418849000 | -0.147156000 | 0.703234000 |
| 6 | 4.075517000 | -2.533017000 | 2.111124000 |
| 6 | 5.520381000 | -0.959834000 | 0.984771000 |
| 6 | 5.353430000 | -2.149801000 | 1.693204000 |
| 1 | 1.980319000 | -2.057152000 | 2.113980000 |
| 1 | 4.566649000 | 0.775992000 | 0.152718000 |
| 1 | 3.934582000 | -3.464349000 | 2.652507000 |
| 1 | 6.508442000 | -0.659332000 | 0.647262000 |
| 1 | 6.210968000 | -2.779421000 | 1.913161000 |
| 1 | 0.448931000 | -3.670390000 | -0.809218000 |
| 1 | 0.118650000 | -1.796849000 | 0.492186000 |

**VI**

E (BS1) = -2103.98016242

E (BS2) = -2104.50369247

$G_{298.15,1M}$ (BS2) = -2103.977759



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| 6 | 0.708296000 | 1.071395000 | -2.227491000 |
| 1 | 1.325580000 | 1.003877000 | -3.127731000 |
| 6 | -1.434338000 | -2.816538000 | 2.331555000 |
| 6 | -1.572532000 | -1.368452000 | 2.013949000 |
| 6 | -1.339036000 | -0.381031000 | 3.190641000 |
| 6 | -0.116701000 | 0.458394000 | 2.842840000 |
| 6 | 1.129491000 | -0.085641000 | 2.535402000 |
| 6 | 1.357429000 | -1.472857000 | 2.172003000 |
| 6 | 0.972868000 | -2.674358000 | 3.063489000 |
| 6 | -0.328929000 | -3.395733000 | 2.820069000 |
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| 1 | -2.200500000 | 0.288639000 | 3.292484000 |
| 1 | 1.007790000 | -2.341899000 | 4.113453000 |
| 1 | -0.341659000 | -4.457163000 | 3.065768000 |
| 1 | -0.152101000 | 1.531592000 | 3.019597000 |
| 1 | -2.562903000 | -1.191754000 | 1.588563000 |
| 1 | -2.304942000 | -3.448822000 | 2.146186000 |
| 1 | 2.368318000 | -1.611811000 | 1.786839000 |
| 1 | 1.938248000 | 0.625683000 | 2.371275000 |
| 6 | 2.641458000 | 1.624406000 | -0.108180000 |
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| 6 | 4.010852000 | 1.474270000 | 0.154911000 |
| 6 | 2.717395000 | 3.824166000 | 0.930378000 |
| 6 | 4.725852000 | 2.491355000 | 0.794039000 |
| 6 | 4.084765000 | 3.669285000 | 1.178468000 |
| 1 | 0.931237000 | 2.927066000 | 0.148943000 |
| 1 | 4.524576000 | 0.564059000 | -0.136571000 |
| 1 | 2.206799000 | 4.734086000 | 1.233626000 |
| 1 | 5.786262000 | 2.359021000 | 0.990257000 |
| 1 | 4.642595000 | 4.458651000 | 1.674106000 |
| 6 | 2.782738000 | -0.874975000 | -1.591650000 |
| 6 | 3.694865000 | -0.416817000 | -2.558631000 |
| 6 | 2.769616000 | -2.236469000 | -1.258702000 |
| 6 | 3.650587000 | -3.124359000 | -1.882733000 |
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| 6 | 4.551106000 | -2.660981000 | -2.842504000 |
| 1 | 3.729399000 | 0.638367000 | -2.816681000 |
| 1 | 2.061268000 | -2.591554000 | -0.517217000 |
| 1 | 3.629521000 | -4.177675000 | -1.617467000 |
| 1 | 5.273931000 | -0.938120000 | -3.924986000 |
| 1 | 5.234804000 | -3.352147000 | -3.327636000 |
| 1 | 0.583975000 | 2.133240000 | -1.992094000 |
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| 1 | -1.254832000 | 0.968087000 | -3.177044000 |
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| 6 | -1.904490000 | 2.730032000 | 0.588217000 |
| 6 | -2.891103000 | 2.685804000 | -1.616953000 |
| 6 | -2.328338000 | 4.051583000 | 0.752433000 |
| 6 | -3.312038000 | 4.005472000 | -1.455002000 |
| 6 | -3.029372000 | 4.692021000 | -0.269944000 |
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| 1 | -3.132805000 | 2.158529000 | -2.535532000 |
| 1 | -2.108868000 | 4.577769000 | 1.677367000 |
| 1 | -3.861818000 | 4.498201000 | -2.252077000 |
| 1 | -3.356585000 | 5.720623000 | -0.146607000 |
| 6 | -3.046532000 | -0.686215000 | -1.164757000 |
| 6 | -2.870701000 | -1.993168000 | -1.650976000 |
| 6 | -4.346254000 | -0.230507000 | -0.901717000 |
| 6 | -3.971777000 | -2.811836000 | -1.895218000 |
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| 6 | -5.264720000 | -2.345919000 | -1.639571000 |
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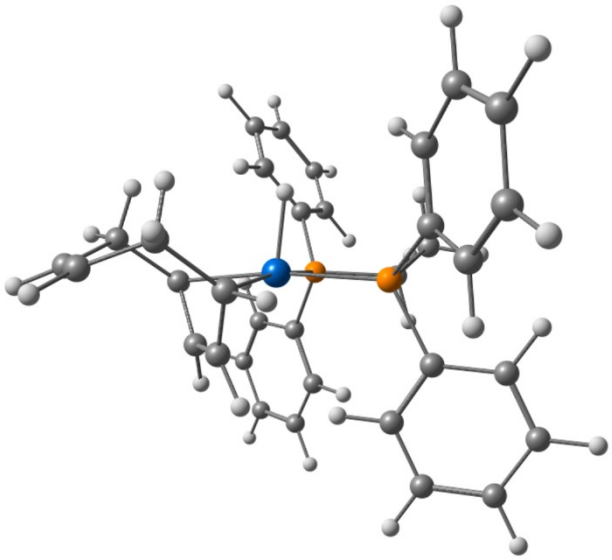
| 1 | -6.448544000 | -0.690863000 | -0.926454000 |
| 1 | -6.122112000 | -2.986860000 | -1.824527000 |
| 1 | -0.150514000 | -1.890127000 | -0.266012000 |
| 1 | 1.782355000 | -3.410448000 | 2.978865000 |

**VII**

E (BS1) = -2103.97050988

E (BS2) = -2104.49495125

$G_{298.15,1M}$ (BS2) = -2103.970085



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| 1 | -1.157922000 | 1.835290000 | 2.860006000 |
| 6 | 0.522832000 | -3.510987000 | -3.430425000 |
| 6 | 1.371466000 | -3.142088000 | -2.238650000 |
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| 6 | -0.744877000 | -0.539507000 | -2.554911000 |
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| 1 | 0.116278000 | -1.813428000 | 0.698924000 |
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| 1 | -1.381372000 | -3.714913000 | -4.293290000 |
| 1 | 1.187354000 | 0.265984000 | -3.039605000 |
| 1 | 2.403396000 | -3.466734000 | -2.419169000 |
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| 1 | -1.241263000 | 0.353226000 | -2.935160000 |
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| 6 | -2.720581000 | -1.787939000 | 1.827887000 |
| 6 | -3.599749000 | -2.489757000 | 2.657418000 |
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| 6 | -4.417007000 | -1.802044000 | 3.555181000 |
| 1 | -3.464341000 | 1.380616000 | 2.834981000 |
| 1 | -2.077148000 | -2.316130000 | 1.132303000 |
| 1 | -3.642270000 | -3.573915000 | 2.600791000 |
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| 1 | -0.413892000 | 2.607097000 | 1.458469000 |
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| 1 | 1.427777000 | 1.725763000 | 2.863590000 |
| 1 | 0.660339000 | 0.128344000 | 2.929696000 |
| 15 | 1.622324000 | 0.480874000 | 0.726279000 |
| 6 | 2.256922000 | 2.104709000 | 0.105541000 |
| 6 | 1.771634000 | 2.606165000 | -1.109509000 |
| 6 | 3.145657000 | 2.892968000 | 0.857017000 |
| 6 | 2.166460000 | 3.865524000 | -1.570013000 |
| 6 | 3.540521000 | 4.149433000 | 0.398258000 |
| 6 | 3.051152000 | 4.638315000 | -0.817118000 |
| 1 | 1.073559000 | 2.005358000 | -1.683204000 |
| 1 | 3.539762000 | 2.519306000 | 1.798104000 |
| 1 | 1.781427000 | 4.239685000 | -2.514621000 |
| 1 | 4.229382000 | 4.747667000 | 0.988195000 |
| 1 | 3.359562000 | 5.617572000 | -1.172425000 |
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| 6 | 4.404851000 | -0.143334000 | 0.752636000 |
| 6 | 4.075705000 | -2.276889000 | 2.521218000 |
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| 6 | 5.344743000 | -1.985233000 | 2.012470000 |
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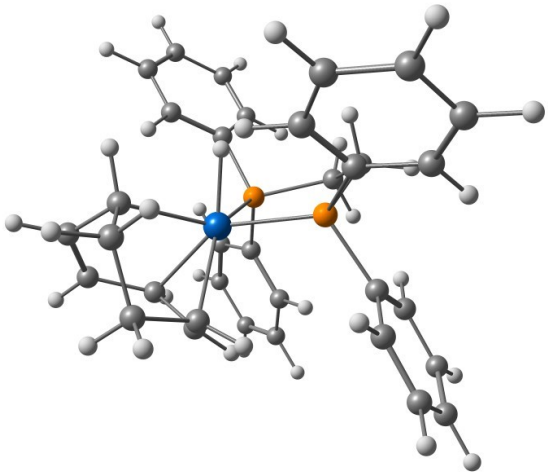
| 1 | 4.546649000 | 0.681877000 | 0.062496000 |
| 1 | 3.940637000 | -3.110537000 | 3.204716000 |
| 1 | 6.484602000 | -0.695260000 | 0.713572000 |
| 1 | 6.200423000 | -2.588713000 | 2.301870000 |
| 1 | 1.028477000 | -3.704249000 | -1.361657000 |
| 1 | -1.242866000 | -3.655494000 | -1.315528000 |

**$TS_{4\text{-}5'}$**

E (BS1) = -2103.955271

E (BS2) = -2104.477955

$G_{298.15,1M}$ (BS2) = -2103.950232



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| 6 | -0.712014000 | 0.116143000 | -2.531399000 |
| 1 | -1.311386000 | 0.668697000 | -3.262071000 |
| 6 | 0.027091000 | -2.178703000 | 2.195567000 |
| 6 | -1.328051000 | -2.172703000 | 2.941460000 |
| 6 | -1.567831000 | -0.764957000 | 3.499862000 |
| 6 | -1.218817000 | 0.305857000 | 2.457660000 |
| 6 | 0.025608000 | 1.014112000 | 2.341877000 |
| 6 | 1.292122000 | 0.333082000 | 2.388508000 |
| 6 | 1.670384000 | -0.756696000 | 3.335621000 |
| 6 | 1.114115000 | -1.963045000 | 3.217075000 |
| 1 | -0.961128000 | -0.614473000 | 4.399086000 |
| 1 | -2.614771000 | -0.640657000 | 3.802845000 |
| 1 | 2.399173000 | -0.522055000 | 4.113247000 |
| 1 | 1.327042000 | -2.751468000 | 3.945777000 |
| 1 | -2.072116000 | 0.912098000 | 2.159235000 |
| 1 | -1.358261000 | -2.921551000 | 3.754294000 |
| 1 | 0.160341000 | -3.149512000 | 1.704156000 |
| 1 | 2.129812000 | 0.962476000 | 2.087883000 |
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E (BS2) = -2104.516146

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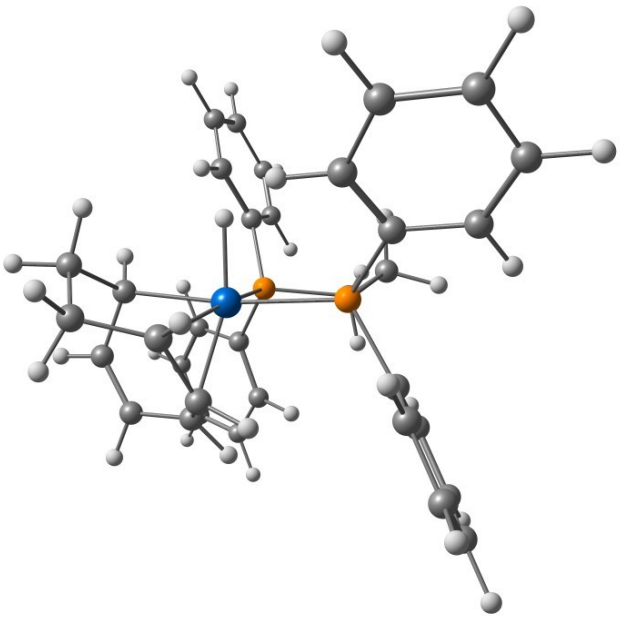

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E (BS2) = -2104.496261

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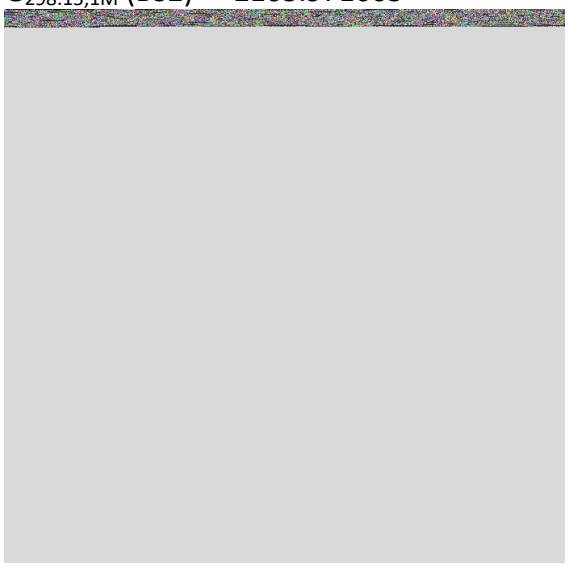

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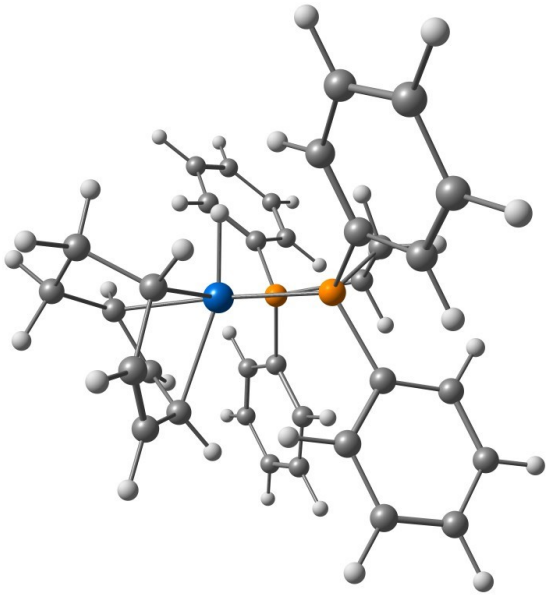

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[4] M. J. Fernandez, M. A. Esteruelas, M. Covarrubias and L. A. Oro, *J. Organomet. Chem.*, 1986, **316**, 343-349.
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