Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Discovery and Mechanistic Investigation of Pt-Catalyzed Oxidative Homocoupling of Benzene with $PhI(OAc)_2$

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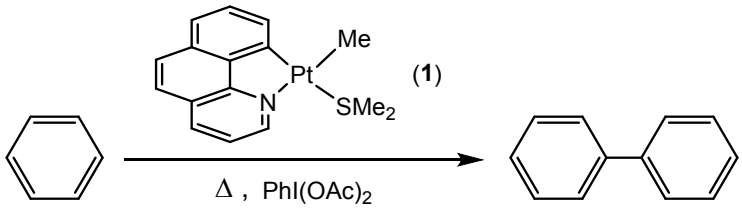
1. Table S1. Crystal data and structure refinement for [PtPh(bhq)(SMe_2)], **4**.

Empirical formula	$C_{21}H_{19}NPtS$	
Formula weight	512.52	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.344(2) Å	α= 68.384(7)°
	b = 9.615(3) Å	β= 78.578(9)°
	c = 11.712(3) Å	γ = 88.123(8)°
Volume	855.4(4) $Å^3$	
Z	2	
Density (calculated)	1.990 Mg/m^3	
Absorption coefficient	8.325 mm^{-1}	
F(000)	492	
Crystal size	0.100 x 0.100 x 0.050 mm^3	
Theta range for data collection	1.909 to 27.099°.	
Reflections collected	5341	
Independent reflections	3603 [R(int) = 0.0353]	
Data / restraints / parameters	3603 / 0 / 219	
Goodness-of-fit on F^2	1.005	
Final R indices [I>2sigma(I)]	R1 = 0.0389, wR2 = 0.0705	
R indices (all data)	R1 = 0.0529, wR2 = 0.0754	

2. Table S2. Optimization of benzene homocoupling

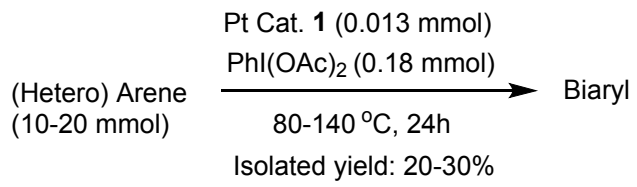


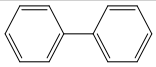
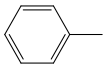
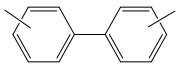
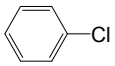
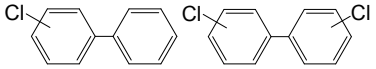
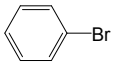
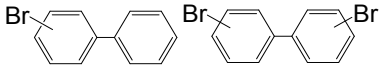
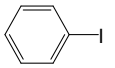
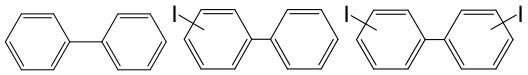
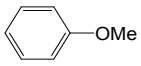
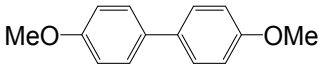
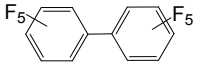
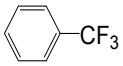
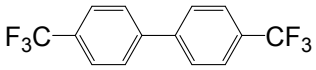
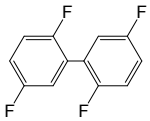
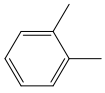
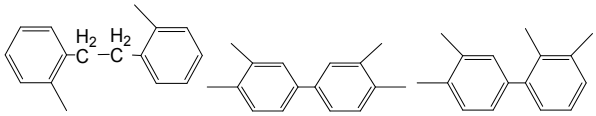
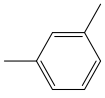
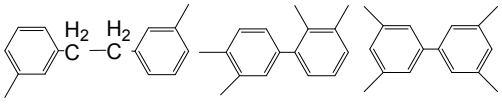
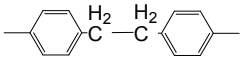
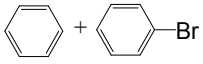
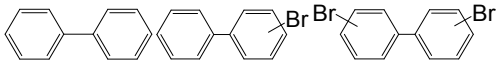
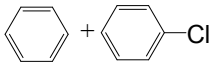
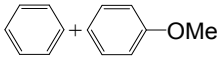
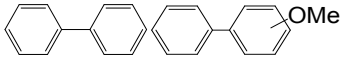
entry	Pt comp. /mmol	$PhI(OAc)_2$ /mmol	Temp. /°C	HOAc /mmol	Yield /%
1	0.013	0.18	100	0	30
2	0.013	0.18	100	30	26
3	0.013	0	100	0	0
4	0	0.18	100	0	0
5	0.013	0	100	15	0
6	0.01	0.15	100	0	25
7	0.013	0.18	70	0	0
8	0.01	0.18	100	0	25
9	0.01	0.1	100	0	15

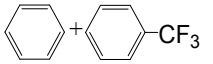
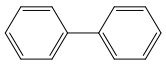
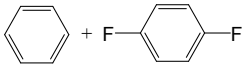
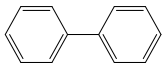
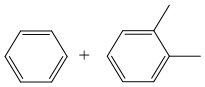
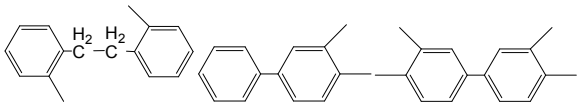
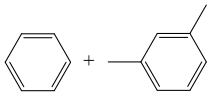
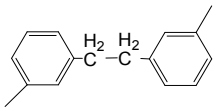
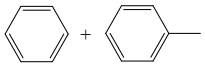
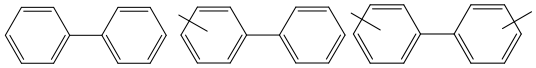
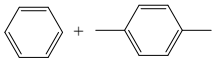
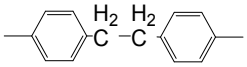
General procedure:

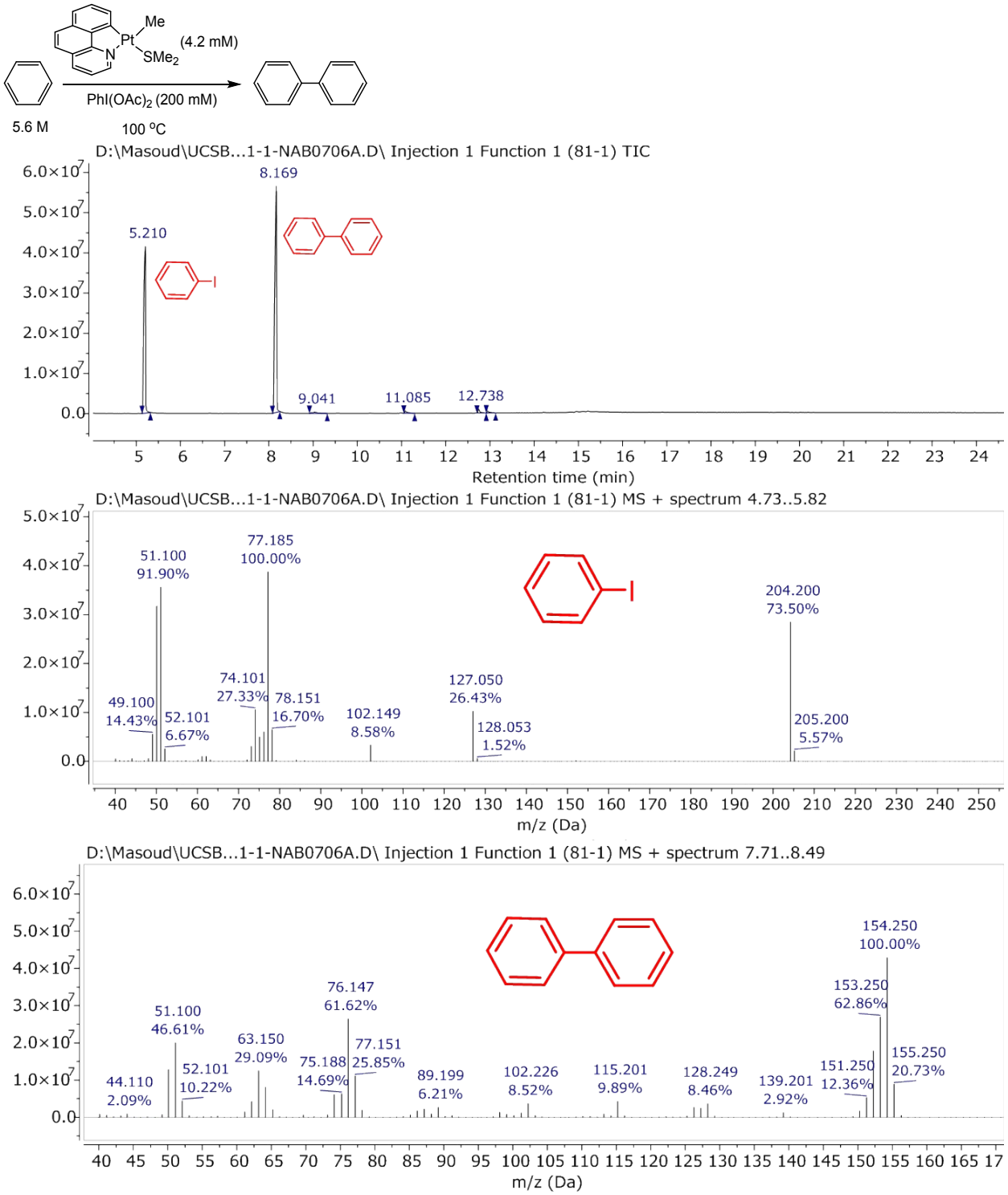
To a 10 mL pressure vessel, benzene (3 mL, 34 mmol), $PhI(OAc)_2$ (as a solide) and Pt complex **1** (as a solid) were added. The mixture was heated for 24 h at 100 (or 70) °C in an oil bath. Then the reaction was allowed to reach to room temperature. The reaction mixture was extracted with 3 mL of hexane and filtered through a Silica gel column. GC was used to calculate the yield based on oxidant. Dodecane or PhBr as GC internal standard was added to extracted product and then the filtrate was analyzed by GC-FID method using GC instrument.

3. Table S3. Pt-catalyzed oxidative homo and hetero-coupling of arenes.



Entry	(Hetero)Arene	Biaryl	Selectivity (%)
1			100
2			85
3			50:34
4			20:80
5			20:45:35
6			100
7			trace
8			trace
9			trace
10			35:55:10
11			50: 15:35
12			100
13			30: 50: 20
14			53:47
15			50:50

16			100
17			100
18			37:33:30
19			100
20			44:44:12
21			100



4. Figure S1. GC-MS data for homocoupling of benzene using **1** as precatalyst

5. Kinetic Data: General comments

[PtMe(bhq)(SMe_2)] was measured from a 0.025 M stock solution (112.5 mg Pt complex dissolved in 10.0 mL benzene or benzene-d^6) using a Hamilton gastight syringe into a J-Young NMR tube. To the NMR tube containing Pt catalyst, $PhI(OAc)_2$ as a solid (see Table S3-S5 for required amount) was added, followed by C_6F_6, C_6H_6 or C_6D_6. Total volume in the NMR tube was 0.6 mL (for the ratio used for C_6H_6 or C_6D_6 and C_6F_6, see Table S3-S5). The NMR tube tightly sealed and heated to 100 °C in a preheated oil bath. After the desired reaction time, the reaction was stopped by putting in a liquid nitrogen bath until frozen solid and then was allowed to reach to room temperature. The reaction mixture was diluted with 1 mL of hexane and filtered through a Silica gel column. Then 10 µL phenyl bromide as GC internal standard was added. The filtrate was analyzed by GC-FID method using GC instrument. Yields and concentrations of biphenyl were used to obtain initial rates and standard error. The rates and standard error were then plotted as a function of concentration of reagents, benzene, $PhI(OAc)_2$ and Pt catalyst and data were fitted using a non-linear least squares method to the equation Rate=$k_{obs}\times$[reagent]^n. Kaleidagraph program was used for data fitting.

6. Order in Pt complex

General method desribed above was used to determine the order of the reaction in Pt complex. C6F6 was used as cosolvent. Table S3 shows the results used to determine the order in Pt. Total volume in the vial is 0.6 mL.

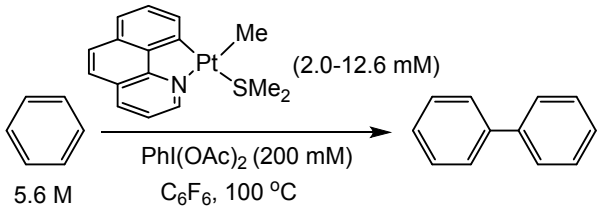
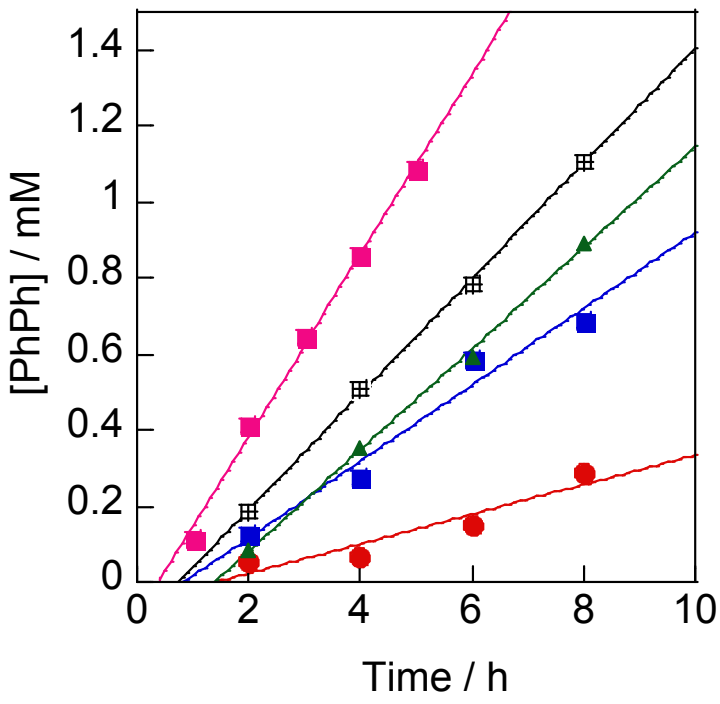


Table S4. Kinetic data for order determination in Pt complex

Entry	[Pt] (mM)	C_6H_6 (mL)	C_6F_6 (mL)	Time (h)	[biphenyl] (mM)
1	2.1	0.3	0.3	2	0.056
2	2.1	0.3	0.3	4	0.066
3	2.1	0.3	0.3	6	0.149
4	2.1	0.3	0.3	8	0.288
5	4.1	0.3	0.3	2	0.124
6	4.1	0.3	0.3	4	0.274
7	4.1	0.3	0.3	6	0.587
8	4.1	0.3	0.3	8	0.690
9	6.3	0.3	0.3	2	0.086
10	6.3	0.3	0.3	4	0.352
11	6.3	0.3	0.3	6	0.593
12	6.3	0.3	0.3	8	0.893
13	8.3	0.3	0.3	2	0.186
14	8.3	0.3	0.3	4	0.510
15	8.3	0.3	0.3	6	0.785
16	8.3	0.3	0.3	8	1.107
17	12.5	0.3	0.3	1	0.116
18	12.5	0.3	0.3	2	0.416
19	12.5	0.3	0.3	3	0.644
20	12.5	0.3	0.3	4	0.859
21	12.5	0.3	0.3	5	1.085



y = m1 + m2 * M0		
	Value	Error
m1	-0.054808	0.055873
m2	0.038999	0.010201
Chisq	0.0041623	NA
R	0.93789	NA

y = m1 + m2 * M0		
	Value	Error
m1	-0.083609	0.075351
m2	0.10051	0.013757
Chisq	0.0075703	NA
R	0.98178	NA

y = m1 + m2 * M0		
	Value	Error
m1	-0.18444	0.02189
m2	0.13313	0.0039966
Chisq	0.00063892	NA
R	0.9991	NA

y = m1 + m2 * M0		
	Value	Error
m1	-0.091509	0.030945
m2	0.23848	0.0093303
Chisq	0.0026116	NA
R	0.99771	NA

y = m1 + m2 * M0		
	Value	Error
m1	-0.11248	0.018698
m2	0.15193	0.0034138
Chisq	0.00046617	NA
R	0.9995	NA

7. Figure S2. Plot of concentration of biphenyl versus time at different concentration of Pt catalyst. The data are fitted to [PhPh]=m1+m2×time.

8. Order in $PhI(OAc)_2$

General method desribed above wes used to determine the order of the reaction in $PhI(OAc)_2$. Table S2 shows the amounts of compounds and results used to determine the order in $PhI(OAc)_2$. Total volume in the vial is 0.6 mL.

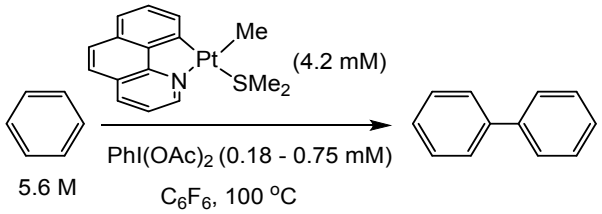
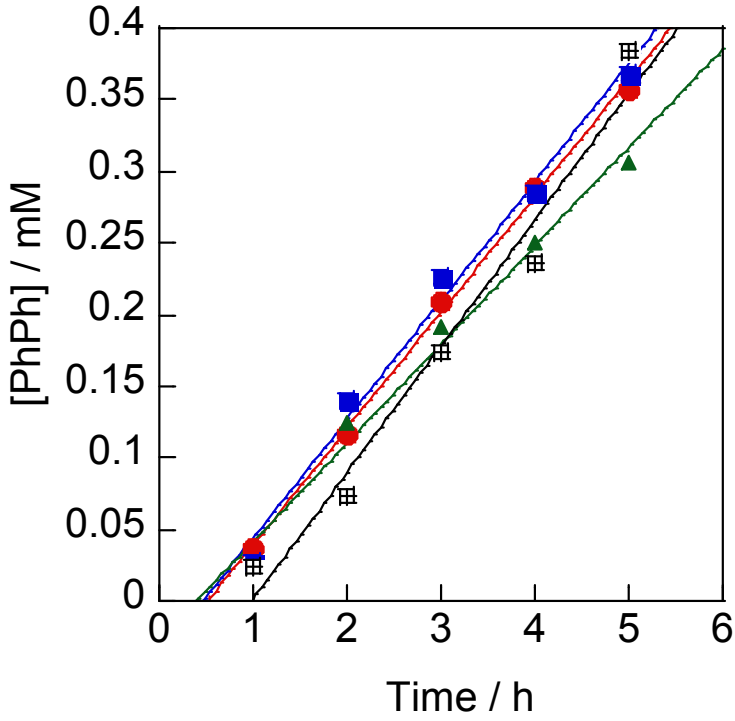


Table S5. Kinetic data for order determination in $PhI(OAc)_2$

Entry	$PhI(OAc)_2$ (M)	C_6F_6 (mL)	Time (h)	[biphenyl] (mM)
1	0.18	0.3	1	0.037
2	0.18	0.3	2	0.116
3	0.18	0.3	3	0.209
4	0.18	0.3	4	0.288
5	0.18	0.3	5	0.357
6	0.37	0.3	1	0.027
7	0.37	0.3	2	0.141
8	0.37	0.3	3	0.226
9	0.37	0.3	4	0.285
10	0.37	0.3	5	0.369
11	0.56	0.3	1	0.025
12	0.56	0.3	2	0.124
13	0.56	0.3	3	0.191
14	0.56	0.3	4	0.250
15	0.56	0.3	5	0.306
16	0.75	0.3	1	0.023
17	0.75	0.3	2	0.073
18	0.75	0.3	3	0.173
19	0.75	0.3	4	0.235
20	0.75	0.3	5	0.383



y = m1 + m2 * M0		
	Value	Error
m1	-0.041979	0.0074093
m2	0.081239	0.002234
Chisq	0.00014972	NA
R	0.99887	NA

y = m1 + m2 * M0		
	Value	Error
m1	-0.038601	0.017575
m2	0.082786	0.005299
Chisq	0.00084238	NA
R	0.99391	NA

y = m1 + m2 * M0		
	Value	Error
m1	-0.086573	0.030461
m2	0.088196	0.0091842
Chisq	0.0025305	NA
R	0.98412	NA

y = m1 + m2 * M0		
	Value	Error
m1	-0.027354	0.016442
m2	0.068868	0.0049573
Chisq	0.00073725	NA
R	0.99232	NA

9. Figure S3. Plot of concentration of biphenyl versus time at different concentration of oxidant $PhI(OAc)_2$. The data are fitted to [PhPh]=m1+m2×time.

10. Order in benzene

General method desribed above wes used to determine the order of the reaction in benzene. C_6F_6 was used as cosolvent. Table S1 shows the amounts of benzene and C_6F_6 and results used to determine the order in benzene. Total volume in the vial is 0.6 mL.

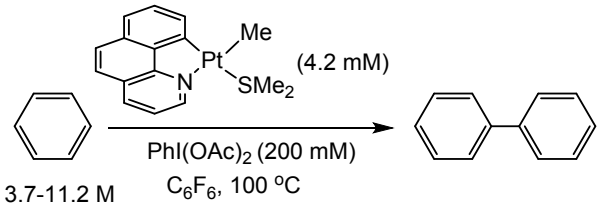
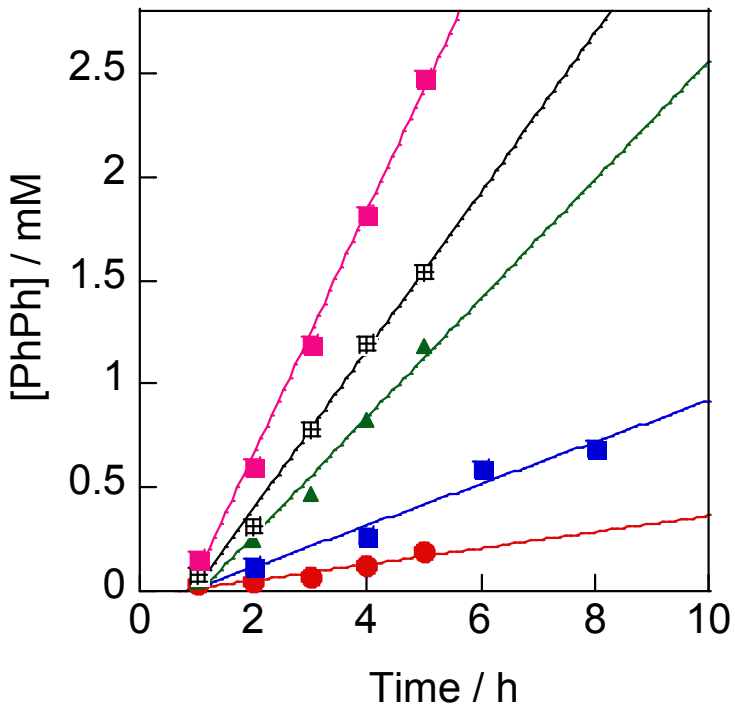


Table S6. Kinetic data for order determination in benzene

Entry	Benzene (mL)	C_6F_6 (mL)	Time (h)	[biphenyl] (mM)
1	0.1	0.4	1	0.035
2	0.1	0.4	2	0.042
3	0.1	0.4	3	0.068
4	0.1	0.4	4	0.121
5	0.1	0.4	5	0.190
6	0.2	0.3	2	0.124
7	0.2	0.3	4	0.274
8	0.2	0.3	6	0.587
9	0.2	0.3	8	0.690
11	0.3	0.2	1	0.047
12	0.3	0.2	2	0.241
13	0.3	0.2	3	0.473
14	0.3	0.2	4	0.828
15	0.3	0.2	5	1.185
16	0.4	0.1	1	0.080
17	0.4	0.1	2	0.312
18	0.4	0.1	3	0.779
19	0.4	0.1	4	1.198
20	0.4	0.1	5	1.546
21	0.5	0	1	0.154
22	0.5	0	2	0.603
23	0.5	0	3	1.200
24	0.5	0	4	1.820
25	0.5	0	5	2.481



$[C_6H_6]$ = 3.74 M		
	Value	Error
m1	-0.025326	0.024795
m2	0.038916	0.0074759
Chisq	0.0016767	NA
R	0.94885	NA

$[C_6H_6]$ = 5.6 M		
	Value	Error
m1	-0.08352	0.075406
m2	0.10048	0.013767
Chisq	0.0075814	NA
R	0.98174	NA

$[C_6H_6]$= 7.47 M		
	Value	Error
m1	-0.30387	0.074791
m2	0.28629	0.02255
Chisq	0.015256	NA
R	0.99082	NA

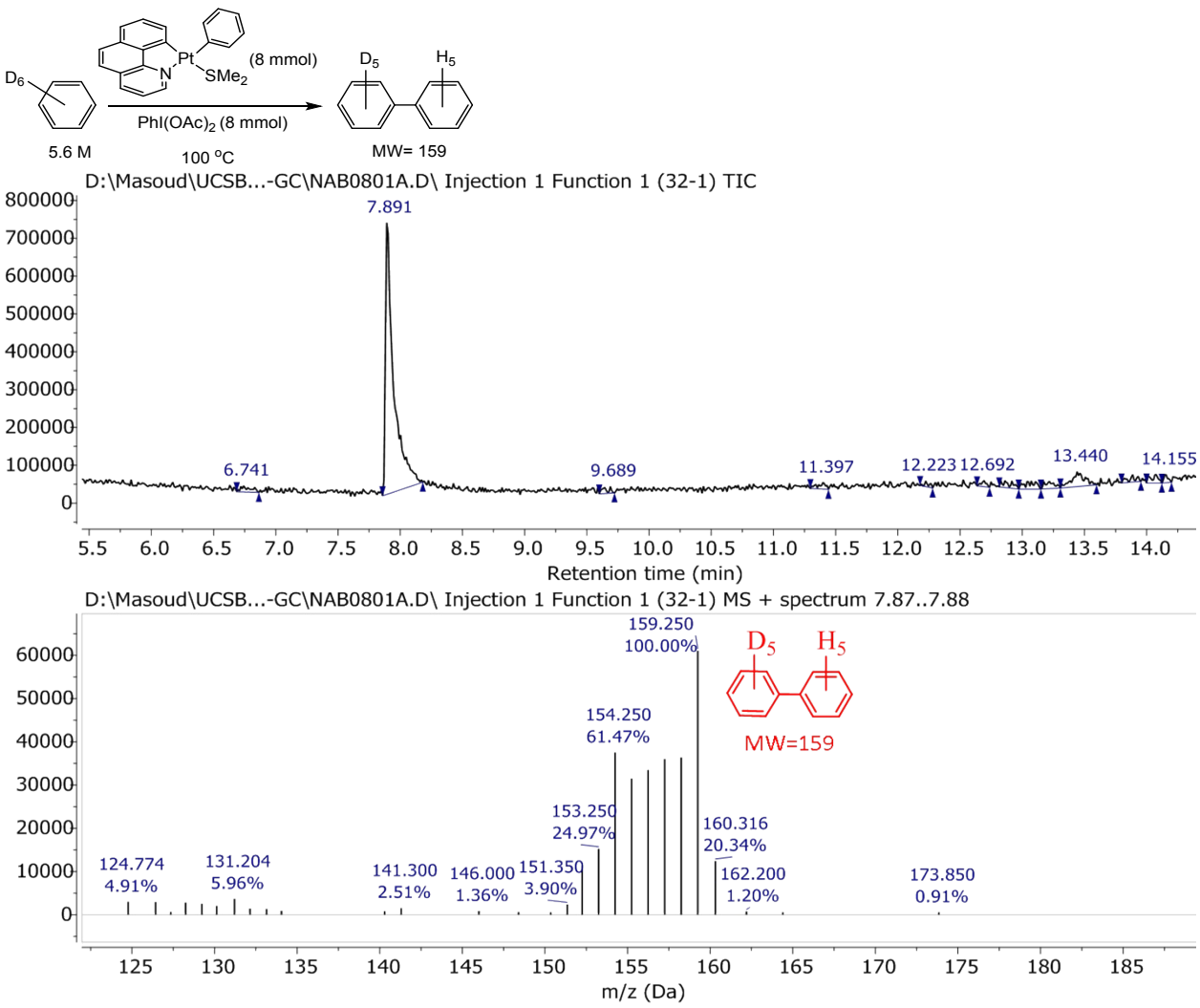
$[C_6H_6]$ = 11.21 M		
	Value	Error
m1	-0.50911	0.076007
m2	0.58692	0.022917
Chisq	0.015756	NA
R	0.99772	NA

$[C_6H_6]$ = 9.33 M		
	Value	Error
m1	-0.36209	0.068186
m2	0.38182	0.020559
Chisq	0.01268	NA
R	0.99568	NA

11. Figure S4. Plot of concentration of biphenyl versus time at different concentration of benzene. The data are fitted to [PhPh]=m1+m2×time.

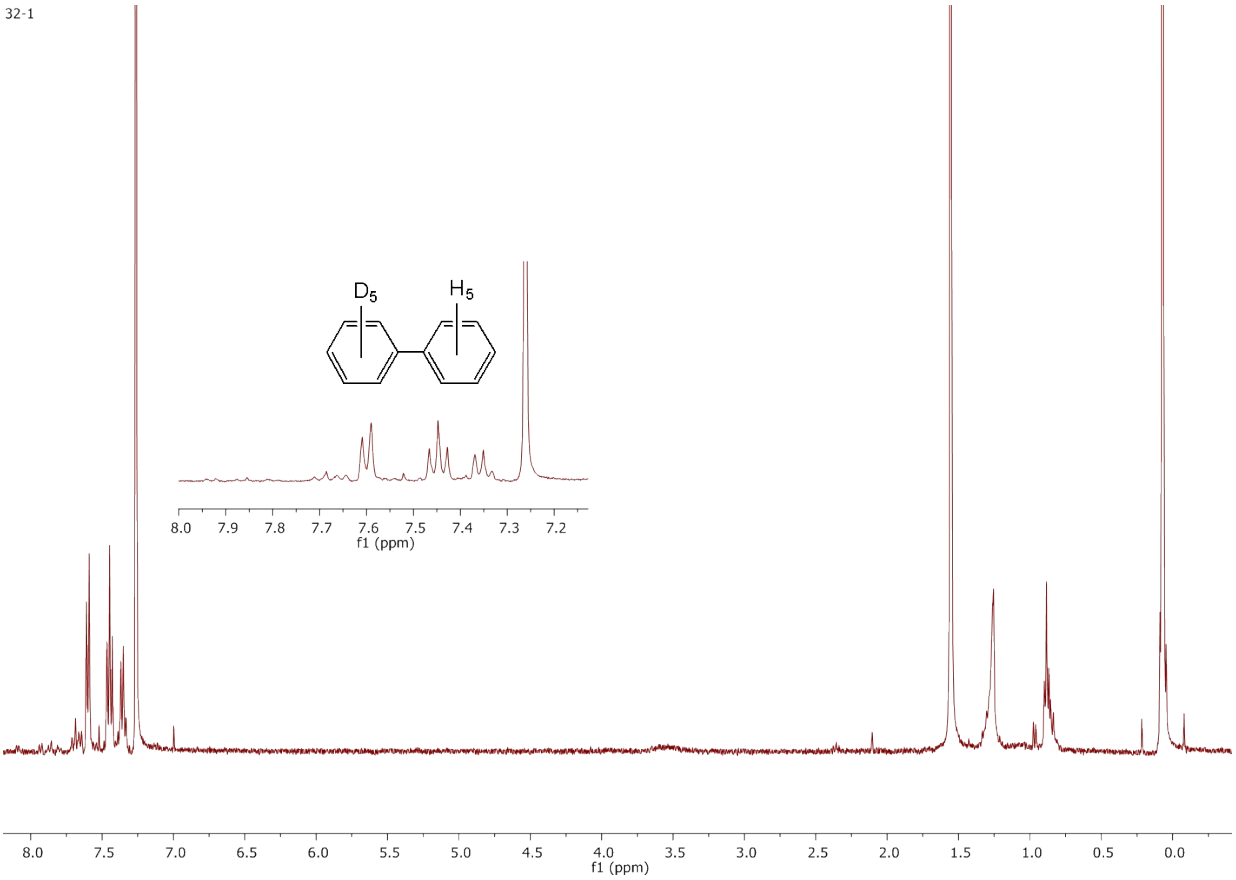
12. Preparation of complex [Pt(bhq)(OAc)(SMe_2)], **3**

2 mL HOAc was added to a solution of [PtMe(bhq)(SMe_2)] (80 mg) in benzene (2 mL) and stirred for 2h at this condition. Then the reaction was stopped and diluted with 1 mL of hexane and filtered through a Silica gel column. The filtrate was removed and then 7 mL CH_2Cl_2 was added to column. The solvent of second collected filtrate was evaporated and the product was obtained a a solid. NMR data in $CDCl_3$: δ 2.10 (s, methyl of OAc group, 3H), 2.86 (s, $^3J_{PtH}$ = 53.8 Hz, SMe_2 *trans* to N, 6H), 9.86 (d, J_{HH} = 7.0 Hz, $^3J_{PtH}$ = 38.7 Hz, the C−H proton adjacent to N of bhq, 1H), other aromatic protons of bhq ligand 7.51−8.42.



13. Figure S5. GC-MS data for homocoupling of C_6D_6 using **4** in the presence of stoichiometric amount of oxidant (1:1)

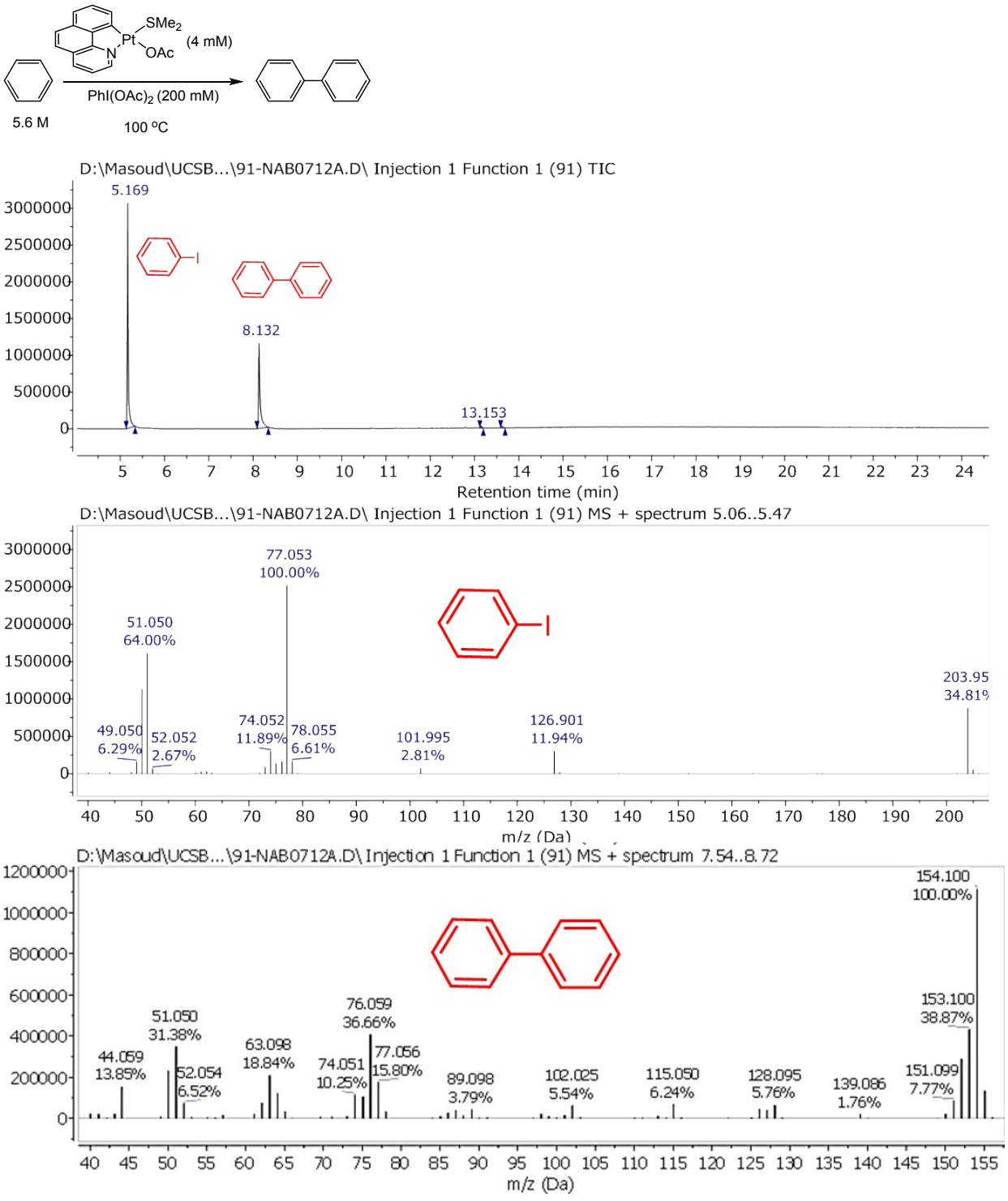
D_5 H_5



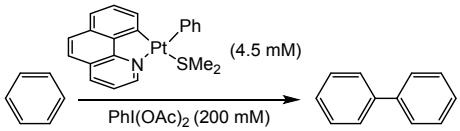
14. Figure S6. ^{1}H NMR of half-deuterated biphenyl ($C_{12}H_5D_5$) (see above experiment)

15. Using complex [Pt(bhq)(OAc)(SMe_2)], **3**, and [PtPh(bhq)(SMe_2)], **4,** as precatalyst for homocoupling of benzene to biphenyl.

6 mg Pt complex was transferred to a vessel pressure containing 2 mL benzene and then 50 mg $PhI(OAc)_2$ was added to the vessel and heated at 100 °C in a preheated oil bath for 24h. The reaction was then stopped and allowed to reach to room temperature. The reaction mixture was diluted with 1 mL of hexane and filtered through a Silica gel column and analyzed by GC-FID method using GC instrument. The GC-MS clearly showed the formation of biphenyl as product.



16. Figure S7. GC-MS data for homocoupling of benzene using **3** as precatalyst



5.6 M

100 °C

```
File       : C:\DOCUME~1\MASSSP~1\DESKTOP\ALLUSE~1\MASOUD\97ANAB~1.D
Operator   : SEYED
Acquired   : 17 Jul 17  10:59     using AcqMethod M006
Instrument :    GC/MS Ins
Sample Name: 97a
Misc Info  : ABU-OMAR
Vial Number: 1
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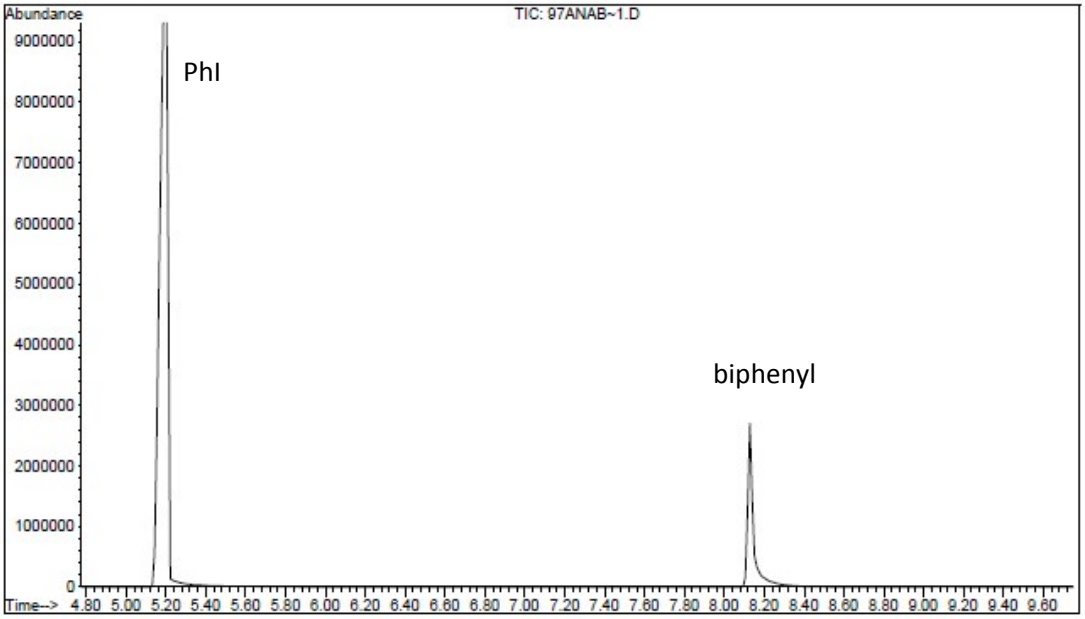
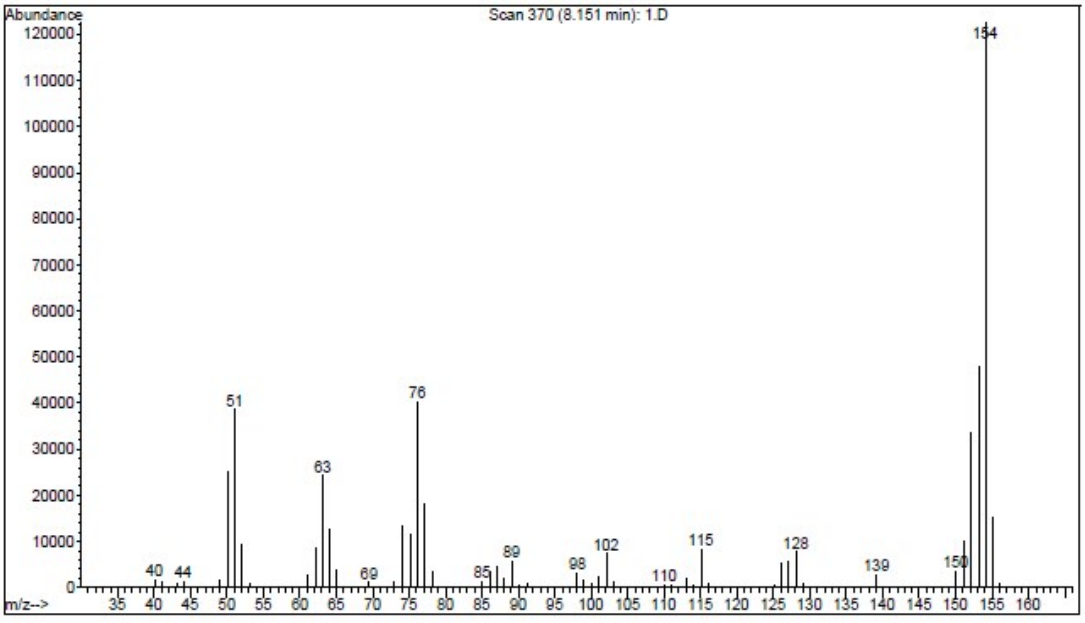
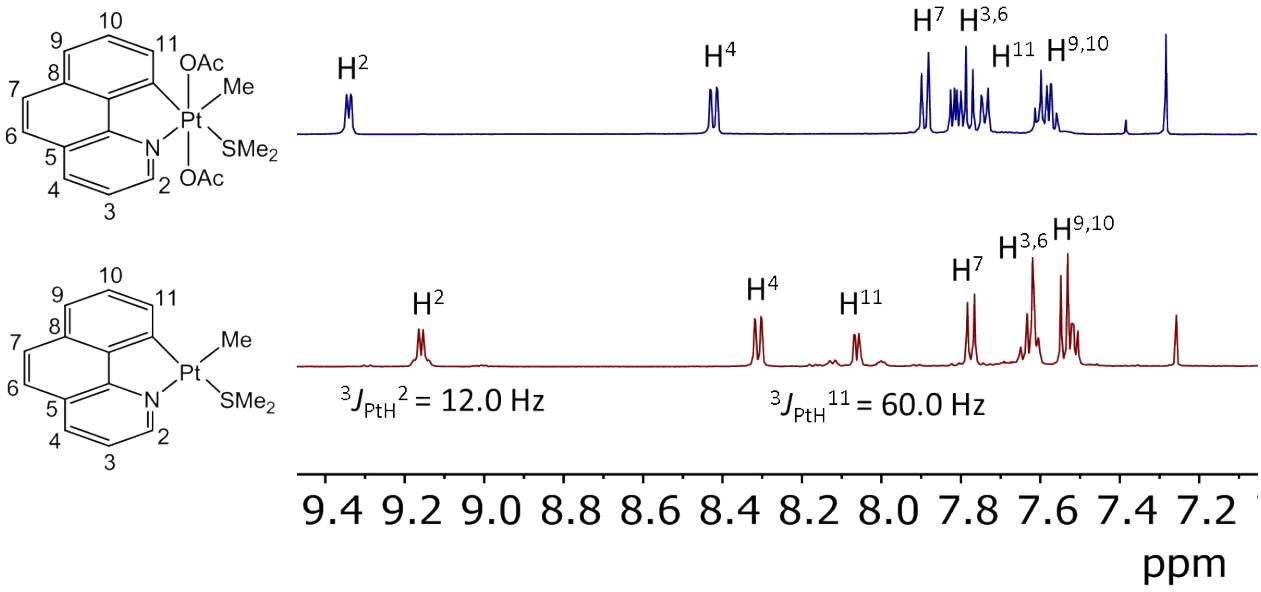




17. Figure S8. GC-MS data for homocoupling of benzene using **4** as precatalyst

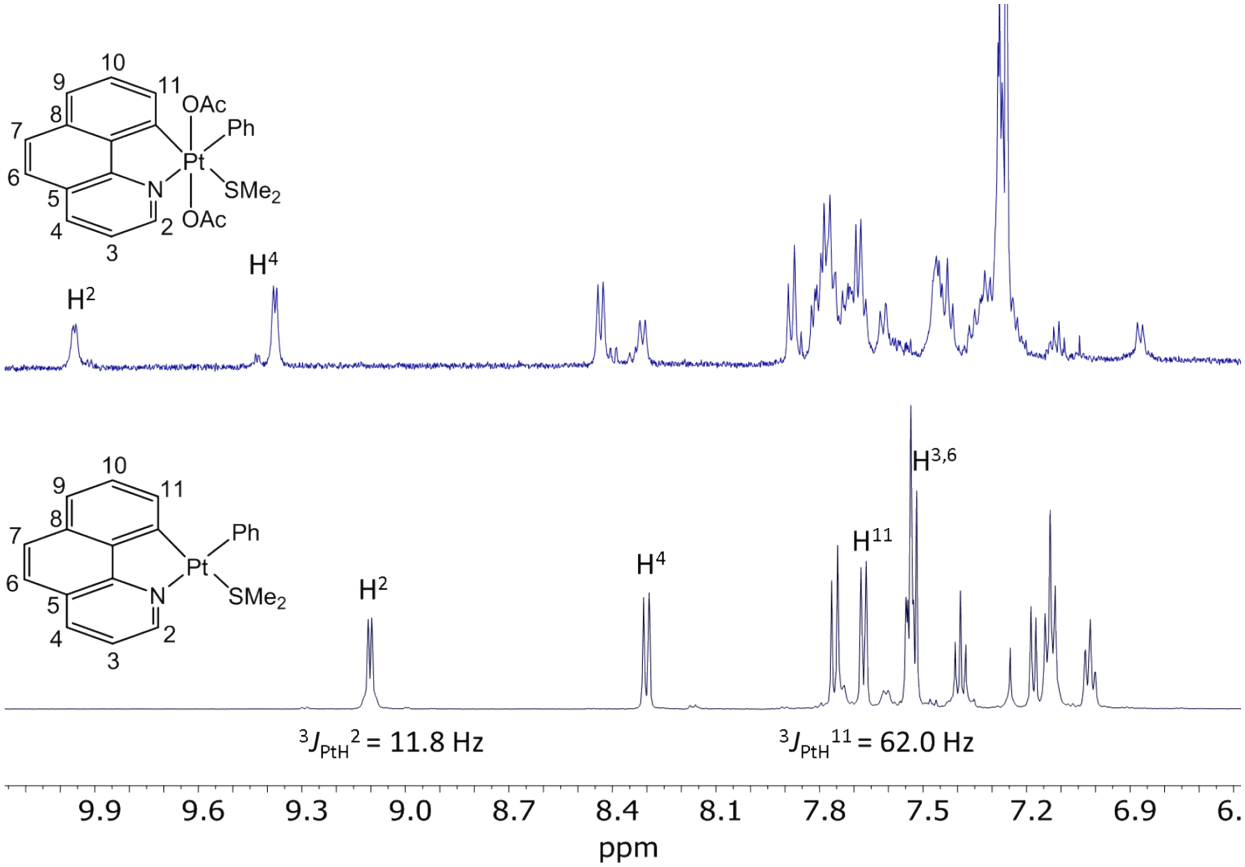
18. Reaction of complex **1** with $PhI(OAc)_2$ (Organometallics, 2018, 37, 87-98) [PtMe(bhq)(SMe_2)] (45 mg, 0.09 mmol), was dissolved in 15 mL CH_2Cl_2 or benzene and $PhI(OAc)_2$ (30 mg, 0.09 mmol) was added to the solution. The mixture was stirred at room temperature over 8 h. The solvent was evaporated from the resulting pale yellow solution, and the residue was washed with ether and hexane. See Figure S7 for ^1H NMR spectra. The comparison of ^1H NMR spectra clearly shows the conversion of Pt(II) to Pt(IV) complex. In the ^1H NMR spectrum, for the Pt(IV), a singlet with platinum satellites at δ = 9.35 ($^3J_{PtH} \approx 4$ Hz) was assigned to the C–H proton adjacent to N of bhq. This $^3J_{PtH}$ value is rather smaller than that for Pt(II) complex (at δ = 9.13 with $^3J_{PtH}$ = 12.0 Hz), confirming oxidation of Pt(II) complex to Pt(IV) complex.



19. Figure S9. Comparison of ^1H NMR spectra in aromatic region for complex **1** and its reaction with $PhI(OAc)_2$ in $CDCl_3$

20. Reaction of complex **4** with $PhI(OAc)_2$

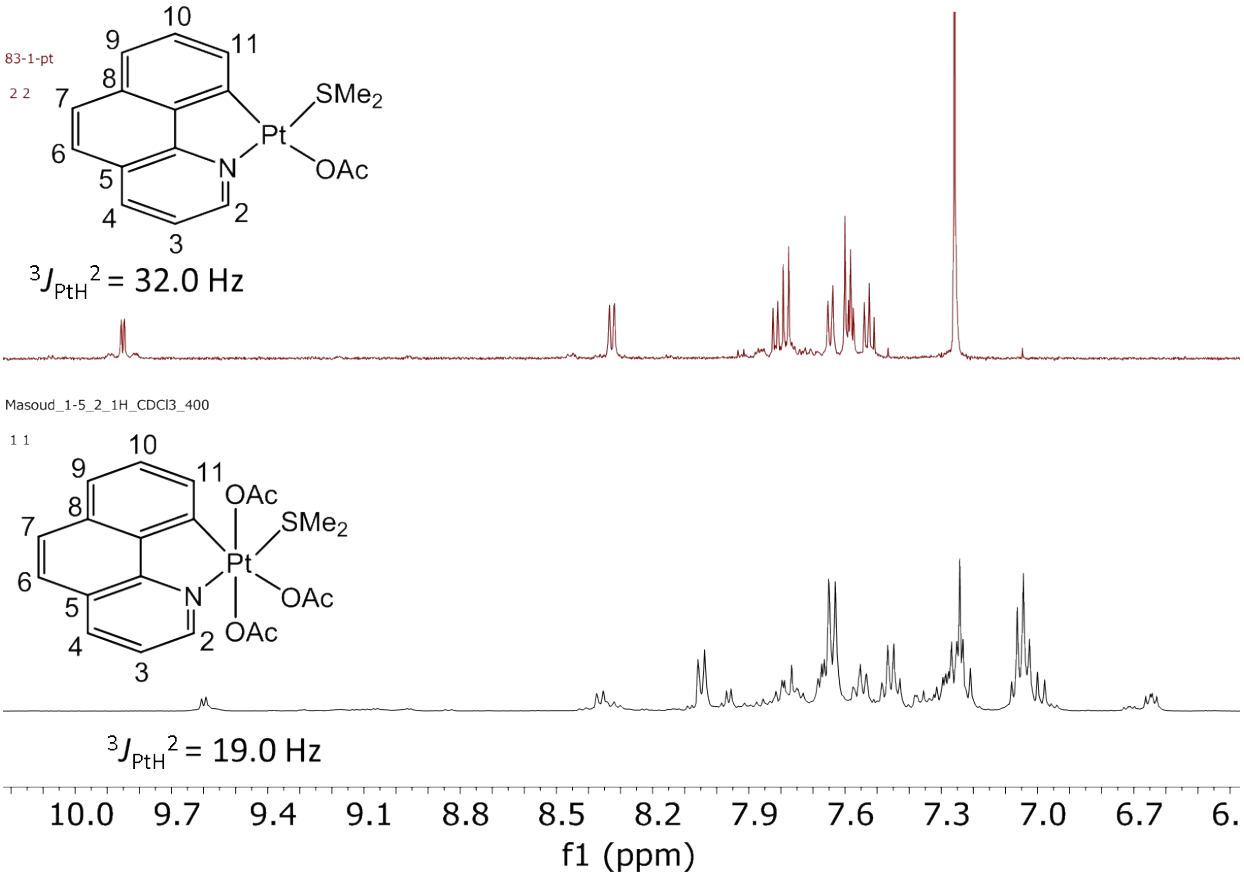
[PtPh(bhq)(SMe_2)] (50 mg, 0.1 mmol), was dissolved in 15 mL CH_2Cl_2 or benzene and $PhI(OAc)_2$ (32 mg, 0.1 mmol) was added to the solution. The mixture was stirred at room temperature over 8 h. The solvent was evaporated from the resulting pale yellow solution. See Figure S8 for ^1H NMR spectra. As is clear from Figure, the product of this reaction is the Pt(IV) complex instead of Pt(II) complex. In the ^1H NMR spectrum, for the Pt(IV), a singlet with platinum satellites at δ = 10.04 ($^3J_{PtH} \approx 5$ Hz) was assigned to the C–H proton adjacent to N of bhq. This $^3J_{PtH}$ value is rather smaller than that for Pt(II) complex (at δ = 9.15 with $^3J_{PtH}$ = 11.8 Hz), confirming oxidation of Pt(II) complex to Pt(IV) complex.



21. Figure S10. Comparison of ^1H NMR spectra in aromatic region for complex **1** and its reaction with $PhI(OAc)_2$ in $CDCl_3$

22. Reaction of complex **3** with $PhI(OAc)_2$

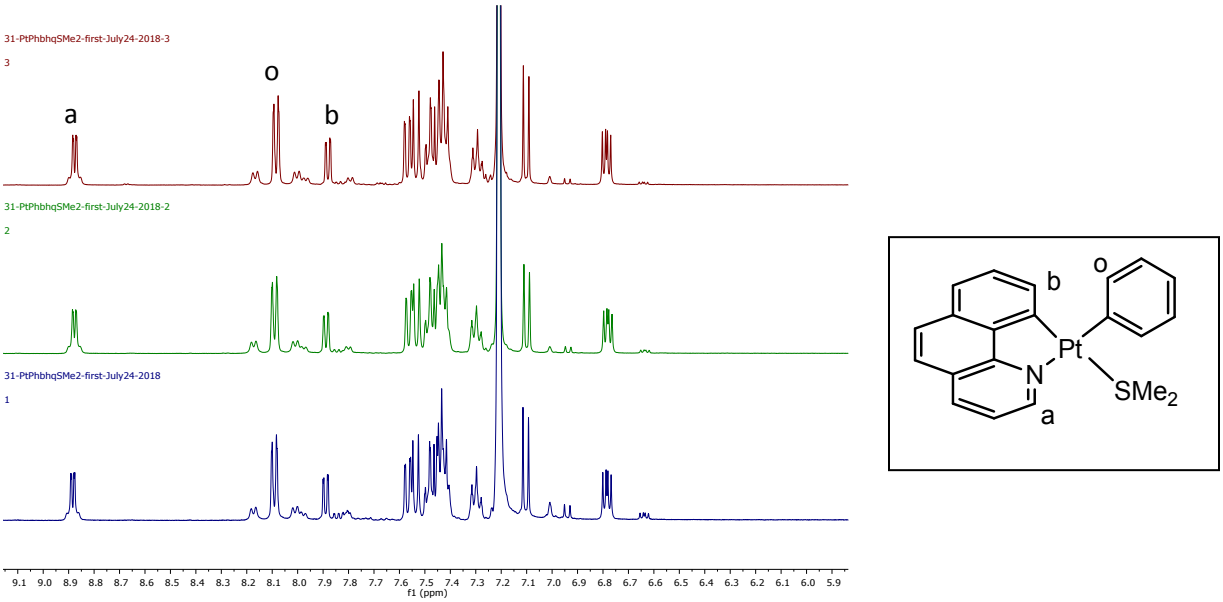
$[PtMe(bhq)(SMe_2)]$ (10 mg), was dissolved in 0.7 mL $CDCl_3$ and 0.1 mL deuterated acetic acid was added to solution to give in situ $[Pt(bhq)(OAc)(SMe_2)]$, **3**. The mixture was stirred at room temperature for 1 h. Then 8 mg $PhI(OAc)_2$ was added to solution and stirred for 8 h. See Figure S11 for ^1H NMR spectra. The comparison of 1H NMR spectra clearly shows the conversion of Pt(II) to Pt(IV) complex. In the ^1H NMR spectrum, for the Pt(IV), a singlet with platinum satellites at δ = 9.68 ($^3J_{PtH} \approx 19$ Hz) was assigned to the C–H proton adjacent to N of bhq. This $^3J_{PtH}$ value is rather smaller than that for Pt(II) complex (at δ = 10.05 with $^3J_{PtH}$ = 32.0 Hz), confirming oxidation of Pt(II) complex to Pt(IV) complex.



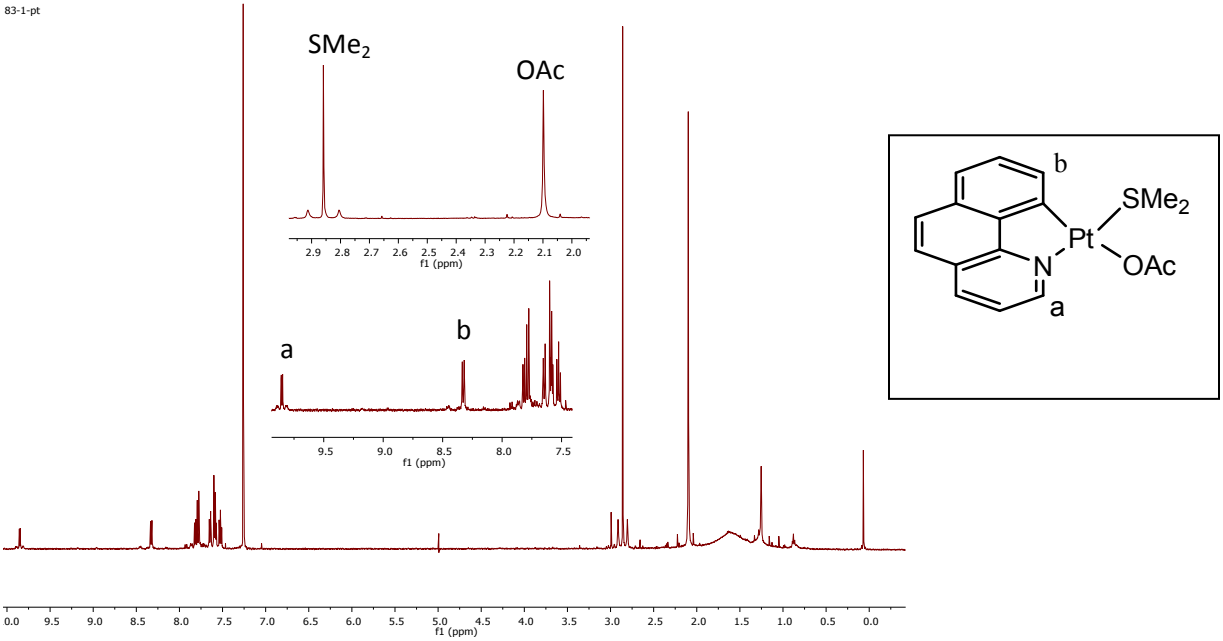
23. Figure S11. Comparison of ^1H NMR spectra in aromatic region for complex **3** and its reaction with $PhI(OAc)_2$ in $CDCl_3$

24. Stability of complexes **3** and **4** in benzene:

10 mg of Pt complex was added into a J-Young NMR tube containing 1 mL C_6D_6. The mixture was heated at 100 °C for 24 h. No change in NMR was found after this time showing no reaction between Pt complex and benzene; see following spectra.



25. Figure S12. ^{1}H NMR monitoring of heating of complex **4** in C_6D_6 at 100 °C.



26. Figure S13. ^{1}H NMR spectrum (in $CDCl_3$) of complex **3** after heating in C_6H_6 at 100 °C for 24 h.

27. H/D exchange experiments:

27.1: 5 mg of [PtMebhq(SMe_2)], 0.3 mL deuterated acetic acid and 0.3 mL C_6H_6 were added into a J-Young NMR tube and the mixture was heated at 100 °C. Then the reaction was cooled to room temperature and 0.1 mL CD_2Cl_2 was added to NMR tube for NMR analysis. The NMR spectrum show no partial depurated benzene. The ^1H and ^2H NMR were shown below:

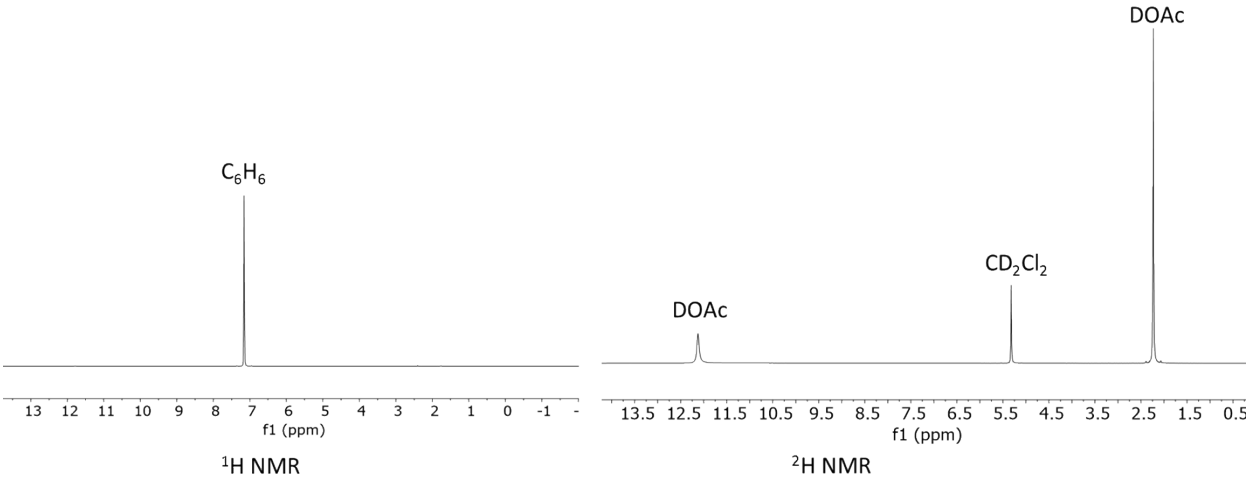


Figure S14. ^1H and ^2H NMR spectra for the reaction of H/D exchange between C_6H_6 and DOAc in the presence of Pt complex **1**.

27-2: 5 mg of [PtMebhq(SMe_2)], 0.3 mL acetic acid and 0.3 mL C_6D_6 were added into a J-Young NMR tube and the mixture was heated at 100 °C. Then the reaction was cooled to room temperature and 0.1 mL CD_2Cl_2 was added to NMR tube for NMR analysis. The NMR spectrum show no partial depurated benzene; see following ^1H NMR spectrum.

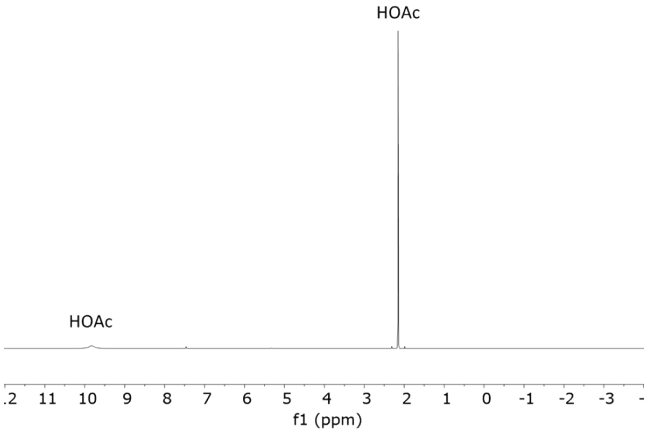


Figure S15. ^1H NMR spectrum for the reaction of H/D exchange between C_6D_6 and HOAc in the presence of Pt complex **1**.

27.3: 5 mg of [PtPhbhq(SMe_2)], **4**, 0.3 mL deuterated acetic acid and 0.3 mL C_6H_6 were added into a J-Young NMR tube and the mixture was heated at 100 °C. Then the reaction was cooled to room temperature and 0.1 mL CD_2Cl_2 was added to NMR tube for NMR analysis. The NMR spectrum show no partial depurated benzene. The ^1H and ^2H NMR were shown below:

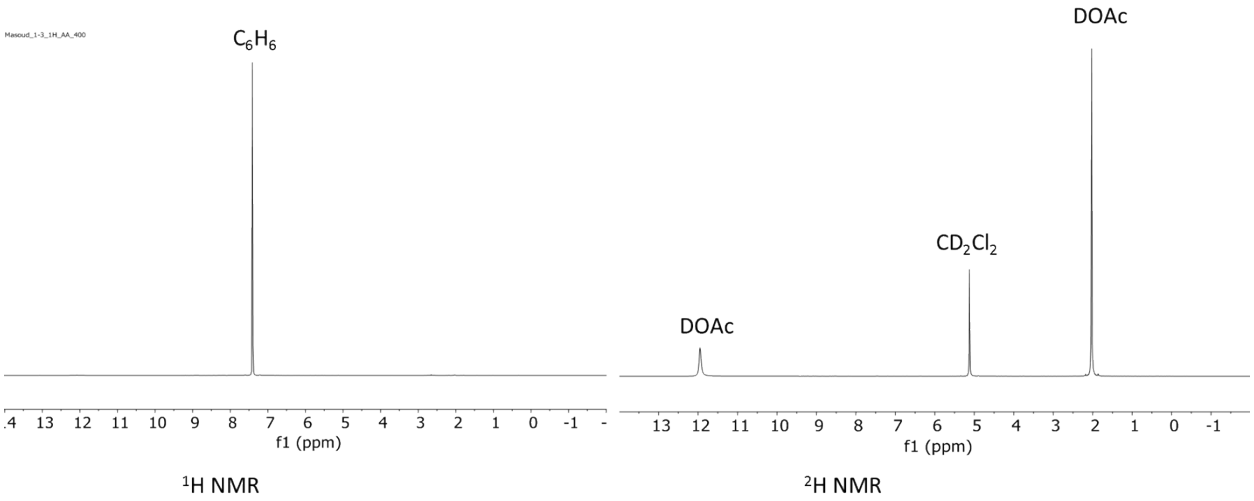


Figure S16. ^1H and ^2H NMR spectra for the reaction of H/D exchange between C_6H_6 and DOAc in the presence of Pt complex **4**.

27.4: 5 mg of [PtPhbhq(SMe_2)], 0.3 mL acetic acid and 0.3 mL C_6D_6 were added into a J-Young NMR tube and the mixture was heated at 100 °C. Then the reaction was cooled to room temperature and 0.1 mL CD_2Cl_2 was added to NMR tube for NMR analysis. The NMR spectrum show no partial depurated benzene; see following ^1H NMR spectrum.

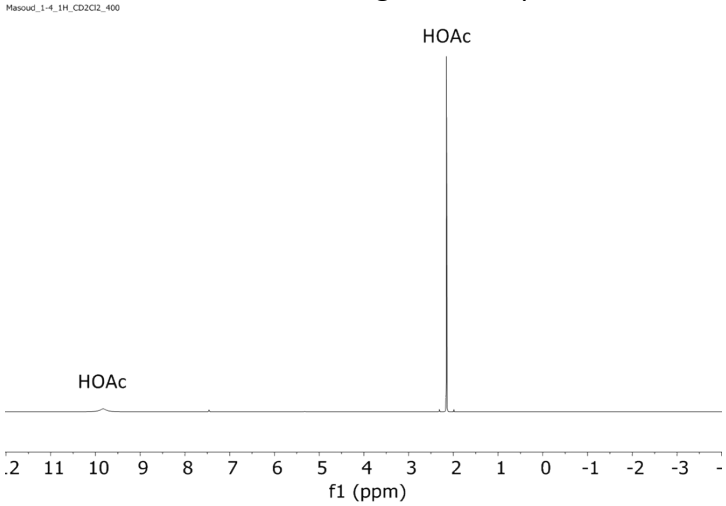
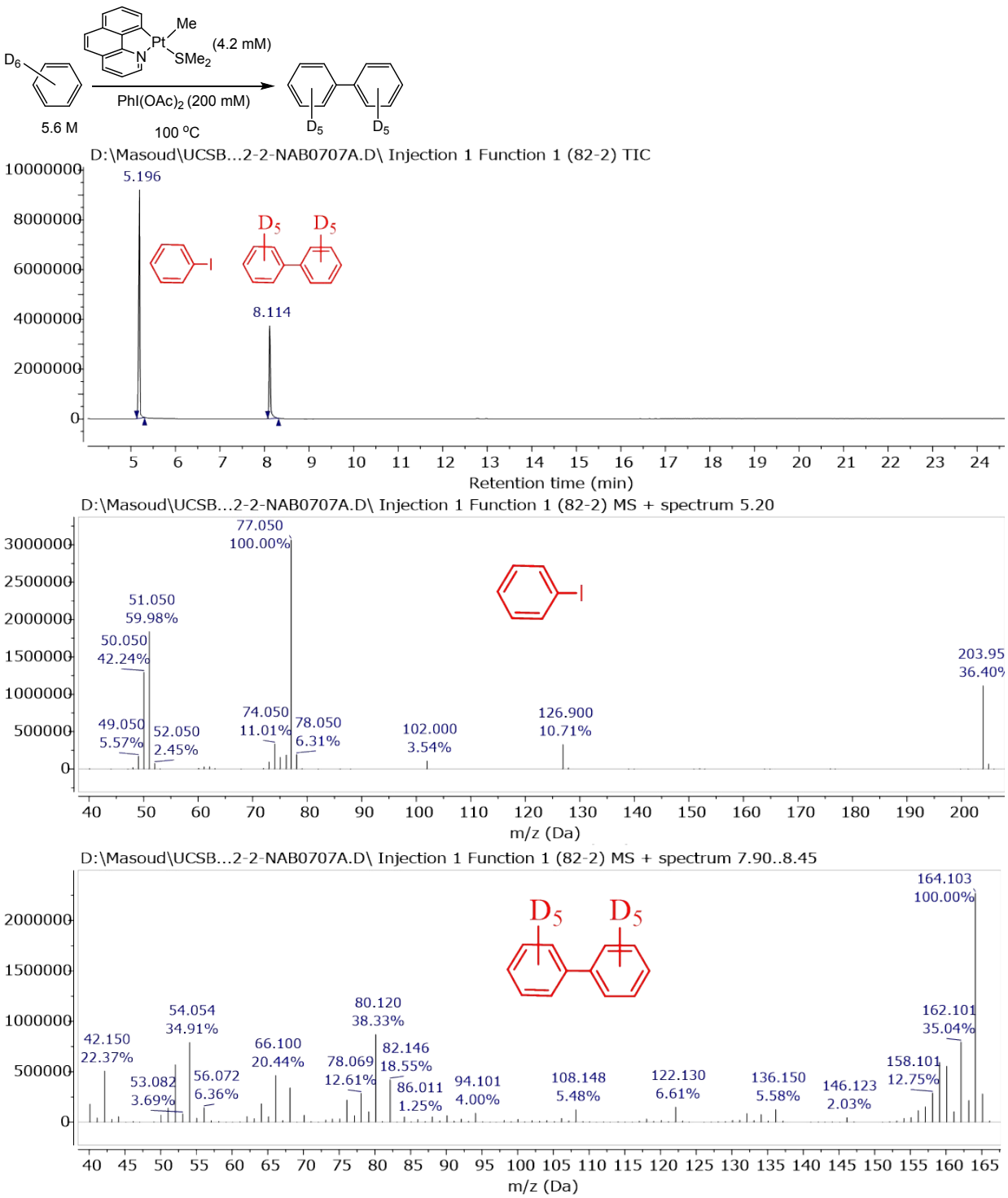
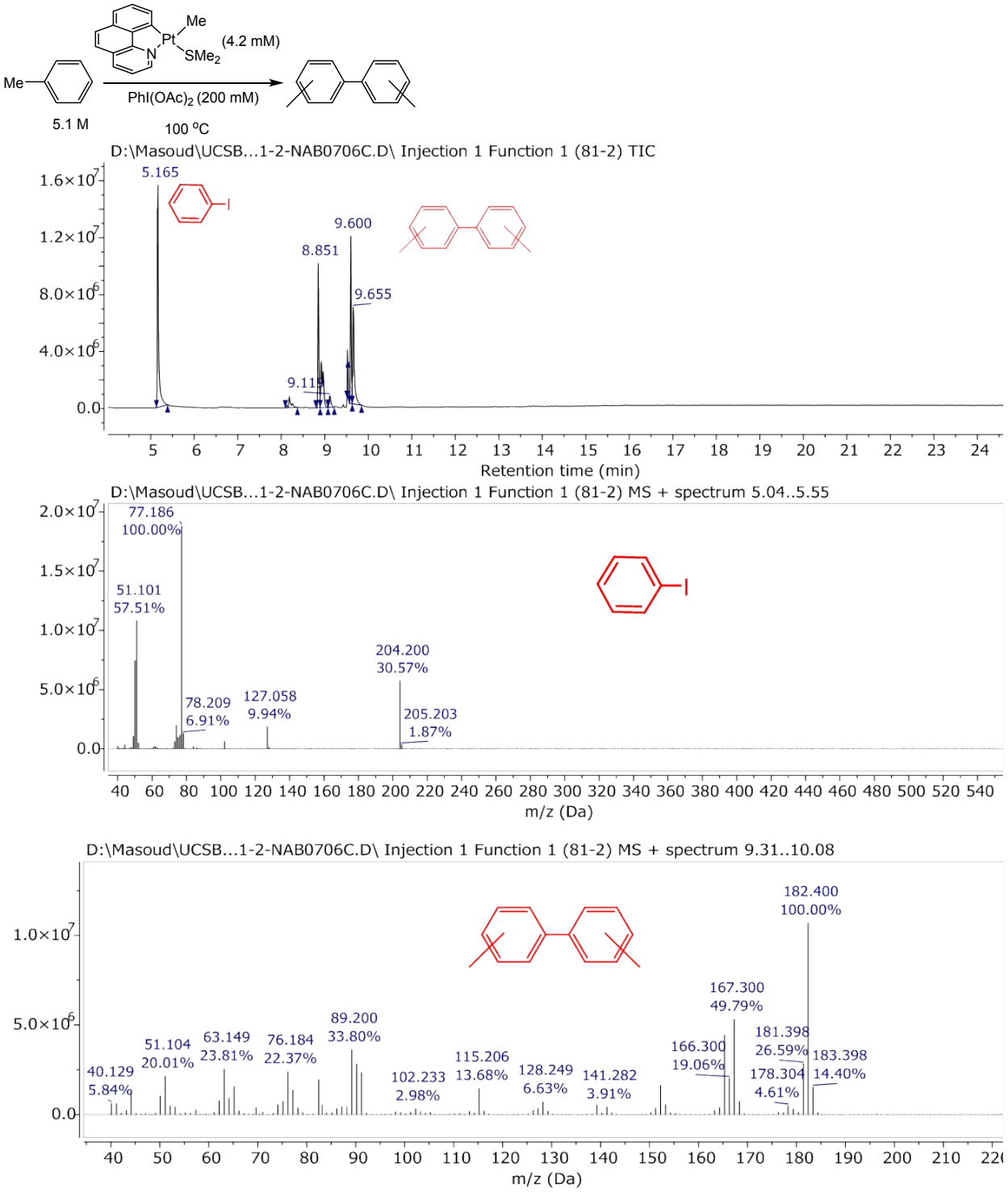


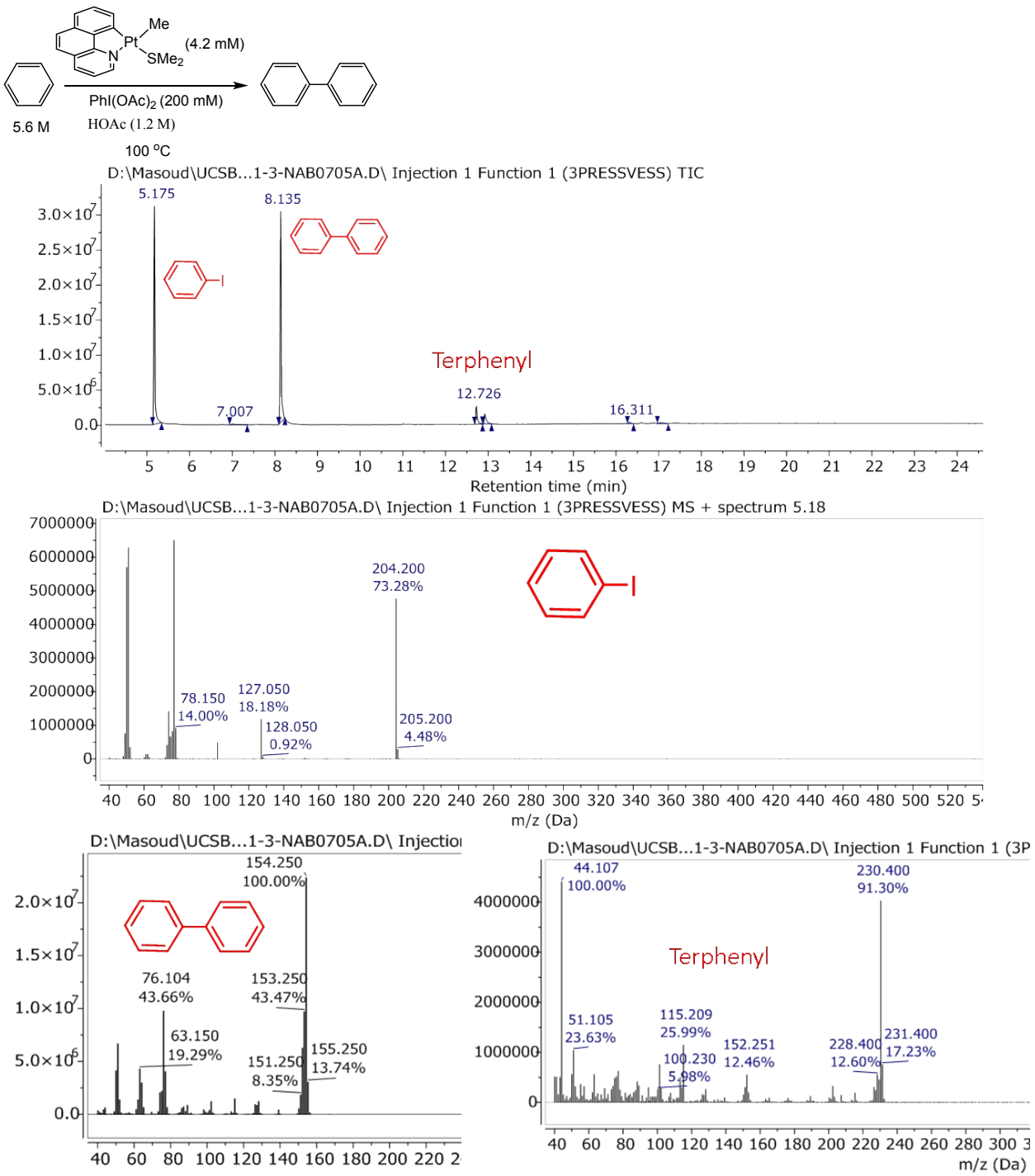
Figure S17. ^1H NMR spectrum for the reaction of H/D exchange between C_6D_6 and HOAc in the presence of Pt complex **4**.



28. Figure S18. GC-MS data for homocoupling of C_6D_6 using **1** as precatalyst



29. Figure S19. GC-MS data for homocoupling of toluene using **1** as precatalyst



30. Figure S20. GC-MS data for homocoupling of benzene using **1** as precatalyst in the presence of HOAc

31. Derivation of equation rate:

Reaction mechanism:

$$\text{IMa} + \text{PhH} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \text{IMb} + \text{HOAc}$$

$$\text{IMb} + \text{PhH} \xrightarrow{k_2} \text{IMc} + \text{HOAc}$$

$$\text{IMc} \xrightarrow{\text{fast}} \text{PhPh} + 3$$

$$\frac{d[PhPh]}{dt} = k_2[PhH][IMb] \quad (1)$$

$$\frac{d[IMb]}{dt} = k_1[IMa][PhH] - k_{-1}[IMb][HOAc] - k_2[IMb][PhH] = 0 \quad (2)$$

$$[Pt]_T = [IMa] + [IMb] \quad so \quad [IMa] = [Pt]_T - [IMb] \quad (3)$$

$$\frac{d[IMb]}{dt} = k_1\{[Pt] - [IMb]\}[PhH] - k_{-1}[IMb][HOAc] - k_2[IMb][PhH] = 0 \quad (4)$$

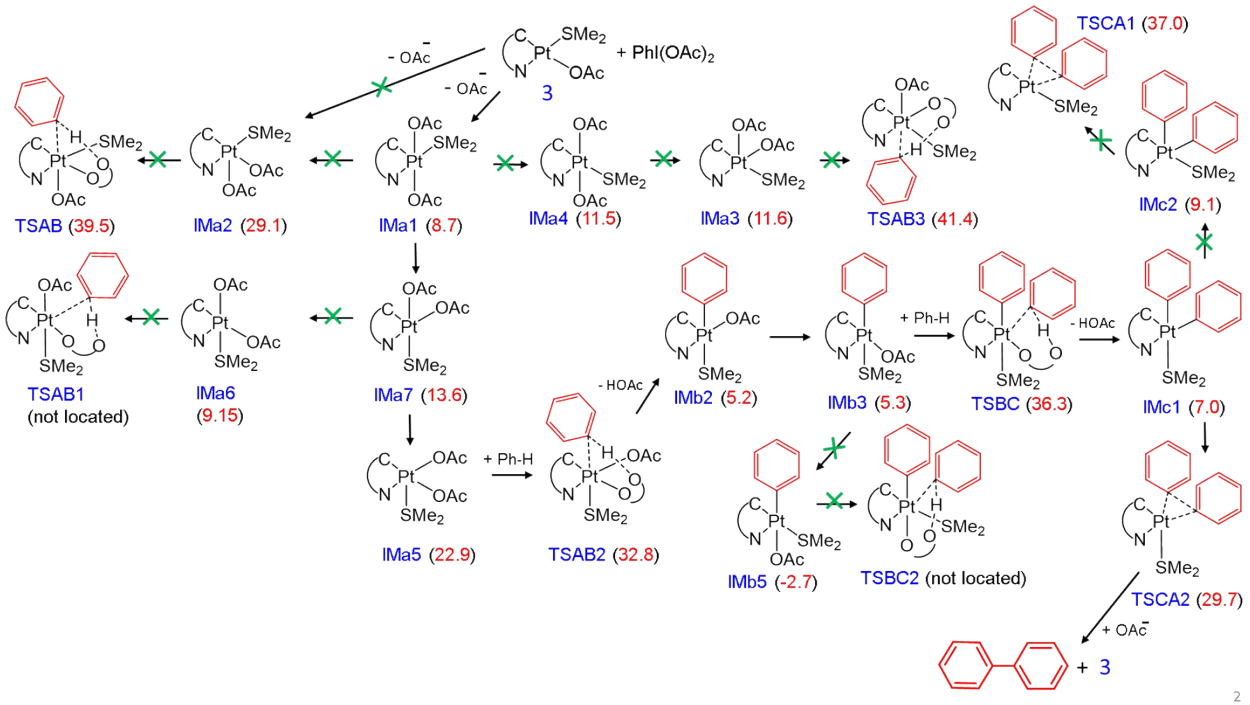
$$[IMb] = \frac{k_1[PhH][Pt]_T}{k_1[PhH] + k_{-1}[HOAc] + k_2[PhH]} \quad (5)$$

$$\frac{d[PhPh]}{dt} = \frac{k_1k_2[PhH]^2[Pt]_T}{k_1[PhH] + k_{-1}[HOAc] + k_2[PhH]} = \frac{k_1k_2[PhH]^2[Pt]_T}{k_{-1}[HOAc] + (k_1 + k_2)[PhH]}$$

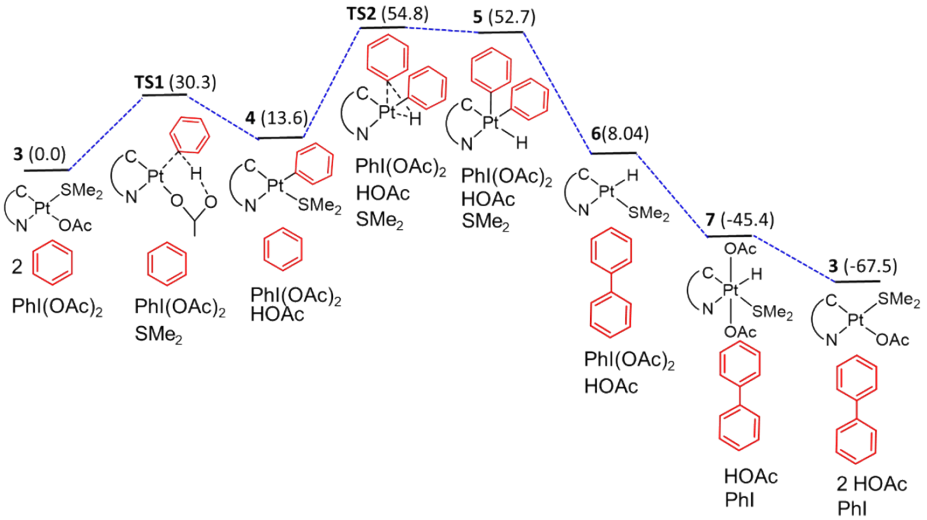
32. *Computational details*

Gaussian 09 was used to fully optimize all the structures in solvent at the B3LYP level of density functional theory. The solvation energies were calculated by CPCM model using the dielectric constant of 2.25 for benzene, respectively. The effective core potential of Hay and Wadt with a double-ξ valence basis set (LANL2DZ) was chosen to describe Pt and I. The 6-31+G* basis set was used for other atoms. This basis set combination will be referred to as BS1. Frequency calculations were carried out at the same level of theory to identify whether the calculated stationary point is a minimum (zero imaginary frequency) or a transition structure (one imaginary frequency). To further refine the energies obtained from the B3LYP/BS1 calculations, we carried out single-point energy calculations in benzene for all the structures with a larger basis set (BS2). BS2 utilizes the quadruple-z valence def2-QZVP basis set on Pt and I and the 6-311+G(2d,p) basis set on other atoms. We have used the energies obtained from B3LYP/BS1 or B3LYP/BS2 throughout the paper as stated in the related reaction profiles. To estimate the corresponding Gibbs free energies and enthalpies, the relevant corrections were calculated at the B3LYP/BS1 level and added to the single-point energies. In this work, "Thermal correction to Gibbs Free Energy" was added to the related energy which is equal to summation of electronic and thermal free energies. Also the free energy was calculated as $G = E(BS2) + G_{corr}(BS1)$, where single point energy correction was used.

The calculated $\Delta G^{\ddagger}$ value of 36.2 kcal mol^{-1} ($\Delta G^{\ddagger} = \Delta G^{\ddagger}_{1} - \Delta G^{\ddagger}_{-1} + \Delta G^{\ddagger}_{2}$; see Figure 7) was in excellent agreement with the experimental value of activation free energy ($\Delta G^{\ddagger}_{exp}$ = 35.9 $kcalmol^{-1}$, obtained from experimental rate constant at 100 °C at the same condition using the equation $\Delta G^{\ddagger}_{exp} = (RT)[\ln(K_B T/h) - \ln(K_{exp})]$).

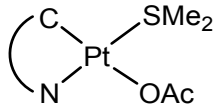
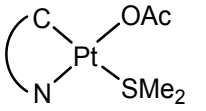
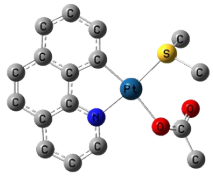
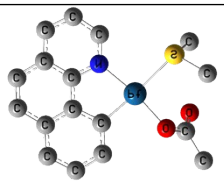


33. Figure S21. Suggested different paths for benzene to biphenyl conversion (5-coordinate Pt(IV) complexes are cationic). Free energy values are shown in parenthesis. Structures are optimized at B3LYP level with lanl2dz (Pt, I) and 6-31+G* basis set.



34. Figure S22. Computed energy (kcal mol^{-1}) pathway for Pt-catalyzed formation of biphenyl from benzene (Path B in Scheme 2). Structures optimized at B3LYP level with lanl2dz (Pt, I) and 6-31+G* basis set. Single point energy calculations conducted at B3LYP with def2-QZVP along with the corresponding ECP (Pt, I) and 6-311+G** basis sets and a solvent correction (benzene, CPCM).

35. Optimized structures (energies in parenthesis are in kcal/mol when E(3) =0)

[Pt(bhq)(SMe_2)(OAc)]	
3	**3′**
	
	
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[Pt(bhq)(SMe_2)($OAc)_2$] (reported energies are for Pt species + OAc^-)			
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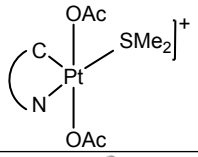	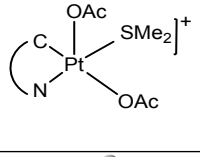	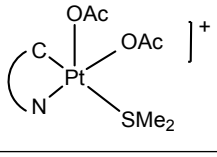	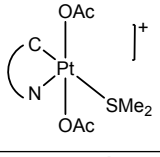
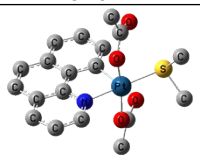	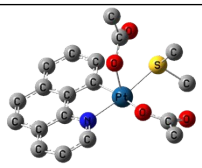	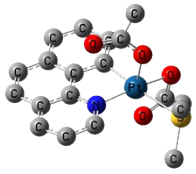	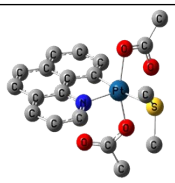
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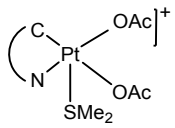	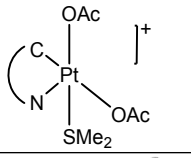	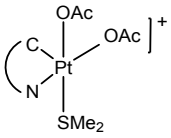	
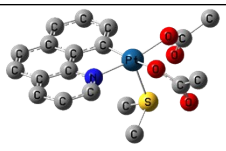	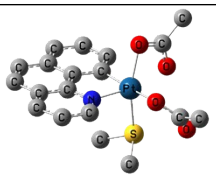	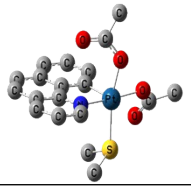	
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[Pt(Ph-H)(bhq)(SMe_2)($OAc)_2$] (reported energies are for Pt species + OAc^-)			
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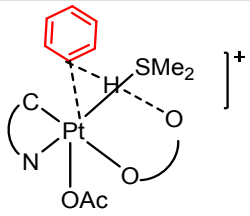
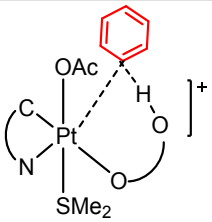
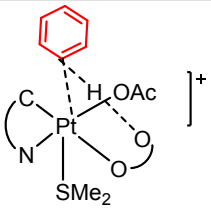
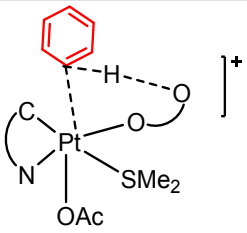
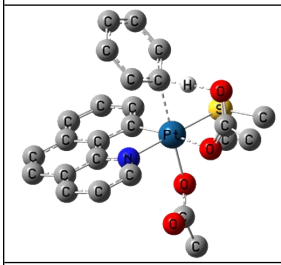
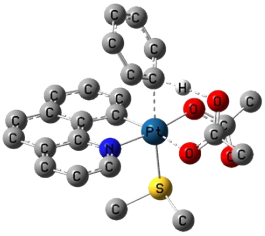
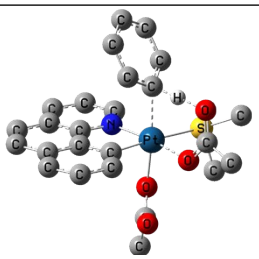
			
	Could not be located		
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[Pt(Ph)(bhq)(SMe_2)(OAc)] (reported energies are for Pt species + OAc^-)				
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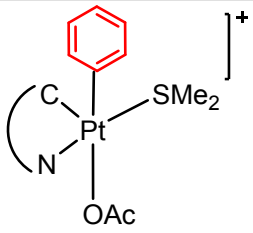	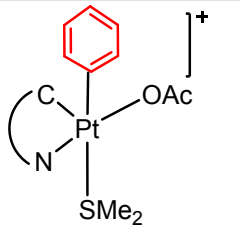	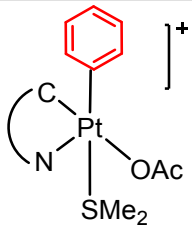	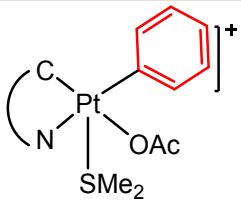	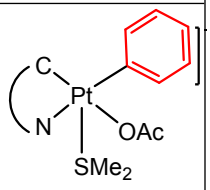
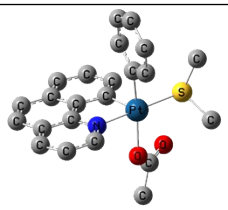	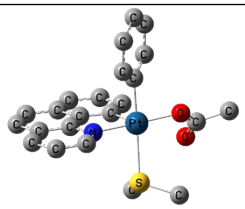	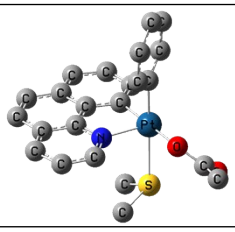	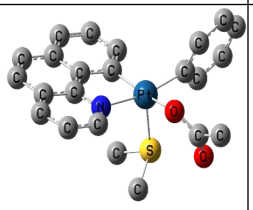	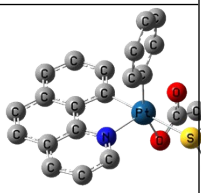
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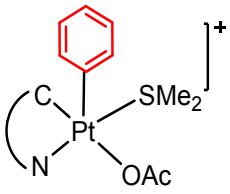
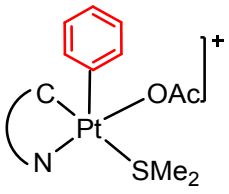
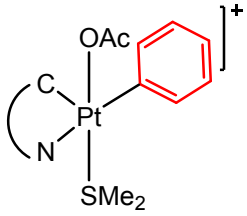
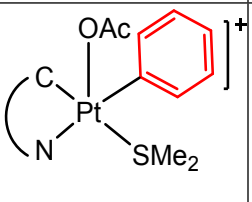
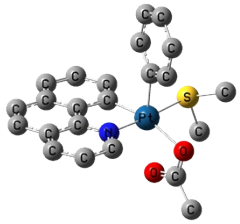
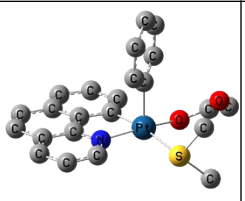
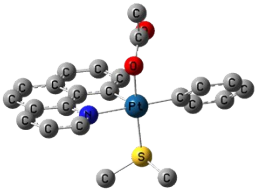
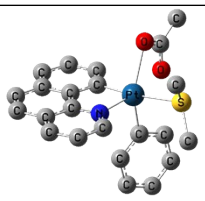
IMb6	IMb7	IMb8	IMb9	
				
				
E=-5.3	E=5.9	E=8.8	E=-0.5	

[Pt(Ph-H)(Ph)(bhq)(SMe_2)(OAc)] (reported energies are for Pt species + OAc^-)		
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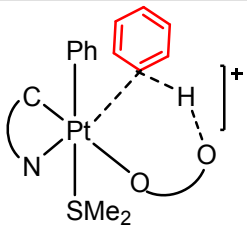
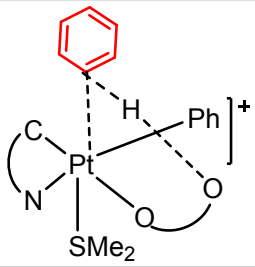
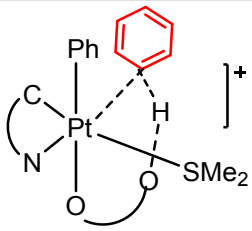
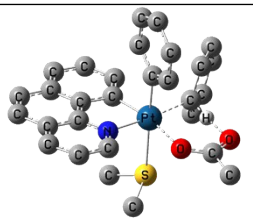
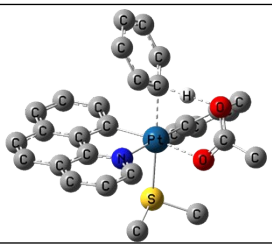
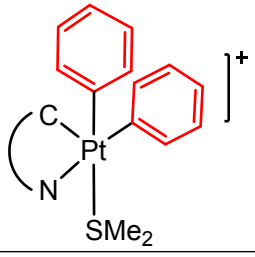
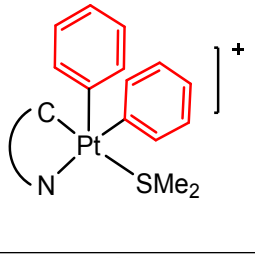
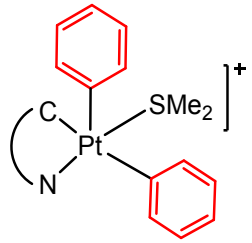
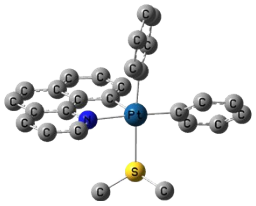
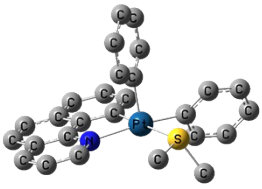
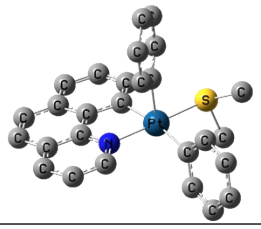
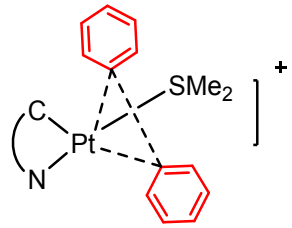
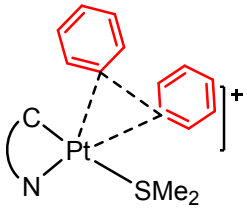
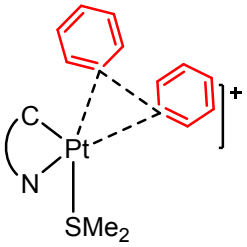
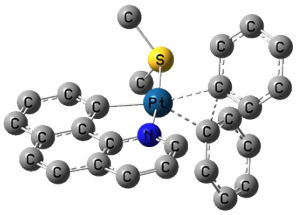
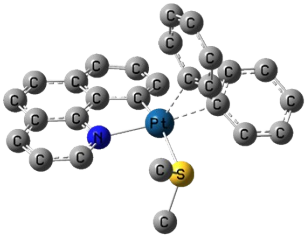
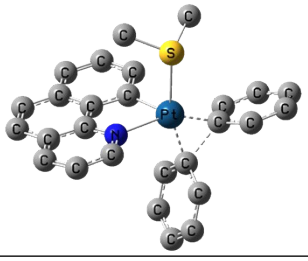
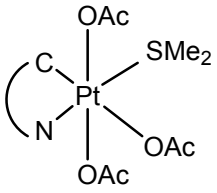
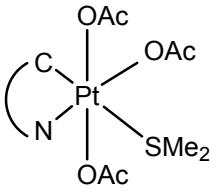
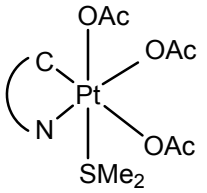
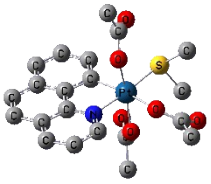
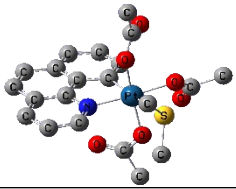
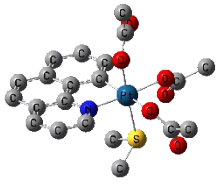
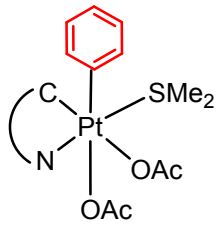
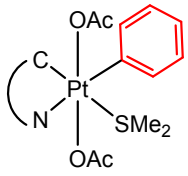
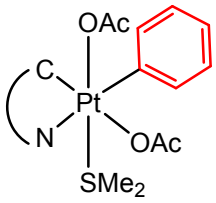
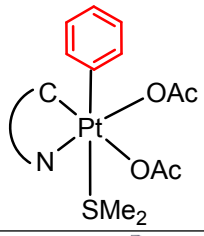
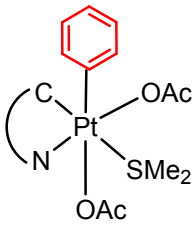
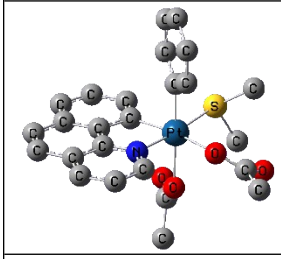
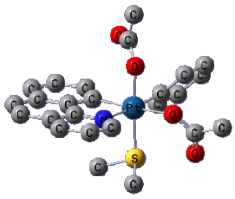
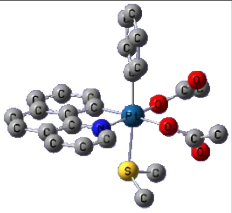
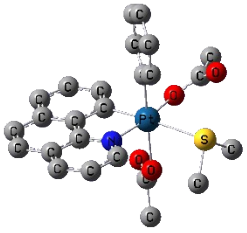
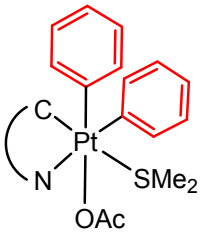
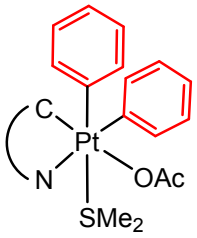
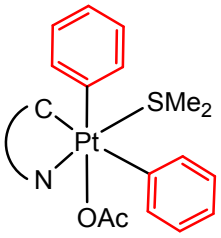
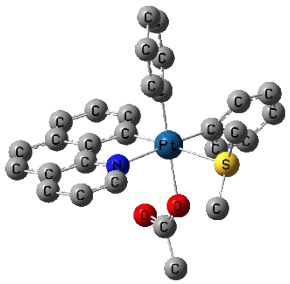
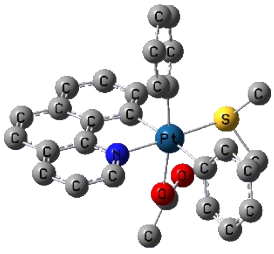
		
		Could not be located
E=36.3	E=37.6	

[$Pt(Ph)_2$(bhq)(SMe_2)] (reported energies are for Pt species + OAc^-)		
IMc1	IMc2	IMc3
		
		
E=7.0	E=9.1	E=24.5

[Pt(Ph)$_2$(bhq)(SMe$_2$)] (reported energies are for Pt species + OAc$^-$)		
TSCA	TSCA1	TSCA2
		
		
E=42.6	E=37.0	E=29.7

[Pt(bhq)(SMe$_2$)(OAc)$_3$]		
A	**A1**	**A2**
		
		
E= 0.00	E = 7.24	E=3.6

[Pt(Ph)(bhq)(SMe$_2$)(OAc)$_2$]				
B	**B1**	**B2**	**B3**	**B4**
				
	Could not located			
E=0.00		E=6.37	E=0.73	E=7.7

[Pt(Ph)$_2$(bhq)(SMe$_2$)(OAc)]		
C	C1	C2
		
	Could not located	
E=0.00		E=15.14

36. Cartesian coordinates and energy of optimized structures

[Pt(bhq)SMe_2OAc], 3

Zero-point correction=	0.303580 (Hartree/Particle)
Thermal correction to Energy=	0.325460
Thermal correction to Enthalpy=	0.326405
Thermal correction to Gibbs Free Energy=	0.250688
Sum of electronic and zero-point Energies=	-1380.434794
Sum of electronic and thermal Energies=	-1380.412913
Sum of electronic and thermal Enthalpies=	-1380.411969
Sum of electronic and thermal Free Energies=	-1380.487685
Entropy=	159.358

Pt	0.593413	-0.125615	-0.194881
C	-1.024619	-1.316708	-0.065967
C	-2.234205	-0.566881	0.039555
C	-1.162507	-2.703926	-0.051788
C	-3.518132	-1.157031	0.163443
C	-2.126106	0.853351	0.005946
C	-2.432497	-3.316115	0.075049
H	-0.293730	-3.349946	-0.146611
C	-3.596346	-2.568893	0.183268
C	-4.665663	-0.290421	0.257675
C	-3.257683	1.697594	0.089024
H	-2.492554	-4.402276	0.084378
H	-4.563316	-3.056682	0.279014
C	-4.546516	1.072417	0.221981
H	-5.648997	-0.744499	0.356998
C	-3.033932	3.090256	0.030922
C	-0.665729	2.668815	-0.179316
H	-5.427422	1.705437	0.291656
H	-3.875705	3.775689	0.091168
C	-1.740263	3.571589	-0.105978
H	0.364485	2.988188	-0.288681
H	-1.539200	4.636518	-0.156871
N	-0.859335	1.350180	-0.120828
O	2.086363	1.442168	-0.393409
C	3.042295	1.662548	0.455773
O	3.348446	0.925415	1.409179
C	3.808130	2.960371	0.205988
H	3.198400	3.809416	0.540809
H	4.747460	2.967380	0.764326
H	4.004679	3.099644	-0.861988

S	2.070764	-1.948291	-0.304897
C	3.649603	-1.398244	-1.040551
H	4.094944	-0.617923	-0.423333
H	4.310002	-2.267287	-1.109204
H	3.432102	-1.019008	-2.040815
C	2.617649	-2.255488	1.416210
H	3.014672	-1.327756	1.832200
H	1.742199	-2.587815	1.978164
H	3.369513	-3.049810	1.400081

[Pt(bhq)SMe_2OAc], 3’

Zero-point correction=	0.303391 (Hartree/Particle)
Thermal correction to Energy=	0.325410
Thermal correction to Enthalpy=	0.326354
Thermal correction to Gibbs Free Energy=	0.250525
Sum of electronic and zero-point Energies=	-1380.429387
Sum of electronic and thermal Energies=	-1380.407367
Sum of electronic and thermal Enthalpies=	-1380.406423
Sum of electronic and thermal Free Energies=	-1380.482252
Entropy=	159.595

Pt	-0.585579	-0.057946	-0.196099
C	0.841728	1.346163	-0.135961
C	2.144268	0.799667	-0.001918
C	0.738424	2.731849	-0.196997
C	3.318138	1.591298	0.079747
C	2.245395	-0.619240	0.039115
C	1.895943	3.542536	-0.117643
H	-0.234544	3.200206	-0.308510
C	3.165765	2.995738	0.020839
C	4.584522	0.918233	0.213260
C	3.495488	-1.270994	0.162190
H	1.785128	4.623679	-0.165507
H	4.041348	3.637487	0.081972
C	4.672410	-0.447095	0.253366
H	5.487909	1.520212	0.281180
C	3.496729	-2.681356	0.182158
C	1.093905	-2.643646	-0.044576
H	5.638976	-0.934304	0.352848
H	4.434791	-3.222622	0.276165
C	2.293808	-3.362798	0.076357
H	0.144486	-3.156927	-0.141688
H	2.257673	-4.447124	0.082284

N	1.061340	-1.306836	-0.058214
O	-2.035142	1.391890	-0.435150
C	-2.891630	1.694085	0.502773
O	-3.028743	1.097367	1.578707
C	-3.744551	2.911761	0.165143
H	-3.936680	2.981903	-0.909286
H	-4.686745	2.878480	0.718130
H	-3.202587	3.816818	0.467822
S	-2.255983	-1.937098	-0.284075
C	-2.884874	-2.156591	1.421036
H	-3.200168	-1.189084	1.815769
H	-3.704653	-2.880541	1.409413
H	-2.059528	-2.551300	2.018784
C	-3.760960	-1.330287	-1.118960
H	-4.158639	-0.460251	-0.595265
H	-3.479156	-1.051821	-2.136532
H	-4.502090	-2.133580	-1.147189

[Pt(bhq)$SMe_2(OAc)_2$], IMa1

Zero-point correction=	0.355644 (Hartree/Particle)
Thermal correction to Energy=	0.381991
Thermal correction to Enthalpy=	0.382935
Thermal correction to Gibbs Free Energy=	0.298293
Sum of electronic and zero-point Energies=	-1608.633073
Sum of electronic and thermal Energies=	-1608.606726
Sum of electronic and thermal Enthalpies=	-1608.605781
Sum of electronic and thermal Free Energies=	-1608.690424
Entropy=	178.144

Pt	0.667775	-0.001369	-0.508484
C	-0.433827	0.004603	1.216548
C	-1.805480	0.003582	0.919237
C	0.038811	0.009596	2.503157
C	-2.766160	0.007274	1.963835
C	-2.228923	-0.000872	-0.435239
C	-0.923444	0.013092	3.546180
H	1.094104	0.010548	2.739892
C	-2.287204	0.011908	3.293238
C	-4.158506	0.006282	1.590657
C	-3.595569	-0.001418	-0.788838
H	-0.563534	0.016656	4.570960
H	-2.993463	0.014642	4.118484

C	-4.557886	0.002249	0.281587
H	-4.902644	0.008940	2.382533
C	-3.896141	-0.005480	-2.168365
C	-1.532244	-0.008202	-2.667909
H	-5.614475	0.001726	0.030185
H	-4.931990	-0.005904	-2.496227
C	-2.867658	-0.008826	-3.101622
H	-0.700746	-0.010813	-3.364904
H	-3.075088	-0.011907	-4.165928
N	-1.241392	-0.004308	-1.367670
S	2.881849	0.005881	0.457972
C	3.765683	-1.386170	-0.341473
H	3.580716	-1.407418	-1.417203
H	4.829905	-1.231766	-0.144865
H	3.432440	-2.304393	0.136687
C	3.767212	1.369698	-0.387592
H	3.580873	1.355451	-1.463281
H	3.436742	2.304033	0.060232
H	4.831515	1.220161	-0.187785
O	0.549542	-2.030664	-0.725141
C	0.857872	-2.897535	0.232098
O	1.395574	-2.594456	1.291504
C	0.467762	-4.316829	-0.132150
H	0.981445	-5.020360	0.525731
H	-0.614627	-4.433799	-0.001578
H	0.700703	-4.534244	-1.178322
O	0.544503	2.027374	-0.731223
C	0.866306	2.897217	0.218836
O	1.421358	2.597560	1.270313
C	0.468020	4.315002	-0.142151
H	-0.611963	4.430933	0.007869
H	0.992584	5.020898	0.504527
H	0.681623	4.529936	-1.192935

[Pt(bhq)$SMe_2(OAc)_2$], IMa2

Zero-point correction=	0.355848 (Hartree/Particle)
Thermal correction to Energy=	0.382864
Thermal correction to Enthalpy=	0.383808
Thermal correction to Gibbs Free Energy=	0.297256
Sum of electronic and zero-point Energies=	-1608.599262
Sum of electronic and thermal Energies=	-1608.572246
Sum of electronic and thermal Enthalpies=	-1608.571302

Sum of electronic and thermal Free Energies= -1608.657854

Entropy= 182.166

Pt	0.489882	-0.002611	-0.369111
C	-1.124595	-1.248598	-0.396526
C	-2.333455	-0.514365	-0.267349
C	-1.202557	-2.625045	-0.569459
C	-3.605397	-1.136015	-0.309997
C	-2.259718	0.897268	-0.112121
C	-2.466063	-3.256070	-0.642264
H	-0.311966	-3.237258	-0.644024
C	-3.644698	-2.539205	-0.504436
C	-4.777725	-0.315312	-0.162311
C	-3.413492	1.698931	0.034782
H	-2.505040	-4.331222	-0.792199
H	-4.603827	-3.048506	-0.540228
C	-4.690004	1.040692	0.010217
H	-5.752302	-0.794737	-0.194272
C	-3.217807	3.092970	0.168740
C	-0.834000	2.759141	-0.023534
H	-5.588345	1.642001	0.115656
H	-4.076340	3.747462	0.292507
C	-1.934756	3.617803	0.136199
H	0.191099	3.108911	-0.061819
H	-1.759508	4.683380	0.234562
N	-1.012160	1.443532	-0.143854
O	1.841811	1.663944	-0.661000
C	3.049833	1.830677	-0.181778
O	3.699386	0.959692	0.406340
C	3.608608	3.227635	-0.402757
H	3.149518	3.915563	0.318287
H	4.689435	3.231601	-0.246906
H	3.370193	3.593213	-1.406038
S	2.026857	-1.819739	-0.809562
C	3.178835	-1.143840	-2.054861
H	3.780891	-0.352828	-1.608710
H	3.805397	-1.974433	-2.392181
H	2.588204	-0.769368	-2.893255
C	3.161520	-2.094230	0.594826
H	3.550275	-1.131919	0.929427
H	2.597161	-2.614852	1.368008
H	3.959470	-2.739520	0.216736
O	0.545334	-0.017459	-2.375101
C	0.310179	-1.126199	-3.082160

O	0.018153	-2.218775	-2.638029
C	0.434257	-0.810685	-4.568843
H	1.115599	-1.545604	-5.008119
H	-0.554821	-0.939475	-5.020523
H	0.794856	0.200045	-4.759739

[Pt(bhq)$SMe_2(OAc)_2$], IMa3

Zero-point correction=	0.355654 (Hartree/Particle)
Thermal correction to Energy=	0.382951
Thermal correction to Enthalpy=	0.383895
Thermal correction to Gibbs Free Energy=	0.295758
Sum of electronic and zero-point Energies=	-1608.625928
Sum of electronic and thermal Energies=	-1608.598632
Sum of electronic and thermal Enthalpies=	-1608.597688
Sum of electronic and thermal Free Energies=	-1608.685824
Entropy=	185.499

Pt	0.693637	0.285466	0.046498
C	-1.086986	1.247353	0.312936
C	-2.152062	0.477369	-0.182574
C	-1.311995	2.494886	0.849176
C	-3.484054	0.954884	-0.167174
C	-1.866117	-0.825309	-0.661303
C	-2.645398	2.984609	0.872053
H	-0.507841	3.102900	1.250614
C	-3.706355	2.244091	0.372729
C	-4.514756	0.089311	-0.680566
C	-2.885749	-1.677859	-1.139155
H	-2.829387	3.968805	1.293903
H	-4.715090	2.646350	0.403512
C	-4.231120	-1.165677	-1.146301
H	-5.540169	0.448867	-0.684316
C	-2.505870	-2.971035	-1.553218
C	-0.217979	-2.456266	-0.983033
H	-5.024938	-1.805566	-1.520529
H	-3.255800	-3.663003	-1.926298
C	-1.175282	-3.357116	-1.469351
H	0.823733	-2.731412	-0.893640
H	-0.855709	-4.349109	-1.768654
N	-0.561044	-1.224313	-0.601951
O	1.763727	2.100567	0.252121
C	1.645569	2.366408	-1.000717
O	1.019117	1.482512	-1.693878

C	2.176232	3.620686	-1.600282
H	3.074876	3.943255	-1.069029
H	2.384586	3.475415	-2.662636
H	1.415482	4.405028	-1.499937
S	3.118072	-0.703836	-0.302525
C	3.355306	-2.191965	0.725422
H	2.666888	-2.993042	0.446756
H	4.388680	-2.529577	0.614490
H	3.173163	-1.893125	1.758766
C	3.304850	-1.370689	-1.993545
H	2.615488	-2.195386	-2.186640
H	3.099758	-0.551494	-2.686140
H	4.335962	-1.708394	-2.123896
O	0.860909	-0.409055	1.938648
C	-0.093742	-1.022020	2.642002
O	-1.182126	-1.364097	2.212091
C	0.343320	-1.225659	4.083271
H	-0.192462	-2.080303	4.502093
H	1.422593	-1.370597	4.169055
H	0.074778	-0.329788	4.655684

[Pt(bhq)(SMe_2)($OAc)_2$], IMa4

Zero-point correction= 0.355657 (Hartree/Particle)
Thermal correction to Energy= 0.382952
Thermal correction to Enthalpy= 0.383896
Thermal correction to Gibbs Free Energy= 0.295770
Sum of electronic and zero-point Energies= -1608.625925
Sum of electronic and thermal Energies= -1608.598631
Sum of electronic and thermal Enthalpies= -1608.597687
Sum of electronic and thermal Free Energies= -1608.685812
Entropy= 185.476

Pt	0.693649	0.285469	-0.046597
C	-1.086972	1.247356	-0.313115
C	-2.152049	0.477462	0.182522
C	-1.311963	2.494819	-0.849528
C	-3.484036	0.954994	0.167080
C	-1.866103	-0.825146	0.661434
C	-2.645361	2.984557	-0.872448
H	-0.507808	3.102768	-1.251060
C	-3.706322	2.244128	-0.373001
C	-4.514733	0.089504	0.680623
C	-2.885731	-1.677623	1.139424
H	-2.829344	3.968696	-1.294435

H	-4.715048	2.646408	-0.403822
C	-4.231096	-1.165421	1.146528
H	-5.540143	0.449069	0.684351
C	-2.505854	-2.970748	1.553643
C	-0.217977	-2.456086	0.983296
H	-5.024912	-1.805246	1.520867
H	-3.255776	-3.662661	1.926838
C	-1.175276	-3.356860	1.469761
H	0.823715	-2.731278	0.893843
H	-0.855709	-4.348827	1.769160
N	-0.561038	-1.224167	0.602101
S	3.118185	-0.703733	0.302460
C	3.304776	-1.370222	1.993646
H	2.614965	-2.194465	2.187062
H	4.335713	-1.708457	2.124013
H	3.100205	-0.550699	2.686007
C	3.355187	-2.192091	-0.725213
H	2.666721	-2.993052	-0.446333
H	3.172954	-1.893416	-1.758589
H	4.388536	-2.529793	-0.614335
O	1.019069	1.482492	1.693683
C	1.645558	2.366438	1.000585
O	1.763795	2.100661	-0.252237
C	2.176252	3.620613	1.600329
H	1.415404	4.404916	1.500519
H	2.385128	3.475033	2.662539
H	3.074637	3.943434	1.068773
O	0.860756	-0.409174	-1.938738
C	-0.093766	-1.022617	-2.641817
O	-1.181909	-1.365160	-2.211641
C	0.342996	-1.226152	-4.083196
H	1.422382	-1.369962	-4.169399
H	-0.192088	-2.081416	-4.501645
H	0.073270	-0.330677	-4.655681

[Pt(bhq)(SMe_2)($OAc)_2$], IMa5

Zero-point correction=	0.356152 (Hartree/Particle)
Thermal correction to Energy=	0.382930
Thermal correction to Enthalpy=	0.383875
Thermal correction to Gibbs Free Energy=	0.298614
Sum of electronic and zero-point Energies=	-1608.610120
Sum of electronic and thermal Energies=	-1608.583342
Sum of electronic and thermal Enthalpies=	-1608.582398

Sum of electronic and thermal Free Energies=			-1608.667658
Entropy=			179.446
Pt	-0.537480	-0.033283	-0.407047
C	0.997998	1.314213	-0.318713
C	2.246258	0.650985	-0.226883
C	0.978462	2.694923	-0.406608
C	3.477118	1.353762	-0.226882
C	2.256571	-0.770953	-0.178442
C	2.201535	3.410968	-0.418224
H	0.046529	3.245429	-0.448103
C	3.424721	2.765650	-0.319943
C	4.698236	0.594415	-0.151224
C	3.459164	-1.510374	-0.127942
H	2.170089	4.494188	-0.495256
H	4.347933	3.338493	-0.316466
C	4.693971	-0.773664	-0.101782
H	5.642255	1.132677	-0.146120
C	3.350054	-2.918687	-0.138406
C	0.946468	-2.717607	-0.267497
H	5.628259	-1.325819	-0.058465
H	4.247731	-3.529559	-0.097730
C	2.099157	-3.515878	-0.219027
H	-0.051427	-3.133186	-0.347700
H	1.992251	-4.594542	-0.248153
N	1.036386	-1.383869	-0.226760
O	-2.019340	1.233645	-0.955455
C	-2.460186	2.264124	-0.252172
O	-1.995161	2.605905	0.833052
C	-3.623434	2.964614	-0.921567
H	-4.539301	2.399397	-0.711191
H	-3.728616	3.971473	-0.512781
H	-3.494609	3.002183	-2.006282
S	-1.112284	0.130555	1.847472
C	-0.691180	-1.472205	2.602378
H	0.377680	-1.681224	2.557971
H	-1.012919	-1.380568	3.646572
H	-1.294745	-2.232727	2.109451
C	0.088614	1.182146	2.728985
H	1.111587	0.816774	2.638333
H	-0.023674	2.190463	2.336337
H	-0.234632	1.146657	3.776047
O	-1.873427	-1.627185	-0.931472
C	-2.999464	-1.886151	-0.309934
O	-3.262267	-1.476219	0.826421

C	-3.962578	-2.748544	-1.103109
H	-3.433422	-3.563150	-1.606658
H	-4.740927	-3.148987	-0.450500
H	-4.432059	-2.133311	-1.880256

[Pt(bhq)(SMe_2)($OAc)_2$], IMa6

Zero-point correction= 0.356811 (Hartree/Particle)
Thermal correction to Energy= 0.383380
Thermal correction to Enthalpy= 0.384324
Thermal correction to Gibbs Free Energy= 0.299241
Sum of electronic and zero-point Energies= -1608.632088
Sum of electronic and thermal Energies= -1608.605520
Sum of electronic and thermal Enthalpies= -1608.604575
Sum of electronic and thermal Free Energies= -1608.689658
Entropy= 179.071

Pt	0.622874	0.235112	0.054303
C	-1.112363	1.248316	-0.319311
C	-2.229514	0.463204	0.040019
C	-1.308958	2.530018	-0.791900
C	-3.557547	0.946808	-0.057614
C	-1.994806	-0.850703	0.529038
C	-2.633788	3.026613	-0.906245
H	-0.474035	3.163261	-1.076749
C	-3.735108	2.261903	-0.549026
C	-4.628523	0.074059	0.352310
C	-3.047770	-1.696512	0.943484
H	-2.782202	4.035716	-1.280725
H	-4.737782	2.669974	-0.641471
C	-4.388854	-1.185468	0.832415
H	-5.649709	0.438665	0.280438
C	-2.692788	-2.966588	1.447251
C	-0.358250	-2.445301	1.097161
H	-5.212848	-1.820710	1.144220
H	-3.468227	-3.651069	1.779999
C	-1.355193	-3.332625	1.528779
H	0.701392	-2.668379	1.154495
H	-1.059934	-4.297173	1.926667
N	-0.689897	-1.251287	0.595975
S	0.800435	-0.504538	-2.211714
C	1.163488	-2.292223	-2.232981
H	0.403037	-2.855941	-1.690927
H	1.172282	-2.588147	-3.286110
H	2.154037	-2.422322	-1.803207

C	-0.867064	-0.554781	-2.961072
H	-1.547304	-1.193385	-2.395790
H	-1.247737	0.464905	-3.013390
H	-0.732991	-0.949546	-3.972463
O	0.877703	1.393174	1.838114
C	1.658028	2.201203	1.218831
O	1.821746	1.957143	-0.035374
C	2.351478	3.325775	1.902214
H	2.508815	4.152325	1.204887
H	1.774500	3.654590	2.769530
H	3.331643	2.974382	2.247471
O	2.299732	-0.902083	0.793975
C	3.409748	-0.967975	0.099577
O	3.501770	-0.626774	-1.085803
C	4.598061	-1.505171	0.877537
H	4.307083	-2.357424	1.498826
H	5.400787	-1.790455	0.194668
H	4.968117	-0.721366	1.549528

[Pt(bhq)(SMe_2)($OAc)_2$],IMa7

Zero-point correction=	0.355817 (Hartree/Particle)
Thermal correction to Energy=	0.379492
Thermal correction to Enthalpy=	0.380436
Thermal correction to Gibbs Free Energy=	0.303192
Sum of electronic and zero-point Energies=	-1608.629871
Sum of electronic and thermal Energies=	-1608.606195
Sum of electronic and thermal Enthalpies=	-1608.605251
Sum of electronic and thermal Free Energies=	-1608.682495
Entropy=	162.573

Pt	0.749067	-0.448973	-0.389114
C	-0.089003	0.639724	1.117712
C	-1.467850	0.806669	0.915025
C	0.553695	1.146327	2.218861
C	-2.254821	1.525230	1.847270
C	-2.072928	0.194077	-0.209408
C	-0.235252	1.872141	3.153016
H	1.617223	1.029908	2.382495
C	-1.596906	2.065267	2.977750
C	-3.668939	1.626850	1.586433
C	-3.462511	0.268528	-0.437904
H	0.260307	2.283410	4.027804
H	-2.166371	2.623328	3.715518
C	-4.247552	1.028332	0.499689

H	-4.283996	2.184266	2.287556
C	-3.963801	-0.434431	-1.554631
C	-1.722877	-1.181214	-2.065483
H	-5.318284	1.107492	0.335915
H	-5.027698	-0.416125	-1.774246
C	-3.095319	-1.162103	-2.358247
H	-1.016139	-1.744547	-2.665873
H	-3.457789	-1.724095	-3.211844
N	-1.235709	-0.503719	-1.023820
O	2.682219	-0.638692	0.203558
C	3.519791	0.360656	0.427680
O	3.200539	1.547540	0.411159
C	4.925390	-0.123662	0.719344
H	5.332170	-0.628998	-0.163567
H	5.560639	0.724276	0.980722
H	4.914061	-0.851228	1.536963
S	1.300524	1.546126	-1.700968
C	0.125445	1.586994	-3.101127
H	-0.908449	1.684066	-2.766463
H	0.399724	2.442954	-3.724260
H	0.259134	0.670352	-3.679010
C	0.819610	3.081805	-0.840465
H	-0.235923	3.067623	-0.565334
H	1.459336	3.160560	0.036517
H	1.024220	3.901069	-1.534926
O	0.669304	-2.294074	0.458784
C	-0.366870	-2.834607	1.096522
O	-1.438986	-2.283366	1.298859
C	-0.040416	-4.238105	1.577893
H	0.663567	-4.175744	2.415540
H	-0.956394	-4.728271	1.913374
H	0.437086	-4.824555	0.787759

[Pt(Ph-H)(bhq)(SMe_2)($OAc)_2$], TSAB

Zero-point correction=	0.455079 (Hartree/Particle)
Thermal correction to Energy=	0.487013
Thermal correction to Enthalpy=	0.487958
Thermal correction to Gibbs Free Energy=	0.390802
Sum of electronic and zero-point Energies=	-1840.764527
Sum of electronic and thermal Energies=	-1840.732593
Sum of electronic and thermal Enthalpies=	-1840.731648
Sum of electronic and thermal Free Energies=	-1840.828804
Entropy=	204.481

Pt	-0.583055	-0.047358	0.151815
C	1.076877	0.388747	1.262857
C	2.247551	-0.102840	0.640938
C	1.197311	1.066440	2.460851
C	3.531789	0.039350	1.225614
C	2.120510	-0.746817	-0.620487
C	2.473694	1.219691	3.058568
H	0.341631	1.506888	2.963273
C	3.619066	0.713517	2.465642
C	4.665167	-0.503785	0.521281
C	3.237732	-1.275268	-1.306100
H	2.546185	1.750309	4.004077
H	4.586828	0.838884	2.943408
C	4.527849	-1.133459	-0.685258
H	5.649450	-0.403497	0.971002
C	2.995968	-1.898372	-2.549005
C	0.638503	-1.440499	-2.298893
H	5.396701	-1.536745	-1.197710
H	3.824769	-2.318358	-3.112542
C	1.700925	-1.978534	-3.040273
H	-0.391509	-1.510085	-2.622994
H	1.486149	-2.464721	-3.985473
N	0.862782	-0.828453	-1.136167
C	-0.385048	1.967367	-0.777905
C	0.421144	2.050641	-1.957156
C	-0.330190	3.078664	0.119103
C	1.211921	3.159073	-2.221529
H	0.372486	1.253510	-2.691176
C	0.457450	4.190188	-0.147370
H	-0.941697	3.075734	1.015205
C	1.239841	4.225011	-1.309934
H	1.799462	3.206934	-3.133554
H	0.469753	5.028664	0.542602
H	1.861976	5.092173	-1.514757
O	-2.206127	-0.679901	-1.205627
C	-2.934874	0.140082	-1.868842
C	-3.960273	-0.453593	-2.811364
H	-4.096530	-1.520367	-2.625730
H	-4.911437	0.076906	-2.708870
H	-3.615206	-0.310043	-3.842322
O	-2.841169	1.397681	-1.782575
H	-1.522676	1.726383	-1.133828
S	-2.144564	0.787465	1.823799
C	-2.028682	-0.322532	3.270698

H	-2.751688	0.049100	4.001602
H	-2.242203	-1.348178	2.974659
H	-1.019042	-0.256987	3.675694
C	-3.835140	0.375254	1.273484
H	-4.500191	0.593010	2.113153
H	-4.077467	1.024566	0.432503
H	-3.896739	-0.676117	0.989927
O	-0.750330	-1.871788	1.186964
C	-0.722871	-3.072641	0.630165
O	-0.551128	-3.317755	-0.557111
C	-0.956464	-4.168782	1.664078
H	-2.024976	-4.213883	1.906736
H	-0.650988	-5.131425	1.248511
H	-0.409710	-3.966301	2.589260

[Pt(Ph-H)(bhq)(SMe_2)($OAc)_2$], TSAB2

Zero-point correction=	0.455705 (Hartree/Particle)
Thermal correction to Energy=	0.487327
Thermal correction to Enthalpy=	0.488271
Thermal correction to Gibbs Free Energy=	0.393150
Sum of electronic and zero-point Energies=	-1840.776822
Sum of electronic and thermal Energies=	-1840.745200
Sum of electronic and thermal Enthalpies=	-1840.744256
Sum of electronic and thermal Free Energies=	-1840.839377
Entropy=	200.199

Pt	0.541938	-0.102466	-0.088370
C	-1.017052	0.322211	-1.322995
C	-2.247294	-0.057510	-0.740490
C	-1.013832	0.895313	-2.579795
C	-3.488256	0.145181	-1.396169
C	-2.219336	-0.693601	0.531998
C	-2.246216	1.101450	-3.249434
H	-0.084162	1.192179	-3.054210
C	-3.459370	0.744489	-2.676809
C	-4.688598	-0.282962	-0.723271
C	-3.400892	-1.127614	1.176246
H	-2.234338	1.552600	-4.238053
H	-4.389603	0.916851	-3.211259
C	-4.650973	-0.888554	0.503749
H	-5.643790	-0.120532	-1.215834
C	-3.255708	-1.772346	2.423108
C	-0.859594	-1.505952	2.263972
H	-5.569417	-1.207706	0.988142

H	-4.135952	-2.121286	2.956282
C	-1.988608	-1.963267	2.960087
H	0.150880	-1.623485	2.640234
H	-1.851931	-2.460488	3.914196
N	-0.985623	-0.887158	1.086014
C	0.337368	1.901679	0.841847
C	-0.427738	1.995493	2.046549
C	0.220245	2.964947	-0.103939
C	-1.231994	3.095465	2.299257
H	-0.330427	1.221270	2.801507
C	-0.580766	4.069368	0.156257
H	0.796555	2.905361	-1.020491
C	-1.314227	4.128143	1.349299
H	-1.786986	3.168407	3.229902
H	-0.645161	4.880991	-0.562399
H	-1.948453	4.988146	1.547873
O	2.023895	-0.719474	1.411127
C	2.906625	0.099256	1.867695
C	4.045401	-0.507270	2.659479
H	4.468876	0.226611	3.348321
H	3.712733	-1.396250	3.201327
H	4.828040	-0.813295	1.954391
O	2.876817	1.342780	1.679138
H	1.490631	1.686802	1.123491
S	0.913110	-2.226988	-1.329757
C	-0.642250	-3.183298	-1.300964
H	-0.447461	-4.131227	-1.810322
H	-0.981192	-3.373200	-0.281172
H	-1.394253	-2.624335	-1.859429
C	1.951924	-3.299871	-0.283471
H	2.063219	-4.251015	-0.811886
H	2.911496	-2.796262	-0.187424
H	1.494618	-3.454617	0.694837
O	1.855244	0.854095	-1.347882
C	3.034039	0.349013	-1.670503
O	3.432841	-0.765841	-1.345892
C	3.869291	1.318007	-2.487143
H	4.314940	2.057883	-1.811538
H	4.670195	0.775835	-2.993802
H	3.255850	1.855925	-3.215129

[Pt(Ph-H)(bhq)(SMe_2)($OAc)_2$], TSAB3

Zero-point correction= 0.453566 (Hartree/Particle)

Thermal correction to Energy= 0.485981

Thermal correction to Enthalpy= 0.486925
Thermal correction to Gibbs Free Energy= 0.388149
Sum of electronic and zero-point Energies= -1840.760278
Sum of electronic and thermal Energies= -1840.727863
Sum of electronic and thermal Enthalpies= -1840.726919
Sum of electronic and thermal Free Energies= -1840.825695
Entropy= 207.893

Pt	0.553961	-0.093930	-0.090048
C	-2.270666	-0.030193	-0.703777
C	-1.092173	0.982394	-2.454207
C	-3.513057	0.158289	-1.352930
C	-2.180816	-0.673484	0.559131
C	-2.284619	1.200576	-3.158257
H	-0.134223	1.290664	-2.855242
C	-3.493714	0.792411	-2.612038
C	-4.694844	-0.316285	-0.681736
C	-3.356368	-1.137544	1.203671
H	-2.239570	1.687465	-4.126194
H	-4.423306	0.956241	-3.150286
C	-4.617209	-0.932291	0.537612
H	-5.656437	-0.176794	-1.167426
C	-3.204502	-1.775449	2.455411
C	-0.771773	-1.482513	2.343087
H	-5.522939	-1.284359	1.024369
H	-4.080979	-2.144073	2.981158
C	-1.939173	-1.940729	3.002948
H	0.201499	-1.664903	2.782791
H	-1.830688	-2.446420	3.958575
C	0.349937	1.920134	0.832853
C	-0.599467	2.097820	1.884253
C	0.517189	3.009110	-0.074800
C	-1.318580	3.279264	2.022521
H	-0.728994	1.311862	2.620027
C	-0.203870	4.188040	0.059938
H	1.237752	2.936802	-0.883550
C	-1.130909	4.320078	1.104161
H	-2.019413	3.396613	2.843854
H	-0.047876	5.005834	-0.637532
H	-1.696197	5.242189	1.209677
O	2.109718	-0.775452	1.089996
C	2.765694	-0.051712	1.934320
C	3.824877	-0.779456	2.728859
H	4.036068	-1.760213	2.300813

H	4.733241	-0.172411	2.774116
H	3.459371	-0.907794	3.754480
O	2.569596	1.173333	2.129342
H	1.410506	1.579666	1.366924
S	2.368103	0.700927	-1.850715
C	3.035689	-0.831636	-2.581733
H	3.854334	-0.560184	-3.253035
H	3.382700	-1.504438	-1.795156
H	2.230455	-1.305092	-3.142918
C	3.865677	1.323520	-1.007502
H	4.580597	1.637888	-1.771853
H	3.589708	2.180996	-0.391548
H	4.305679	0.543307	-0.383448
O	0.556424	-1.862752	-1.215135
C	0.665615	-3.087031	-0.715189
O	0.812323	-3.373936	0.463742
C	0.554929	-4.142356	-1.810548
H	1.102831	-3.848821	-2.710401
H	0.930673	-5.096602	-1.435234
H	-0.499671	-4.260836	-2.086539
C	-0.907553	-0.843125	1.130251
N	-1.094293	0.385506	-1.258939

[Pt(Ph)(bhq)(SMe_2)(OAc)], IMb1

Zero-point correction=	0.394894 (Hartree/Particle)
Thermal correction to Energy=	0.422162
Thermal correction to Enthalpy=	0.423106
Thermal correction to Gibbs Free Energy=	0.335847
Sum of electronic and zero-point Energies=	-1611.755869
Sum of electronic and thermal Energies=	-1611.728601
Sum of electronic and thermal Enthalpies=	-1611.727656
Sum of electronic and thermal Free Energies=	-1611.814916
Entropy=	183.652

Pt	-0.630783	-0.164272	-0.369515
C	0.597361	-0.485304	1.214340
C	1.925846	-0.147568	0.893271
C	0.268096	-1.001752	2.445303
C	2.967756	-0.308311	1.841171
C	2.220617	0.334965	-0.408539
C	1.309814	-1.156802	3.398082
H	-0.739980	-1.302597	2.703731
C	2.623603	-0.817628	3.114893

C	4.304409	0.047346	1.435500
C	3.535471	0.665638	-0.801385
H	1.054643	-1.559817	4.374054
H	3.395913	-0.951066	3.867060
C	4.578978	0.510572	0.177284
H	5.108867	-0.066759	2.156976
C	3.713096	1.113320	-2.128623
C	1.342025	0.857585	-2.509955
H	5.596675	0.765261	-0.104262
H	4.705234	1.380581	-2.481605
C	2.619299	1.204214	-2.978801
H	0.464167	0.914553	-3.144688
H	2.730027	1.539840	-4.003954
N	1.164429	0.441069	-1.256958
S	-2.660659	-0.919017	0.690911
C	-3.730430	0.528142	1.026824
H	-3.898376	1.127012	0.130836
H	-4.675343	0.130577	1.407809
H	-3.249455	1.132633	1.796201
C	-3.619733	-1.669192	-0.672462
H	-3.708290	-0.977588	-1.513138
H	-3.103420	-2.583960	-0.956780
H	-4.609842	-1.906655	-0.273988
O	-0.116837	-2.070982	-1.258164
C	-0.428918	-3.229954	-0.736106
O	-1.182468	-3.377860	0.234210
C	0.222404	-4.414497	-1.431542
H	1.304705	-4.388985	-1.258607
H	-0.180725	-5.352319	-1.044341
H	0.064521	-4.358027	-2.513540
C	-0.990132	1.800837	0.114286
C	-1.580161	2.545965	-0.916770
C	-0.680587	2.431763	1.323259
C	-1.875411	3.903305	-0.736946
H	-1.823653	2.081129	-1.872697
C	-0.974020	3.790996	1.500157
H	-0.217097	1.884555	2.137538
C	-1.572424	4.529060	0.475584
H	-2.337058	4.464566	-1.545331
H	-0.730300	4.269432	2.445410
H	-1.797918	5.582211	0.618329

[Pt(Ph)(bhq)(SMe_2)(OAc)], IMb2

Zero-point correction= 0.394540 (Hartree/Particle)

Thermal correction to Energy= 0.422059
Thermal correction to Enthalpy= 0.423004
Thermal correction to Gibbs Free Energy= 0.335098
Sum of electronic and zero-point Energies= -1611.757548
Sum of electronic and thermal Energies= -1611.730029
Sum of electronic and thermal Enthalpies= -1611.729084
Sum of electronic and thermal Free Energies= -1611.816991
Entropy= 185.014

Pt	-0.607340	0.050668	-0.497513
C	0.326266	-0.324832	1.269575
C	1.720704	-0.429668	1.107453
C	-0.255800	-0.468430	2.507477
C	2.574370	-0.684477	2.209454
C	2.261552	-0.316358	-0.197234
C	0.596630	-0.720625	3.615436
H	-1.328205	-0.422273	2.651760
C	1.973412	-0.821290	3.482063
C	3.988006	-0.794500	1.948478
C	3.644787	-0.448684	-0.448229
H	0.141259	-0.835876	4.595012
H	2.594218	-1.011263	4.353054
C	4.501743	-0.682557	0.684318
H	4.654011	-0.978598	2.787150
C	4.061476	-0.352931	-1.793064
C	1.760865	-0.036524	-2.460813
H	5.570501	-0.777199	0.515734
H	5.115001	-0.443634	-2.042678
C	3.118603	-0.154273	-2.793893
H	0.997979	0.113735	-3.217745
H	3.411041	-0.088213	-3.836046
N	1.354944	-0.105012	-1.189995
O	-2.562855	0.372238	-0.061168
C	-3.360576	-0.390020	0.669297
O	-3.005967	-1.404031	1.265269
C	-4.778320	0.147300	0.716709
H	-5.130397	0.409851	-0.285380
H	-5.440399	-0.594296	1.167543
H	-4.798573	1.061791	1.320927
S	-0.827542	-2.458826	-1.251443
C	-0.716099	-3.518489	0.233698
H	-1.447899	-3.189675	0.972101
H	-0.891073	-4.553764	-0.070204
H	0.297485	-3.423739	0.628704

C	-2.551555	-2.772246	-1.766960
H	-3.231377	-2.610831	-0.930182
H	-2.783603	-2.087790	-2.586030
H	-2.622764	-3.802535	-2.124953
C	-0.384407	2.067220	-0.161073
C	0.218252	2.845742	-1.155019
C	-0.907757	2.675350	0.983777
C	0.279025	4.238768	-1.008910
H	0.633438	2.398772	-2.052557
C	-0.830653	4.064462	1.129674
H	-1.385672	2.085555	1.757507
C	-0.238891	4.849243	0.134713
H	0.737362	4.837072	-1.792087
H	-1.239724	4.530296	2.022448
H	-0.183263	5.928045	0.250655

[Pt(Ph)(bhq)(SMe_2)(OAc)], IMb3

Zero-point correction=	0.395335 (Hartree/Particle)
Thermal correction to Energy=	0.422461
Thermal correction to Enthalpy=	0.423406
Thermal correction to Gibbs Free Energy=	0.336974
Sum of electronic and zero-point Energies=	-1611.758430
Sum of electronic and thermal Energies=	-1611.731304
Sum of electronic and thermal Enthalpies=	- 1611.730359
Sum of electronic and thermal Free Energies=	-1611.816791
Entropy=	185.910

Pt	-0.605249	0.052467	-0.504349
C	1.727904	-0.431093	1.092208
C	-0.244085	-0.472302	2.498514
C	2.585090	-0.688047	2.190974
C	2.264560	-0.315384	-0.213999
C	0.611884	-0.726654	3.603248
H	-1.316015	-0.426318	2.646336
C	1.988219	-0.827194	3.465253
C	3.997867	-0.797709	1.925241
C	3.646966	-0.447365	-0.469695
H	0.159658	-0.843701	4.584067
H	2.611808	-1.018858	4.333882
C	4.507542	-0.683441	0.659646
H	4.666552	-0.983442	2.761417
C	4.059332	-0.349126	-1.815683

C	1.756613	-0.031256	-2.475425
H	5.575742	-0.777864	0.487444
H	5.112039	-0.439456	-2.068858
C	3.113260	-0.148504	-2.813096
H	0.991309	0.120493	-3.229613
H	3.402348	-0.080515	-3.856059
O	-2.559317	0.373396	-0.061106
C	-3.354756	-0.390159	0.670493
O	-2.998329	-1.405319	1.263416
C	-4.772288	0.147201	0.723478
H	-5.127564	0.411664	-0.276978
H	-5.432984	-0.595180	1.175049
H	-4.790506	1.060558	1.329473
S	-0.828122	-2.455587	-1.262273
C	-0.712000	-3.518046	0.220510
H	-1.441386	-3.190552	0.961882
H	-0.888052	-4.552733	-0.084769
H	0.302860	-3.424130	0.612427
C	-2.553816	-2.767882	-1.772823
H	-3.230924	-2.607976	-0.933559
H	-2.788434	-2.081869	-2.589856
H	-2.626278	-3.797491	-2.132518
C	-0.381037	2.068364	-0.164845
C	0.218494	2.848695	-1.159264
C	-0.900639	2.674392	0.982824
C	0.279872	4.241439	-1.010737
H	0.630744	2.403372	-2.058971
C	-0.822930	4.063220	1.131078
H	-1.376117	2.083189	1.756981
C	-0.234299	4.849813	0.135691
H	0.735743	4.841170	-1.794262
H	-1.229079	4.527415	2.026037
H	-0.178193	5.928391	0.253477
C	1.354780	-0.102092	-1.203437
N	0.334006	-0.326434	1.259016

[Pt(Ph)(bhq)(SMe_2)(OAc)], IMb4

Zero-point correction=	0.394976 (Hartree/Particle)
Thermal correction to Energy=	0.421970
Thermal correction to Enthalpy=	0.422914
Thermal correction to Gibbs Free Energy=	0.337250
Sum of electronic and zero-point Energies=	-1611.732787
Sum of electronic and thermal Energies=	-1611.705793

Sum of electronic and thermal Enthalpies= -1611.704849
Sum of electronic and thermal Free Energies= -1611.790513
Entropy= 180.295

Pt	-0.423520	-0.158416	-0.169878
C	0.903354	1.388723	-0.006794
C	2.251512	0.970319	-0.182618
C	0.639801	2.738910	0.165436
C	3.321735	1.904789	-0.182576
C	2.544285	-0.414221	-0.406473
C	1.699824	3.677280	0.162301
H	-0.375414	3.096700	0.296047
C	3.014799	3.274568	0.002340
C	4.664051	1.424945	-0.385674
C	3.867963	-0.866598	-0.621941
H	1.468713	4.731348	0.289830
H	3.818985	4.005442	0.009346
C	4.930453	0.100428	-0.594010
H	5.475556	2.147893	-0.380798
C	4.048410	-2.246082	-0.871932
C	1.667251	-2.561400	-0.691586
H	5.949763	-0.239321	-0.754638
H	5.049024	-2.634691	-1.042207
C	2.949828	-3.091140	-0.912497
H	0.774196	-3.177418	-0.727803
H	3.061389	-4.150479	-1.117002
N	1.481548	-1.266733	-0.432545
S	-0.745091	-0.357033	2.121876
C	-0.196399	-2.042772	2.547476
H	0.839045	-2.202030	2.246124
H	-0.294175	-2.112978	3.636143
H	-0.886390	-2.734146	2.068050
C	0.565600	0.570109	3.002343
H	1.563541	0.263577	2.687494
H	0.413328	1.634169	2.826309
H	0.411842	0.342266	4.062188
O	-1.533188	-1.881416	-0.804001
C	-2.559270	-2.366952	-0.149257
O	-2.841335	-2.056184	1.014791
C	-3.392867	-3.359649	-0.938434
H	-2.761115	-3.998243	-1.562398
H	-3.999869	-3.967523	-0.264227
H	-4.062982	-2.803799	-1.606038
C	-2.108164	0.988622	-0.346141
C	-2.616612	0.943731	-1.650963

C	-2.693988	1.824400	0.606790
C	-3.667275	1.796772	-2.019416
H	-2.219043	0.248335	-2.386895
C	-3.757375	2.655954	0.238269
H	-2.341160	1.856644	1.633392
C	-4.240787	2.649532	-1.074992
H	-4.046459	1.765336	-3.037252
H	-4.203713	3.311065	0.981831
H	-5.070431	3.293189	-1.353484

[Pt(Ph)(bhq)(SMe_2)(OAc)], IMb5

Zero-point correction=	0.395400 (Hartree/Particle)
Thermal correction to Energy=	0.422570
Thermal correction to Enthalpy=	0.423514
Thermal correction to Gibbs Free Energy=	0.336700
Sum of electronic and zero-point Energies=	-1611.770847
Sum of electronic and thermal Energies=	-1611.743678
Sum of electronic and thermal Enthalpies=	-1611.742733
Sum of electronic and thermal Free Energies=	-1611.829548
Entropy=	182.716

Pt	0.548281	-0.179889	0.248220
C	-1.019373	-1.255043	-0.473991
C	-2.253470	-0.682025	-0.106386
C	-1.003877	-2.412569	-1.226082
C	-3.492184	-1.269119	-0.466027
C	-2.232594	0.515177	0.659161
C	-2.234772	-3.009157	-1.598863
H	-0.072384	-2.873013	-1.539447
C	-3.453659	-2.458507	-1.230533
C	-4.701946	-0.621725	-0.027849
C	-3.426368	1.135322	1.096521
H	-2.215340	-3.920960	-2.189598
H	-4.382879	-2.936482	-1.528102
C	-4.673442	0.523462	0.720335
H	-5.655469	-1.066333	-0.300325
C	-3.300698	2.302763	1.877352
C	-0.899241	2.126048	1.712687
H	-5.598017	0.990885	1.046773
H	-4.190599	2.813016	2.235479
C	-2.038443	2.789802	2.188331
H	0.098183	2.492751	1.924202
H	-1.911443	3.682173	2.791237
N	-0.999495	1.024012	0.961102

O	1.105768	-1.965864	1.749244
C	1.852527	-2.370943	0.825017
O	1.923894	-1.654737	-0.264824
C	2.642118	-3.643614	0.896280
H	2.032573	-4.456954	0.483185
H	3.557417	-3.570940	0.303860
H	2.874077	-3.885310	1.935896
S	2.473666	1.300762	1.163956
C	3.204223	0.451285	2.607716
H	3.549029	-0.548660	2.340157
H	4.037535	1.053335	2.978226
H	2.430875	0.379537	3.374950
C	3.824788	1.142332	-0.054680
H	4.023949	0.090243	-0.268105
H	3.503493	1.653162	-0.963846
H	4.713123	1.634173	0.348852
C	0.635059	0.867696	-1.512056
C	0.248643	2.204383	-1.622967
C	1.169206	0.183510	-2.606177
C	0.420103	2.866967	-2.847002
H	-0.172681	2.750169	-0.787770
C	1.333159	0.856572	-3.823380
H	1.469844	-0.855168	-2.521636
C	0.959929	2.197732	-3.947028
H	0.125780	3.910089	-2.928466
H	1.752203	0.322282	-4.671981
H	1.087189	2.715826	-4.893316

[Pt(Ph)(bhq)(SMe_2)(OAc)], IMb6

Zero-point correction=	0.395788 (Hartree/Particle)
Thermal correction to Energy=	0.422727
Thermal correction to Enthalpy=	0.423671
Thermal correction to Gibbs Free Energy=	0.337438
Sum of electronic and zero-point Energies=	-1611.775427
Sum of electronic and thermal Energies=	-1611.748488
Sum of electronic and thermal Enthalpies=	-1611.747544
Sum of electronic and thermal Free Energies=	-1611.833777
Entropy=	181.492

Pt	-0.594170	0.194954	-0.185735
C	0.884940	-0.784048	-1.187000
C	2.160313	-0.348624	-0.758304
C	0.802014	-1.697605	-2.220971
C	3.357795	-0.828464	-1.346369

C	2.230849	0.610861	0.288741
C	1.991171	-2.178887	-2.825080
H	-0.151078	-2.073565	-2.579842
C	3.243654	-1.763828	-2.400988
C	4.611847	-0.332357	-0.839264
C	3.465152	1.092313	0.780418
H	1.908587	-2.895607	-3.637621
H	4.140617	-2.152747	-2.874953
C	4.667142	0.581061	0.177606
H	5.531398	-0.701133	-1.285809
C	3.418071	2.042339	1.822904
C	1.006409	1.952833	1.769006
H	5.624600	0.940284	0.543787
H	4.342289	2.438441	2.234751
C	2.191857	2.467663	2.314744
H	0.028535	2.265392	2.116464
H	2.128541	3.196704	3.114998
N	1.039971	1.052762	0.783829
O	-1.982049	1.779893	0.618293
C	-1.726890	2.583383	-0.352688
O	-0.942790	2.195379	-1.276424
C	-2.327898	3.961087	-0.372265
H	-1.665270	4.642918	0.175267
H	-2.417286	4.326920	-1.397719
H	-3.301485	3.964914	0.123890
S	-2.373777	-0.940898	-1.322322
C	-3.808041	-0.863707	-0.192879
H	-3.985840	0.163414	0.128765
H	-4.668512	-1.264483	-0.734769
H	-3.579740	-1.499053	0.663708
C	-2.936125	0.157011	-2.669562
H	-3.285419	1.111765	-2.277128
H	-2.092864	0.314025	-3.343759
H	-3.741512	-0.365117	-3.192660
C	-0.670440	-1.285054	1.240357
C	-1.192609	-0.858614	2.466374
C	-0.293412	-2.616931	1.056701
C	-1.337740	-1.775093	3.515504
H	-1.506119	0.171634	2.611322
C	-0.444297	-3.526416	2.113312
H	0.112072	-2.962879	0.113560
C	-0.961576	-3.109947	3.341895
H	-1.746327	-1.437448	4.464409
H	-0.150957	-4.562566	1.965664

H	-1.072771	-3.819215	4.157276

[Pt(Ph)(bhq)(SMe_2)(OAc)], IMb7

Zero-point correction=	0.394753 (Hartree/Particle)
Thermal correction to Energy=	0.422193
Thermal correction to Enthalpy=	0.423137
Thermal correction to Gibbs Free Energy=	0.335866
Sum of electronic and zero-point Energies=	-1611.756943
Sum of electronic and thermal Energies=	-1611.729503
Sum of electronic and thermal Enthalpies=	-1611.728559
Sum of electronic and thermal Free Energies=	-1611.815830
Entropy=	183.677

Pt	-0.425197	0.038734	-0.524494
C	1.056008	-1.353390	-0.489388
C	2.327561	-0.764913	-0.332496
C	0.948235	-2.723461	-0.624675
C	3.512094	-1.542963	-0.299290
C	2.407755	0.652510	-0.247909
C	2.124352	-3.513682	-0.594241
H	-0.018058	-3.197308	-0.757893
C	3.378697	-2.945614	-0.427652
C	4.771023	-0.860164	-0.151184
C	3.653096	1.313098	-0.129473
H	2.033238	-4.591164	-0.700999
H	4.265383	-3.572956	-0.400671
C	4.840867	0.503390	-0.069029
H	5.681123	-1.452908	-0.113506
C	3.638994	2.723174	-0.098551
C	1.236656	2.674731	-0.314738
H	5.801145	1.000631	0.033198
H	4.571993	3.272337	-0.005788
C	2.431701	3.398667	-0.200129
H	0.282393	3.179693	-0.402960
H	2.389112	4.482265	-0.193283
N	1.224264	1.336490	-0.324137
S	-2.087101	2.058897	-0.835863
C	-3.210747	1.611519	-2.204554
H	-3.815405	0.747066	-1.927997
H	-3.848904	2.471079	-2.424161
H	-2.595735	1.384463	-3.078315
C	-3.267168	2.254694	0.545450
H	-3.809145	1.322288	0.699022
H	-2.690098	2.509282	1.436099

H	-3.938163	3.081036	0.297142
O	-1.733098	-1.441757	-1.027938
C	-2.993657	-1.574969	-0.641983
O	-3.578777	-0.820691	0.125603
C	-3.641543	-2.811315	-1.240779
H	-3.323933	-3.691429	-0.668249
H	-4.728121	-2.726552	-1.174730
H	-3.333055	-2.961242	-2.278950
C	-0.604437	-0.144764	1.513038
C	-0.399269	0.976469	2.313568
C	-0.948958	-1.381376	2.053577
C	-0.581038	0.856802	3.699297
H	-0.110662	1.935502	1.901888
C	-1.123972	-1.480558	3.439723
H	-1.092201	-2.254527	1.431037
C	-0.943152	-0.367045	4.263530
H	-0.431924	1.732238	4.325733
H	-1.403291	-2.440549	3.865231
H	-1.080145	-0.453723	5.337454

[Pt(Ph)(bhq)(SMe_2)(OAc)], IMb8

Zero-point correction=	0.394355 (Hartree/Particle)
Thermal correction to Energy=	0.421818
Thermal correction to Enthalpy=	0.422763
Thermal correction to Gibbs Free Energy=	0.334416
Sum of electronic and zero-point Energies=	-1611.751257
Sum of electronic and thermal Energies=	-1611.723794
Sum of electronic and thermal Enthalpies=	-1611.722850
Sum of electronic and thermal Free Energies=	-1611.811196
Entropy=	185.940

Pt	0.492125	0.345728	-0.314033
C	-0.557377	-0.820133	0.989330
C	-1.953349	-0.719832	0.806526
C	-0.014137	-1.663904	1.930918
C	-2.831148	-1.482041	1.627605
C	-2.498875	0.113927	-0.219035
C	-0.892955	-2.409408	2.754173
H	1.053598	-1.798298	2.031402
C	-2.267807	-2.322350	2.614073
C	-4.248986	-1.370998	1.398761
C	-3.894972	0.191486	-0.439848
H	-0.462851	-3.074258	3.497778
H	-2.921868	-2.912101	3.250242

C	-4.761668	-0.576746	0.411788
H	-4.916300	-1.950953	2.030750
C	-4.333375	1.020460	-1.495896
C	-2.037000	1.577593	-1.968000
H	-5.834637	-0.519182	0.251991
H	-5.396074	1.110236	-1.704805
C	-3.404907	1.708589	-2.263095
H	-1.281335	2.099285	-2.548176
H	-3.715046	2.344619	-3.085214
N	-1.605956	0.810461	-0.968214
S	0.616932	2.102099	1.339760
C	1.607805	3.395405	0.508044
H	1.163495	3.670710	-0.450801
H	1.647498	4.261465	1.173795
H	2.612091	2.992906	0.365666
C	-1.003364	2.938465	1.440976
H	-1.334543	3.285192	0.461223
H	-1.716790	2.226239	1.858649
H	-0.888457	3.780837	2.128207
O	0.466857	-0.972503	-1.859562
C	0.794929	-2.263945	-1.791490
O	1.102093	-2.861663	-0.772752
C	0.732370	-2.916417	-3.163209
H	0.984191	-3.974852	-3.076439
H	-0.270503	-2.808193	-3.589673
H	1.434646	-2.425787	-3.845950
C	2.443851	-0.053797	0.139985
C	3.297787	-0.129659	-0.971708
C	2.989648	-0.116884	1.428141
C	4.680519	-0.265000	-0.792709
H	2.896715	-0.100609	-1.980844
C	4.370517	-0.268268	1.601604
H	2.359692	-0.047230	2.309678
C	5.219695	-0.341284	0.493313
H	5.327724	-0.326007	-1.663813
H	4.778451	-0.324711	2.607553
H	6.290557	-0.461135	0.631702

[Pt(Ph)(bhq)(SMe_2)(OAc)], IMb9

Zero-point correction= 0.395116 (Hartree/Particle)

Thermal correction to Energy= 0.422468

Thermal correction to Enthalpy= 0.423412

Thermal correction to Gibbs Free Energy= 0.336263

Sum of electronic and zero-point Energies= -1611.767222
Sum of electronic and thermal Energies= -1611.739870
Sum of electronic and thermal Enthalpies= -1611.738926
Sum of electronic and thermal Free Energies= -1611.826075
Entropy= 183.420

Pt	0.557988	0.231377	0.239073
C	-1.077060	1.308103	-0.286847
C	-2.271065	0.621131	0.012086
C	-1.134211	2.571248	-0.840416
C	-3.545278	1.200111	-0.211616
C	-2.172695	-0.692560	0.545593
C	-2.402200	3.162390	-1.071408
H	-0.231380	3.114881	-1.098316
C	-3.582959	2.501877	-0.763980
C	-4.710528	0.426860	0.132260
C	-3.324224	-1.447142	0.870330
H	-2.442646	4.159221	-1.501838
H	-4.541390	2.978571	-0.949991
C	-4.608017	-0.835684	0.650142
H	-5.691015	0.866906	-0.029312
C	-3.123666	-2.745448	1.384414
C	-0.740340	-2.423179	1.196586
H	-5.500218	-1.401492	0.902430
H	-3.978975	-3.361277	1.648736
C	-1.832794	-3.229458	1.545613
H	0.276121	-2.777791	1.298195
H	-1.648303	-4.225082	1.933660
N	-0.908203	-1.190402	0.710009
S	2.771034	-0.919908	1.014642
C	2.612073	-1.359722	2.780925
H	1.812238	-2.084288	2.948344
H	3.565120	-1.765946	3.128732
H	2.388810	-0.433654	3.314595
C	3.049308	-2.550412	0.240553
H	2.254698	-3.261175	0.478637
H	3.088951	-2.390588	-0.838786
H	4.010542	-2.937960	0.587262
O	1.805022	1.865883	-0.041089
C	1.806296	2.374446	1.161963
O	1.157353	1.789015	2.060342
C	2.567852	3.647482	1.386299
H	2.886527	3.713917	2.428924
H	3.428889	3.711746	0.716748

H	1.905068	4.495624	1.174620
C	0.746776	-0.472321	-1.677664
C	1.835115	0.032333	-2.392922
C	-0.130509	-1.390537	-2.255752
C	2.061445	-0.417725	-3.700483
H	2.500633	0.768355	-1.954517
C	0.107595	-1.828524	-3.566056
H	-0.992366	-1.773594	-1.724403
C	1.201359	-1.348212	-4.289050
H	2.911714	-0.027291	-4.253464
H	-0.575948	-2.544491	-4.014912
H	1.378077	-1.690145	-5.304850

[Pt(Ph-H)(Ph)(bhq)(SMe_2)(OAc)], TSBC

Zero-point correction=	0.494270 (Hartree/Particle)
Thermal correction to Energy=	0.526525
Thermal correction to Enthalpy=	0.527469
Thermal correction to Gibbs Free Energy=	0.429578
Sum of electronic and zero-point Energies=	-1843.890254
Sum of electronic and thermal Energies=	-1843.857999
Sum of electronic and thermal Enthalpies=	-1843.857055
Sum of electronic and thermal Free Energies=	-1843.954946
Entropy=	206.029

Pt	0.389702	-0.223346	-0.160709
C	-0.783024	1.436663	-0.052245
C	-2.157548	1.093328	0.020640
C	-0.445214	2.779751	-0.062777
C	-3.184332	2.071381	0.084687
C	-2.513741	-0.286153	0.043444
C	-1.459254	3.767891	-0.008244
H	0.587913	3.104071	-0.101733
C	-2.802028	3.432063	0.064583
C	-4.551995	1.626863	0.172778
C	-3.858458	-0.713425	0.144737
H	-1.167434	4.814851	-0.018424
H	-3.562924	4.206336	0.112418
C	-4.878335	0.299041	0.204390
H	-5.336020	2.378160	0.220067
C	-4.093741	-2.104706	0.184188
C	-1.716691	-2.490601	0.016775
H	-5.916604	-0.012239	0.277260
H	-5.111295	-2.477355	0.265791
C	-3.025027	-2.988126	0.124681

H	-0.848043	-3.136659	-0.037668
H	-3.178969	-4.061132	0.160348
N	-1.486032	-1.177592	-0.032830
C	2.315035	0.922473	-0.212478
C	2.810668	1.419155	1.032206
C	2.541685	1.738234	-1.364900
C	3.454078	2.647623	1.123017
H	2.713680	0.806251	1.920162
C	3.188927	2.963364	-1.277240
H	2.245878	1.373216	-2.343020
C	3.632006	3.426014	-0.028837
H	3.828679	2.998306	2.080248
H	3.361137	3.556980	-2.170360
H	4.137240	4.385812	0.041520
O	1.304326	-2.221815	-0.477288
C	2.560182	-2.431483	-0.666405
C	2.991898	-3.871442	-0.859948
H	2.158966	-4.495474	-1.191031
H	3.817128	-3.924132	-1.574524
H	3.356292	-4.257423	0.100128
O	3.431269	-1.526347	-0.673020
H	2.745088	-0.187153	-0.407241
C	0.450715	-0.391496	1.914932
C	0.831792	-1.629831	2.443551
C	0.089317	0.644931	2.783170
C	0.864581	-1.822778	3.831874
H	1.108233	-2.448894	1.790524
C	0.121610	0.443949	4.169202
H	-0.203130	1.616100	2.404084
C	0.509344	-0.788687	4.700058
H	1.168788	-2.789635	4.225337
H	-0.157058	1.261901	4.829163
H	0.534061	-0.940772	5.775640
S	0.291783	-0.284691	-2.798003
C	-0.510655	-1.856928	-3.258410
H	-1.533643	-1.902246	-2.878903
H	-0.509629	-1.940804	-4.348136
H	0.085477	-2.661264	-2.825059
C	-0.941231	0.909668	-3.421722
H	-1.016740	0.795087	-4.505999
H	-1.915010	0.748924	-2.954252
H	-0.583249	1.913225	-3.184954

[Pt(Ph-H)(Ph)(bhq)(SMe_2)(OAc)], TSBC1

Zero-point correction=			0.493897 (Hartree/Particle)
Thermal correction to Energy=			0.525790
Thermal correction to Enthalpy=			0.526734
Thermal correction to Gibbs Free Energy=			0.431408
Sum of electronic and zero-point Energies=			-1843.890348
Sum of electronic and thermal Energies=			-1843.858454
Sum of electronic and thermal Enthalpies=			-1843.857510
Sum of electronic and thermal Free Energies=			-1843.952836
Entropy=			200.630
Pt	0.430360	-0.213997	-0.074798
C	-0.865543	1.202899	-0.776212
C	-2.218594	0.767300	-0.739878
C	-0.598663	2.485059	-1.225928
C	-3.277764	1.593614	-1.209832
C	-2.541434	-0.514523	-0.186817
C	-1.645684	3.314521	-1.692330
H	0.410868	2.877594	-1.225547
C	-2.960218	2.880339	-1.699394
C	-4.627529	1.094986	-1.153603
C	-3.879593	-0.980695	-0.122657
H	-1.403971	4.312461	-2.048538
H	-3.754383	3.526071	-2.064434
C	-4.921196	-0.135327	-0.637305
H	-5.425393	1.730378	-1.529511
C	-4.098979	-2.248006	0.459303
C	-1.730306	-2.449515	0.838521
H	-5.947662	-0.489332	-0.598509
H	-5.110627	-2.639287	0.529083
C	-3.025267	-2.982080	0.942116
H	-0.860289	-2.989171	1.198628
H	-3.167227	-3.956439	1.397436
N	-1.503611	-1.254991	0.291513
C	0.300451	0.851558	1.862298
C	-0.869152	0.606159	2.649158
C	0.844343	2.171409	1.911164
C	-1.432971	1.594241	3.443145
H	-1.291420	-0.391961	2.671811
C	0.281230	3.159067	2.709824
H	1.729066	2.404146	1.330704
C	-0.862701	2.875848	3.467083
H	-2.306272	1.375008	4.050643
H	0.723209	4.150707	2.741318
H	-1.306307	3.651499	4.085777

O	1.528090	-1.984311	0.687471
C	2.007829	-2.055116	1.872905
C	2.733429	-3.327625	2.256121
H	2.531930	-3.578582	3.300692
H	2.450848	-4.154908	1.601717
H	3.812239	-3.155830	2.156433
O	1.934559	-1.122249	2.722343
H	1.115512	-0.014181	2.192695
S	0.573987	-1.273503	-2.327186
C	-0.563647	-2.700281	-2.387548
H	-0.408080	-3.196733	-3.349363
H	-0.367282	-3.393540	-1.568135
H	-1.586240	-2.324400	-2.338683
C	2.167140	-2.169480	-2.368988
H	2.196421	-2.738571	-3.301894
H	2.961802	-1.423311	-2.363129
H	2.252170	-2.822078	-1.499810
C	2.199744	0.725548	-0.594574
C	2.359590	1.340437	-1.846210
C	3.308938	0.675546	0.263504
C	3.588700	1.895325	-2.226984
H	1.534483	1.394303	-2.549359
C	4.536752	1.233664	-0.115771
H	3.238308	0.212796	1.241346
C	4.683764	1.847178	-1.362023
H	3.680743	2.363981	-3.203787
H	5.376840	1.183448	0.572684
H	5.636928	2.278924	-1.654681

$[Pt(Ph)_2(bhq)(SMe_2)]$, IMC1

Zero-point correction=	0.433553 (Hartree/Particle)
Thermal correction to Energy=	0.461148
Thermal correction to Enthalpy=	0.462092
Thermal correction to Gibbs Free Energy=	0.374098
Sum of electronic and zero-point Energies=	-1614.875702
Sum of electronic and thermal Energies=	-1614.848106
Sum of electronic and thermal Enthalpies=	-1614.847162
Sum of electronic and thermal Free Energies=	-1614.935156
Entropy=	185.199

Pt	-0.471538	-0.153380	-0.361625
C	0.546194	-0.045399	1.387539
C	1.950213	-0.032798	1.210487
C	-0.000503	0.016398	2.653052

C	2.816220	0.012579	2.337869
C	2.514206	-0.057743	-0.103520
C	0.863852	0.055957	3.774602
H	-1.071075	0.042522	2.811592
C	2.240183	0.051547	3.628185
C	4.238551	0.026758	2.111511
C	3.916467	-0.035961	-0.304007
H	0.423518	0.097297	4.766936
H	2.886045	0.087683	4.501075
C	4.768726	0.005884	0.852373
H	4.895082	0.059718	2.976937
C	4.379200	-0.056041	-1.637729
C	2.093428	-0.129371	-2.389864
H	5.845110	0.021966	0.706128
H	5.447144	-0.035642	-1.838061
C	3.467214	-0.101760	-2.681495
H	1.352853	-0.170600	-3.183535
H	3.793843	-0.117580	-3.715827
N	1.635377	-0.106330	-1.138785
S	-0.495676	-2.761565	-0.431787
C	-1.717227	-3.166568	-1.732082
H	-1.434545	-2.715800	-2.686644
H	-1.779136	-4.253222	-1.830958
H	-2.681048	-2.773380	-1.403632
C	1.028802	-3.413346	-1.198838
H	1.196900	-2.977069	-2.185755
H	1.862173	-3.169937	-0.536641
H	0.939228	-4.499835	-1.279163
C	-0.586896	1.884169	-0.437855
C	-0.282562	2.473457	-1.673411
C	-1.013817	2.693655	0.621695
C	-0.425826	3.855832	-1.852521
H	0.060014	1.873138	-2.511773
C	-1.138902	4.076027	0.444275
H	-1.262904	2.259969	1.583700
C	-0.847916	4.661115	-0.791961
H	-0.195942	4.296595	-2.819295
H	-1.471245	4.692899	1.275389
H	-0.948300	5.734552	-0.926995
C	-2.402796	-0.274372	0.281849
C	-2.825016	-1.161650	1.285653
C	-3.378971	0.451953	-0.423161
C	-4.184773	-1.319406	1.576922
H	-2.103944	-1.750401	1.845084

C	-4.740963	0.279991	-0.140712
H	-3.092939	1.163993	-1.191098
C	-5.148764	-0.599851	0.863968
H	-4.486377	-2.010912	2.359805
H	-5.477232	0.851710	-0.700098
H	-6.204030	-0.721028	1.092698

$[Pt(Ph)_2(bhq)(SMe_2)]$, IMC2

Zero-point correction=	0.433790 (Hartree/Particle)
Thermal correction to Energy=	0.461280
Thermal correction to Enthalpy=	0.462224
Thermal correction to Gibbs Free Energy=	0.374613
Sum of electronic and zero-point Energies=	-1614.872599
Sum of electronic and thermal Energies=	-1614.845110
Sum of electronic and thermal Enthalpies=	-1614.844166
Sum of electronic and thermal Free Energies=	-1614.931776
Entropy=	184.392

Pt	0.397919	-0.161508	-0.314100
C	-0.814888	1.467548	-0.159978
C	-2.192339	1.165719	-0.308069
C	-0.435008	2.784482	0.045929
C	-3.178135	2.190300	-0.262980
C	-2.607907	-0.190450	-0.514317
C	-1.408093	3.809563	0.085048
H	0.607020	3.052545	0.176457
C	-2.754407	3.524411	-0.063519
C	-4.563318	1.833245	-0.419960
C	-3.979183	-0.518238	-0.670777
H	-1.085120	4.835431	0.240351
H	-3.494391	4.319285	-0.024650
C	-4.950904	0.538561	-0.613720
H	-5.307003	2.624963	-0.381099
C	-4.308444	-1.874212	-0.880716
C	-1.968971	-2.411896	-0.767685
H	-6.001105	0.285890	-0.730438
H	-5.349007	-2.162999	-1.003109
C	-3.300815	-2.823062	-0.932085
H	-1.164608	-3.135437	-0.802813
H	-3.518935	-3.873063	-1.095149
N	-1.628073	-1.138985	-0.560397
S	2.099135	-2.154459	-0.589892
C	1.385474	-3.803672	-0.929154
H	0.740455	-3.789068	-1.811020

H	2.211013	-4.502172	-1.090680
H	0.826661	-4.124973	-0.047582
C	2.921820	-1.866691	-2.199692
H	2.195370	-1.878562	-3.016047
H	3.412727	-0.894309	-2.149468
H	3.670249	-2.649097	-2.348380
C	0.357213	-0.354089	1.720579
C	0.014640	-1.612816	2.218133
C	0.652173	0.702189	2.582955
C	-0.008519	-1.820489	3.604058
H	-0.237337	-2.435351	1.558957
C	0.620174	0.480618	3.966043
H	0.912570	1.682535	2.207060
C	0.292871	-0.776042	4.480254
H	-0.267889	-2.804255	3.986194
H	0.853673	1.304333	4.635457
H	0.270749	-0.939538	5.553849
C	2.128791	0.919690	-0.384098
C	2.279876	1.723427	-1.527077
C	3.194094	0.818861	0.520351
C	3.479081	2.406742	-1.765119
H	1.465539	1.829346	-2.240954
C	4.388215	1.513493	0.285685
H	3.110875	0.198792	1.406566
C	4.535770	2.307112	-0.855377
H	3.577541	3.022289	-2.655758
H	5.204655	1.425343	0.998129
H	5.463434	2.844129	-1.033276

$[Pt(Ph)_2(bhq)(SMe_2)]$, IMC3

Zero-point correction=			0.433541 (Hartree/Particle)
Thermal correction to Energy=			0.460893
Thermal correction to Enthalpy=			0.461837
Thermal correction to Gibbs Free Energy=			0.374962
Sum of electronic and zero-point Energies=			-1614.848660
Sum of electronic and thermal Energies=			-1614.821308
Sum of electronic and thermal Enthalpies=			-1614.820364
Sum of electronic and thermal Free Energies=			-1614.907239
Entropy=			182.844
Pt	-0.361108	-0.194521	-0.376544
C	1.556468	-1.056425	-0.682299
C	2.571525	-0.082482	-0.493125
C	1.965231	-2.326402	-1.068399

C	3.953066	-0.360405	-0.674094
C	2.177452	1.238825	-0.117094
C	3.335283	-2.629396	-1.260776
H	1.241263	-3.123920	-1.225853
C	4.316558	-1.670297	-1.065593
C	4.910910	0.692133	-0.459005
C	3.130318	2.269455	0.082409
H	3.619448	-3.633909	-1.564587
H	5.365459	-1.914957	-1.211486
C	4.520881	1.950450	-0.095787
H	5.966114	0.468956	-0.594864
C	2.652083	3.548706	0.433431
C	0.399880	2.702726	0.348205
H	5.255828	2.735381	0.058948
H	3.356430	4.360053	0.596858
C	1.288205	3.764306	0.561946
H	-0.671914	2.831468	0.432498
H	0.890835	4.738621	0.824375
N	0.835888	1.479402	0.025062
S	-1.487108	-2.208378	-1.021103
C	-3.129289	-2.324430	-0.235083
H	-3.746265	-1.463943	-0.491899
H	-3.583033	-3.257030	-0.580779
H	-2.969753	-2.369879	0.843450
C	-1.962485	-1.892979	-2.757005
H	-2.571667	-0.989745	-2.827024
H	-1.043205	-1.786144	-3.336744
H	-2.519021	-2.764507	-3.111609
C	-0.324743	-0.756833	1.600779
C	-0.572418	0.205016	2.578498
C	-0.024855	-2.076822	1.939193
C	-0.536770	-0.175427	3.927504
H	-0.808235	1.229559	2.322514
C	-0.005630	-2.441026	3.292975
H	0.210834	-2.820266	1.187763
C	-0.258564	-1.495038	4.288314
H	-0.734493	0.574778	4.688619
H	0.224068	-3.470299	3.555377
H	-0.233777	-1.782209	5.335506
C	-2.192202	0.902633	-0.333080
C	-2.439741	1.652895	-1.499695
C	-3.168899	0.943396	0.674538
C	-3.608702	2.411068	-1.657196
H	-1.709367	1.666369	-2.311262

C	-4.337907	1.703405	0.530390
H	-3.033881	0.376053	1.592041
C	-4.563533	2.439705	-0.636846
H	-3.766190	2.980338	-2.570538
H	-5.073698	1.716149	1.331500
H	-5.469567	3.029452	-0.748777

$[Pt(Ph)_2(bhq)(SMe_2)]$, TSCA

Zero-point correction=	0.433978 (Hartree/Particle)
Thermal correction to Energy=	0.460553
Thermal correction to Enthalpy=	0.461497
Thermal correction to Gibbs Free Energy=	0.377192
Sum of electronic and zero-point Energies=	-1614.821572
Sum of electronic and thermal Energies=	-1614.794997
Sum of electronic and thermal Enthalpies=	-1614.794053
Sum of electronic and thermal Free Energies=	-1614.878358
Entropy=	177.436

Pt	-0.165809	0.322185	-0.173330
C	-1.807274	-0.043271	1.200757
C	-2.989180	0.695626	1.337132
H	-3.422487	1.220130	0.493346
C	-3.653895	0.725959	2.568498
H	-4.571554	1.301567	2.657687
C	-3.163790	0.005735	3.660675
C	-2.004711	-0.759727	3.509276
H	-1.608911	-1.329557	4.345941
C	-1.334777	-0.804813	2.281059
H	-0.439833	-1.409970	2.194863
C	-1.988547	-0.857758	-0.810575
C	-2.381878	-0.335234	-2.054780
C	-3.212015	-1.069276	-2.912879
C	-3.697419	-2.320596	-2.533406
C	-3.349378	-2.828732	-1.279835
C	-2.516808	-2.101189	-0.424064
H	-2.035993	0.628719	-2.406082
H	-3.472632	-0.647649	-3.880256
H	-3.741802	-3.785958	-0.946362
H	-2.329301	-2.503298	0.565489
H	-4.350730	-2.882283	-3.194941
H	-3.687071	0.026629	4.612200
N	1.021560	-1.459852	-0.014024
C	2.366048	-1.203130	0.061233
C	0.612769	-2.732420	-0.030428

C	2.760575	0.163391	0.001332
C	3.322525	-2.243837	0.175586
C	1.499032	-3.814372	0.068731
H	-0.445836	-2.905890	-0.132289
C	4.142797	0.482527	0.096440
C	1.746887	1.149869	-0.156762
C	4.711380	-1.889134	0.266381
C	2.856281	-3.574033	0.182837
H	1.098322	-4.822069	0.053213
C	4.520823	1.843363	0.050829
C	5.100772	-0.581349	0.232820
C	2.179203	2.471075	-0.185395
H	5.444464	-2.685395	0.360290
H	3.563519	-4.394668	0.267298
C	3.547251	2.815746	-0.081863
H	5.570951	2.113338	0.123068
H	6.154155	-0.323139	0.303427
H	1.484906	3.293870	-0.280451
H	3.829034	3.865065	-0.110194
S	-1.290511	2.398974	-0.638637
C	-0.572749	3.241316	-2.094171
H	0.499615	3.405271	-2.009525
H	-0.781645	2.605863	-2.957184
H	-1.102161	4.191046	-2.208062
C	-1.049283	3.604523	0.712424
H	0.001562	3.762785	0.950483
H	-1.522208	4.539997	0.402402
H	-1.571851	3.198972	1.580652

$[Pt(Ph)_2(bhq)(SMe_2)]$, TSCA1

Zero-point correction=	0.433200 (Hartree/Particle)
Thermal correction to Energy=	0.460227
Thermal correction to Enthalpy=	0.461171
Thermal correction to Gibbs Free Energy=	0.375409
Sum of electronic and zero-point Energies=	-1614.829539
Sum of electronic and thermal Energies=	-1614.802512
Sum of electronic and thermal Enthalpies=	-1614.801568
Sum of electronic and thermal Free Energies=	-1614.887330
Entropy=	180.501

Pt	0.215294	-0.172617	-0.347728
C	1.614473	0.019041	1.293520
C	2.672762	-0.874472	1.513400
H	3.218919	-1.308932	0.684139

C	3.073927	-1.165337	2.821690
H	3.903449	-1.850250	2.977234
C	2.441261	-0.563668	3.912116
C	1.406388	0.348885	3.685030
H	0.904642	0.829264	4.520811
C	0.999016	0.656524	2.384117
H	0.199589	1.372074	2.230614
C	2.012595	1.023855	-0.408571
C	2.917073	0.574910	-1.398098
C	3.889653	1.427076	-1.926889
C	4.022318	2.733272	-1.450370
C	3.167498	3.180432	-0.436923
C	2.181889	2.339720	0.075169
H	2.870863	-0.437093	-1.777962
H	4.547464	1.059599	-2.709962
H	3.276521	4.182252	-0.030408
H	1.565744	2.704703	0.887446
H	4.793057	3.387718	-1.847561
H	2.762125	-0.788128	4.925113
C	-1.001614	1.472329	-0.295675
C	-2.358134	1.131490	-0.027947
C	-0.735141	2.801084	-0.602072
C	-2.717882	-0.244719	0.035611
C	-3.381960	2.111074	0.081817
C	-1.750456	3.785297	-0.519885
H	0.246599	3.119763	-0.919498
C	-4.049517	-0.654634	0.297134
N	-1.718509	-1.141002	-0.222934
C	-4.723470	1.683380	0.380433
C	-3.042704	3.463788	-0.148083
H	-1.494099	4.815731	-0.751936
C	-4.316186	-2.038884	0.322098
C	-5.045490	0.361080	0.497159
C	-2.003993	-2.445423	-0.202034
H	-5.491529	2.443308	0.498958
H	-3.806439	4.232439	-0.066441
C	-3.288792	-2.934498	0.073348
H	-5.323342	-2.392292	0.526028
H	-6.064660	0.055360	0.716409
H	-1.191960	-3.124401	-0.409971
H	-3.457713	-4.005884	0.077084
S	1.476110	-2.416976	-1.069046
C	0.703352	-3.029529	-2.606750
H	-0.345170	-3.300150	-2.464625

H	0.774965	-2.222218	-3.339170
H	1.268669	-3.893507	-2.965372
C	1.371388	-3.875568	0.028338
H	0.356580	-4.269704	0.109001
H	2.037771	-4.649117	-0.361467
H	1.717272	-3.556829	1.013535

$[Pt(Ph)_2(bhq)(SMe_2)]$, TSCA2

Zero-point correction=	0.431265 (Hartree/Particle)
Thermal correction to Energy=	0.458824
Thermal correction to Enthalpy=	0.459768
Thermal correction to Gibbs Free Energy=	0.370660
Sum of electronic and zero-point Energies=	-1614.829090
Sum of electronic and thermal Energies=	-1614.801531
Sum of electronic and thermal Enthalpies=	-1614.800586
Sum of electronic and thermal Free Energies=	-1614.898969
Entropy=	187.544

Pt	-0.481603	-0.158841	0.527744
C	-1.289556	1.685997	-0.221654
C	-0.865600	2.141424	-1.490198
H	-0.676007	1.433933	-2.289954
C	-0.690660	3.502203	-1.740833
H	-0.368911	3.823850	-2.727905
C	-0.923143	4.446804	-0.735728
C	-1.331544	4.012128	0.531885
H	-1.517369	4.733311	1.323438
C	-1.510223	2.654687	0.787715
H	-1.845978	2.351377	1.775712
C	-2.476531	0.233325	-0.205475
C	-2.968411	-0.158494	-1.468600
C	-4.281031	-0.605753	-1.620388
C	-5.142319	-0.682581	-0.520203
C	-4.673661	-0.291483	0.739081
C	-3.365484	0.166351	0.894803
H	-2.342112	-0.076399	-2.349463
H	-4.633606	-0.887483	-2.609267
H	-5.328802	-0.333829	1.605252
H	-3.046387	0.483356	1.885594
H	-6.164665	-1.027471	-0.643793
H	-0.792467	5.506231	-0.936270
N	1.685967	0.450816	1.256322
C	2.538089	0.278486	0.212547
C	2.127546	1.015454	2.376557

C	2.001667	-0.337461	-0.966975
C	3.902213	0.658868	0.282176
C	3.460018	1.440800	2.529324
H	1.406135	1.133817	3.180964
C	2.872236	-0.622796	-2.057438
C	0.629532	-0.690782	-1.048824
C	4.745980	0.400504	-0.852028
C	4.347725	1.259178	1.480891
H	3.774310	1.897556	3.462031
C	2.353513	-1.297011	-3.187608
C	4.251902	-0.220760	-1.963259
C	0.150012	-1.378800	-2.147567
H	5.790199	0.697221	-0.803976
H	5.384797	1.571162	1.573385
C	1.024601	-1.681209	-3.219301
H	3.010681	-1.518743	-4.024015
H	4.904093	-0.426670	-2.807982
H	-0.887800	-1.685266	-2.207998
H	0.631479	-2.215620	-4.079942
S	-0.243101	-2.477508	1.585975
C	1.453306	-3.134665	1.422448
H	1.760456	-3.150174	0.374812
H	2.113772	-2.481532	1.995967
H	1.482966	-4.143151	1.842933
C	-1.163476	-3.655533	0.538528
H	-0.759618	-3.662250	-0.476386
H	-1.096940	-4.652928	0.980960
H	-2.205575	-3.329606	0.522741

[OAc^-]

Zero-point correction=	0.048349 (Hartree/Particle)
Thermal correction to Energy=	0.052813
Thermal correction to Enthalpy=	0.053757
Thermal correction to Gibbs Free Energy=	0.019973
Sum of electronic and zero-point Energies=	-228.549431
Sum of electronic and thermal Energies=	-228.544967
Sum of electronic and thermal Enthalpies=	-228.544023
Sum of electronic and thermal Free Energies=	-228.577807
Entropy=	71.105

C	0.196571	0.000148	-0.004586
O	0.715957	1.154423	0.000890
C	-1.353053	-0.042158	-0.001765
H	-1.733377	-1.060433	-0.135672

H	-1.725842	0.351945	0.953339
H	-1.750871	0.604403	-0.794020
O	0.802666	-1.109905	0.000918

C_6H_6

Zero-point correction=	0.100589 (Hartree/Particle)
Thermal correction to Energy=	0.104986
Thermal correction to Enthalpy=	0.105930
Thermal correction to Gibbs Free Energy=	0.073118
Sum of electronic and zero-point Energies=	-232.159978
Sum of electronic and thermal Energies=	-232.155581
Sum of electronic and thermal Enthalpies=	-232.154637
Sum of electronic and thermal Free Energies=	-232.187450
Entropy=	69.059

C	-0.978229	-1.000648	0.000002
C	0.377612	-1.347366	0.000076
C	1.355747	-0.346823	-0.000064
C	0.978145	1.000730	0.000008
C	-0.377500	1.347395	0.000067
C	-1.355776	0.346713	-0.000063
H	-1.737936	-1.778112	-0.000063
H	0.670776	-2.394126	0.000078
H	2.408872	-0.616094	-0.000145
H	1.738044	1.777997	0.000009
H	-0.670907	2.394080	0.000019
H	-2.408843	0.616246	-0.000055

HOAc

Zero-point correction=	0.061574 (Hartree/Particle)
Thermal correction to Energy=	0.066192
Thermal correction to Enthalpy=	0.067137
Thermal correction to Gibbs Free Energy=	0.034023
Sum of electronic and zero-point Energies=	-229.038875
Sum of electronic and thermal Energies=	-229.034256
Sum of electronic and thermal Enthalpies=	-229.033312
Sum of electronic and thermal Free Energies=	-229.066426
Entropy=	69.694

C	-0.088090	0.123101	0.000019
O	-0.634472	1.209124	-0.000003
C	1.396994	-0.120534	-0.000018
H	1.679487	-0.703447	-0.883198
H	1.926856	0.832494	0.000555

H	1.679421	-0.704341	0.882625
O	-0.790395	-1.037821	0.000021
H	-1.740246	-0.810530	-0.000134

$C_{12}H_{10}$

Zero-point correction=	0.181655 (Hartree/Particle)
Thermal correction to Energy=	0.190561
Thermal correction to Enthalpy=	0.191506
Thermal correction to Gibbs Free Energy=	0.147007
Sum of electronic and zero-point Energies=	-463.144168
Sum of electronic and thermal Energies=	-463.135261
Sum of electronic and thermal Enthalpies=	-463.134317
Sum of electronic and thermal Free Energies=	-463.178815
Entropy=	93.654

C	-0.743900	-0.000001	0.000000
C	-1.467382	-1.136682	-0.405183
C	-2.864046	-1.137581	-0.404673
C	-3.569463	0.000001	-0.000001
C	-2.864045	1.137582	0.404674
C	-1.467382	1.136681	0.405184
C	0.743900	-0.000001	0.000000
C	1.467382	-1.136682	0.405182
C	2.864046	-1.137581	0.404674
C	3.569463	0.000001	0.000001
C	2.864045	1.137582	-0.404674
C	1.467381	1.136681	-0.405184
H	-0.932434	-2.019538	-0.745242
H	-3.400965	-2.025371	-0.729601
H	-4.656376	0.000002	-0.000001
H	-3.400964	2.025372	0.729602
H	-0.932431	2.019535	0.745246
H	0.932434	-2.019539	0.745241
H	3.400966	-2.025371	0.729602
H	4.656376	0.000002	0.000002
H	3.400964	2.025372	-0.729603
H	0.932431	2.019536	-0.745245

PhI

Zero-point correction=	0.090038 (Hartree/Particle)
Thermal correction to Energy=	0.095948
Thermal correction to Enthalpy=	0.096892
Thermal correction to Gibbs Free Energy=	0.058258

Sum of electronic and zero-point Energies=	-242.943456
Sum of electronic and thermal Energies=	-242.937546
Sum of electronic and thermal Enthalpies=	-242.936601
Sum of electronic and thermal Free Energies=	-242.975235
Entropy=	81.311

C	-0.577394	-0.000005	0.000001
C	-1.261152	1.217415	0.000002
C	-2.661352	1.209247	0.000003
C	-3.363177	0.000002	0.000004
C	-2.661360	-1.209242	0.000004
C	-1.261155	-1.217416	0.000002
H	-0.721259	2.158661	0.000001
H	-3.198412	2.154347	0.000003
H	-4.449760	0.000008	0.000005
H	-3.198417	-2.154344	0.000005
H	-0.721273	-2.158668	0.000001
I	1.566088	0.000000	-0.000002

$PhI(OAc)_2$

Zero-point correction=	0.192460 (Hartree/Particle)
Thermal correction to Energy=	0.209332
Thermal correction to Enthalpy=	0.210277
Thermal correction to Gibbs Free Energy=	0.144120
Sum of electronic and zero-point Energies=	-699.721263
Sum of electronic and thermal Energies=	-699.704390
Sum of electronic and thermal Enthalpies=	-699.703446
Sum of electronic and thermal Free Energies=	-699.769602
Entropy=	139.238

C	1.436616	3.843960	0.396359
C	2.280310	2.875558	-0.153892
C	1.806051	1.583922	-0.417995
C	0.479616	1.317293	-0.106597
C	-0.397467	2.248607	0.430515
C	0.105560	3.531589	0.684379
H	1.814768	4.842438	0.596098
H	3.314035	3.112758	-0.388740
H	2.454372	0.825910	-0.840637
H	-1.435106	2.007637	0.622305
H	-0.558165	4.280389	1.107152
I	-0.267031	-0.705851	-0.519014
O	1.805978	-1.351370	-0.640037
O	-2.256083	0.204321	-0.500755

C	2.544323	-1.897776	0.340065
C	-3.325703	-0.227912	0.178071
O	3.704460	-2.193346	0.101685
O	-4.348607	0.440283	0.157383
C	-3.226134	-1.536216	0.941137
H	-2.950954	-2.361235	0.273486
H	-2.464537	-1.472487	1.727139
H	-4.190310	-1.759349	1.400573
C	1.908667	-2.125095	1.698574
H	1.554191	-1.181855	2.129688
H	1.049237	-2.800769	1.622030
H	2.648092	-2.566042	2.368726