

SUPPLEMENTARY MATERIAL FOR:

# **Phenyl-Group Exchange in Triphenylphosphine Mediated by Cationic Gold-Platinum Complexes – A Gas-Phase Mimetic Approach**

Konstantin Koessler, Harald Scherer, and Burkhard Butschke\*

*Albert-Ludwigs-Universität Freiburg, Institut für Anorganische und Analytische Chemie,  
Albertstr. 21, 79104 Freiburg*

**Contents:**

1. NMR Spectra
2. X-Ray Structural Data for Complexes **1**[BAr<sub>4</sub><sup>F</sup>] and **4**[BAr<sub>4</sub><sup>F</sup>]
3. Validation of the Degree of Deuterium Labeling in Purchased PPh<sub>3</sub>-d<sub>15</sub>
4. Dependency of the Signal Intensities of the LTQ XL on the Capillary Temperature
5. Details of the Models Describing the Phenyl-Group Exchange in the Gas Phase
  - 5.1 General Considerations
  - 5.2 Model 1
  - 5.3 Model 2
6. Phenyl Group Exchange in Solution
  - 6.1 Time-Dependent Phosphine-Exchange in Solution
  - 6.2 Stoichiometric Experiments
  - 6.3 Quantification of the Phenyl-Group Exchange in Solution
  - 6.4 Test on Phenyl-Group Exchange employing Mononuclear Complexes
7. DFT Calculations
8. Cartesian Coordinates and Energies of the DFT Calculations

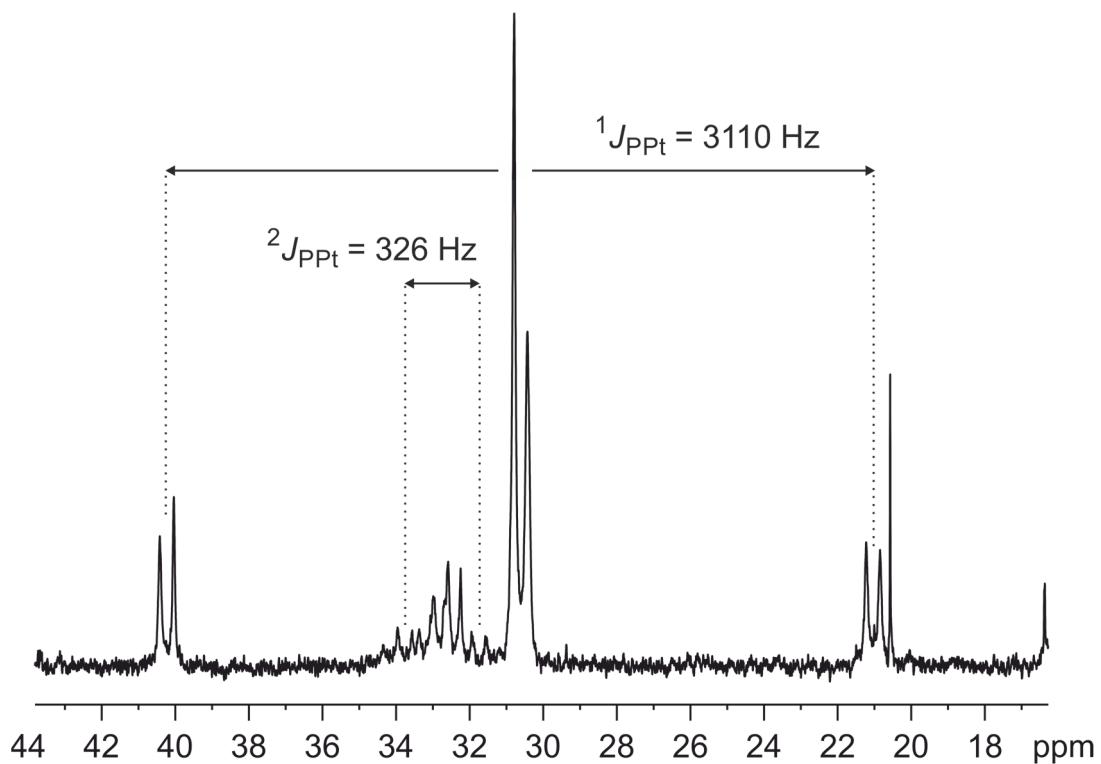
## 1. NMR Spectra

### 1.1. General Remark

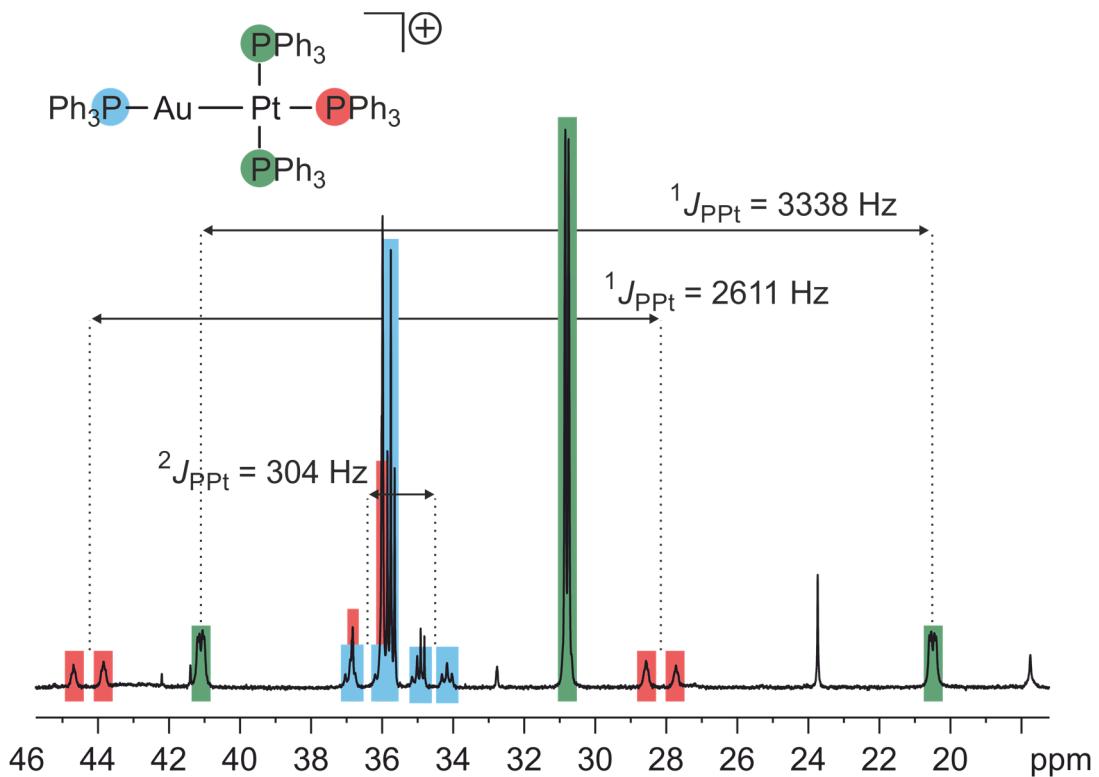
Note that in the  $^{31}\text{P}\{^1\text{H}\}$ -NMR spectrum of **1**[ $\text{BAr}_4^{\text{F}}$ ] (Figure 2 in the main text), the homonuclear spin system differs for the main signals and the platinum satellites. The frequency difference  $\Delta\nu$  of the signals of the coupling partners in the main resonances results only from the chemical-shift difference of the coalescence signal of the phosphine ligands bound to the platinum atom (34.3 ppm) and the resonance of the phosphine ligand bound to the gold atom (36.7 ppm). At 161.99 MHz,  $\Delta\nu$  amounts to 356 Hz, and with a  $^3J_{\text{PP}}$  coupling of 60 Hz the result is a spectrum with pronounced effects of higher order ( $\Delta\nu/J = 5.9$ ). In the platinum satellites,  $\Delta\nu$  of the coupling partners is increased by the great difference of the absolute values of the  $^1J_{\text{PPt}}$  and  $^2J_{\text{PPt}}$  coupling constants. In this molecule the signs of the  $^1J_{\text{PPt}}$  and  $^2J_{\text{PPt}}$  couplings are equal. Consequently, the downfield satellite of the resonance at 34.3 ppm and the downfield satellite of the signal at 36.7 ppm are the one pair of coupling partners and the respective highfield satellites the other. For the downfield satellites  $\Delta\nu$  is 1012 Hz and for the highfield satellites 1772 Hz, thus leading to spin systems with much smaller effects of higher order.

Moreover, it is noticeable that in the coalescence signal of the phosphine ligands bound to the platinum atom the FWHM of the main signal and of both platinum satellites is different. This observation is due to the fact that the  $^1J_{\text{PPt}}$  couplings of the phosphine ligands in the *cis*-position to the gold and the phosphine ligand in the *trans*-position to the gold are different. Therefore, the frequency difference of the signals that are averaged by the fast intramolecular chemical exchange of the phosphine ligands bound to the platinum atom is not the same for the main signals and the platinum satellites, which leads to different FWHMs in the respective coalescence signals.

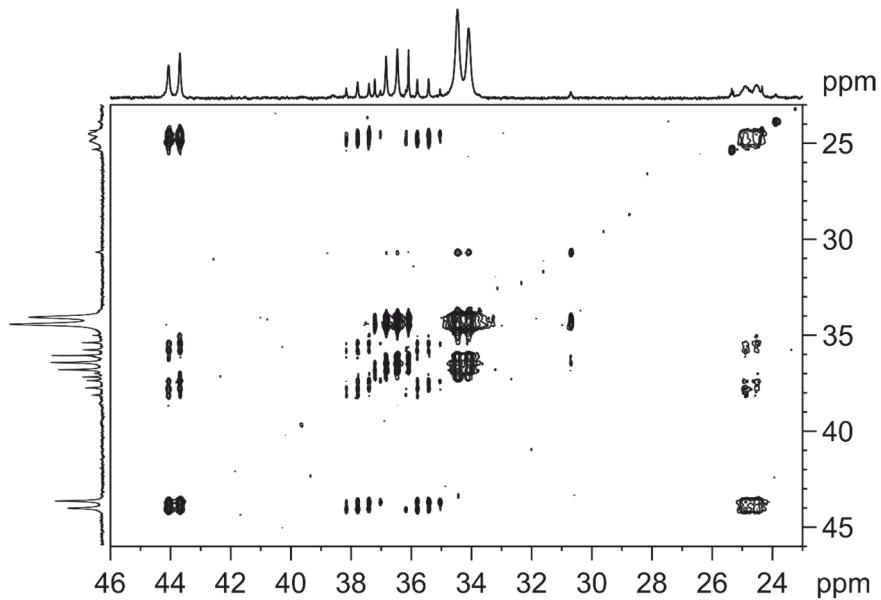
## 1.2. Spectra



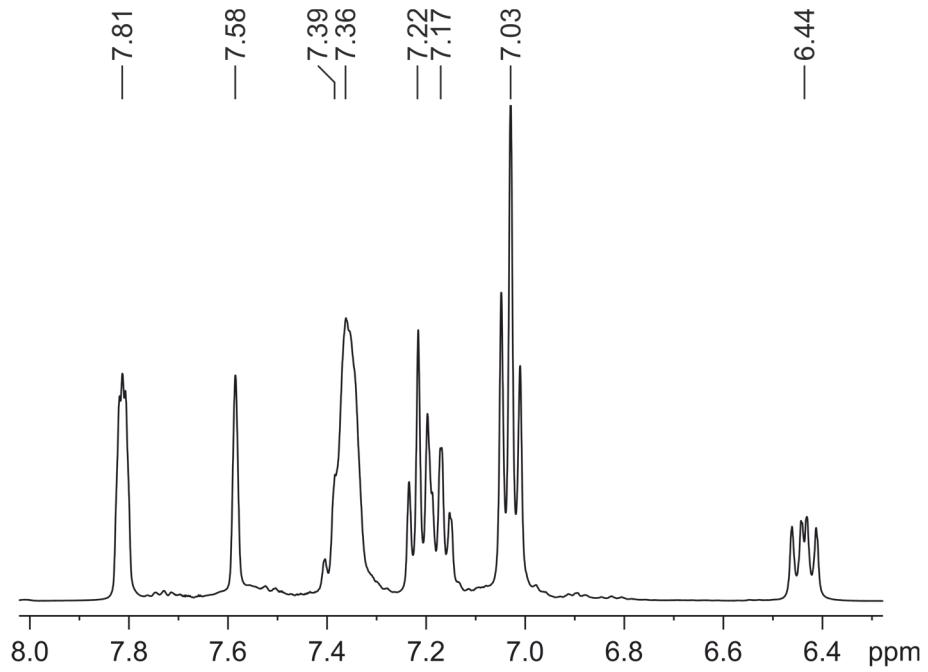
**Figure S1:**  $^{31}\text{P}\{\text{H}\}$ -NMR spectrum (161.99 MHz, 328 K, THF- $d_8$ ) of  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_3][\text{BAr}_4^{\text{F}}]$  (**1**). The doublet with pronounced roof tilt at 30.6 ppm corresponds to the coalescence signal of the three Pt-bound triphenylphosphine ligands. The multiplet at 32.8 ppm corresponds to the gold-bound triphenylphosphine ligand, thus indicating an intact AuPt bond even at elevated temperature. Both signals show platinum satellites of which the  $^1J_{\text{PPt}}$  and  $^2J_{\text{PPt}}$  coupling constants are provided in the spectrum.



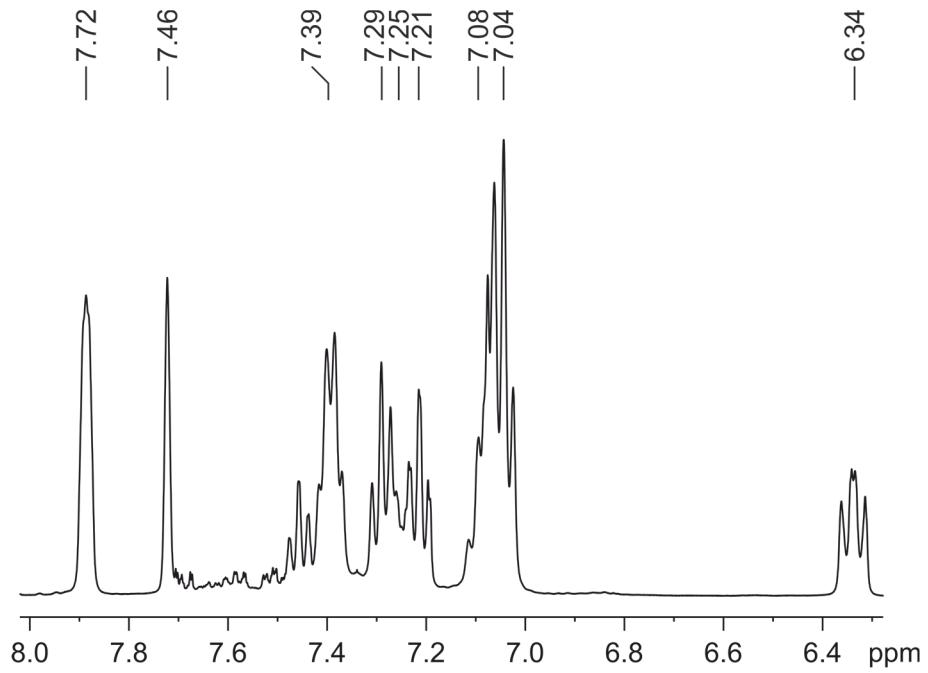
**Figure S2:**  $^{31}\text{P}\{^1\text{H}\}$ -NMR spectrum (161.99 MHz, 208 K, THF-*d*<sub>8</sub>) of  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_3]\text{[BAr}_4^{\text{F}}]$  (**1[BAr<sub>4</sub>F]**). All signals show platinum satellites (indicated in the same color) of which the  $^1J_{\text{PPt}}$  and  $^2J_{\text{PPt}}$  coupling constants are provided in the spectrum.



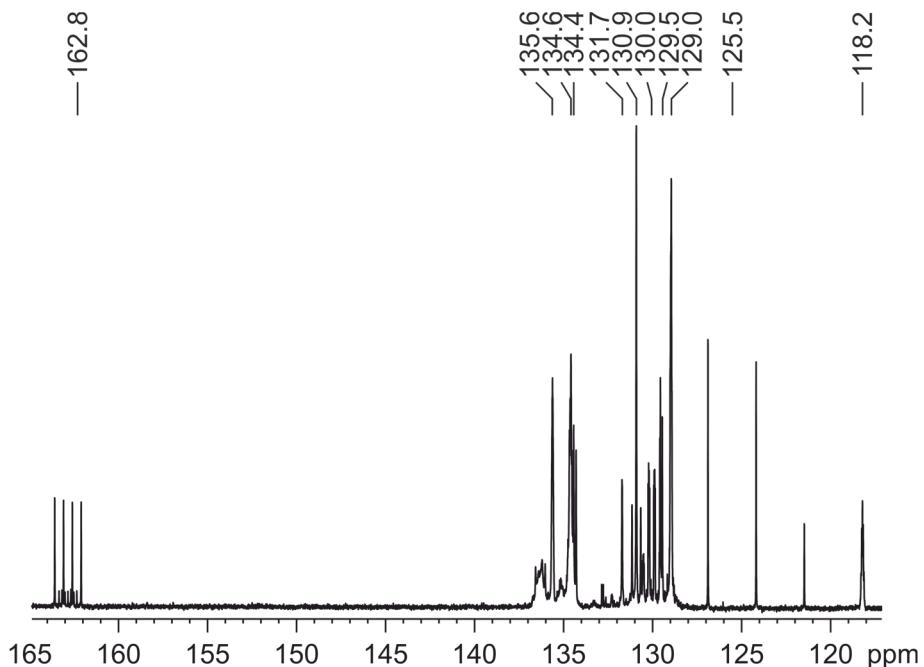
**Figure S3:**  $^{31}\text{P}$ ,  $^{31}\text{P}$ -EXSY NMR spectrum (161.99 MHz, 298 K, THF-*d*<sub>8</sub>, mixing time: 0.5 s) of  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_3]\text{[BAr}_4^{\text{F}}]$  (**1[BAr<sub>4</sub>F]**) showing cross peaks between the main signals at 34.3 and 36.7 ppm as well as for their platinum satellites, thus indicating chemical exchange of the PPh<sub>3</sub> ligands between the gold and the platinum atom at room temperature.



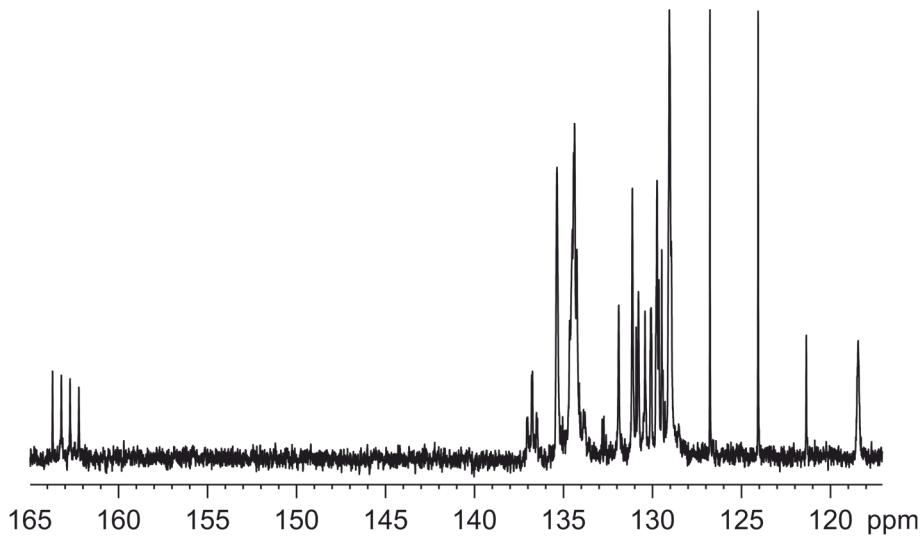
**Figure S4:** <sup>1</sup>H-NMR spectrum (400.17 MHz, 298 K, THF-*d*<sub>8</sub>) of [(Ph<sub>3</sub>P)AuPt(PPh<sub>3</sub>)<sub>3</sub>][BAr<sub>4</sub>F]  
(**1**[BAr<sub>4</sub>F]).



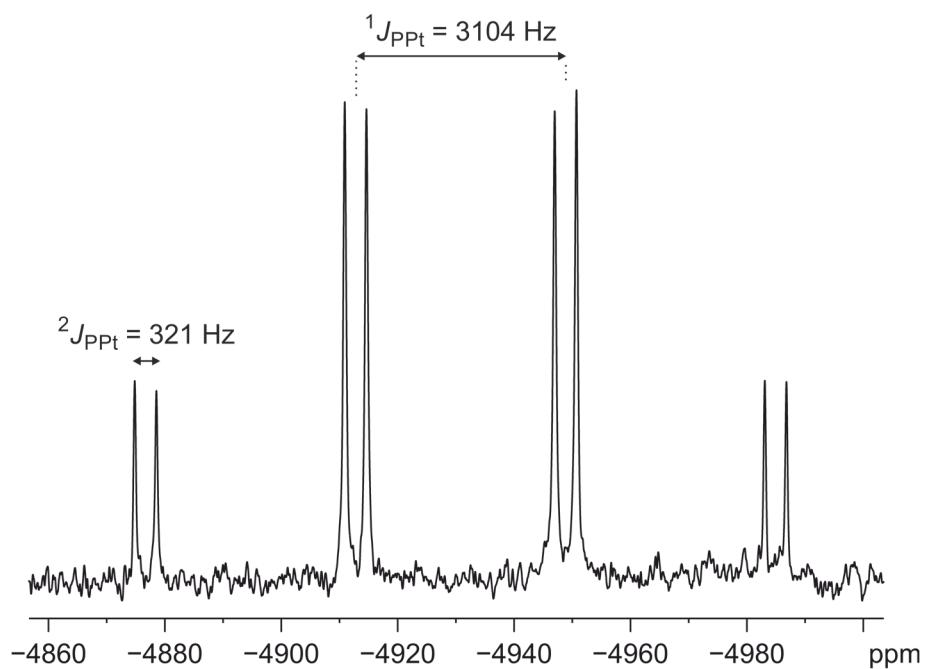
**Figure S5:** <sup>1</sup>H-NMR spectrum (400.17 MHz, 208 K, THF-*d*<sub>8</sub>) of [(Ph<sub>3</sub>P)AuPt(PPh<sub>3</sub>)<sub>3</sub>][BAr<sub>4</sub>F]  
(**1**[BAr<sub>4</sub>F]).



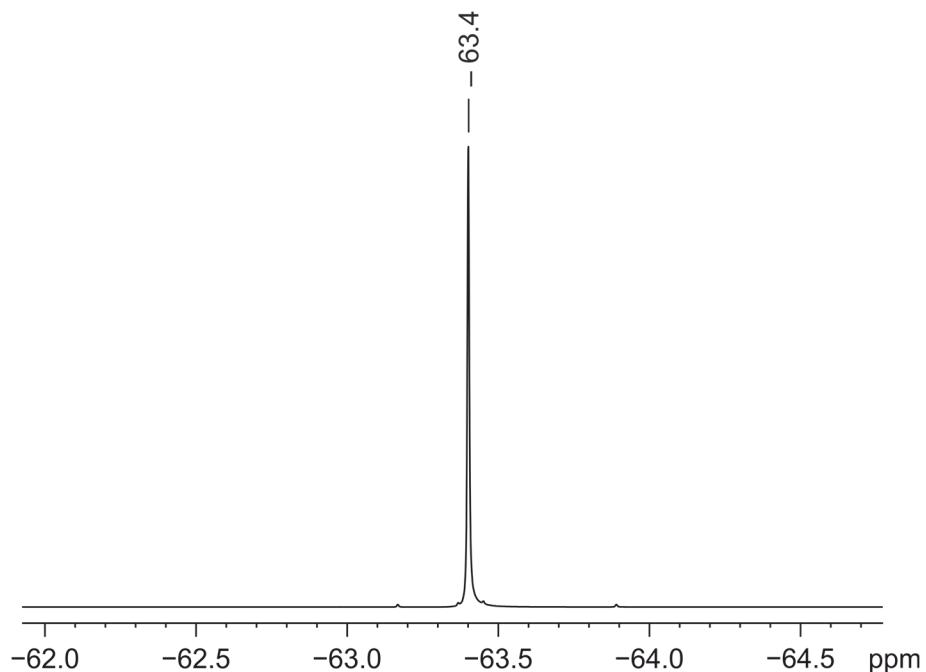
**Figure S6:**  $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100.62 MHz, 298 K, THF- $d_8$ ) of  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_3][\text{BAr}_4^{\text{F}}]$  (**1**[ $\text{BAr}_4^{\text{F}}$ ]).



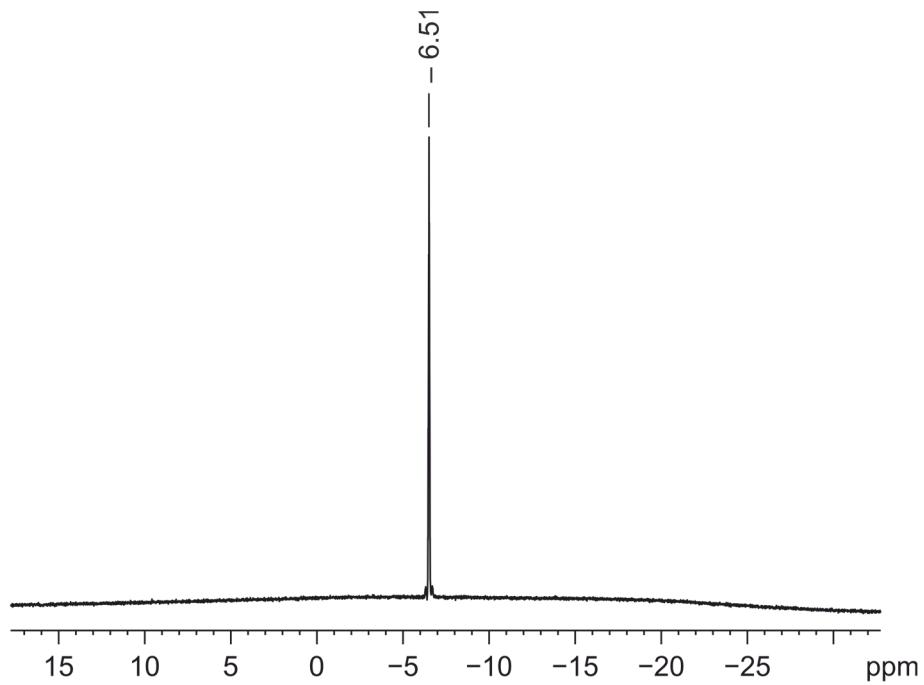
**Figure S7:**  $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum (100.62 MHz, 208 K, THF- $d_8$ ) of  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_3][\text{BAr}_4^{\text{F}}]$  (**1**[ $\text{BAr}_4^{\text{F}}$ ]).



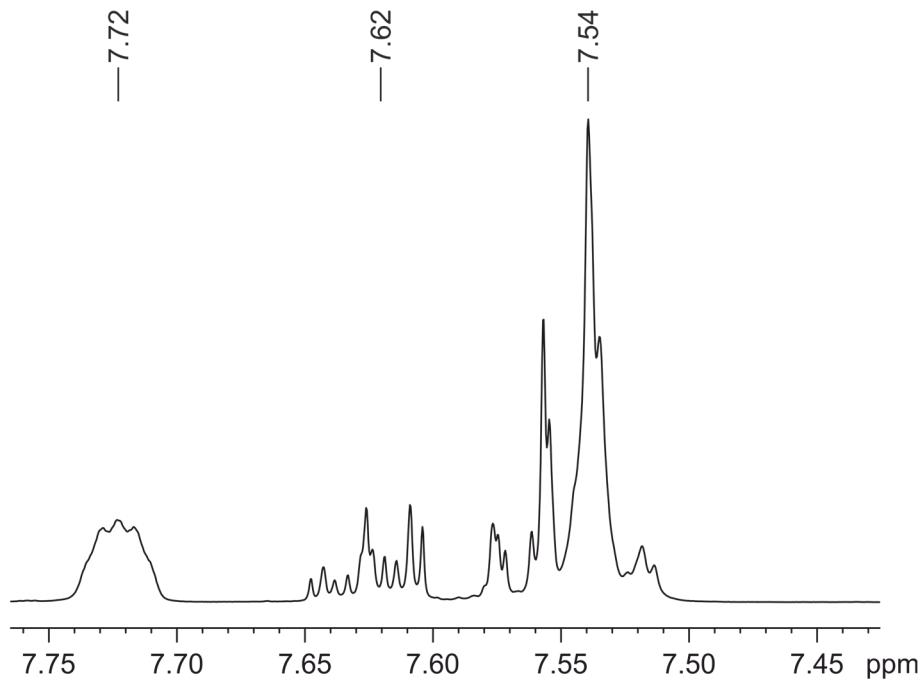
**Figure S8:**  $^{195}\text{Pt}$ -NMR spectrum (86.02 MHz, 298 K, THF- $d_8$ ) of  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_3][\text{BAr}_4^{\text{F}}]$  (**1**[ $\text{BAr}_4^{\text{F}}$ ]).



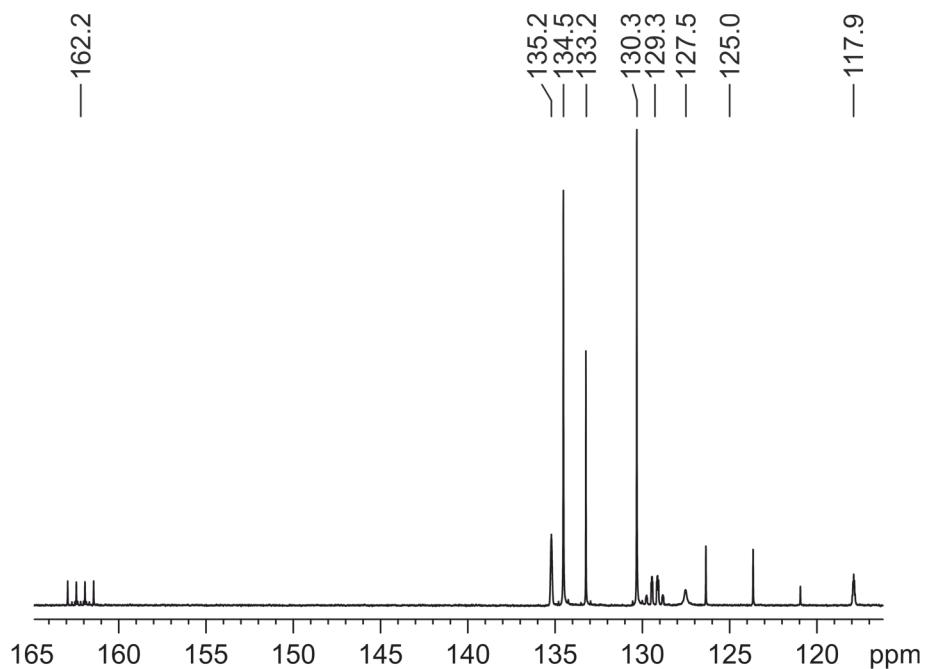
**Figure S9:**  $^{19}\text{F}\{^{11}\text{B}\}$ -NMR spectrum (376.54 MHz, 298 K, THF- $d_8$ ) of  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_3][\text{BAr}_4^{\text{F}}]$  (**1**[ $\text{BAr}_4^{\text{F}}$ ]).



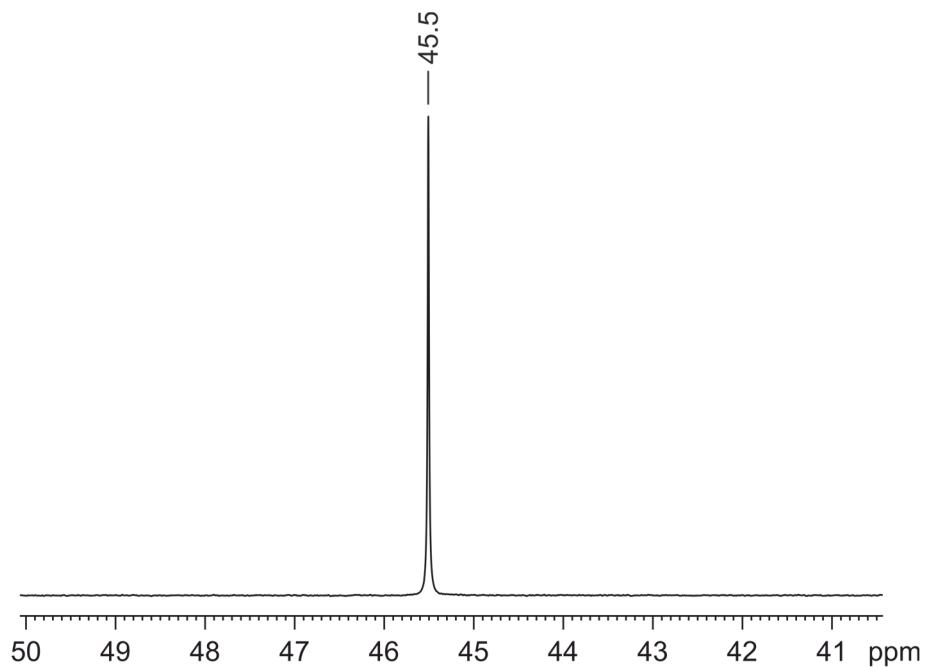
**Figure S10:** <sup>11</sup>B-NMR spectrum (128.39 MHz, 298 K, THF-*d*<sub>8</sub>) of [(Ph<sub>3</sub>P)AuPt(PPh<sub>3</sub>)<sub>3</sub>][BAr<sub>4</sub><sup>F</sup>] (**1**[BAr<sub>4</sub><sup>F</sup>]).



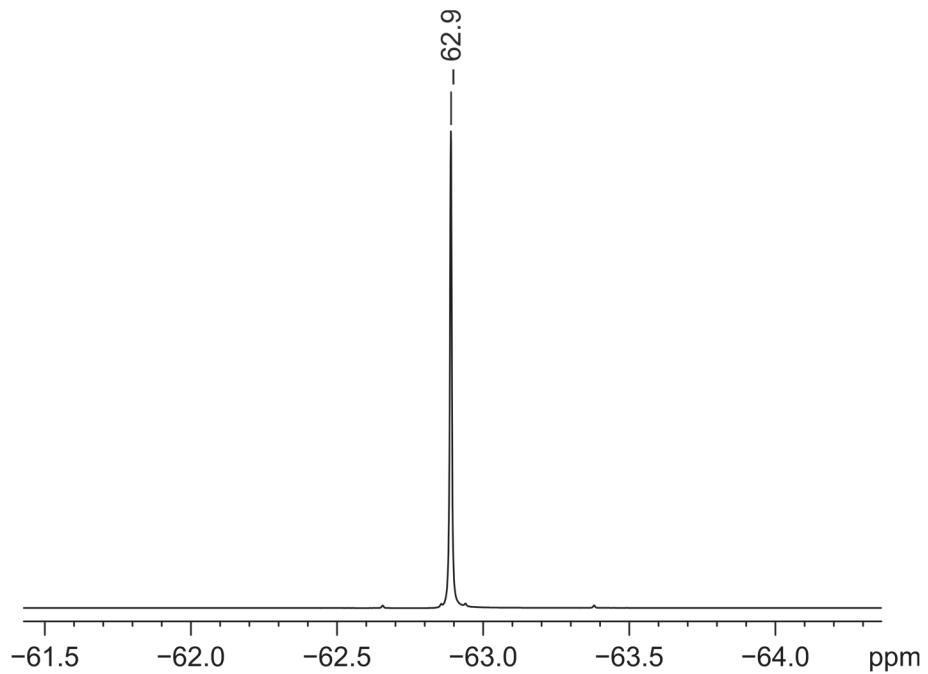
**Figure S11:** <sup>1</sup>H-NMR spectrum (400.17 MHz, 298 K, CD<sub>2</sub>Cl<sub>2</sub>) of [Au(PPh<sub>3</sub>)<sub>2</sub>][BAr<sub>4</sub><sup>F</sup>] (**3**[BAr<sub>4</sub><sup>F</sup>]).



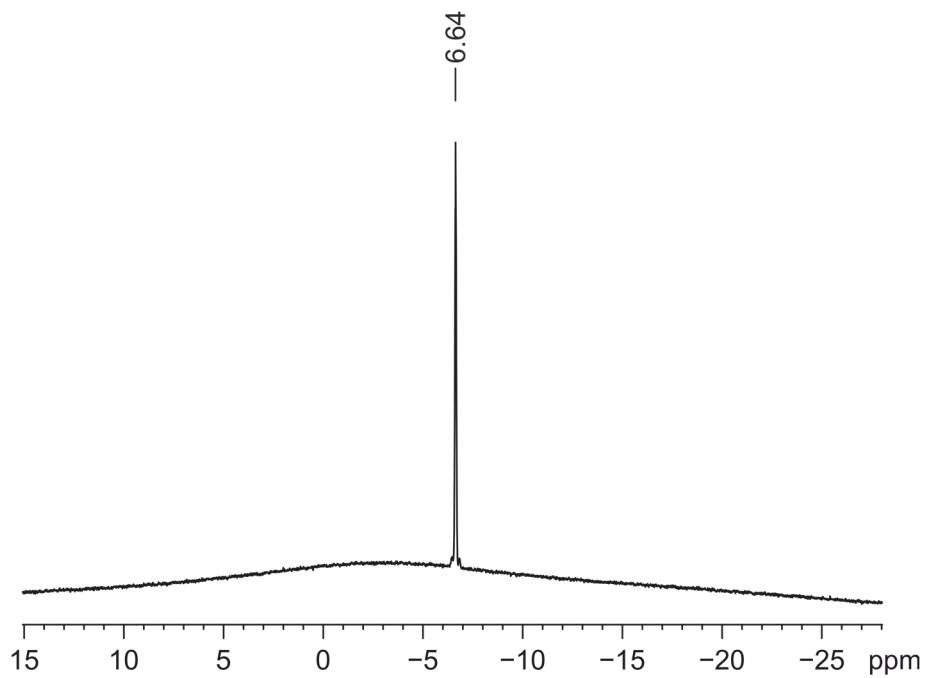
**Figure S12:**  $^{13}\text{C}\{\text{H}\}$ -NMR spectrum (100.62 MHz, 298 K,  $\text{CD}_2\text{Cl}_2$ ) of  $[\text{Au}(\text{PPh}_3)_2]\text{[BAr}_4^{\text{F}}]$  (**3[BAr<sub>4</sub>F]**).



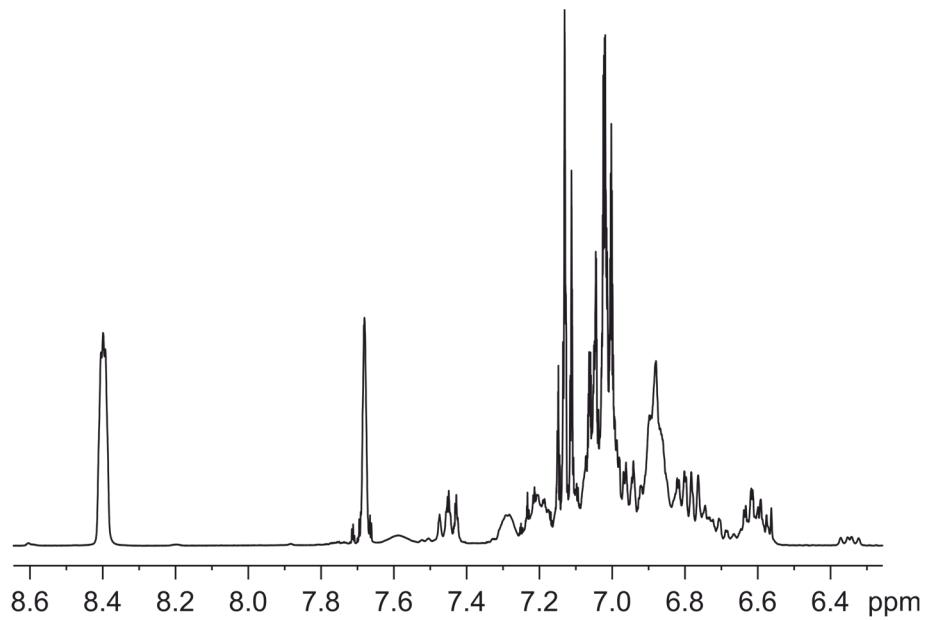
**Figure S13:**  $^{31}\text{P}\{\text{H}\}$ -NMR spectrum (161.99 MHz, 298 K,  $\text{CD}_2\text{Cl}_2$ ) of  $[\text{Au}(\text{PPh}_3)_2]\text{[BAr}_4^{\text{F}}]$  (**3[BAr<sub>4</sub>F]**).



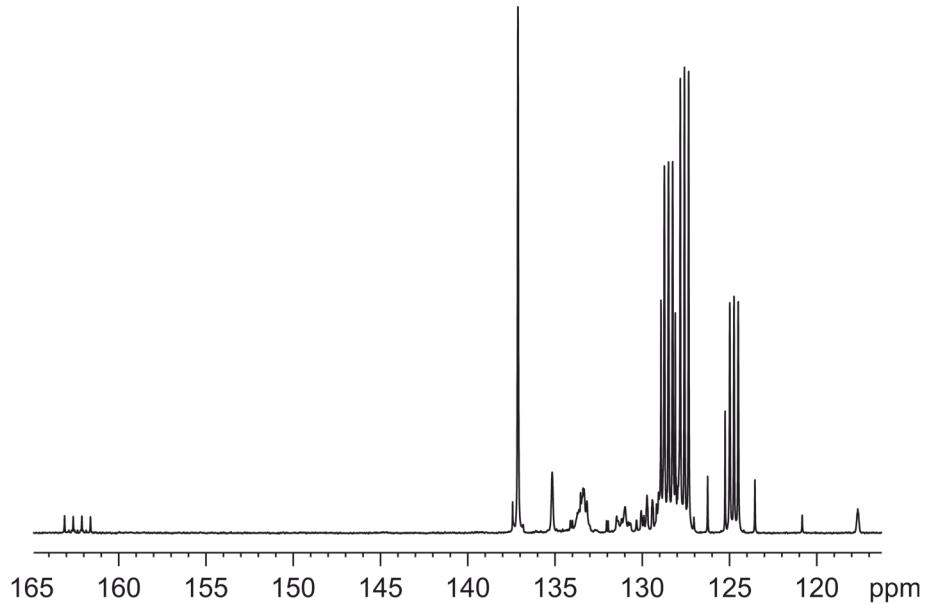
**Figure S14:**  $^{19}\text{F}\{^{11}\text{B}\}$ -NMR spectrum (376.54 MHz, 298 K,  $\text{CD}_2\text{Cl}_2$ ) of  $[\text{Au}(\text{PPh}_3)_2][\text{BAr}_4^{\text{F}}]$  (**3**[ $\text{BAr}_4^{\text{F}}$ ]).



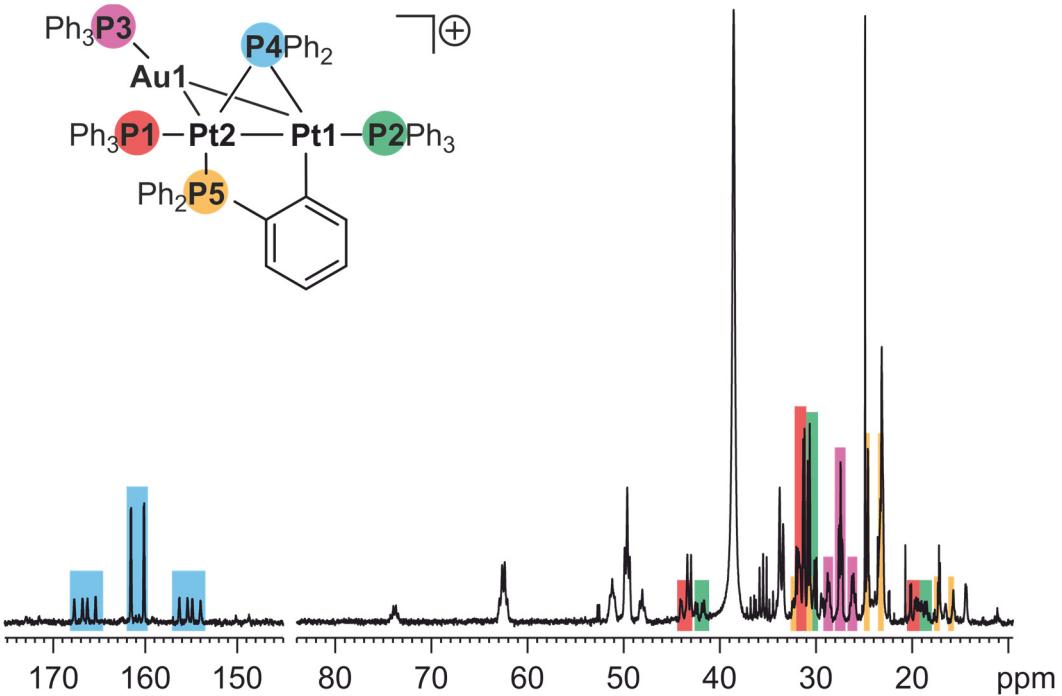
**Figure S15:**  $^{11}\text{B}$ -NMR spectrum (128.39 MHz, 298 K,  $\text{CD}_2\text{Cl}_2$ ) of  $[\text{Au}(\text{PPh}_3)_2][\text{BAr}_4^{\text{F}}]$  (**3**[ $\text{BAr}_4^{\text{F}}$ ]).



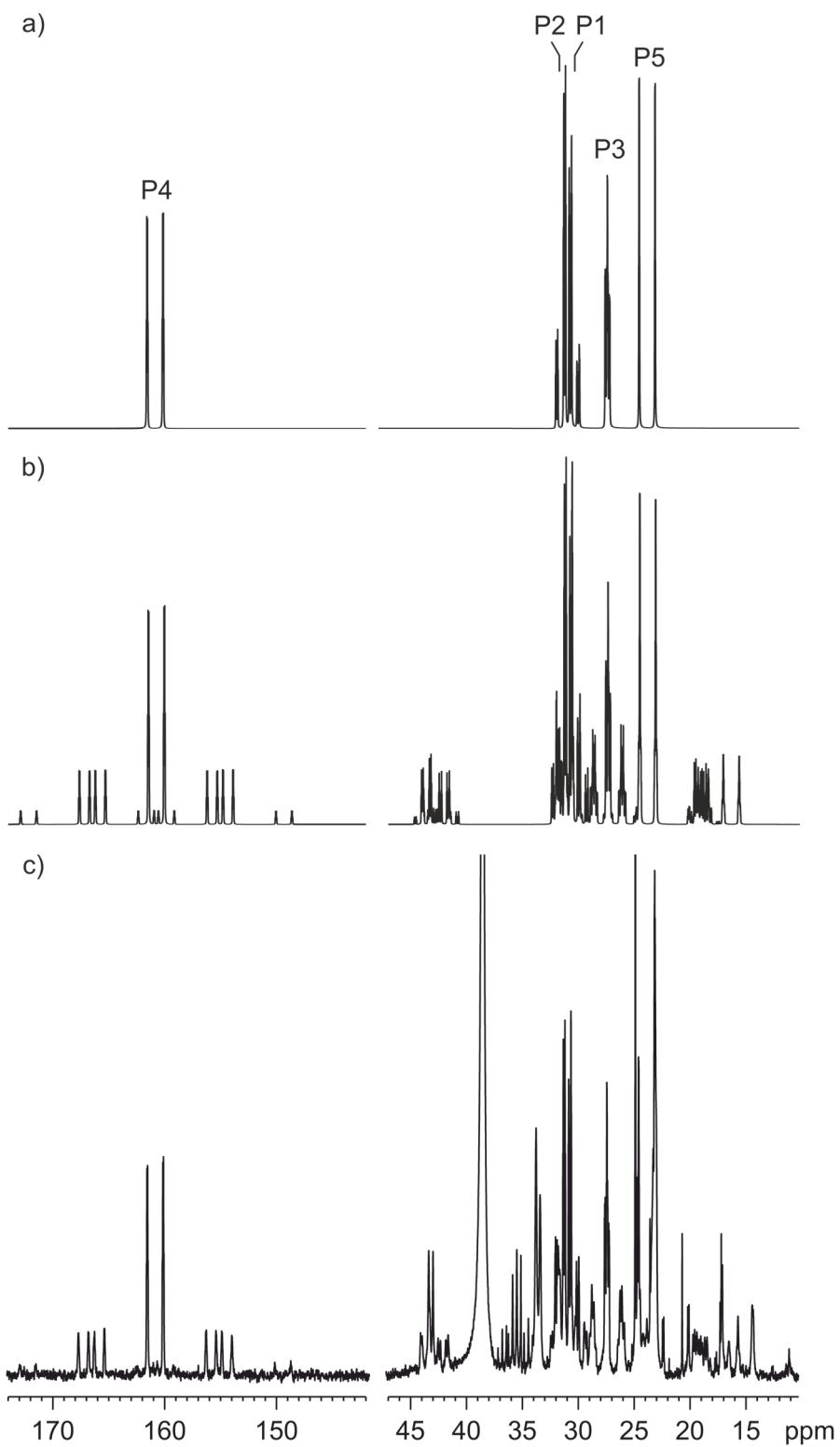
**Figure S16:** <sup>1</sup>H-NMR spectrum (400.17 MHz, 298 K, toluene-*d*<sub>8</sub>) of [AuPt<sub>2</sub>(PPh<sub>3</sub>)<sub>3</sub>(PPh<sub>2</sub>)(PPh<sub>2</sub>{C<sub>6</sub>H<sub>4</sub>})][BAr<sub>4</sub><sup>F</sup>] (**4**[BAr<sub>4</sub><sup>F</sup>]).



**Figure S17:** <sup>13</sup>C{<sup>1</sup>H}-NMR spectrum (100.62 MHz, 298 K, toluene-*d*<sub>8</sub>) of [AuPt<sub>2</sub>(PPh<sub>3</sub>)<sub>3</sub>(PPh<sub>2</sub>)(PPh<sub>2</sub>{C<sub>6</sub>H<sub>4</sub>})][BAr<sub>4</sub><sup>F</sup>] (**4**[BAr<sub>4</sub><sup>F</sup>]).



**Figure S18:**  $^{31}\text{P}\{\text{H}\}$ -NMR spectrum (161.99 MHz 298 K, toluene-*d*<sub>8</sub>) of the product mixture after heating  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_3][\text{BAr}_4^F]$  **1** [ $\text{BAr}_4^F$ ] in toluene to 165 °C in a closed vessel and evaporation of all volatiles. The ABCDE spin system of the five distinguishable phosphor atoms in  $[\text{AuPt}_2(\text{PPh}_3)_3(\text{PPh}_2\{\text{C}_6\text{H}_4\})][\text{BAr}_4^F]$  (**4** [ $\text{BAr}_4^F$ ]) is highlighted by different colors together with their platinum satellites. The signals at 49.6 ppm (t) and 62.5 ppm (q) belong to an A<sub>2</sub>B<sub>3</sub> spin system ( $J_{\text{PP}} = 44$  Hz) and carry platinum satellites with  ${}^1J_{\text{PPt}} = 3668$  Hz and  ${}^3J_{\text{PPt}} = 506$  Hz, respectively. The identity of this impurity is unknown.



**Figure S19:** a) Simulated  $^{31}\text{P}\{\text{H}\}$ -NMR spectrum of  $[\text{AuPt}_2(\text{PPh}_3)_3(\text{PPh}_2)(\text{PPh}_2\{\text{C}_6\text{H}_4\})][\text{BAr}_4^{\text{F}}]$  (**4**)[ $\text{BAr}_4^{\text{F}}$ ]) without  $^{195}\text{Pt}$  satellites. b) Simulated  $^{31}\text{P}\{\text{H}\}$ -NMR spectrum of **4**( $\text{BAr}_4^{\text{F}}$ ) with  $^{195}\text{Pt}$  satellites. c)  $^{31}\text{P}\{\text{H}\}$ -NMR spectrum of **4**[ $\text{BAr}_4^{\text{F}}$ ] (161.99 MHz, 298 K, toluene- $d_8$ ).

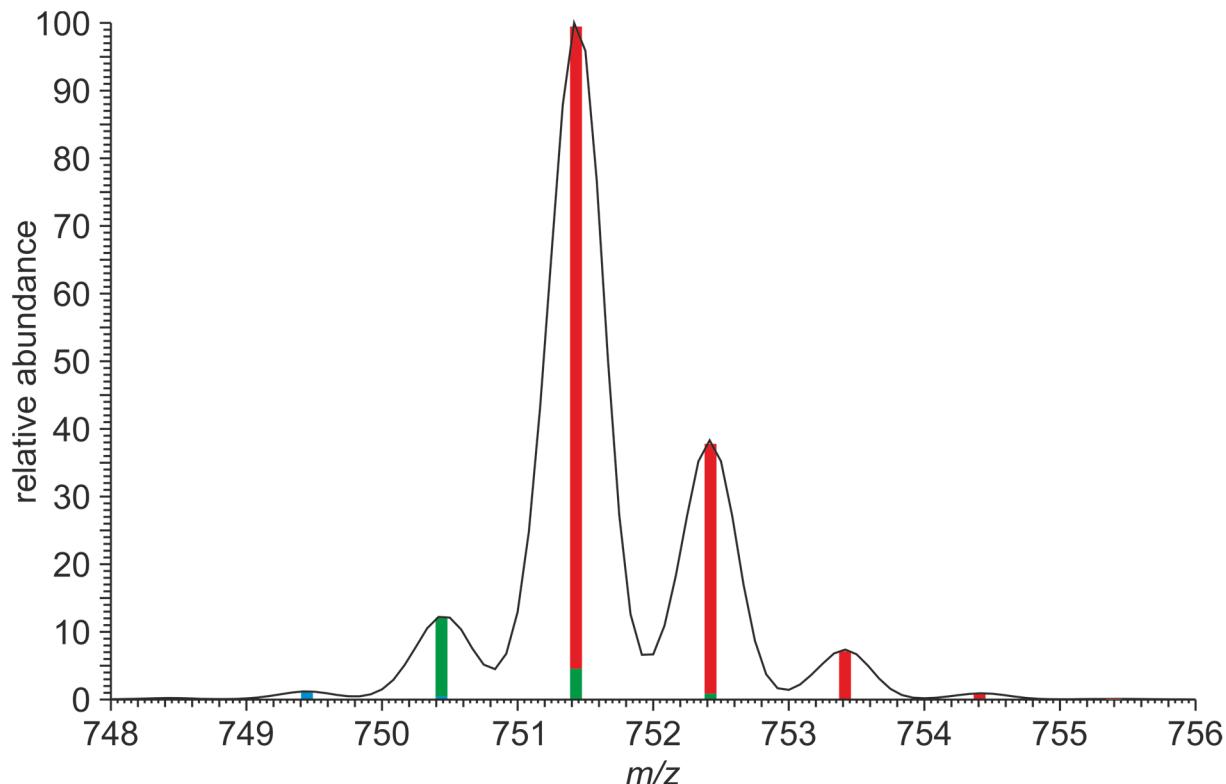
## 2. X-Ray Structural Data for Complexes **1**[BAr<sub>4</sub><sup>F</sup>] and **4**[BAr<sub>4</sub><sup>F</sup>]

**Table S1:** Crystal data and summary of the data collection and refinement for complexes **1**[BAr<sub>4</sub><sup>F</sup>] and **4**[BAr<sub>4</sub><sup>F</sup>].

Complex	<b>1</b> [BAr <sub>4</sub> <sup>F</sup> ]	<b>4</b> [BAr <sub>4</sub> <sup>F</sup> ]
CCDC number	1966138	1966139
Empirical formula	C <sub>104</sub> H <sub>72</sub> AuBF <sub>24</sub> P <sub>4</sub> Pt	C <sub>126</sub> H <sub>105</sub> AuBF <sub>24</sub> P <sub>5</sub> Pt <sub>2</sub>
Formula weight	2304.36	2827.90
Temperature [K]	100.0	100.0
Crystal system	triclinic	triclinic
Space group (number)	<i>P</i> -1 (2)	<i>P</i> -1 (2)
<i>a</i> [Å]	12.933(8)	14.263(7)
<i>b</i> [Å]	16.688(9)	19.629(10)
<i>c</i> [Å]	22.016(14)	23.155(12)
$\alpha$ [Å]	99.442(16)	106.433(7)
$\beta$ [Å]	90.871(11)	96.835(15)
$\gamma$ [Å]	96.698(9)	100.593(8)
Volume [Å <sup>3</sup> ]	4652(5)	6011(5)
<i>Z</i>	2	2
$\rho_{\text{calc}}$ [g/cm <sup>3</sup> ]	1.645	1.562
$\mu$ [mm <sup>-1</sup> ]	3.242	3.690
<i>F</i> (000)	2268	2784
Crystal size [mm <sup>3</sup> ]	0.168×0.136×0.057	0.290×0.170×0.070
Crystal colour	Colourless	red
Crystal shape	block	block
Radiation	MoK $\alpha$ ( $\lambda$ =0.71073)	MoK $\alpha$ ( $\lambda$ =0.71073)
2 $\Theta$ range [°]	1.88 to 60.37	1.86 to 55.08
Index ranges	-18 ≤ <i>h</i> ≤ 18	-18 ≤ <i>h</i> ≤ 18
	-23 ≤ <i>k</i> ≤ 23	-25 ≤ <i>k</i> ≤ 25
	-31 ≤ <i>l</i> ≤ 31	-30 ≤ <i>l</i> ≤ 30
Reflections collected	242221	196592
Independent reflections	27512	27681
	<i>R</i> <sub>int</sub> = 0.0424	<i>R</i> <sub>int</sub> = 0.0388
	<i>R</i> <sub>sigma</sub> = 0.0247	<i>R</i> <sub>sigma</sub> = 0.0253
Completeness to $\theta$ = 25.242°	100.00	100.00
Data / Restraints / Parameters	27512/1976/1467	27681/847/1587
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.030	1.045
Final <i>R</i> indexes	<i>R</i> <sub>1</sub> = 0.0220	<i>R</i> <sub>1</sub> = 0.0324
[ <i>I</i> ≥ 2σ( <i>I</i> )]	w <i>R</i> <sub>2</sub> = 0.0457	w <i>R</i> <sub>2</sub> = 0.0820
Final <i>R</i> indexes	<i>R</i> <sub>1</sub> = 0.0324	<i>R</i> <sub>1</sub> = 0.0427
[all data]	w <i>R</i> <sub>2</sub> = 0.0493	w <i>R</i> <sub>2</sub> = 0.0883
Largest peak/hole [eÅ <sup>-3</sup> ]	1.07/-0.77	6.55/-0.97

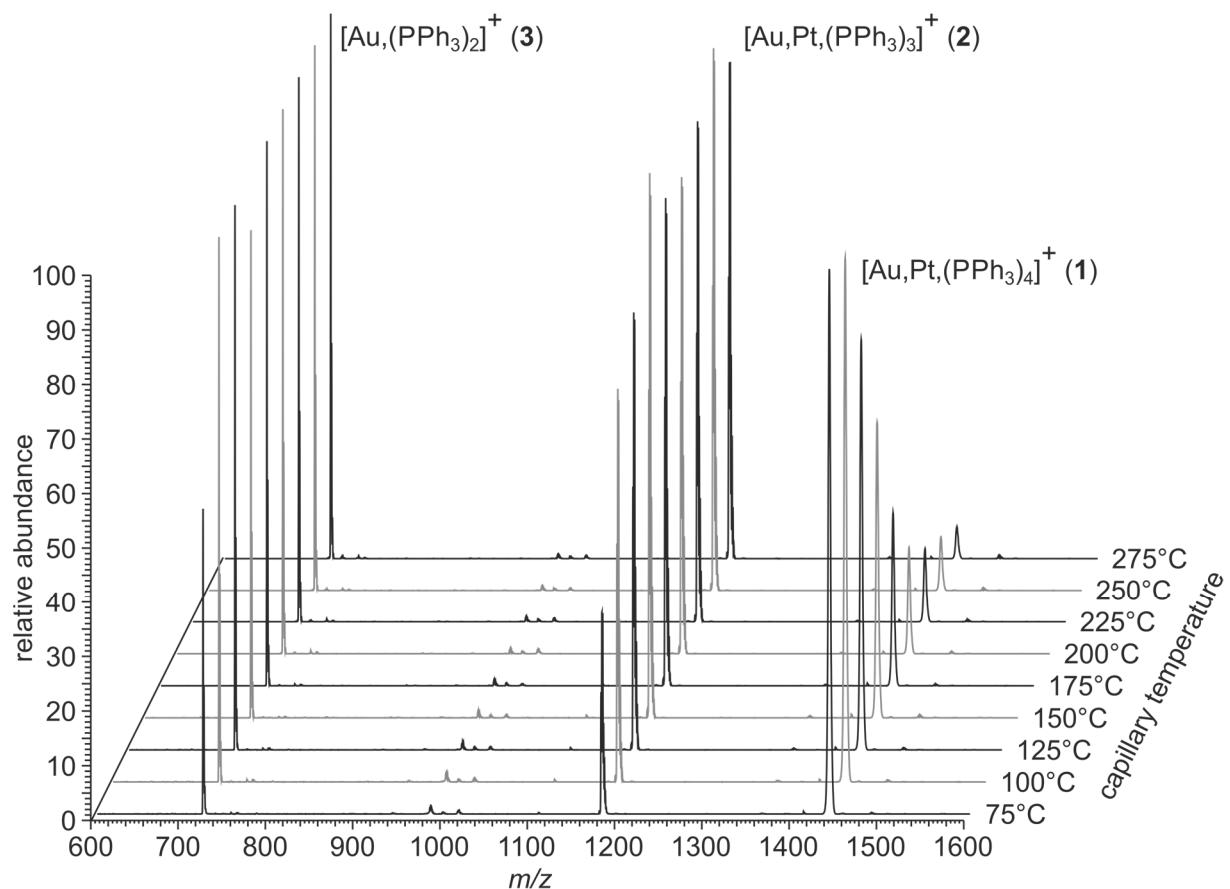
### 3. Validation of the Degree of Deuterium Labeling in Purchased PPh<sub>3</sub>-d<sub>15</sub>

The degree of deuterium labeling in PPh<sub>3</sub>-d<sub>15</sub> (purchased from Sigma-Aldrich; 99 atom%D according to the label) was validated by modelling the isotope pattern of [Au(PPh<sub>3</sub>)<sub>2</sub>]<sup>+</sup>-d<sub>n</sub> ( $n \leq 30$ ) in the ESI-MS spectra of a solution of [(Ph<sub>3</sub>P-d<sub>15</sub>)AuPt(PPh<sub>3</sub>-d<sub>15</sub>)<sub>3</sub>][BAr<sub>4</sub><sup>F</sup>] in methanol. The signal of pure [Au(PPh<sub>3</sub>)<sub>2</sub>]<sup>+</sup>-d<sub>30</sub> amounts to 87.8 %. This value translates to a deuterium content of (0.878)<sup>1/30</sup>, and thus 99.6 atom% D.

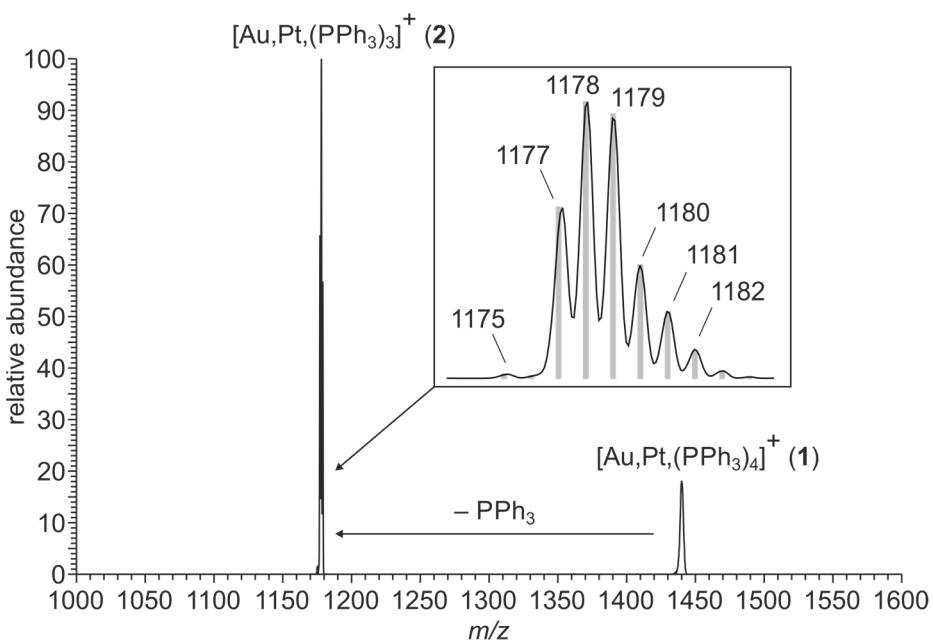


**Figure S20:** Parts of the ESI-MS spectrum of a solution of [(Ph<sub>3</sub>P)AuPt(PPh<sub>3</sub>)<sub>3</sub>]-d<sub>60</sub>[BAr<sub>4</sub><sup>F</sup>] in methanol highlighting the isotope pattern [Au(PPh<sub>3</sub>)<sub>2</sub>]<sup>+</sup>-d<sub>n</sub>. The colored bars indicate the isotope patterns of the compounds [Au(PPh<sub>3</sub>)<sub>2</sub>]<sup>+</sup>-d<sub>30</sub> (87.8 %, red bars), [Au(PPh<sub>3</sub>)<sub>2</sub>]<sup>+</sup>-d<sub>29</sub> (10.8 %, green bars), and [Au(PPh<sub>3</sub>)<sub>2</sub>]<sup>+</sup>-d<sub>28</sub> (1.04 %, blue bars).

#### 4. Dependency of the Signal Intensities of the LTQ XL on the Capillary Temperature



**Figure S21:** Cation-mode ESI mass spectra of  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_3][\text{BAr}_4^{\text{F}}]$  (**1**) dissolved in diethyl ether at capillary temperatures varying between 75 °C and 275 °C.

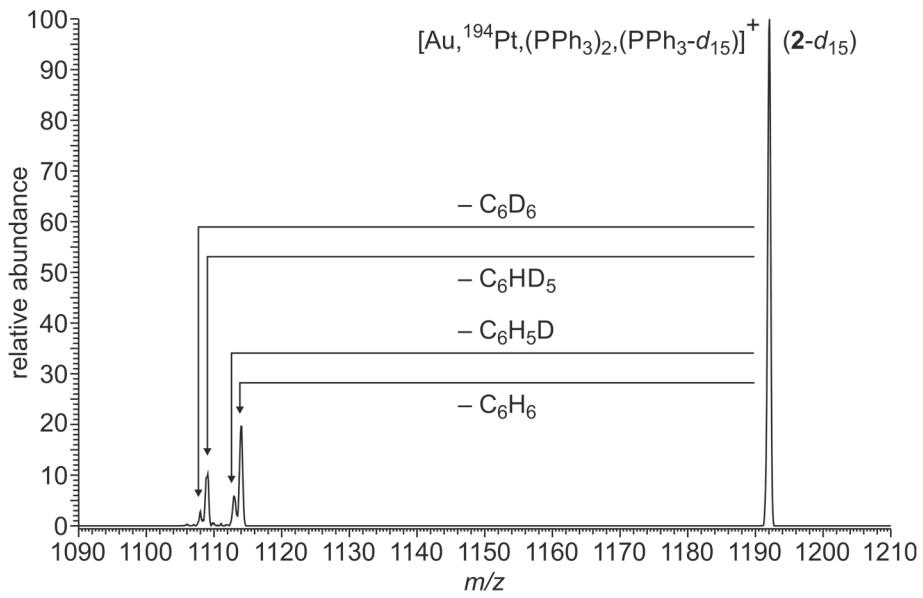


**Figure S22:** CID spectrum of  $[\text{Au},\text{Pt},(\text{PPh}_3)_4]^+ (1)$  (mass-selected with an isolation width of 14 centered around  $m/z$  1439). The resulting isotope pattern of  $[\text{Au},\text{Pt},(\text{PPh}_3)_3]^+ (2)$  is well-resolved in contrast to that of the mass-selected parent ion 1. The inset shows the enlarged isotope pattern of the product ion 2 together with the simulated isotope pattern.

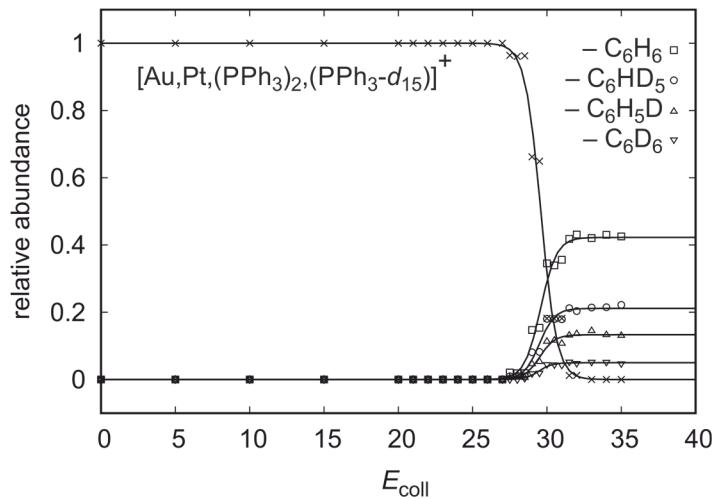
## 5. Details of the Models Describing the Phenyl-Group Exchange in the Gas Phase

### 5.1 General Considerations

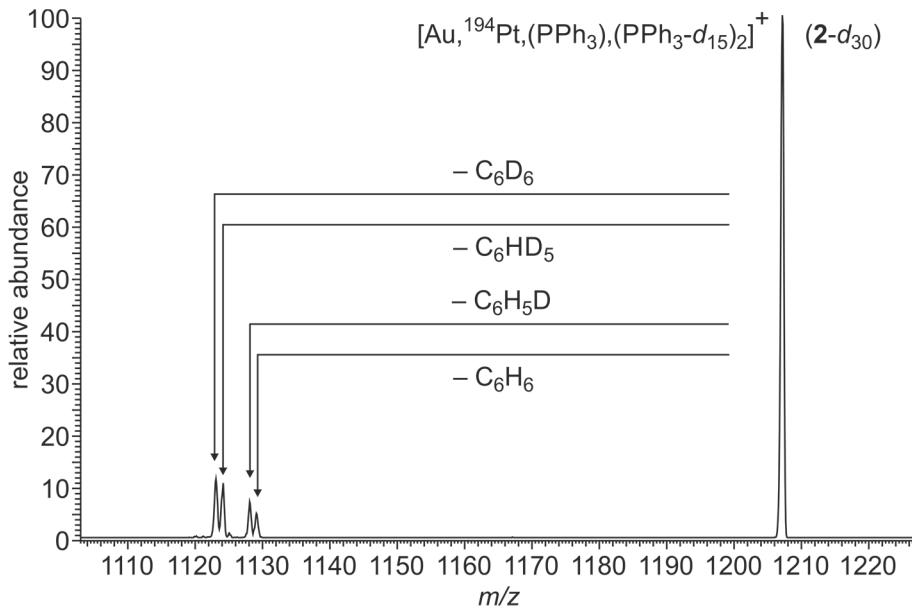
To describe the benzene isotopologue distribution in the CID experiments employing mass-selected  $[\text{Au},\text{Pt},(\text{PPh}_3)_2,(\text{PPh}_3-d_{15})]^+ (2-d_{15})$  and  $[\text{Au},\text{Pt},(\text{PPh}_3),(\text{PPh}_3-d_{15})_2]^+ (2-d_{30})$  (see Table 2 in the main text; the respective spectra are provided in Figure S23 and Figure S25 together with the respective breakdown curves given in Figure S24 and Figure S26) two statistical models (Model 1 and Model 2) were applied to the data. Both models assume that the  $\text{PPh}_3$  ligands are not statically bound to certain positions of the AuPt core but that they are mobile on it.



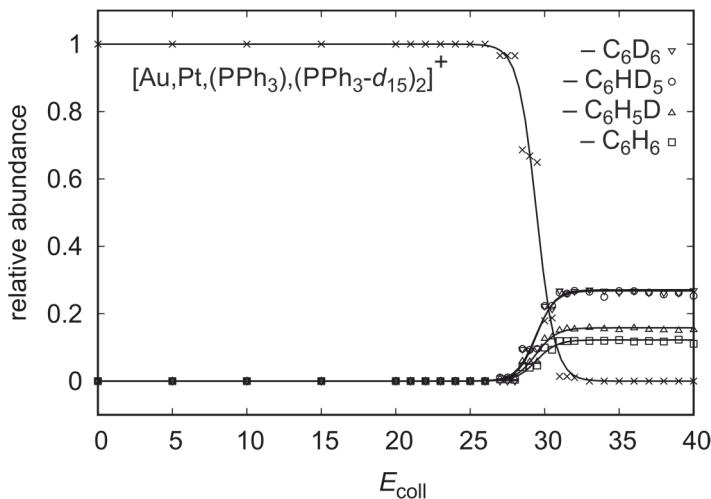
**Figure S23:** CID spectrum of mass-selected  $[Au,^{194}\text{Pt},(\text{PPh}_3)_2,(\text{PPh}_3-d_{15})]^+$  (**2-d<sub>15</sub>**) (at a Normalized Collision Energy of 29.5) showing the losses of  $C_6\text{H}_6$ ,  $C_6\text{H}_5\text{D}$ ,  $C_6\text{D}_5\text{H}$ , and  $C_6\text{D}_6$ .



**Figure S24:** Breakdown graph for the CID of mass selected  $[Au,\text{Pt},(\text{PPh}_3)_2,(\text{PPh}_3-d_{15})]^+$  (**2-d<sub>15</sub>**). Appearance energies for the fragmentations are summarized in Table S2.



**Figure S25:** CID spectrum of mass-selected  $[Au,^{194}Pt,(PPh_3),(PPh_3-d_{15})_2]^+$  (**2-d<sub>30</sub>**) (at a normalized collision energy of 29.5) showing the losses of  $C_6H_6$ ,  $C_6H_5D$ ,  $C_6D_5H$ , and  $C_6D_6$ .



**Figure S26:** Breakdown graph for the CID of mass selected  $[Au,Pt,(PPh_3),(PPh_3-d_{15})_2]^+$  (**2-d<sub>30</sub>**). Appearance energies for the fragmentations are summarized in Table S2.

The breakdown curves were fitted with equation 1, a sigmoid-type function, using the least-square criterion. The parameter  $E_{coll}^{0.5}$  is the energy of the sigmoid midpoint and  $k$  the steepness of the curve.

$$f(E_{coll}) = \frac{1}{(1 + e^{k(-E_{coll} + E_{coll}^{0.5})})} \quad (1)$$

To obtain the appearance energies, the tangent through the inflection point of the sigmoid function was extrapolated to the base line.

**Table S2:** Appearance energies for the fragmentation of mass selected  $[\text{Au},\text{Pt},(\text{PPh}_3)_2,(\text{PPh}_3-d_{15})]^+$  (**2**- $d_{15}$ ) and  $[\text{Au},\text{Pt},(\text{PPh}_3),(\text{PPh}_3-d_{15})_2]^+$  (**2**- $d_{30}$ ). Values are given as Normalized Collision Energies (NCE, in arbitrary units).

	<b>2</b> - $d_{15}$	<b>2</b> - $d_{30}$
C <sub>6</sub> H <sub>6</sub>	28.49	28.11
C <sub>6</sub> HD <sub>5</sub>	28.46	28.12
C <sub>6</sub> H <sub>5</sub> D	28.50	28.05
C <sub>6</sub> D <sub>6</sub>	28.58	28.21

## 5.2 Model 1

Within Model 1, we assume that the energy supplied by collision-induced dissociation (CID) is inducing reversible phenyl-group exchange between the PPh<sub>3</sub> ligands in  $[\text{Au},\text{Pt},(\text{PPh}_3)_3]^+$  (**2**) (in addition to the positional change of the PPh<sub>3</sub> ligands on the “AuPt” core). Thus, within this model, the phenyl groups are indistinguishable (because they are detached from their originating phosphorous atoms). As a consequence, one out of nine phenyl groups and one hydrogen atom out of the remaining eight phenyl groups, each chosen randomly, form the eliminated benzene molecule. For the partially deuterated complexes  $[\text{Au},\text{Pt},(\text{PPh}_3)_2,(\text{PPh}_3-d_{15})]^+$  (**2**- $d_{15}$ ) and  $[\text{Au},\text{Pt},(\text{PPh}_3),(\text{PPh}_3-d_{15})_2]^+$  (**2**- $d_{30}$ ) the calculated and the modeled isotopologue distributions, taking into account a primary KIE of 1.74 and a secondary KIE of 1.18, are given in Table S3. The two KIEs were optimized for the experimental data of **2**- $d_{15}$  and **2**- $d_{30}$  together, using the least-square criterion.

**Table S3:** Benzene isotopologue distributions resulting from Model 1 (with and without the involvement of a KIE) together with the CID data. Primary and secondary kinetic isotope effects of 1.74 and 1.18, respectively, are considered.

	“Model 1”		“Model 1” (+ KIE)		Experiment	
	<b>2</b> - $d_{15}$	<b>2</b> - $d_{15}$	<b>2</b> - $d_{15}$	<b>2</b> - $d_{30}$	<b>2</b> - $d_{15}$	<b>2</b> - $d_{30}$
C <sub>6</sub> H <sub>6</sub>	0.417	0.083	0.513	0.130	0.513	0.148
C <sub>6</sub> H <sub>5</sub> D	0.250	0.250	0.177	0.224	0.164	0.192
C <sub>6</sub> HD <sub>5</sub>	0.250	0.250	0.261	0.330	0.261	0.328
C <sub>6</sub> D <sub>6</sub>	0.083	0.417	0.050	0.316	0.063	0.332

### 5.3 Model 2

As an alternative to Model 1, one might assume that two different scenarios apply for the loss of benzene from  $[\text{Au},\text{Pt},(\text{PPh}_3)_3]^+$  (**2**) and that the data are the result of linear combination of both scenarios. In the first scenario, the phenyl group and the hydrogen atom might originate from the same  $\text{PPh}_3$  ligand (scenario 1), whereas in the second scenario the phenyl group and the hydrogen atom stem from two different  $\text{PPh}_3$  ligands (scenario 2). Considering the partial deuteration in  $[\text{Au},\text{Pt},(\text{PPh}_3)_2,(\text{PPh}_3-d_{15})]^+$  (**2-d<sub>15</sub>**) and  $[\text{Au},\text{Pt},(\text{PPh}_3),(\text{PPh}_3-d_{15})_2]^+$  (**2-d<sub>30</sub>**) and assuming positional flexibility of the  $\text{PPh}_3$  ligand on the “AuPt” core (but not of the Ph groups on the “AuPtP<sub>3</sub>“ core within this model), defined distributions of  $\text{C}_6\text{H}_6$ ,  $\text{C}_6\text{H}_5\text{D}$ ,  $\text{C}_6\text{HD}_5$ , and  $\text{C}_6\text{D}_6$  are expected for both scenarios (see Table S4).

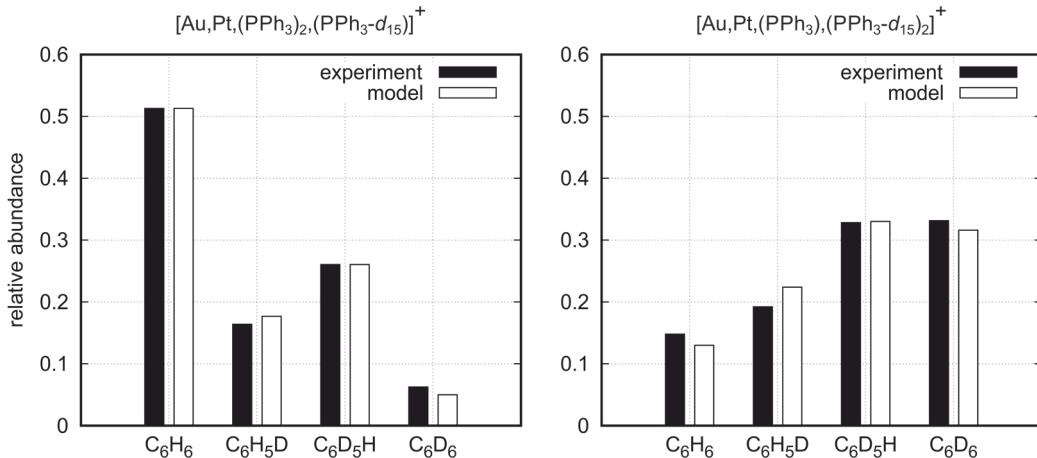
**Table S4:** Benzene-isotopologue distributions in the CID of **2-d<sub>15</sub>** and **2-d<sub>30</sub>** as expected for scenario 1 (loss of benzene from one  $\text{PPh}_3$  ligand) and scenario 2 (loss of benzene from two different  $\text{PPh}_3$  ligands).

	<b>2-d<sub>15</sub></b>		<b>2-d<sub>30</sub></b>	
	scenario 1	scenario 2	scenario 1	scenario 2
$\text{C}_6\text{H}_6$	2/3	1/3	1/3	0
$\text{C}_6\text{H}_5\text{D}$	0	1/3	0	1/3
$\text{C}_6\text{HD}_5$	0	1/3	0	1/3
$\text{C}_6\text{D}_6$	1/3	0	2/3	1/3

While none of the scenarios alone gives a satisfactory result (as detailed in the *Results and Discussion* section), a linear combination of both scenarios, thus accepting both mechanisms to compete, provides values, which are in good agreement with the experimental data. Furthermore, primary and secondary kinetic isotope effects (KIEs) have to be considered to optimize the model. The KIEs and the weighting factor  $N$  have been optimized for the CID experiments employing mass selected **2-d<sub>15</sub>** and **2-d<sub>30</sub>** together using the least-square criterion (see Table S5 and Figure S27). While both Model 1 and Model 2 describe the observed isotopologue distributions satisfactorily, the observation of phenyl-group exchange in solution and the structural features in **4[BAr<sub>4</sub>F]** let us believe that Model 1 describes the underlying processes better. On the other hand, it is important to note that both models are mathematically synonymous for  $N = 0.25$  but that the experimental data are described better with  $N = 0.34$  together with the altered isotope effects (see Table S5).

**Table S5:** Benzene isotopologue distributions in the CID of **2-d<sub>15</sub>** and **2-d<sub>30</sub>** for scenario 1 and scenario 2 considering primary and secondary kinetic isotope effects of 1.46 (KIE<sub>prim</sub>) and 0.92 (KIE<sub>sec</sub>); linear combination of both scenarios weighted with  $N = 0.34$ ; experimental data.

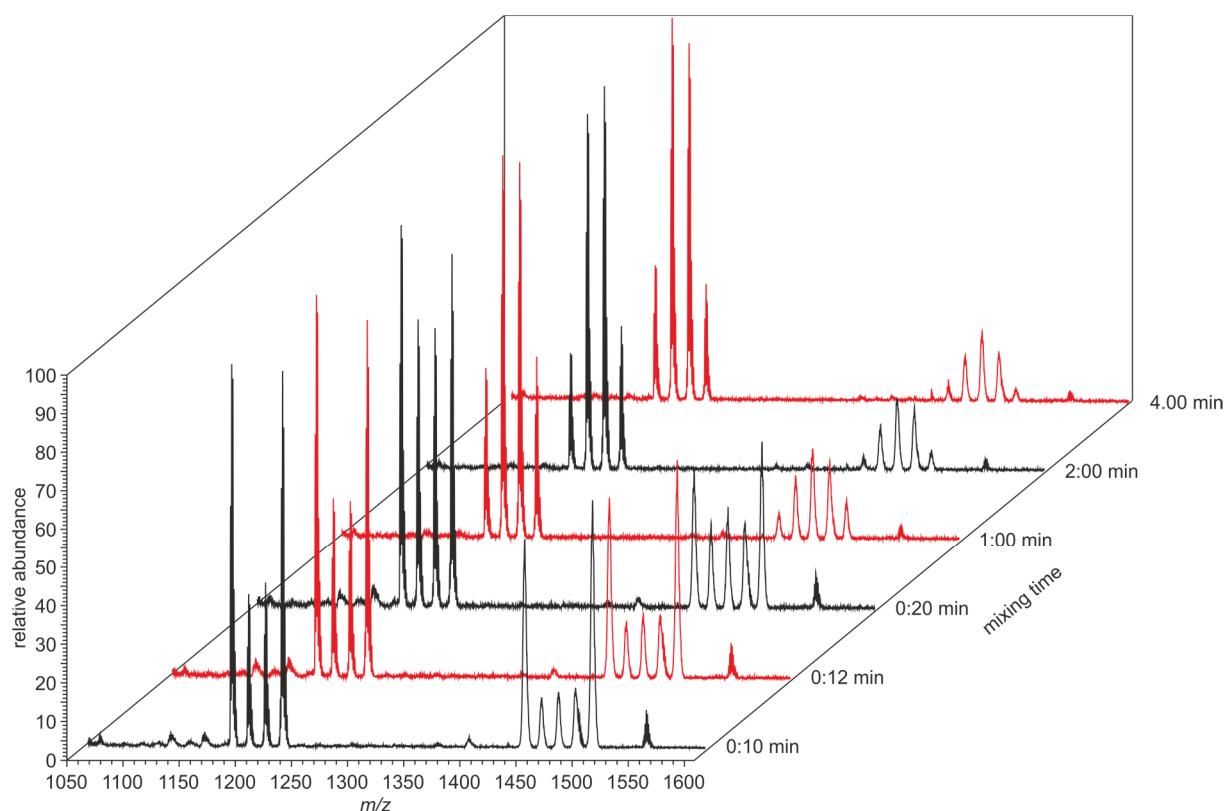
<b>2-d<sub>15</sub> (+ KIEs)</b>		<b>2-d<sub>30</sub> (+ KIEs)</b>		<b>2-d<sub>15</sub></b>	<b>2-d<sub>30</sub></b>	<b>2-d<sub>15</sub></b>	<b>2-d<sub>30</sub></b>
scenario	scenario	scenario	scenario	$N(\text{scenario 1}) +$	$(1-N)(\text{scenario 2})$	experiment	
1	2	1	2				
C <sub>6</sub> H <sub>6</sub>	0.667	0.333	0.333	0.000	0.485	0.135	0.513 0.148
C <sub>6</sub> H <sub>5</sub> D	0.000	0.228	0.000	0.228	0.164	0.181	0.164 0.192
C <sub>6</sub> HD <sub>5</sub>	0.000	0.362	0.000	0.362	0.260	0.287	0.261 0.328
C <sub>6</sub> D <sub>6</sub>	0.248	0.000	0.495	0.248	0.091	0.397	0.063 0.332



**Figure S27:** Benzene isotopologue distributions in the CID of mass-selected  $[\text{Au},\text{Pt},(\text{PPh}_3)_2,(\text{PPh}_3-\text{d}_{15})]^+$  (**2-d<sub>15</sub>**) and  $[\text{Au},\text{Pt},(\text{PPh}_3),(\text{PPh}_3-\text{d}_{15})_2]^+$  (**2-d<sub>30</sub>**). The black bars indicate the experimental results, while the white bars result from linear combination of two mechanistic scenarios, scenario 1 (involving just one PPh<sub>3</sub> ligand) and scenario 2 (involving two PPh<sub>3</sub> ligands). We further assume that the losses of the hydrogen atom and of the phenyl group are associated with a primary and secondary kinetic isotope effect of 1.46 (KIE<sub>prim</sub>) and 0.92 (KIE<sub>sec</sub>), respectively.

## 6. Phenyl Group Exchange in Solution

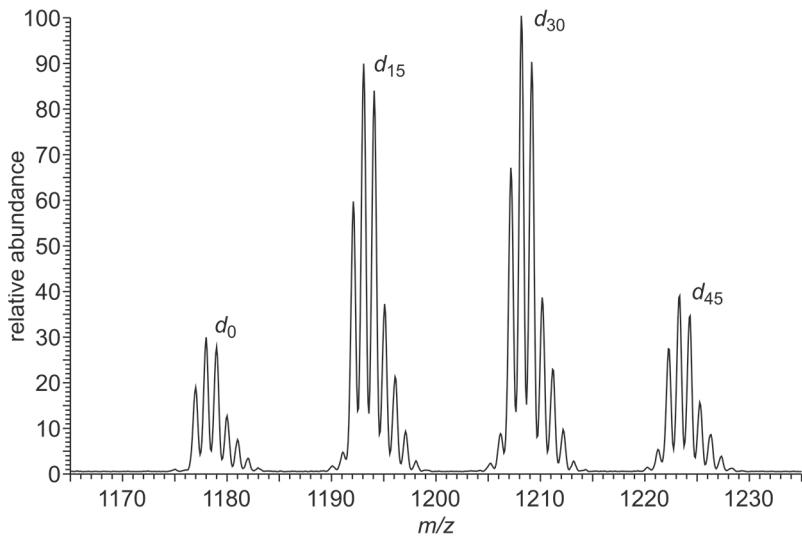
### 6.1 Time-dependent Phosphine-Exchange in Solution



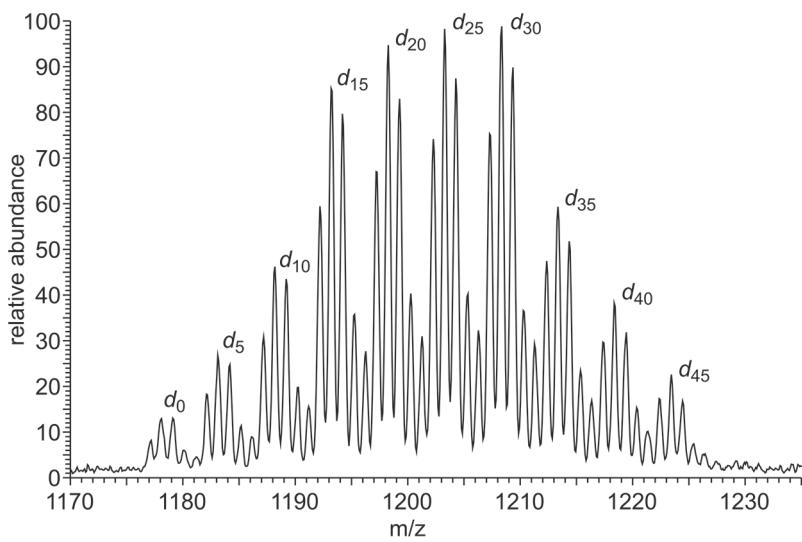
**Figure S28:** Cation-mode ESI mass spectra for different mixing times of  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_3][\text{BAr}_4^{\text{F}}]$  (**1[BAr<sub>4</sub><sup>F</sup>]**) and  $[(\text{Ph}_3\text{P}-d_{15})\text{AuPt}(\text{PPh}_3-d_{15})_3][\text{BAr}_4^{\text{F}}]$  (**1-d<sub>60</sub>[BAr<sub>4</sub><sup>F</sup>]**) dissolved in methanol. The two sets of signals correspond to  $[\text{Au},\text{Pt},(\text{PPh}_3)_{3-m},(\text{PPh}_3-d_{15})_m]^+$  ( $m = 0, 1, 2, 3$ ) and  $[\text{Au},\text{Pt},(\text{PPh}_3)_{4-n},(\text{PPh}_3-d_{15})_n]^+$  ( $n = 0, 1, 2, 3, 4$ ). The PPh<sub>3</sub> exchange is complete after 1 – 2 minutes.

## 6.2 Stoichiometric Experiments

Mass spectra before and after heating a mixture of **1**[BAr<sub>4</sub><sup>F</sup>] and **1-d**<sub>60</sub>[BAr<sub>4</sub><sup>F</sup>] in toluene are shown in Figure S29 and Figure S30, respectively.



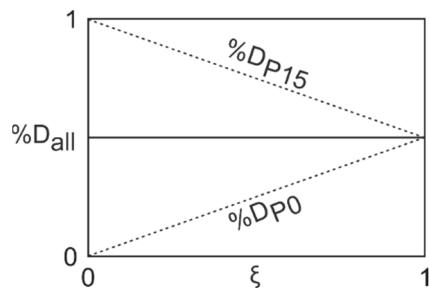
**Figure S29:** Isotopologue distribution of  $[\text{Au},\text{Pt},(\text{PPh}_3)_3]^+$  (**2**) as a result of electrospray ionization of a mixture of **1**[BAr<sub>4</sub><sup>F</sup>] and **1-d**<sub>60</sub>[BAr<sub>4</sub><sup>F</sup>] in methanol. The spectrum is measured ca. five minutes after mixing both components and shows the isotopologues **2-d**<sub>n</sub> ( $n = 0, 15, 30$ , and  $45$ ). Note that signals, which are located one mass unit below the expected patterns, do not indicate H/D exchange between the phenyl groups but are the consequence of the incomplete deuterium labeling (99.6 atom% D) of the employed PPh<sub>3</sub>-d<sub>15</sub> (see Figure S20).



**Figure S30:** Isotopologue distribution of  $[\text{Au},\text{Pt},(\text{PPh}_3)_3]^+$  (**2**) as generated by electrospray ionization of an equimolar mixture of  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_3][\text{BAr}_4^{\text{F}}]$  (**1**[BAr<sub>4</sub><sup>F</sup>]) und PPh<sub>3</sub>-d<sub>15</sub>, which was heated to 165 °C in toluene in a closed vessel. The mixture was sprayed from methanol. The spectrum shows the isotopologues **2-d**<sub>n</sub> ( $n = 0, 5, 10, 15, 20, 25, 30, 35, 40$ , and  $45$ ), and the isotope patterns are consistent with this interpretation.

### 6.3 Quantification of the Phenyl-Group Exchange in Solution

The degree of the phenyl-group exchange in the phenyl-group exchange reactions is quantified by the extent of reaction  $\xi$  ranging between 0 and 1.  $\xi = 0$  indicates the complete absence of phenyl-group exchange, while  $\xi = 1$  indicates statistical exchange of the deuterated and non-deuterated phenyl groups among the triphenylphosphine ligands. Towards the determination of  $\xi$ , we distinguish between the phosphorus atoms that carry only C<sub>6</sub>H<sub>5</sub> and C<sub>6</sub>D<sub>5</sub> groups in the beginning. The mole fractions of the two types of phosphorus atoms are denoted as  $x_{P0}$  and  $x_{P15}$  and correspond to the mole fractions of P(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub> and P(C<sub>6</sub>D<sub>5</sub>)<sub>3</sub> contained in the reaction mixture before heating. During the reaction the number of phosphorus atoms does not change, and consequently  $x_{P0}$  and  $x_{P15}$  are constant. Also the overall deuterium content %D<sub>all</sub> (or in other words the fraction of deuterated phenyl groups) in the mixture is constant. What changes, however, are the degrees of deuteration %D<sub>P0</sub> and %D<sub>P15</sub> within the two mole fractions  $x_{P0}$  and  $x_{P15}$ , respectively. Before the reaction mixture is heated, %D<sub>P0</sub> = 0 and %D<sub>P15</sub> = 1, thus  $\xi = 0$ . During the reaction, the overall deuterium content %D<sub>all</sub> =  $x_{P0} \cdot \%D_{P0} + x_{P15} \cdot \%D_{P15}$  is a constant and equals  $x_{P15}$ . If the reaction leads to statistical exchange of the deuterated and non-deuterated phenyl groups within the fractions  $x_{P0}$  and  $x_{P15}$ , %D<sub>P0</sub> = %D<sub>P15</sub> is valid and therefore  $\xi = 1$ . These relationships are summarized in Figure S31.



**Figure S31:** Illustration of the relationship of the extent of reaction  $\xi$ , the mole fractions  $x_{P0}$  and  $x_{P15}$  (which correspond to the mole fractions of P(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub> and P(C<sub>6</sub>D<sub>5</sub>)<sub>3</sub> contained in the reaction mixture), the respective deuterium contents %D<sub>P0</sub> and %D<sub>P15</sub>, and the overall deuterium content %D<sub>all</sub>.

The deuterium content within the two fractions  $x_{P0}$  and  $x_{P15}$  is thus a function of  $x_{P15}$  and  $\xi$  according to equations (2) and (3).

$$\%D_{P0} = x_{P15} \cdot \xi \quad (2)$$

$$\%D_{P15} = 1 - (1 - x_{P15}) \cdot \xi \quad (3)$$

The mass spectra of the product mixture were modeled accordingly employing  $x_{P15}$  and  $\xi$  as parameters.

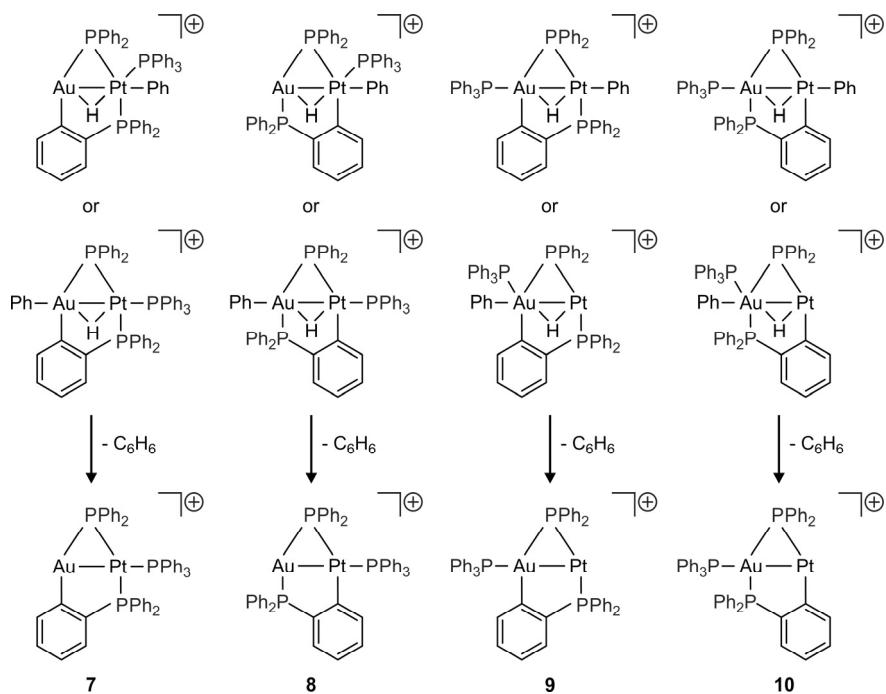
#### 6.4 Test on Phenyl-Group Exchange employing Mononuclear Complexes

To verify that phenyl-group exchange between triphenylphosphine is exclusively mediated by the cationic, bimetallic AuPt complex  $[\text{AuPt}(\text{PPh}_3)_3]^+$  (**2**), experiments employing  $[(\text{Ph}_3\text{P})\text{AuCl}]$ ,  $[\text{Pt}(\text{PPh}_3)_3]$ , and  $[\text{Au}(\text{PPh}_3)_2]^+$  have been conducted (see Table S5). However, phenyl-group exchange is not observed for any of these complexes when mixed with  $\text{PPh}_3-d_{15}$  and heated to 165 °C in toluene in a closed vessel.

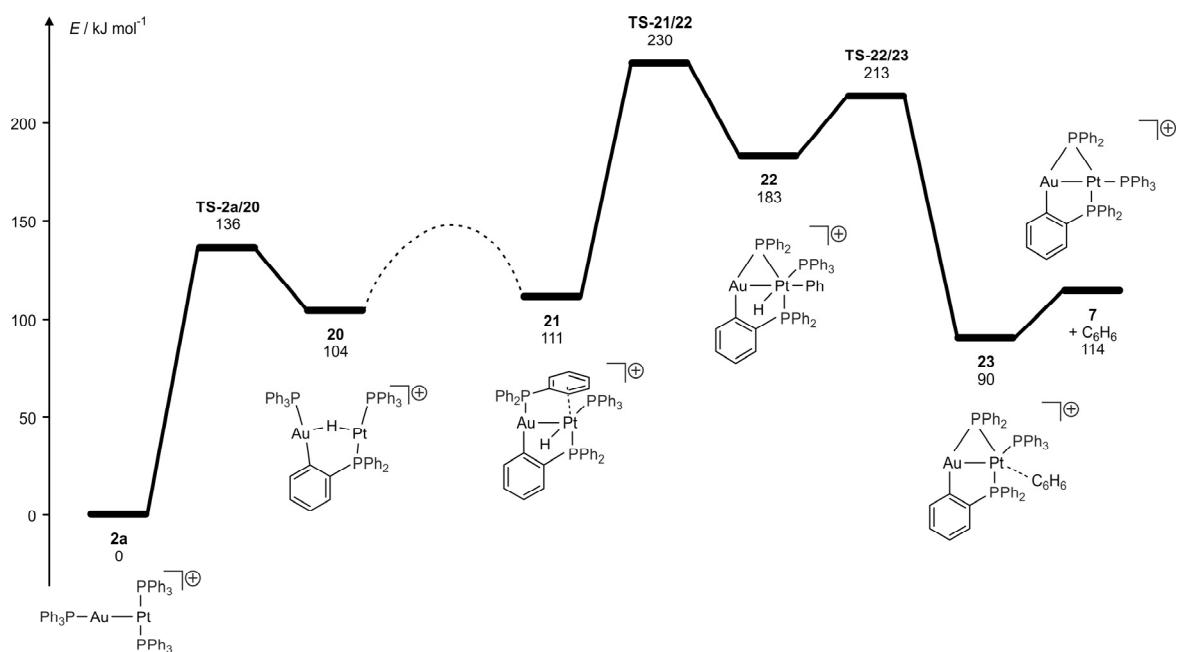
**Table S5:** Mixtures of  $\text{PPh}_3-d_{15}$  and different gold and platinum complexes, of which was suspected that phenyl-group exchange might be mediated, heated to 165 °C in toluene (ca. 2 ml) in a closed vessel.

entry	compounds	amount of substance	Reaction time
1	$[\text{Pt}(\text{PPh}_3)_3]$	9.9 mg, 0.01 mmol	2 h
	$\text{PPh}_3-d_{15}$	8.4 mg, 0.03 mmol	
2	$[\text{Au}(\text{PPh}_3)_2][\text{BAr}_4^F]$	15.9 mg, 0.01 mmol	2 h
	$\text{PPh}_3-d_{15}$	5.6 mg, 0.02 mmol	
3	$[(\text{Ph}_3\text{P})\text{AuCl}]$	5.0 mg, 0.01 mmol	2 h
	$\text{Pt}(\text{PPh}_3)_3$	9.8 mg, 0.01 mmol	
	$\text{PPh}_3-d_{15}$	11.5 mg, 0.04 mmol	
4	$[(\text{Ph}_3\text{P})\text{AuCl}]$	5.2 mg, 0.01 mmol	2 h
	$\text{PPh}_3-d_{15}$	3.1 mg, 0.01 mmol	

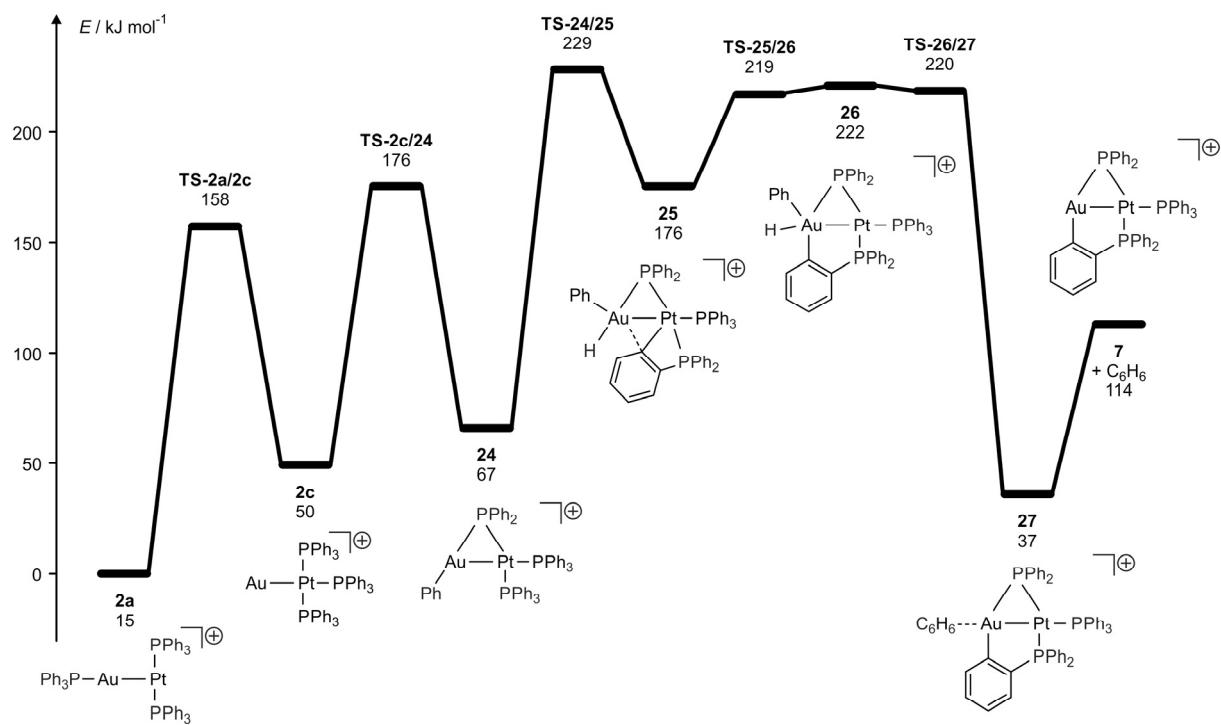
## 7. DFT Calculations



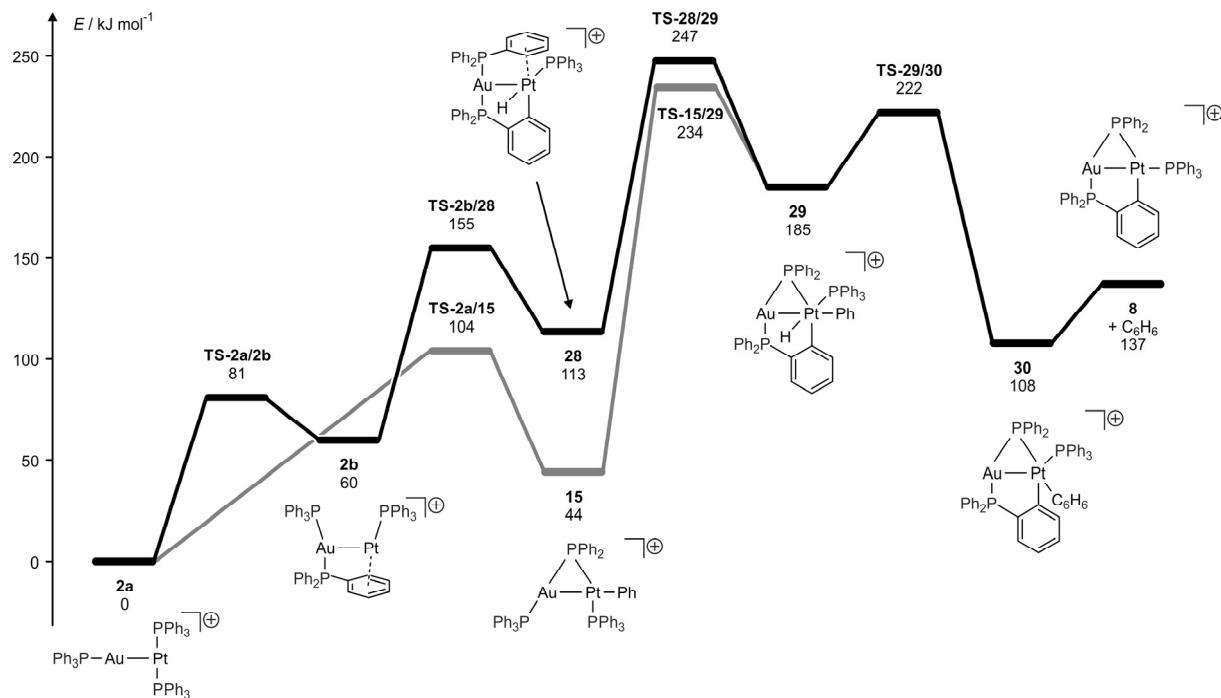
**Scheme S1:** Summary of the eight hydride intermediates, which have been chosen as starting points for the elucidation of reaction pathways towards the formation of the possible product ions **7 – 10** in the CID of mass-selected  $[Au,Pt,(PPh_3)_3]^+$  (**2**).



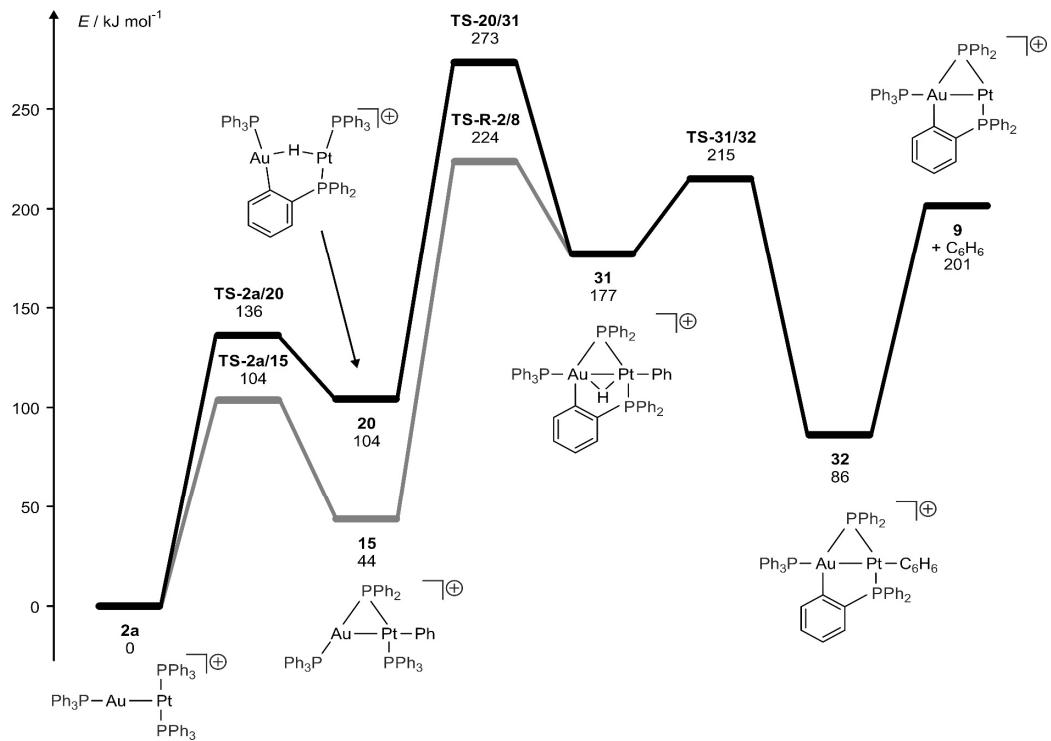
**Figure S32:** Energy profile for the formation of **7** and  $C_6H_6$  upon CID of mass-selected  $[(Ph_3P)AuPt(PPh_3)_2]^+$  (**2**). Both the hydride and phenyl-group transfer occur *at the platinum atom*. A transition state for the transformation of **20** to **21** could not be located even after several attempts. The corresponding barriers, however, will most probably not exceed **TS-21/22**. Zero-point corrected electronic energies are given in  $\text{kJ mol}^{-1}$  relative to **2a**.



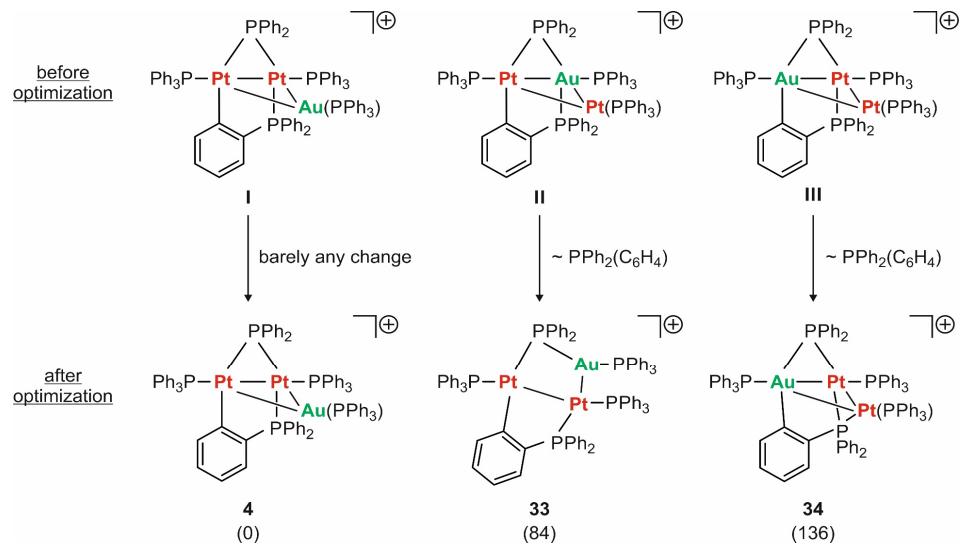
**Figure S33:** Energy profile for the formation of **7** and  $\text{C}_6\text{H}_6$  upon CID of mass-selected  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_2]^+$  (**2**). Both the hydride and phenyl-group transfer occur *at the gold atom*. Zero-point corrected electronic energies are given in kJ mol<sup>-1</sup> relative to **2a**.



**Figure S34:** Energy profiles for the formation of **8** and  $\text{C}_6\text{H}_6$  upon CID of mass-selected  $[(\text{Ph}_3\text{P})\text{AuPt}(\text{PPh}_3)_2]^+$  (**2**). Zero-point corrected electronic energies are given in kJ mol<sup>-1</sup> relative to **2a**.



**Figure S35:** Energy profiles for the formation of **9** and C<sub>6</sub>H<sub>6</sub> upon CID of mass-selected [(Ph<sub>3</sub>P)AuPt(PPh<sub>3</sub>)<sub>2</sub>]<sup>+</sup> (**2**). Zero-point corrected electronic energies are given in kJ mol<sup>-1</sup> relative to **2a**.



**Scheme S2:** Schematic representation of the outcome of the geometry optimizations of the three possible metallomers of **4** together with the zero-point corrected electronic energies in kJ mol<sup>-1</sup>. The crystal structure of **4[BAr<sub>4</sub>F]** served as the input structure. Metallomer **I** converges to the topology observed in the crystal structure of **4[BAr<sub>4</sub>F]**. Metallomer **II** undergoes quite a severe rearrangement resulting in a structure that is by 84 kJ mol<sup>-1</sup> less stable than **4**. The rearrangement, which is observed upon optimization of metallomers **III** is only minor, but the energy of the resulting structure is 136 kJ mol<sup>-1</sup> higher in energy than **4** and the corresponding topology is thus excluded as the structure of **4**.

## 8 Cartesian Coordinates and Energies of the DFT Calculations

### 2a

ZPE(BP86/def2-SVP) = 0.8060780 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0449719 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.05730330401 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.15774	-0.03447	2.28090
Au	-0.00388	-0.32686	-0.29389
C	1.25919	-1.64326	-3.16646
P	-0.05666	-0.54280	-2.55083
P	0.15830	-2.33507	2.35359
C	1.58313	-2.78434	-2.40278
C	2.57332	-3.66762	-2.85403
P	0.00070	2.19455	1.73339
C	3.24505	-3.41178	-4.06257
C	2.92546	-2.27212	-4.82085
C	1.93291	-1.38376	-4.37707
C	0.17049	1.07051	-3.37326
C	-0.64808	1.48776	-4.44017
C	-0.45629	2.75979	-5.00527
C	0.54587	3.61075	-4.50946
C	1.36817	3.18860	-3.44862
C	1.18018	1.92311	-2.87847
C	-1.63581	-1.21769	-3.16078
C	-1.68566	-2.28120	-4.08175
C	-2.93125	-2.75928	-4.52121
C	-4.11904	-2.17489	-4.05036
C	-4.06499	-1.11408	-3.12815
C	-2.82727	-0.64223	-2.67220
C	1.75560	-3.12974	1.92803
C	2.58387	-2.51659	0.96421
C	3.76731	-3.14431	0.55075
C	4.13931	-4.37978	1.10898
C	3.32494	-4.98547	2.08100
C	-1.00387	-2.98608	1.08172
C	-0.65053	-4.03829	0.21516
C	-1.52471	-4.41828	-0.81805
C	-2.75734	-3.76747	-0.97601
C	-3.12553	-2.73729	-0.09291
C	-2.25179	-2.33927	0.92678
C	-0.35594	-3.09965	3.93156
C	0.21199	-2.59580	5.12187
C	-0.13597	-3.16122	6.35648
C	-1.05755	-4.22216	6.40915
C	-1.62970	-4.71837	5.22611
C	-1.28147	-4.16064	3.98517
C	-0.38730	3.36595	3.08494
C	-1.36733	4.37051	2.95870
C	-1.59950	5.25432	4.02527
C	-0.85939	5.13807	5.21333
C	0.11580	4.13301	5.34129
C	0.35038	3.24492	4.28246
C	-1.35630	2.41919	0.50684
C	-2.61544	1.85871	0.82202
C	-3.67665	1.96347	-0.08698

C	-3.48612	2.60878	-1.32380
C	-2.23313	3.15410	-1.64389
C	-1.17141	3.06850	-0.72855
C	1.49230	2.89449	0.92863
C	2.71659	4.78650	0.00415
C	3.73815	3.91804	-0.42117
C	3.64804	2.54162	-0.15344
C	2.52905	2.02970	0.52221
C	2.13365	-4.36542	2.49152
H	-3.43144	-4.05374	-1.79584
H	-4.09171	-2.22743	-0.21494
H	-2.51705	-1.50774	1.59808
H	0.31620	-4.54812	0.33766
H	-1.23537	-5.22618	-1.50632
H	-4.31731	2.68071	-2.04099
H	-2.97274	-3.59144	-5.23963
H	-5.09213	-2.54966	-4.40148
H	-4.99429	-0.65872	-2.75412
H	-2.78125	0.17205	-1.93355
H	-0.75461	-2.73493	-4.45188
H	-4.65754	1.53471	0.16757
H	2.15087	3.85041	-3.04923
H	-2.36500	6.03845	3.92668
H	0.68688	4.60842	-4.95140
H	-1.09695	3.08816	-5.83727
H	-1.44003	0.82578	-4.81984
H	1.80156	1.60731	-2.02707
H	-1.04601	5.83139	6.04693
H	0.69276	4.03883	6.27327
H	1.11095	2.45313	4.37858
H	-1.95109	4.45891	2.03022
H	5.07266	-4.86884	0.79194
H	4.40323	-2.66402	-0.20750
H	3.61879	-5.94845	2.52462
H	2.28380	-1.54688	0.53349
H	4.02688	-4.10172	-4.41380
H	2.82917	-4.55154	-2.25128
H	3.45500	-2.07090	-5.76393
H	1.68562	-0.48740	-4.96535
H	1.05975	-2.97014	-1.45323
H	-2.07040	3.64680	-2.61321
H	-0.19294	3.49093	-0.99070
H	-1.33413	-4.66124	7.37927
H	-2.35315	-5.54624	5.26814
H	0.30902	-2.76969	7.28330
H	0.92994	-1.76097	5.07531
H	-2.75192	1.33508	1.78125
H	2.44593	0.95483	0.74713
H	4.61693	4.31999	-0.94752
H	-1.72942	-4.54742	3.05764
H	4.45606	1.86337	-0.46562
H	1.49559	-4.84199	3.25087
C	1.59891	4.27975	0.68440
H	2.79558	5.86699	-0.18776
H	0.80798	4.96257	1.03076

## 2b

ZPE(BP86/def2-SVP) = 0.8054293 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0220383 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.03375117600 Hartree (single point)

Cartesian coordinates in Å:

Pt	1.36929	0.40160	-0.97681
Au	-1.27610	0.75319	0.31049
C	1.09406	3.01392	1.78128
P	-0.00233	2.73642	0.34762
P	1.94419	-1.56594	-0.07724
C	2.27783	2.25872	1.93727
C	3.05339	2.40353	3.09536
P	-2.78566	-0.97584	-0.06608
C	2.65472	3.29602	4.10534
C	1.47783	4.04818	3.95219
C	0.69558	3.91123	2.79479
C	1.08400	2.64173	-1.13621
C	2.35644	3.29589	-1.20314
C	3.05850	3.33811	-2.40518
C	2.53408	2.73223	-3.57388
C	1.29079	2.10357	-3.53990
C	0.53867	2.05488	-2.33144
C	-1.00256	4.25623	0.17186
C	-0.39997	5.47313	-0.21190
C	-1.18632	6.62617	-0.34285
C	-2.56955	6.56951	-0.09166
C	-3.17018	5.35796	0.28739
C	-2.38960	4.19796	0.41573
C	3.75778	-1.86412	-0.10512
C	4.61904	-0.74810	-0.12928
C	6.00958	-0.93093	-0.09007
C	6.54639	-2.22818	-0.03748
C	5.69095	-3.34361	-0.03113
C	1.49534	-1.82172	1.69000
C	1.75120	-3.05142	2.33426
C	1.51089	-3.18788	3.70854
C	1.02938	-2.09740	4.45647
C	0.76615	-0.87493	3.81967
C	0.99248	-0.74338	2.44083
C	1.23571	-2.98969	-0.98545
C	0.13405	-3.71432	-0.49378
C	-0.44929	-4.71857	-1.28336
C	0.05937	-5.00295	-2.55882
C	1.16168	-4.28066	-3.05035
C	1.74567	-3.27326	-2.27165
C	-2.65711	-2.42053	1.03994
C	-2.10846	-2.24026	2.32504
C	-2.00039	-3.33221	3.19863
C	-2.43698	-4.60377	2.79220
C	-2.99478	-4.78235	1.51401
C	-3.10744	-3.69435	0.63606
C	-4.51420	-0.39276	0.06643
C	-5.45962	-1.02793	0.89378
C	-6.77138	-0.52813	0.96229
C	-7.13959	0.59743	0.20896
C	-6.19333	1.23350	-0.61589

C	-4.88208	0.74582	-0.68437
C	-2.61713	-1.58546	-1.78032
C	-3.53888	-2.70527	-3.73453
C	-2.29577	-2.59320	-4.38142
C	-1.21918	-1.96514	-3.73412
C	-1.37421	-1.46378	-2.43460
C	4.29972	-3.16553	-0.06502
H	0.86291	-2.20420	5.53912
H	0.39112	-0.01372	4.39245
H	0.79011	0.21037	1.93526
H	2.14484	-3.90575	1.76474
H	1.71202	-4.14976	4.20319
H	-8.16796	0.98424	0.26486
H	-0.71903	7.57546	-0.64412
H	-3.18231	7.47731	-0.19634
H	-4.25209	5.31324	0.48144
H	-2.85073	3.23860	0.70295
H	0.68151	5.51828	-0.41227
H	-7.50935	-1.02487	1.60957
H	0.86296	1.65669	-4.44902
H	-1.56374	-3.18676	4.19614
H	3.10778	2.76731	-4.51140
H	4.03498	3.84321	-2.44387
H	2.77504	3.75740	-0.29716
H	-0.51959	1.75152	-2.37004
H	-2.34403	-5.46146	3.47486
H	-3.34156	-5.77751	1.19772
H	-3.52479	-3.83859	-0.37084
H	-1.75069	-1.24730	2.63413
H	7.63690	-2.37242	-0.01270
H	6.67784	-0.05710	-0.11208
H	6.11077	-4.36032	-0.00516
H	4.18154	0.26115	-0.20166
H	3.26432	3.40740	5.01439
H	3.97226	1.80961	3.20905
H	1.16504	4.75078	4.73881
H	-0.22404	4.50356	2.67830
H	2.57179	1.54775	1.14685
H	-6.48006	2.11607	-1.20691
H	-4.13778	1.24638	-1.32418
H	-0.40216	-5.78955	-3.17377
H	1.56592	-4.50212	-4.04948
H	-1.30811	-5.28134	-0.89172
H	-0.27161	-3.49469	0.50314
H	-5.17251	-1.90987	1.48480
H	-0.52450	-0.96109	-1.93159
H	-2.17137	-2.98843	-5.40076
H	2.59996	-2.69781	-2.66059
H	-0.24764	-1.86231	-4.23790
H	3.63572	-4.04294	-0.08179
C	-3.70706	-2.19517	-2.43815
H	-4.38742	-3.18216	-4.24736
H	-4.68906	-2.25453	-1.94408

## 2c

ZPE(BP86/def2-SVP) = 0.8073764 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0409545 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.03939711884 Hartree (single point)

Cartesian coordinates in Å:

C	-2.30905	1.79796	-1.07487
P	-1.48359	0.17595	-1.29685
P	1.90055	-0.60702	-1.33229
C	-1.46958	2.90655	-0.83514
C	-2.00586	4.20016	-0.77475
P	-1.03036	0.44022	2.14513
C	-3.38681	4.39282	-0.94357
C	-4.22610	3.28775	-1.15900
C	-3.69313	1.99163	-1.22917
C	-2.72114	-1.16579	-1.13116
C	-3.79188	-1.28445	-2.04380
C	-4.72007	-2.32702	-1.90326
C	-4.57472	-3.27099	-0.87120
C	-3.49291	-3.17538	0.01960
C	-2.57122	-2.12623	-0.11100
C	-1.14538	0.16168	-3.10506
C	-1.05548	1.36247	-3.83853
C	-0.82237	1.32318	-5.22060
C	-0.66966	0.09326	-5.88091
C	-0.75176	-1.10440	-5.15194
C	-0.99525	-1.07345	-3.77176
C	3.64152	-0.76010	-0.75118
C	4.56735	0.28736	-0.90414
C	5.85602	0.16394	-0.35680
C	6.22555	-1.00300	0.32845
C	5.30718	-2.06213	0.45621
C	2.00184	0.68474	-2.62552
C	1.91353	2.01705	-2.16368
C	2.05513	3.08593	-3.05934
C	2.28386	2.83102	-4.42215
C	2.36166	1.50724	-4.88308
C	2.22309	0.43304	-3.99048
C	1.60929	-2.24983	-2.07851
C	2.48125	-2.77989	-3.05379
C	2.23203	-4.04893	-3.59660
C	1.13684	-4.80912	-3.14779
C	0.29905	-4.30621	-2.13896
C	0.53738	-3.03110	-1.60511
C	-1.27390	-1.04705	3.19210
C	-0.51559	-2.21318	2.95569
C	-0.71629	-3.35707	3.74293
C	-1.66841	-3.34388	4.77573
C	-2.42656	-2.18523	5.01561
C	-2.23913	-1.04253	4.22324
C	-2.74663	1.10292	2.00759
C	-3.82948	0.22864	1.77282
C	-5.13641	0.72790	1.68472
C	-5.37785	2.10289	1.83542
C	-4.30349	2.97668	2.06621
C	-2.99326	2.48331	2.15144
C	4.01927	-1.94409	-0.07962

H	2.39525	3.66750	-5.12791
H	2.52323	1.30444	-5.95195
H	2.25824	-0.59677	-4.36894
H	1.74436	2.20236	-1.09038
H	1.98851	4.12102	-2.69263
H	-6.40464	2.49370	1.77677
H	-0.76106	2.26522	-5.78459
H	-0.49034	0.06803	-6.96609
H	-0.63944	-2.07380	-5.65961
H	-1.08713	-2.01661	-3.21839
H	-1.17695	2.33070	-3.33508
H	-5.97081	0.03266	1.50935
H	-3.36357	-3.91513	0.82351
H	-0.12091	-4.26181	3.54986
H	-5.30150	-4.09086	-0.77055
H	-5.55679	-2.41051	-2.61270
H	-3.88768	-0.57525	-2.87924
H	-1.72732	-2.04432	0.59013
H	-1.82248	-4.23997	5.39531
H	-3.17410	-2.17097	5.82261
H	-2.85488	-0.14870	4.40000
H	0.24332	-2.20786	2.15659
H	7.23456	-1.09478	0.75700
H	6.57530	0.98841	-0.47200
H	5.59731	-2.98548	0.97922
H	4.28664	1.20481	-1.44007
H	-3.81245	5.40605	-0.89475
H	-1.34382	5.05945	-0.59153
H	-5.31083	3.43285	-1.26837
H	-4.36136	1.13384	-1.38211
H	-0.38992	2.74158	-0.70603
H	-4.48356	4.05490	2.18658
H	-2.16266	3.17603	2.34333
H	0.94990	-5.80619	-3.57371
H	-0.544476	-4.90481	-1.76495
H	2.90600	-4.45470	-4.36567
H	3.36862	-2.21324	-3.37208
H	-3.66060	-0.85135	1.68210
H	-0.11126	-2.62481	-0.81589
H	-0.67443	0.85598	5.09321
H	0.47003	2.65991	6.38200
C	-0.19127	1.68640	4.55943
C	0.45853	2.70016	5.28263
C	-0.19018	1.72308	3.15310
C	1.09213	3.75726	4.61020
H	1.60009	4.54799	5.18194
C	0.45196	2.78304	2.47724
C	1.08373	3.79978	3.20461
H	0.47020	2.78971	1.37737
H	1.58602	4.62184	2.67332
H	3.29932	-2.76855	0.03198
Pt	0.24378	-0.04372	0.22037
Au	2.12049	-0.20287	2.00733

**4**

ZPE(BP86/def2-SVP) = 1.2447442 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -5322.4071397 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -5320.84364520672 Hartree (single point)

Cartesian coordinates in Å:

P	1.15812	-0.70239	-0.04656
P	-4.33743	2.94858	2.20485
P	-0.44378	4.33280	-2.19498
P	-1.32255	0.97717	2.19420
P	-2.34467	-0.35150	-1.76526
C	1.69201	-1.36605	1.57373
C	0.75203	-2.12892	2.29937
C	1.04381	-2.55535	3.60171
C	2.27849	-2.22101	4.18673
C	3.22339	-1.47552	3.46045
C	2.93426	-1.04534	2.15483
C	1.49663	-2.00696	-1.28033
C	1.79087	-3.33455	-0.91180
C	1.90149	-4.32584	-1.90192
C	1.73425	-3.99566	-3.25681
C	1.45403	-2.66765	-3.62657
C	1.32361	-1.67891	-2.64339
C	2.34084	0.65046	-0.42727
C	3.45862	0.47541	-1.26866
C	4.30333	1.56440	-1.54501
C	4.04485	2.82505	-0.98004
C	2.94347	2.99728	-0.12464
C	2.09329	1.91759	0.14632
C	-4.08776	4.72576	1.82147
C	-3.71546	5.07825	0.50505
C	-3.55122	6.42644	0.15336
C	-3.73573	7.43132	1.11830
C	-4.09443	7.08606	2.43312
C	-4.27547	5.73902	2.78611
C	-6.14345	2.64389	2.14099
C	-7.10000	3.64640	2.39325
C	-8.46775	3.33717	2.32805
C	-8.88333	2.03009	2.02131
C	-7.92989	1.02849	1.76998
C	-6.56250	1.33502	1.81990
C	-3.90730	2.75152	3.97899
C	-4.62156	1.84161	4.78413
C	-4.21331	1.60105	6.10545
C	-3.09720	2.26753	6.63500
C	-2.37640	3.16740	5.83113
C	-2.77419	3.40591	4.50821
C	0.53909	3.69330	-3.59718
C	1.38617	2.58762	-3.36695
C	2.16541	2.07693	-4.41370
C	2.09493	2.65633	-5.69276
C	1.24033	3.74778	-5.92582
C	0.46095	4.27018	-4.88073
C	0.61100	5.54537	-1.33130
C	1.91795	5.84049	-1.76333
C	2.69816	6.75875	-1.04080
C	2.17364	7.38900	0.09947

C	0.86404	7.09788	0.52507
C	0.08635	6.16837	-0.17802
C	-1.83451	5.28498	-2.89692
C	-1.71481	6.66068	-3.18507
C	-2.82112	7.36422	-3.68739
C	-4.04150	6.69973	-3.90109
C	-4.15807	5.32805	-3.61689
C	-3.05984	4.61737	-3.11309
C	-0.03031	2.05442	2.87730
C	-0.02206	3.41409	2.49220
C	1.06827	4.23182	2.82012
C	2.16063	3.70004	3.52868
C	2.15922	2.34626	3.90586
C	1.07128	1.52202	3.58238
C	-1.75127	-0.29297	3.41978
C	-1.47522	-0.16817	4.79468
C	-1.89558	-1.16636	5.68752
C	-2.59844	-2.28834	5.21925
C	-2.89396	-2.40561	3.84770
C	-2.47690	-1.41429	2.95198
C	-2.97717	-1.88813	-0.99440
C	-2.07236	-2.95967	-0.79344
C	-2.45647	-4.06229	-0.01839
C	-3.73418	-4.10177	0.56970
C	-4.63121	-3.03816	0.37333
C	-4.25753	-1.93078	-0.40538
C	-1.79047	-0.75041	-3.45750
C	-2.02785	-1.98740	-4.08557
C	-1.58004	-2.19806	-5.40038
C	-0.90176	-1.17907	-6.08974
C	-0.66507	0.05852	-5.46259
C	-1.10541	0.27069	-4.14999
C	-3.78874	0.76001	-2.00722
C	-4.47978	0.73725	-3.23715
C	-5.59055	1.57059	-3.43547
C	-6.01119	2.41309	-2.39346
C	-5.31933	2.42841	-1.17114
C	-4.18667	1.61312	-0.92965
H	-0.93230	5.92668	0.16342
H	0.44633	7.59657	1.41266
H	2.78567	8.11252	0.65840
H	3.72089	6.98729	-1.37599
H	2.32663	5.34579	-2.65653
H	-0.21301	5.12025	-5.06405
H	1.17729	4.19576	-6.92870
H	2.70244	2.24976	-6.51521
H	2.82176	1.21515	-4.22552
H	1.41981	2.12236	-2.37087
H	-3.16191	3.54906	-2.86275
H	-0.76388	7.18214	-2.99883
H	-2.73129	8.43860	-3.90686
H	-4.90895	7.25699	-4.28513
H	-5.11132	4.80283	-3.77098
H	-5.68616	3.09935	-0.38083
H	1.22564	2.05781	0.80163
H	2.73049	3.97661	0.32626
H	4.70482	3.67555	-1.20731
H	5.17055	1.42518	-2.20790
H	3.66390	-0.50932	-1.71376
H	3.66262	-0.43913	1.59652
H	4.19032	-1.21689	3.91783
H	2.50332	-2.53960	5.21562

H	0.29187	-3.12456	4.16785
H	-0.22679	-2.35613	1.85044
H	-6.77760	4.67169	2.62776
H	-9.21451	4.12285	2.51720
H	-9.95657	1.79296	1.97021
H	-8.25428	0.00743	1.51962
H	-5.80247	0.57110	1.58827
H	-2.70464	-1.50413	1.87755
H	-3.45117	-3.27545	3.46966
H	-2.92359	-3.06949	5.92274
H	-1.67645	-1.06083	6.76069
H	-0.94745	0.71780	5.17277
H	-2.19884	4.10505	3.88642
H	-5.50009	1.31938	4.37825
H	-4.77549	0.88650	6.72451
H	-2.78356	2.08091	7.67290
H	-1.49458	3.68837	6.23322
H	-3.54833	4.28854	-0.24184
H	-3.27435	6.68681	-0.87853
H	-3.60091	8.48867	0.84484
H	-4.23907	7.87146	3.19016
H	-4.55237	5.47360	3.81738
H	-0.91380	1.23265	-3.64925
H	-0.13154	0.86131	-5.99174
H	-0.55623	-1.34850	-7.12067
H	-1.76521	-3.16605	-5.88970
H	-2.56377	-2.78435	-3.54949
H	1.07153	-0.64859	-2.93370
H	1.31705	-2.39948	-4.68380
H	1.82276	-4.77507	-4.02825
H	2.12765	-5.36268	-1.61080
H	1.92933	-3.59183	0.14880
H	-1.06521	-2.92133	-1.23573
H	-1.75024	-4.89226	0.13295
H	-4.03139	-4.96714	1.18095
H	-5.63023	-3.06812	0.83338
H	-4.94812	-1.08672	-0.54769
H	-6.88980	3.06330	-2.52890
H	-6.12585	1.55585	-4.39664
H	-4.14274	0.07205	-4.04618
H	-0.86569	3.80960	1.90203
H	1.07377	5.28471	2.50504
H	3.02016	4.34059	3.77613
H	3.01985	1.92034	4.44297
H	1.09361	0.45557	3.84814
Pt	-0.98862	0.15229	0.03605
Au	-1.21051	2.67671	-0.86956
Pt	-3.07833	1.62444	0.83629

ZPE(BP86/def2-SVP) = 0.7068918 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3130.8947537 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3129.95849695169 Hartree (single point)

Cartesian coordinates in Å:

Pt	3.33824	4.74363	4.15768
Au	5.40501	6.06446	5.08931
P	4.22171	5.23338	2.03741
P	1.44807	3.53929	4.01212
P	3.44406	5.32098	6.39541
C	6.02430	5.60355	2.17335
C	6.83904	5.44135	1.03183
C	8.19210	5.80966	1.07297
C	8.73432	6.33583	2.25583
C	7.93029	6.47647	3.40070
C	3.46384	6.82641	1.53029
C	4.17770	7.76679	0.75927
C	3.56907	8.97706	0.39088
C	2.25437	9.26265	0.79718
C	1.54605	8.33688	1.58182
C	2.14932	7.12614	1.95106
C	4.04189	4.08187	0.63566
C	3.82161	4.52043	-0.68462
C	3.68753	3.57754	-1.71636
C	3.76605	2.20436	-1.43197
C	3.97957	1.76692	-0.11271
C	4.11619	2.70209	0.92064
C	1.06658	2.81614	2.37929
C	1.01488	3.64530	1.23705
C	0.70384	3.10037	-0.01454
C	0.47896	1.72003	-0.14447
C	0.55965	0.88694	0.98256
C	0.84824	1.42905	2.24441
C	0.01427	4.55366	4.51906
C	-0.78772	5.23246	3.57802
C	-1.80539	6.09299	4.01860
C	-2.03895	6.27128	5.39234
C	-1.25160	5.58527	6.33138
C	-0.22112	4.74254	5.89849
C	1.54867	2.13970	5.17824
C	0.38887	1.55665	5.73087
C	0.51006	0.46114	6.59950
C	1.77835	-0.05896	6.90875
C	2.93259	0.51618	6.35160
C	2.82124	1.61777	5.49378
C	3.59348	4.02094	7.65143
C	2.48893	3.51787	8.37582
C	2.65054	2.42088	9.23204
C	3.91057	1.81515	9.37621
C	5.01192	2.30618	8.65499
C	4.85588	3.40107	7.79352
C	2.19670	6.54883	6.87032
C	1.67741	7.36335	5.83521
C	0.72447	8.34500	6.12257
C	0.27744	8.52729	7.44371
C	0.80458	7.73569	8.47815

C	1.76769	6.75298	8.19982
C	6.56809	6.11202	3.38960
H	1.78545	10.21590	0.51121
H	0.52266	8.56052	1.91849
H	1.60708	6.41678	2.59515
H	5.21654	7.55912	0.46251
H	4.13076	9.70745	-0.21023
H	-0.47625	9.29612	7.66973
H	0.32279	8.96798	5.31032
H	1.78447	2.03349	9.78827
H	4.03373	0.95623	10.05241
H	6.00031	1.83632	8.76700
H	5.71548	3.78326	7.22001
H	1.49828	3.98158	8.27143
H	-2.84094	6.94299	5.73203
H	9.79448	6.62940	2.29337
H	8.82163	5.68248	0.17981
H	8.38283	6.87375	4.32265
H	6.41497	5.02290	0.10651
H	-2.43131	6.61480	3.27955
H	-0.63844	5.07396	2.50122
H	0.40310	4.21672	6.63207
H	-1.42638	5.72144	7.40805
H	-0.39364	0.00860	7.03405
H	0.47127	7.89067	9.51522
H	2.19172	6.15410	9.01872
H	1.86734	-0.91688	7.59159
H	3.92599	0.11685	6.59969
H	3.71985	2.09546	5.07170
H	-0.60525	1.95731	5.48331
H	3.65398	1.46883	-2.24237
H	0.25035	1.29121	-1.13119
H	0.66364	3.75470	-0.89659
H	0.39364	-0.19592	0.88272
H	1.24008	4.71776	1.31575
H	0.90473	0.77256	3.12401
H	4.02855	0.69159	0.11200
H	3.51672	3.91847	-2.74842
H	3.74421	5.59589	-0.90354
H	2.02331	7.20904	4.80098
H	4.26116	2.36933	1.96052

## 8

ZPE(BP86/def2-SVP) = 0.7064282 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3130.8780144 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3129.94914776000 Hartree (single point)

Cartesian coordinates in Å:

Au	-0.36815	-1.81646	-0.77546
Pt	0.61238	0.38888	0.39915
C	0.12991	2.27222	3.25782
P	-0.01274	2.24991	1.43775
P	0.22657	-0.80777	-2.82832
C	0.51241	1.11984	3.96836
C	0.56180	1.14074	5.37050
P	-0.61202	-1.24290	1.55786
C	0.23163	2.31422	6.06741
C	-0.13399	3.47375	5.36018
C	-0.17985	3.46069	3.95861
C	-1.79213	2.39890	1.02573
C	-2.76313	2.68711	2.00426
C	-4.11013	2.81296	1.63110
C	-4.49454	2.65196	0.29111
C	-3.53180	2.33288	-0.68080
C	-2.18661	2.19340	-0.31615
C	0.79917	3.79029	0.89427
C	1.97912	4.20537	1.55065
C	2.70049	5.30467	1.06279
C	2.25638	5.98621	-0.08317
C	1.08282	5.57268	-0.73630
C	0.35335	4.47743	-0.25262
C	1.55723	0.41905	-2.48268
C	2.43805	0.71194	-3.54989
C	3.44440	1.67432	-3.39427
C	3.58036	2.33883	-2.16530
C	2.70932	2.04426	-1.10539
C	-1.21247	0.17387	-3.38510
C	-2.46373	-0.46728	-3.50812
C	-3.57377	0.24777	-3.97978
C	-3.44303	1.60743	-4.31599
C	-2.20287	2.25225	-4.17209
C	-1.08489	1.53950	-3.70836
C	0.75595	-1.78926	-4.26877
C	1.66988	-2.84195	-4.04795
C	2.12923	-3.60376	-5.13087
C	1.67102	-3.32629	-6.43127
C	0.75447	-2.28456	-6.64935
C	0.29444	-1.51127	-5.57145
C	0.15318	-2.30525	2.82138
C	1.55928	-2.24785	2.95700
C	2.20955	-3.06273	3.89378
C	1.46343	-3.94211	4.69871
C	0.06651	-4.00938	4.55885
C	-0.59165	-3.19792	3.62218
C	-2.32834	-0.91505	2.05672
C	-3.34463	-0.83719	1.08116
C	-4.65250	-0.49994	1.45416
C	-4.95745	-0.23483	2.79943
C	-3.94400	-0.28702	3.77087

C	-2.63167	-0.61948	3.40560
C	1.68376	1.07884	-1.21857
H	-4.31408	2.16786	-4.68707
H	-2.10247	3.31759	-4.42745
H	-0.11092	2.03877	-3.59827
H	-2.56364	-1.53253	-3.24451
H	-4.54564	-0.25676	-4.08494
H	-5.98741	0.01899	3.09087
H	3.61620	5.62865	1.57919
H	2.82536	6.84626	-0.46637
H	0.73047	6.11034	-1.62897
H	-0.56427	4.15800	-0.76647
H	2.33510	3.66472	2.44054
H	-5.43988	-0.44724	0.68837
H	-3.82203	2.17658	-1.72888
H	3.30358	-3.01122	3.99764
H	-5.55209	2.75580	0.00625
H	-4.86481	3.03239	2.40028
H	-2.47487	2.80297	3.05767
H	-1.44090	1.90411	-1.07096
H	1.97379	-4.58055	5.43505
H	-0.51687	-4.70339	5.18224
H	-1.68440	-3.25859	3.51168
H	2.13687	-1.55440	2.32268
H	4.37256	3.09041	-2.02749
H	4.11941	1.90092	-4.23280
H	2.84032	2.58034	-0.15533
H	2.33246	0.18561	-4.51036
H	0.26971	2.33200	7.16682
H	0.86686	0.23494	5.91507
H	-0.38086	4.39764	5.90400
H	-0.45210	4.37433	3.40891
H	0.77972	0.20831	3.41919
H	-4.17529	-0.06706	4.82384
H	-1.84070	-0.64824	4.16914
H	2.02769	-3.93009	-7.27889
H	0.39413	-2.07004	-7.66640
H	2.84287	-4.42316	-4.95953
H	2.02030	-3.06129	-3.02678
H	-3.10411	-1.04248	0.02605
H	-0.42078	-0.69315	-5.74209

**9**

ZPE(BP86/def2-SVP) = 0.7064002 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3130.8539965 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3129.92490973983 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.71526	0.82675	-1.65380
Au	0.23637	-0.28883	0.62918
C	-1.70073	-1.71866	3.13744
P	-0.28555	-0.60526	2.87419
P	-0.09419	-1.12010	-2.53885
C	-2.29818	-1.76923	4.41766
C	-3.37954	-2.63194	4.64382
P	0.56962	2.07349	0.29328
C	-3.87516	-3.43128	3.59792
C	-3.29155	-3.36541	2.32241
C	-2.20509	-2.50980	2.08628
C	-0.72271	0.93103	3.74749
C	-0.00681	1.38469	4.87310
C	-0.39318	2.58013	5.50082
C	-1.47109	3.32768	4.99851
C	-2.18801	2.86916	3.87775
C	-1.82225	1.66863	3.25755
C	1.18992	-1.27157	3.69910
C	1.14420	-2.42429	4.50791
C	2.32553	-2.89744	5.10182
C	3.54089	-2.22484	4.89215
C	3.58290	-1.07487	4.08317
C	2.41303	-0.59801	3.47862
C	-1.91242	-1.00905	-2.27560
C	-2.62927	-2.03481	-1.62756
C	-4.00001	-1.87502	-1.36498
C	-4.66154	-0.69838	-1.75240
C	-3.95195	0.32080	-2.41280
C	0.41538	-2.51174	-1.44141
C	0.71173	-3.77998	-1.98058
C	1.09203	-4.83101	-1.13096
C	1.17913	-4.61289	0.25235
C	0.88039	-3.34699	0.78893
C	0.49538	-2.27976	-0.04179
C	0.14176	-1.70603	-4.25055
C	1.41497	-1.54372	-4.83663
C	1.65090	-2.01712	-6.13522
C	0.61628	-2.64031	-6.85503
C	-0.65484	-2.79212	-6.27580
C	-0.89677	-2.32765	-4.97331
C	1.89698	2.59380	1.41632
C	3.21659	2.22782	1.05943
C	4.26819	2.41622	1.96737
C	4.01390	2.97117	3.23474
C	2.70440	3.33848	3.59042
C	1.64541	3.15123	2.69072
C	-0.88309	3.14067	0.48248
C	-1.98475	5.23712	1.05147
C	-3.22664	4.68896	0.68820
C	-3.29583	3.37075	0.19928
C	-2.13195	2.60088	0.09147

C	-2.58159	0.17003	-2.66900
H	1.48429	-5.43101	0.92256
H	0.96314	-3.20057	1.87646
H	0.64930	-3.94274	-3.06712
H	1.32335	-5.81995	-1.55380
H	4.83972	3.12082	3.94602
H	2.29462	-3.79870	5.73170
H	4.46316	-2.60165	5.35867
H	4.53303	-0.54761	3.91370
H	2.45127	0.29548	2.83642
H	0.19227	-2.95192	4.66733
H	5.29252	2.13306	1.68295
H	-3.03206	3.44999	3.47900
H	-1.75951	4.27086	5.48576
H	0.15856	2.93216	6.38508
H	0.84970	0.81071	5.25393
H	-2.38870	1.30557	2.38816
H	-5.73465	-0.57580	-1.54280
H	-4.55569	-2.67598	-0.85507
H	-4.46699	1.24171	-2.72469
H	-2.10957	-2.95612	-1.32553
H	-4.72698	-4.10355	3.77927
H	-3.84315	-2.67568	5.64041
H	-3.68357	-3.98467	1.50227
H	-1.74580	-2.45107	1.08985
H	-1.92271	-1.12880	5.23019
H	2.50110	3.76760	4.58272
H	0.62192	3.41608	2.98813
H	0.80067	-3.00403	-7.87686
H	-1.46512	-3.27496	-6.84218
H	2.64402	-1.89244	-6.59174
H	2.21748	-1.04475	-4.27006
H	3.40299	1.78250	0.06903
H	-2.18303	1.57104	-0.29810
H	-4.14150	5.29413	0.77351
H	-1.89148	-2.44559	-4.51808
H	-4.26263	2.93994	-0.10115
H	-2.01846	0.97801	-3.16196
C	-0.81311	4.47169	0.94558
H	-1.92519	6.27397	1.41458
H	0.15577	4.91469	1.21715

## 10

ZPE(BP86/def2-SVP) = 0.7064202 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3130.8510171 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3129.91464393097 Hartree (single point)

Cartesian coordinates in Å:

Au	3.40413	4.70659	4.15481
Pt	5.44812	6.00305	5.05175
P	4.26917	5.27286	1.96262
P	1.42364	3.45706	4.07467
P	3.68097	5.48043	6.45489
C	6.05760	5.55535	2.09429
C	6.89137	5.40881	0.96468
C	8.26486	5.66311	1.07829
C	8.79924	6.04753	2.32130
C	7.96855	6.16921	3.44749
C	3.48830	6.89471	1.63293
C	4.23930	7.96293	1.10288
C	3.62729	9.20805	0.88745
C	2.27163	9.39710	1.20509
C	1.52247	8.33738	1.74518
C	2.12939	7.09288	1.96386
C	3.99434	4.21706	0.50628
C	3.63342	4.74359	-0.74951
C	3.46294	3.87657	-1.84125
C	3.64699	2.49322	-1.68003
C	4.00106	1.96838	-0.42409
C	4.17253	2.82646	0.66898
C	1.08467	2.68224	2.45772
C	1.01985	3.48286	1.29565
C	0.71404	2.90302	0.05847
C	0.51708	1.51588	-0.03824
C	0.62009	0.71069	1.10729
C	0.89549	1.28814	2.35670
C	-0.01268	4.48702	4.52345
C	-0.83043	5.09296	3.54703
C	-1.85832	5.96400	3.94072
C	-2.08590	6.22338	5.30205
C	-1.28150	5.60954	6.27614
C	-0.23985	4.75782	5.89044
C	1.54431	2.10602	5.28638
C	0.39376	1.53302	5.86814
C	0.53007	0.44981	6.74931
C	1.80347	-0.06842	7.04029
C	2.94852	0.49965	6.45752
C	2.82305	1.59127	5.58915
C	3.65545	4.10905	7.64401
C	2.50741	3.64100	8.32292
C	2.59866	2.54147	9.18559
C	3.83183	1.89497	9.37925
C	4.97612	2.34551	8.69851
C	4.89016	3.44336	7.83213
C	2.26478	6.58566	6.74151
C	1.79476	7.34949	5.64526
C	0.78039	8.29472	5.82317
C	0.22806	8.50457	7.09929
C	0.70786	7.77155	8.19755

C	1.72267	6.81694	8.02641
C	6.57276	5.93520	3.37149
H	1.79978	10.37709	1.04009
H	0.46345	8.48052	2.00739
H	1.54385	6.28027	2.42058
H	5.30626	7.82032	0.87576
H	4.21775	10.03998	0.47585
H	-0.56894	9.24950	7.24046
H	0.42135	8.87356	4.95977
H	1.69977	2.18436	9.70895
H	3.89990	1.03416	10.06096
H	5.94249	1.84125	8.84734
H	5.77902	3.80108	7.28664
H	1.54003	4.14215	8.18634
H	-2.89750	6.90090	5.60542
H	9.87773	6.24761	2.41571
H	8.91899	5.55803	0.20018
H	8.42390	6.45636	4.41026
H	6.46568	5.09617	-0.00125
H	-2.49750	6.42816	3.17510
H	-0.68773	4.86795	2.48124
H	0.39554	4.28657	6.65014
H	-1.45535	5.80493	7.34340
H	-0.36564	0.00324	7.20590
H	0.29620	7.95062	9.20216
H	2.10983	6.27231	8.89953
H	1.90415	-0.91918	7.73040
H	3.94583	0.10288	6.69305
H	3.72019	2.05432	5.14820
H	-0.60386	1.93100	5.63059
H	3.51013	1.81805	-2.53778
H	0.29316	1.05963	-1.01367
H	0.65888	3.53589	-0.83796
H	0.47699	-0.37747	1.03310
H	1.22522	4.56058	1.34695
H	0.96075	0.65494	3.25286
H	4.13552	0.88447	-0.29604
H	3.18707	4.28547	-2.82481
H	3.48761	5.82756	-0.87089
H	2.23713	7.20483	4.64735
H	4.43678	2.42148	1.65860

# 11

ZPE(BP86/def2-SVP) = 0.8044849 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0074126 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.01864065128 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.06785	-1.29454	-2.02774
Au	-0.21318	0.17240	0.43013
C	-0.96317	1.83990	3.53332
P	-0.06994	2.04966	1.95891
P	-0.27405	-1.91319	1.56526
C	-2.07824	2.63372	3.86618
C	-2.80382	2.36078	5.03820
P	-0.10675	0.89345	-1.84167
C	-2.41490	1.30928	5.88311
C	-1.29835	0.51977	5.55468
C	-0.58286	0.77207	4.37884
C	-0.65605	3.58437	1.16728
C	0.06725	4.79141	1.24131
C	-0.35626	5.90118	0.49219
C	-1.49523	5.81137	-0.32732
C	-2.22673	4.61171	-0.39041
C	-1.80614	3.50080	0.35283
C	1.69128	2.30524	2.36467
C	2.13040	2.64242	3.66137
C	3.50429	2.78091	3.91729
C	4.43974	2.59138	2.88539
C	4.00228	2.26192	1.59023
C	2.63387	2.11225	1.32830
C	1.30962	-2.40360	2.31411
C	1.62831	-3.76288	2.52472
C	2.85015	-4.10547	3.12351
C	3.75530	-3.09992	3.50742
C	3.44581	-1.74767	3.28411
C	-0.64998	-3.13848	0.26450
C	-1.93135	-3.65551	0.07041
C	-2.26495	-4.27757	-1.15941
C	-1.32718	-4.37121	-2.18621
C	-0.00327	-3.88946	-1.99069
C	0.34628	-3.26831	-0.76538
C	-1.58268	-1.99869	2.83023
C	-2.68683	-1.13140	2.67857
C	-3.71080	-1.12460	3.63414
C	-3.62942	-1.97219	4.75200
C	-2.52662	-2.82841	4.91108
C	-1.50155	-2.84660	3.95231
C	0.42577	-1.53065	-4.00203
C	1.67058	-2.01343	-4.45784
C	1.91444	-2.15112	-5.83650
C	0.92306	-1.80536	-6.76936
C	-0.31342	-1.31581	-6.31759
C	-0.56229	-1.16891	-4.94097
C	1.32587	1.97275	-2.11346
C	2.56519	1.40262	-2.47357
C	3.72037	2.20006	-2.48382
C	3.64395	3.56042	-2.13760
C	2.40662	4.12942	-1.78710

C	1.24701	3.34277	-1.77177
C	-1.58676	1.68500	-2.53113
C	-2.69134	3.29790	-3.97916
C	-3.94349	2.85579	-3.52110
C	-4.02003	1.81236	-2.57899
C	-2.84733	1.22564	-2.08765
C	2.22755	-1.39724	2.68368
H	-1.59351	-4.83594	-3.14596
H	0.76777	-4.08375	-2.74905
H	1.40237	-3.05339	-0.53146
H	-2.69276	-3.54423	0.85708
H	-3.27960	-4.67735	-1.30334
H	4.55191	4.18168	-2.14477
H	3.84532	3.04273	4.93006
H	5.51486	2.70122	3.09208
H	4.72690	2.11363	0.77636
H	2.29658	1.84362	0.31585
H	1.39928	2.78973	4.46992
H	4.68536	1.75695	-2.77179
H	-3.11048	4.52812	-1.03977
H	2.88823	-2.53314	-6.18057
H	-1.81217	6.67978	-0.92365
H	0.21253	6.84163	0.54311
H	0.97216	4.85360	1.86366
H	-2.35351	2.54985	0.27179
H	1.11577	-1.91375	-7.84709
H	-1.09429	-1.03604	-7.04187
H	-1.53052	-0.76920	-4.60211
H	2.45986	-2.29017	-3.73988
H	4.71303	-3.37495	3.97382
H	3.09995	-5.16423	3.28760
H	4.15735	-0.95782	3.56629
H	0.92602	-4.54976	2.20825
H	-2.98367	1.10187	6.80153
H	-3.67385	2.98304	5.29581
H	-0.99394	-0.30967	6.20895
H	0.27446	0.13496	4.11472
H	-2.37634	3.46574	3.21100
H	2.34237	5.19263	-1.51257
H	0.28660	3.78624	-1.47351
H	-4.42634	-1.95803	5.51020
H	-2.46173	-3.48635	5.79043
H	-4.56387	-0.44077	3.51812
H	-2.72289	-0.44262	1.81913
H	2.60803	0.33666	-2.74372
H	-2.89475	0.40287	-1.35553
H	-4.86497	3.31721	-3.90622
H	-0.63244	-3.50752	4.08564
H	-5.00024	1.45519	-2.22959
H	1.99935	-0.33957	2.48487
C	-1.51145	2.71431	-3.49107
H	-2.63042	4.10144	-4.72818
H	-0.53338	3.05778	-3.85733

## 12

ZPE(BP86/def2-SVP) = 0.8019500 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9764696 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.98350510582 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.21383	1.88565	-1.60010
Au	-0.37488	-0.38000	-0.05652
C	-1.49337	-3.19273	2.04523
P	-0.35436	-1.77199	1.92690
P	-0.05857	-1.56871	-2.07910
C	-2.23578	-3.45275	3.21541
C	-3.08017	-4.57348	3.26858
P	-0.00331	1.84850	0.69929
C	-3.18237	-5.43667	2.16473
C	-2.44117	-5.17837	0.99842
C	-1.60428	-4.05612	0.93476
C	-0.60885	-0.79612	3.45318
C	0.26251	-0.88895	4.55648
C	0.05692	-0.06552	5.67561
C	-1.00555	0.85453	5.69379
C	-1.88188	0.94043	4.59675
C	-1.68609	0.11349	3.48263
C	1.33071	-2.46199	2.08921
C	1.55863	-3.78118	2.52871
C	2.87607	-4.24530	2.67749
C	3.96137	-3.39846	2.39518
C	3.73152	-2.08527	1.95047
C	2.42141	-1.61821	1.79102
C	1.64809	-2.20466	-1.94677
C	2.70532	-1.50401	-2.56146
C	4.02857	-1.93111	-2.36661
C	4.29928	-3.05732	-1.57232
C	3.24476	-3.75434	-0.95777
C	-0.14031	-0.51558	-3.56075
C	-0.37293	-1.13065	-4.81073
C	-0.42755	-0.35789	-5.97623
C	-0.24717	1.03142	-5.88424
C	-0.00600	1.63738	-4.64137
C	0.04727	0.89236	-3.43435
C	-1.16340	-2.98795	-2.38411
C	-2.53554	-2.80453	-2.10699
C	-3.44290	-3.84772	-2.33239
C	-2.98511	-5.08220	-2.82642
C	-1.62003	-5.26817	-3.10163
C	-0.70622	-4.22272	-2.88755
C	0.03897	3.89764	-0.97986
C	1.08942	4.67798	-0.46803
C	0.85076	6.01681	-0.10493
C	-0.43036	6.57195	-0.24532
C	-1.47445	5.78942	-0.76822
C	-1.24510	4.45272	-1.13213
C	1.54455	1.89267	1.63658
C	2.76383	1.81659	0.92425
C	3.97312	1.69592	1.62242
C	3.97261	1.63975	3.02793
C	2.76015	1.71011	3.73466

C	1.54456	1.83890	3.04709
C	-1.27435	2.80106	1.55806
C	-1.99318	4.66690	2.93707
C	-3.33547	4.33830	2.68089
C	-3.64979	3.24776	1.84974
C	-2.62199	2.48263	1.28407
C	1.92365	-3.32215	-1.12845
H	-0.29253	1.65434	-6.79061
H	0.12816	2.72849	-4.60953
H	1.01438	2.80107	-2.59501
H	-0.52595	-2.21923	-4.86580
H	-0.61400	-0.83672	-6.94870
H	4.92201	1.54003	3.57460
H	3.05433	-5.27472	3.02266
H	4.99098	-3.76730	2.51509
H	4.57429	-1.41977	1.71463
H	2.24844	-0.59318	1.43448
H	0.70887	-4.44134	2.75710
H	4.92088	1.64428	1.06633
H	-2.70997	1.66444	4.59779
H	1.67721	6.62293	0.29669
H	-1.15197	1.50823	6.56643
H	0.73850	-0.13741	6.53630
H	1.10891	-1.59037	4.53216
H	-2.36331	0.18865	2.61984
H	-0.61664	7.61534	0.04918
H	-2.48045	6.21810	-0.89143
H	-2.07427	3.84132	-1.51941
H	2.09269	4.24920	-0.33312
H	5.33686	-3.39446	-1.43049
H	4.85225	-1.38491	-2.85003
H	3.45068	-4.63172	-0.32880
H	2.48817	-0.62797	-3.19057
H	-3.84533	-6.31334	2.21265
H	-3.65990	-4.77444	4.18176
H	-2.52021	-5.84329	0.12633
H	-1.04455	-3.84654	0.01296
H	-2.15122	-2.78171	4.08264
H	2.75571	1.65744	4.83321
H	0.59829	1.87650	3.60453
H	-3.69685	-5.90357	-2.99755
H	-1.26200	-6.23216	-3.49281
H	-4.51064	-3.70178	-2.11268
H	-2.88589	-1.84179	-1.70218
H	2.74469	1.83358	-0.17765
H	-2.85529	1.63598	0.61825
H	-4.14241	4.94182	3.12246
H	0.36113	-4.36871	-3.10908
H	-4.70015	2.99813	1.63873
H	1.10841	-3.85625	-0.61953
C	-0.95882	3.90432	2.37657
H	-1.74868	5.53275	3.56986
H	0.09028	4.17976	2.55340

## 13

ZPE(BP86/def2-SVP) = 0.8055066 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0125994 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.01855715296 Hartree (single point)

Cartesian coordinates in Å:

Pt	-0.02814	1.91211	-1.50984
Au	-0.42841	-0.16715	0.04073
C	-1.37829	-3.19631	1.78935
P	-0.37051	-1.67735	1.90140
P	-0.24224	-1.46639	-1.93679
C	-2.67159	-3.24306	2.34772
C	-3.46333	-4.39046	2.18025
P	0.04997	2.06989	0.79685
C	-2.97003	-5.49292	1.46374
C	-1.68158	-5.44678	0.90494
C	-0.89080	-4.30139	1.05811
C	-0.85300	-0.82927	3.44680
C	-0.15317	-1.01313	4.65607
C	-0.50335	-0.25265	5.78270
C	-1.54584	0.68818	5.70812
C	-2.25324	0.86272	4.50639
C	-1.90553	0.10709	3.37795
C	1.35774	-2.22333	2.11193
C	1.67997	-3.38268	2.85176
C	3.02373	-3.74491	3.02810
C	4.04733	-2.95388	2.47665
C	3.72695	-1.80241	1.74075
C	2.38708	-1.43941	1.55268
C	1.52182	-1.94370	-1.90984
C	2.47691	-0.97768	-2.29459
C	3.84399	-1.24630	-2.13581
C	4.26826	-2.47349	-1.59680
C	3.31931	-3.43296	-1.20936
C	-0.54976	-0.44894	-3.41594
C	-0.87886	-1.09456	-4.62774
C	-1.12012	-0.34070	-5.78164
C	-1.03576	1.05986	-5.71165
C	-0.71048	1.69211	-4.50174
C	-0.45373	0.97477	-3.30634
C	-1.27313	-2.96123	-2.05086
C	-2.54761	-2.90193	-1.44658
C	-3.42794	-3.98540	-1.55519
C	-3.03576	-5.14021	-2.25312
C	-1.76501	-5.20776	-2.84825
C	-0.88318	-4.11901	-2.75661
C	0.98415	3.73364	-2.51022
C	2.07058	4.19149	-1.70358
C	1.83741	5.00473	-0.59605
C	0.51629	5.38785	-0.25247
C	-0.56472	4.94111	-1.00687
C	-0.35468	4.10312	-2.14650
C	1.54386	1.95461	1.82516
C	2.79620	2.02896	1.17547
C	3.97681	1.79295	1.89529
C	3.91589	1.47102	3.26199
C	2.67084	1.39288	3.91049
C	1.48707	1.63573	3.20129

C	-1.23770	2.91646	1.74954
C	-1.98899	4.47718	3.46420
C	-3.31951	4.30109	3.04938
C	-3.61044	3.44326	1.97116
C	-2.57645	2.75887	1.32059
C	1.95010	-3.16849	-1.35694
H	-1.23023	1.66799	-6.60864
H	-0.66650	2.79271	-4.50414
H	1.19884	3.31699	-3.50449
H	-0.96038	-2.19145	-4.66461
H	-1.37860	-0.84096	-6.72643
H	4.84148	1.27744	3.82413
H	3.27334	-4.64960	3.60230
H	5.09952	-3.24263	2.61865
H	4.51904	-1.18303	1.29807
H	2.14461	-0.54515	0.96121
H	0.88080	-4.00516	3.28124
H	4.95021	1.85863	1.38629
H	-3.05923	1.60736	4.43416
H	2.68343	5.36375	0.00819
H	-1.80436	1.29233	6.59039
H	0.04972	-0.38841	6.72407
H	0.68295	-1.72520	4.70877
H	-2.43055	0.27337	2.42571
H	0.34423	6.04011	0.61609
H	-1.58917	5.24266	-0.74596
H	-1.18567	3.95942	-2.85311
H	3.09847	3.93103	-1.99660
H	5.34184	-2.68179	-1.47756
H	4.58478	-0.49291	-2.44294
H	3.64443	-4.39144	-0.77918
H	2.14063	-0.01402	-2.70841
H	-3.59127	-6.39236	1.34100
H	-4.46886	-4.42601	2.62525
H	-1.29189	-6.30512	0.33901
H	0.11688	-4.26706	0.62214
H	-3.05516	-2.39031	2.92764
H	2.61848	1.13186	4.97788
H	0.51715	1.55763	3.71085
H	-3.72393	-5.99501	-2.33134
H	-1.46008	-6.11097	-3.39758
H	-4.41819	-3.93472	-1.08051
H	-2.84125	-2.00173	-0.88426
H	2.82616	2.26070	0.10041
H	-2.79403	2.09454	0.46824
H	-4.13231	4.83816	3.56049
H	0.10518	-4.16984	-3.23709
H	-4.65026	3.31113	1.63649
H	1.21249	-3.91933	-1.04243
C	-0.94822	3.79161	2.81794
H	-1.75716	5.15664	4.29803
H	0.09140	3.94037	3.14307

## 15

ZPE(BP86/def2-SVP) = 0.8047265 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0265374 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.03927934243 Hartree (single point)

Cartesian coordinates in Å:

Pt	-0.29637	0.49570	1.57839
Au	-0.12159	0.99674	-1.27186
C	1.16041	-1.94036	-2.86080
P	0.06087	-0.50360	-3.09413
P	0.00145	-1.78808	1.87914
C	0.74381	-2.98126	-2.00438
C	1.58450	-4.07737	-1.77729
P	-0.36068	2.51568	0.56090
C	2.84641	-4.13645	-2.39101
C	3.26488	-3.09740	-3.23854
C	2.42659	-1.99694	-3.47728
C	0.70721	0.38883	-4.55029
C	0.37624	-0.01566	-5.85977
C	0.92630	0.66449	-6.95627
C	1.80511	1.74269	-6.75143
C	2.13357	2.14831	-5.44697
C	1.58265	1.47654	-4.34505
C	-1.57398	-1.16356	-3.56809
C	-1.72953	-2.44986	-4.12271
C	-3.00655	-2.89609	-4.49769
C	-4.12552	-2.06362	-4.32729
C	-3.97063	-0.77863	-3.77701
C	-2.69904	-0.32961	-3.39280
C	1.68648	-2.28176	1.35275
C	2.36087	-1.48038	0.40670
C	3.64166	-1.83652	-0.03436
C	4.25630	-2.99805	0.46202
C	3.58866	-3.80088	1.40198
C	-1.14296	-2.75900	0.82818
C	-1.02199	-4.16085	0.72161
C	-1.85298	-4.86866	-0.15890
C	-2.80536	-4.18302	-0.93579
C	-2.94039	-2.79083	-0.81890
C	-2.11273	-2.07830	0.06313
C	-0.20335	-2.40918	3.57747
C	0.75885	-2.03352	4.54086
C	0.52919	-2.29987	5.89584
C	-0.65602	-2.94065	6.29804
C	-1.61072	-3.31910	5.34118
C	-1.39181	-3.04842	3.98078
C	-0.40426	0.80481	3.55472
C	-1.53570	0.39344	4.28235
C	-1.56676	0.58205	5.67483
C	-0.47664	1.16994	6.33732
C	0.64329	1.58730	5.60042
C	0.68442	1.41225	4.20457
C	-1.87655	3.50341	0.40564
C	-2.82925	3.44498	1.44531
C	-4.02448	4.17291	1.33471
C	-4.27166	4.95418	0.19356
C	-3.32447	5.01000	-0.84486

C	-2.12851	4.28482	-0.74426
C	1.07354	3.63022	0.64296
C	2.08711	5.83811	0.77984
C	3.36083	5.25247	0.86078
C	3.49308	3.85147	0.83893
C	2.35640	3.04073	0.73293
C	2.30739	-3.44446	1.85209
H	-3.44679	-4.73866	-1.63557
H	-3.68181	-2.25417	-1.42718
H	-2.19902	-0.98284	0.15650
H	-0.26853	-4.69673	1.31775
H	-1.75454	-5.96110	-0.24503
H	-5.20915	5.52417	0.11096
H	-3.12698	-3.90131	-4.92819
H	-5.12436	-2.41780	-4.62270
H	-4.84557	-0.12623	-3.63970
H	-2.57641	0.67029	-2.94562
H	-0.85615	-3.10589	-4.24973
H	-4.76544	4.13178	2.14684
H	2.81557	2.99619	-5.28580
H	-2.44890	0.25137	6.24380
H	2.23166	2.27416	-7.61512
H	0.66521	0.35239	-7.97832
H	-0.31581	-0.85584	-6.02030
H	1.82960	1.79664	-3.31929
H	-0.50156	1.30564	7.42868
H	1.49746	2.05963	6.10974
H	1.56210	1.74934	3.63221
H	-2.38061	-0.09683	3.77691
H	5.26315	-3.27762	0.11777
H	4.15931	-1.20744	-0.77262
H	4.07304	-4.70601	1.79778
H	1.87136	-0.57008	0.02362
H	3.50810	-4.99512	-2.20577
H	1.25228	-4.88177	-1.10599
H	4.25126	-3.14357	-3.72350
H	2.75264	-1.18901	-4.14861
H	-0.24027	-2.93572	-1.52219
H	-3.52124	5.62025	-1.73901
H	-1.38747	4.32136	-1.55793
H	-0.83626	-3.14283	7.36428
H	-2.53744	-3.82264	5.65431
H	1.27413	-1.99382	6.64453
H	1.67557	-1.51093	4.23050
H	-2.62414	2.82946	2.33488
H	2.45065	1.94250	0.73005
H	4.25452	5.88820	0.94666
H	-2.15110	-3.32457	3.23417
H	4.48926	3.38972	0.91038
H	1.79941	-4.05771	2.61187
C	0.94127	5.03347	0.67115
H	1.98088	6.93292	0.80557
H	-0.05526	5.49575	0.61745

## 16

ZPE(BP86/def2-SVP) = 0.8061626 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0341286 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.02934577531 Hartree (single point)

Cartesian coordinates in Å:

Pt	-0.07948	0.05816	0.15887
Au	-0.22161	2.01019	-3.25198
C	0.26064	-3.09988	-1.66848
P	-0.19261	-1.32221	-1.79625
P	-0.29777	-1.68077	1.70403
C	-0.72860	-4.06106	-1.37099
C	-0.36934	-5.40143	-1.16994
P	-0.27868	2.12657	-0.95994
C	0.97458	-5.79772	-1.25939
C	1.95897	-4.84895	-1.57757
C	1.60534	-3.50867	-1.78775
C	1.07927	-0.66137	-2.95880
C	2.31007	-0.23333	-2.41927
C	3.29530	0.32544	-3.24874
C	3.05280	0.48557	-4.62325
C	1.82500	0.07289	-5.16894
C	0.83912	-0.50440	-4.34439
C	-1.75706	-1.31660	-2.74829
C	-2.01834	-2.27757	-3.74820
C	-3.20920	-2.21269	-4.48846
C	-4.14248	-1.19128	-4.23996
C	-3.88609	-0.23327	-3.24469
C	-2.69927	-0.29770	-2.50029
C	1.18563	-2.72590	1.89011
C	2.30618	-2.45567	1.08246
C	3.48231	-3.20519	1.22828
C	3.54306	-4.23292	2.18186
C	2.43549	-4.49269	3.00897
C	-1.75041	-2.70776	1.25601
C	-1.88328	-4.06237	1.61557
C	-3.02754	-4.77820	1.23247
C	-4.04197	-4.15225	0.48676
C	-3.91786	-2.79801	0.13351
C	-2.77865	-2.07878	0.52274
C	-0.66102	-1.12032	3.40548
C	0.40683	-0.76770	4.25692
C	0.14014	-0.18825	5.50354
C	-1.18655	0.03814	5.90886
C	-2.24971	-0.32232	5.06577
C	-1.99124	-0.89919	3.81243
C	0.40489	1.27506	1.76301
C	-0.52013	1.91523	2.60820
C	-0.07929	2.71533	3.67607
C	1.29376	2.88445	3.91399
C	2.22520	2.24708	3.07744
C	1.78333	1.45070	2.00838
C	-1.89883	2.87023	-0.54427
C	-2.85070	2.11765	0.17432
C	-4.11282	2.66010	0.45987
C	-4.42791	3.96055	0.03377
C	-3.48065	4.71624	-0.68172

C	-2.22273	4.17397	-0.97779
C	0.98477	3.35292	-0.47349
C	1.77343	5.08128	1.04305
C	3.06710	4.96246	0.51019
C	3.31806	4.04438	-0.52457
C	2.28112	3.24094	-1.01733
C	1.26409	-3.73415	2.87662
H	-4.93020	-4.72340	0.17832
H	-4.69928	-2.30092	-0.45968
H	-2.66028	-1.02566	0.22814
H	-1.08146	-4.57453	2.16355
H	-3.12167	-5.83914	1.50793
H	-5.41580	4.38949	0.25848
H	-3.40990	-2.96643	-5.26437
H	-5.07462	-1.14511	-4.82264
H	-4.61116	0.56851	-3.04108
H	-2.51010	0.44365	-1.71267
H	-1.29463	-3.08332	-3.94157
H	-4.84845	2.06746	1.02379
H	1.62801	0.19756	-6.24403
H	-0.81822	3.20512	4.32823
H	3.81907	0.93679	-5.27034
H	4.25218	0.65221	-2.81535
H	2.47516	-0.29384	-1.33168
H	-0.11372	-0.84139	-4.77888
H	1.63873	3.51177	4.74956
H	3.30434	2.37612	3.25115
H	2.52776	0.97475	1.35112
H	-1.60009	1.78814	2.45301
H	4.46349	-4.82469	2.29595
H	4.35456	-2.98504	0.59514
H	2.49137	-5.28095	3.77426
H	2.24410	-1.63947	0.34810
H	1.25335	-6.84896	-1.09435
H	-1.15163	-6.13899	-0.93840
H	3.01221	-5.15281	-1.66700
H	2.38428	-2.78016	-2.05186
H	-1.78431	-3.76672	-1.30369
H	-3.72827	5.73405	-1.01781
H	-1.48753	4.75927	-1.55097
H	-1.39180	0.49613	6.88783
H	-3.28929	-0.15539	5.38492
H	0.97546	0.09722	6.15927
H	1.44576	-0.92248	3.93371
H	-2.57801	1.10666	0.51819
H	2.47086	2.52162	-1.82863
H	3.88249	5.59061	0.89854
H	-2.82564	-1.17641	3.15152
H	4.32743	3.95882	-0.95414
H	0.42330	-3.90275	3.56557
C	0.72909	4.28381	0.55364
H	1.57250	5.79497	1.85534
H	-0.27296	4.35939	0.99640

ZPE(BP86/def2-SVP) = 0.8045862 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0029697 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.99794853113 Hartree (single point)

Cartesian coordinates in Å:

Pt	-0.19410	0.18195	0.99097
Au	0.87899	0.88396	-2.24020
C	0.28060	-2.45280	-1.54933
P	-0.41849	-0.85445	-1.09130
P	-0.23596	-1.76675	2.29523
C	-0.35021	-3.39923	-2.38411
C	0.29589	-4.60988	-2.66753
P	0.12855	2.15337	-0.31918
C	1.55586	-4.89132	-2.11278
C	2.17248	-3.96394	-1.25352
C	1.54032	-2.74879	-0.97498
C	1.30368	-0.30064	-3.86078
C	0.58880	-0.06843	-5.05479
C	0.88186	-0.81564	-6.21014
C	1.87957	-1.80350	-6.17468
C	2.59622	-2.03401	-4.98762
C	2.30311	-1.29143	-3.83214
C	-2.00299	-0.58134	-1.92572
C	-2.23125	-0.84814	-3.29576
C	-3.47079	-0.53075	-3.86557
C	-4.48142	0.05876	-3.08347
C	-4.25223	0.34101	-1.72631
C	-3.01526	0.03170	-1.14863
C	1.46656	-2.30362	2.67831
C	2.55425	-1.57976	2.14793
C	3.86984	-1.97416	2.43601
C	4.10261	-3.08905	3.25852
C	3.02032	-3.79997	3.80741
C	-1.06945	-3.12254	1.38567
C	-0.47506	-4.37538	1.14669
C	-1.13821	-5.32204	0.34962
C	-2.39414	-5.03053	-0.20726
C	-2.98812	-3.77879	0.02285
C	-2.32568	-2.82612	0.80962
C	-1.04655	-1.64208	3.92696
C	-0.32459	-1.03212	4.97607
C	-0.95181	-0.78536	6.20338
C	-2.29741	-1.14313	6.39361
C	-3.01326	-1.75901	5.35417
C	-2.39286	-2.00897	4.11966
C	-0.16254	1.27150	2.73670
C	-1.37662	1.56397	3.39485
C	-1.38721	2.31948	4.57937
C	-0.18063	2.77463	5.13630
C	1.03406	2.46964	4.50084
C	1.04325	1.72566	3.30828
C	-1.50193	2.89973	-0.67732
C	-2.43559	3.12287	0.36009
C	-3.71994	3.59946	0.05891
C	-4.08970	3.84219	-1.27590
C	-3.16728	3.61773	-2.31100

C	-1.87690	3.15449	-2.01388
C	1.18785	3.35244	0.54335
C	1.52396	5.22491	2.05734
C	2.90412	4.96409	2.08105
C	3.43025	3.90239	1.32497
C	2.57641	3.09908	0.55589
C	1.70347	-3.40605	3.52737
H	-2.90578	-5.77704	-0.83257
H	-3.96501	-3.53524	-0.42020
H	-2.77888	-1.83583	0.96511
H	0.51687	-4.60545	1.55918
H	-0.66090	-6.29337	0.15397
H	-5.10011	4.21015	-1.50927
H	-3.64614	-0.73178	-4.93280
H	-5.44906	0.31319	-3.54108
H	-5.03120	0.82121	-1.11775
H	-2.81024	0.27799	-0.09516
H	-1.42730	-1.26189	-3.92036
H	-4.43963	3.77700	0.87229
H	3.38611	-2.79980	-4.95852
H	-2.34388	2.53869	5.07762
H	2.09970	-2.39610	-7.07531
H	0.32515	-0.62396	-7.14025
H	-0.20084	0.69906	-5.09566
H	2.86041	-1.49865	-2.90650
H	-0.18723	3.36167	6.06694
H	1.98568	2.81984	4.92882
H	2.00511	1.51521	2.81824
H	-2.32820	1.17624	2.99795
H	5.13358	-3.39797	3.48701
H	4.71582	-1.40286	2.02586
H	3.20419	-4.66123	4.46674
H	2.34905	-0.69463	1.52242
H	2.05520	-5.84446	-2.34208
H	-0.19459	-5.34570	-3.32142
H	3.14969	-4.18701	-0.80082
H	2.01805	-2.01823	-0.30675
H	-1.34711	-3.19899	-2.79681
H	-3.45199	3.80760	-3.35645
H	-1.15313	2.97936	-2.82487
H	-2.78919	-0.94475	7.35754
H	-4.06260	-2.05349	5.50459
H	-0.38650	-0.30020	7.01219
H	0.72089	-0.72867	4.82508
H	-2.15534	2.90323	1.40090
H	2.98430	2.26315	-0.03576
H	3.57348	5.59419	2.68531
H	-2.95786	-2.49984	3.31444
H	4.51236	3.70303	1.33040
H	0.85775	-3.94465	3.98125
C	0.66366	4.42408	1.29217
H	1.10962	6.05663	2.64605
H	-0.41648	4.62645	1.28942

## 18

ZPE(BP86/def2-SVP) = 0.8044918 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9976863 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.99681386017 Hartree (single point)

Cartesian coordinates in Å:

Pt	-0.12112	-0.53261	0.06945
Au	0.13107	2.82005	-0.56283
C	0.87687	0.47936	-3.27340
P	-0.28354	0.85909	-1.92636
P	0.01285	-2.65522	-0.90268
C	0.58460	-0.49937	-4.24752
C	1.57343	-0.89909	-5.15787
P	0.06153	1.34406	1.35770
C	2.85853	-0.33389	-5.10576
C	3.14971	0.65317	-4.14809
C	2.16352	1.06274	-3.23931
C	0.55079	4.34128	0.75290
C	-0.42794	4.99679	1.51902
C	-0.05062	6.03797	2.38689
C	1.29879	6.41131	2.49800
C	2.27577	5.74988	1.73387
C	1.90677	4.70450	0.87161
C	-1.99190	0.87558	-2.56362
C	-2.30026	1.14333	-3.91267
C	-3.63942	1.18363	-4.33170
C	-4.68061	0.97682	-3.41101
C	-4.37823	0.72999	-2.05956
C	-3.04271	0.67510	-1.63863
C	1.75378	-3.02677	-1.30533
C	2.63694	-1.96145	-1.57330
C	3.95471	-2.22521	-1.97216
C	4.39960	-3.55201	-2.09486
C	3.52435	-4.61687	-1.81784
C	-0.92326	-2.88476	-2.45499
C	-0.37979	-3.56080	-3.56586
C	-1.13023	-3.67024	-4.74658
C	-2.41487	-3.10390	-4.82647
C	-2.96325	-2.44278	-3.71436
C	-2.21988	-2.33738	-2.53022
C	-0.55065	-3.99234	0.20896
C	0.27794	-4.38040	1.28412
C	-0.20305	-5.27120	2.25121
C	-1.50894	-5.78217	2.15350
C	-2.32840	-5.41034	1.07654
C	-1.85385	-4.51564	0.10389
C	-0.26836	-1.39397	1.97190
C	-1.56282	-1.76914	2.39214
C	-1.76358	-2.35388	3.65094
C	-0.67545	-2.55174	4.52042
C	0.61264	-2.16625	4.11902
C	0.81411	-1.58657	2.85240
C	-1.34051	1.76062	2.41281
C	-1.32982	1.38255	3.77425
C	-2.49661	1.52936	4.53764
C	-3.66525	2.04811	3.95547
C	-3.67853	2.40912	2.59590

C	-2.52265	2.25798	1.81964
C	1.61134	1.63459	2.22588
C	2.97207	2.79060	3.86963
C	4.11799	2.15148	3.36303
C	4.01529	1.26285	2.27690
C	2.76436	1.00287	1.70421
C	2.20188	-4.36001	-1.42504
H	-2.99086	-3.17878	-5.76077
H	-3.96380	-1.99014	-3.76858
H	-2.63899	-1.80383	-1.66665
H	0.63645	-3.97669	-3.51799
H	-0.70339	-4.19277	-5.61562
H	-4.57538	2.16478	4.56229
H	-3.87097	1.38472	-5.38843
H	-5.72820	1.01172	-3.74502
H	-5.18807	0.56806	-1.33223
H	-2.79763	0.44703	-0.58742
H	-1.49313	1.32071	-4.63842
H	-2.49275	1.22474	5.59442
H	3.33405	6.04067	1.81492
H	-2.77618	-2.65899	3.95543
H	1.59150	7.21887	3.18562
H	-0.81918	6.55462	2.98173
H	-1.48590	4.70255	1.45866
H	2.68608	4.17031	0.30537
H	-0.83452	-3.00587	5.50997
H	1.47051	-2.31510	4.79287
H	1.83124	-1.29030	2.55670
H	-2.42490	-1.61966	1.72358
H	5.43448	-3.75976	-2.40544
H	4.63321	-1.38806	-2.19170
H	3.87337	-5.65620	-1.90916
H	2.27933	-0.92627	-1.48086
H	3.63150	-0.65429	-5.81979
H	1.33590	-1.66564	-5.91050
H	4.14781	1.11544	-4.11703
H	2.38701	1.83932	-2.48995
H	-0.41409	-0.95288	-4.29039
H	-4.59519	2.80913	2.13808
H	-2.53273	2.52545	0.75105
H	-1.88612	-6.47746	2.91806
H	-3.34589	-5.81938	0.98871
H	0.44398	-5.56165	3.09154
H	1.29451	-3.97284	1.37206
H	-0.42982	0.93618	4.22102
H	2.66171	0.31082	0.85208
H	5.10155	2.35505	3.81204
H	-2.50071	-4.22825	-0.73734
H	4.91409	0.77009	1.87808
H	1.51782	-5.19385	-1.20729
C	1.71706	2.54490	3.29932
H	3.05958	3.50094	4.70447
H	0.82906	3.08272	3.66032

## 19

ZPE(BP86/def2-SVP) = 0.8063658 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0325867 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.02756562660 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.13529	-0.26531	0.60591
Au	1.90509	1.39319	-2.14038
C	0.80468	-1.68111	-2.74667
P	0.30659	-0.21776	-1.76346
P	0.28936	-2.58162	0.79738
C	-0.09554	-2.30665	-3.63368
C	0.29598	-3.46171	-4.32694
P	-0.10920	2.07364	0.88059
C	1.57659	-4.00498	-4.13827
C	2.47698	-3.38087	-3.25727
C	2.09803	-2.21851	-2.57509
C	0.09193	3.22800	-0.54859
C	-1.01039	3.43854	-1.39966
C	-0.86977	4.19418	-2.57516
C	0.36903	4.75945	-2.91307
C	1.46870	4.59040	-2.05273
C	1.33864	3.82320	-0.87659
C	-1.17040	0.42703	-2.63569
C	-1.10604	0.87644	-3.97231
C	-2.24591	1.41038	-4.58698
C	-3.45861	1.49802	-3.87676
C	-3.53084	1.04096	-2.55103
C	-2.38866	0.50746	-1.93333
C	2.03218	-3.11828	0.78200
C	3.03766	-2.15536	0.55908
C	4.38826	-2.53323	0.55622
C	4.74101	-3.87489	0.77820
C	3.74343	-4.83455	1.02463
C	-0.64550	-3.46060	-0.50898
C	-0.21178	-4.65794	-1.10561
C	-1.03804	-5.31287	-2.03188
C	-2.29503	-4.78275	-2.36504
C	-2.72160	-3.57592	-1.78658
C	-1.89780	-2.91504	-0.86515
C	-0.39077	-3.25882	2.35821
C	0.44094	-3.35920	3.49281
C	-0.10769	-3.71641	4.73124
C	-1.48241	-3.98155	4.84649
C	-2.30860	-3.89728	3.71445
C	-1.76762	-3.53576	2.47108
C	0.23431	-0.26859	2.68739
C	-0.88986	-0.30634	3.53403
C	-0.74134	-0.29431	4.93165
C	0.53765	-0.25351	5.50808
C	1.66797	-0.23982	4.67510
C	1.51526	-0.25366	3.27941
C	-1.78218	2.50842	1.46745
C	-2.78148	1.51759	1.51529
C	-4.09025	1.85207	1.89435
C	-4.40367	3.17938	2.22974
C	-3.41071	4.17400	2.17633

C	-2.10395	3.84493	1.78879
C	1.10951	2.62168	2.12635
C	1.70571	3.36689	4.36180
C	3.06581	3.18371	4.06702
C	3.45064	2.69899	2.80556
C	2.47618	2.39965	1.84414
C	2.39185	-4.45900	1.03878
H	-2.93782	-5.30399	-3.08982
H	-3.69527	-3.14215	-2.05856
H	-2.21571	-1.95961	-0.42144
H	0.77830	-5.07074	-0.86979
H	-0.68992	-6.24360	-2.50336
H	-5.42855	3.44342	2.53028
H	-2.18917	1.76848	-5.62569
H	-4.34979	1.92346	-4.36200
H	-4.47488	1.10847	-1.99019
H	-2.42541	0.17550	-0.88652
H	-0.15377	0.82066	-4.52127
H	-4.86658	1.07350	1.93102
H	2.43271	5.06789	-2.28320
H	-1.63595	-0.32361	5.57215
H	0.47635	5.35072	-3.83413
H	-1.74257	4.33848	-3.22805
H	-1.98806	3.00687	-1.14933
H	2.18639	3.75165	-0.18072
H	0.65352	-0.24052	6.60225
H	2.67840	-0.21718	5.11101
H	2.41627	-0.24089	2.64982
H	-1.90355	-0.36491	3.11599
H	5.80006	-4.17305	0.77501
H	5.16859	-1.77734	0.38303
H	4.02093	-5.88107	1.21941
H	2.74150	-1.10699	0.38938
H	1.87734	-4.91130	-4.68458
H	-0.41242	-3.94340	-5.01680
H	3.48716	-3.79109	-3.11134
H	2.81784	-1.71193	-1.91876
H	-1.10614	-1.90019	-3.77430
H	-3.65862	5.21496	2.43146
H	-1.33486	4.62943	1.72417
H	-1.91025	-4.25852	5.82142
H	-3.38339	-4.11768	3.79655
H	0.54477	-3.77904	5.61421
H	1.51231	-3.13118	3.41545
H	-2.51386	0.48295	1.25049
H	2.77206	1.94342	0.88537
H	3.82882	3.40302	4.82848
H	-2.42111	-3.47495	1.58907
H	4.51368	2.53006	2.57804
H	1.61779	-5.20446	1.27441
C	0.72597	3.09328	3.39491
H	1.39951	3.71893	5.35777
H	-0.33744	3.21211	3.64368

## 20

ZPE(BP86/def2-SVP) = 0.8019652 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0063104 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.01351810817 Hartree (single point)

Cartesian coordinates in Å:

Pt	-0.27223	0.56486	-1.39877
Au	0.82010	-1.79244	0.76041
C	-2.25905	-1.19794	2.42026
P	-0.47031	-1.39923	2.70897
P	-0.00690	-1.42281	-2.55996
C	-3.10620	-0.69211	3.43150
C	-4.49273	-0.65831	3.22965
P	-0.32368	2.57073	-0.26749
C	-5.03877	-1.11809	2.01839
C	-4.19562	-1.59362	1.00137
C	-2.80649	-1.63743	1.19719
C	0.05247	0.04892	3.69869
C	1.10857	-0.07169	4.62512
C	1.57673	1.06508	5.30066
C	0.99579	2.32161	5.05919
C	-0.05837	2.43982	4.14074
C	-0.52750	1.31064	3.45546
C	-0.27150	-2.84868	3.81412
C	-1.28889	-3.27839	4.68939
C	-1.06517	-4.37531	5.53517
C	0.16956	-5.04609	5.51551
C	1.18354	-4.62582	4.63906
C	0.96242	-3.53522	3.78453
C	-1.28083	-2.67098	-2.14281
C	-0.95969	-3.89269	-1.51947
C	-1.98573	-4.78231	-1.15709
C	-3.32512	-4.46970	-1.43732
C	-3.64459	-3.25801	-2.07753
C	1.61460	-2.18926	-2.20016
C	2.44022	-2.62595	-3.25571
C	3.68795	-3.20318	-2.97408
C	4.10151	-3.34842	-1.64143
C	3.27038	-2.91651	-0.59163
C	2.01475	-2.32111	-0.84290
C	-0.11241	-1.20136	-4.36804
C	0.34066	0.02085	-4.91038
C	0.30631	0.22793	-6.29705
C	-0.18152	-0.78144	-7.14472
C	-0.63423	-1.99872	-6.60660
C	-0.60192	-2.21284	-5.22015
C	-0.28411	3.91680	-1.50766
C	0.91159	4.11140	-2.23663
C	0.95999	5.07526	-3.25287
C	-0.18156	5.83969	-3.55502
C	-1.37246	5.63905	-2.83818
C	-1.42933	4.67797	-1.81579
C	1.10601	2.89117	0.82862
C	1.45921	4.20967	1.18822
C	2.51975	4.43149	2.07943
C	3.24144	3.34451	2.60185
C	2.90877	2.03374	2.22491

C	1.84508	1.80580	1.34167
C	-1.84155	2.85889	0.71368
C	-3.15543	4.13881	2.31452
C	-4.22357	3.23774	2.15584
C	-4.10479	2.15373	1.27177
C	-2.91337	1.95580	0.55736
C	-2.62966	-2.35129	-2.41307
H	5.08050	-3.79730	-1.41392
H	3.62058	-3.04153	0.44518
H	0.09756	-0.30373	-0.12409
H	2.10984	-2.51124	-4.29890
H	4.33540	-3.53804	-3.79799
H	4.07567	3.52292	3.29659
H	-1.86379	-4.71032	6.21361
H	0.33897	-5.90597	6.18050
H	2.14774	-5.15470	4.61271
H	1.75039	-3.21589	3.08244
H	-2.26154	-2.76622	4.70342
H	2.79251	5.46046	2.35738
H	-0.51828	3.41821	3.94369
H	1.89438	5.23300	-3.81193
H	1.36630	3.21071	5.58998
H	2.39838	0.96656	6.02561
H	1.55886	-1.05499	4.82710
H	-1.34727	1.41404	2.73182
H	-0.14105	6.59589	-4.35306
H	-2.26547	6.23713	-3.07326
H	-2.36203	4.52234	-1.25401
H	1.80460	3.51302	-1.99695
H	-4.12434	-5.17333	-1.16097
H	-1.73203	-5.73115	-0.66169
H	-4.69223	-3.01832	-2.31484
H	0.09058	-4.14644	-1.31768
H	-6.12827	-1.09727	1.86444
H	-5.15026	-0.27018	4.02155
H	-4.61372	-1.94162	0.04709
H	-2.14993	-2.01870	0.40017
H	-2.67909	-0.32060	4.37483
H	3.47744	1.17986	2.61989
H	1.59496	0.77715	1.04230
H	-0.21171	-0.61775	-8.23228
H	-1.01568	-2.78752	-7.27196
H	0.65821	1.18149	-6.71769
H	0.72499	0.80716	-4.23891
H	0.92199	5.06525	0.75103
H	-2.79653	1.09389	-0.11961
H	-5.15459	3.38595	2.72309
H	-0.95845	-3.16393	-4.79729
H	-4.93772	1.45014	1.14159
H	-2.87984	-1.39260	-2.89425
C	-1.96855	3.95684	1.59045
H	-3.25044	4.99133	3.00346
H	-1.13691	4.66506	1.71488

## 21

ZPE(BP86/def2-SVP) = 0.8044284 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0148661 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.01325745534 Hartree (single point)

Cartesian coordinates in Å:

Au	1.04575	0.83077	0.86721
Pt	-1.51899	-0.26623	-0.48002
C	1.16970	-3.00182	-0.06751
P	-0.19667	-2.22914	-1.02706
P	-0.68296	1.27465	-1.89817
C	1.62367	-2.44083	1.13709
C	2.67793	-3.02558	1.85507
P	-0.10449	0.45588	2.89334
C	3.29378	-4.18767	1.36632
C	2.86413	-4.74763	0.14918
C	1.81462	-4.15739	-0.56944
C	0.58147	-2.07523	-2.69282
C	-0.21625	-2.03815	-3.85350
C	0.37448	-1.86249	-5.11352
C	1.76863	-1.74297	-5.22777
C	2.56643	-1.78080	-4.07307
C	1.97935	-1.93239	-2.80900
C	-1.45266	-3.57152	-1.23008
C	-1.28619	-4.87949	-0.73457
C	-2.32214	-5.82075	-0.85459
C	-3.53385	-5.47121	-1.47207
C	-3.71237	-4.16537	-1.96044
C	-2.68383	-3.22225	-1.82931
C	1.11790	1.15454	-2.15754
C	1.68202	1.28250	-3.44091
C	3.07678	1.31118	-3.57983
C	3.89352	1.19326	-2.44442
C	3.32027	1.04683	-1.16851
C	-0.93646	2.98607	-1.25763
C	0.14241	3.81107	-0.88678
C	-0.10283	5.11399	-0.41941
C	-1.41474	5.60386	-0.34126
C	-2.49230	4.78521	-0.72831
C	-2.25598	3.47892	-1.17528
C	-1.53710	1.33867	-3.51171
C	-1.25856	2.39065	-4.41207
C	-1.90262	2.43018	-5.65695
C	-2.83904	1.43883	-6.00068
C	-3.14479	0.41378	-5.09075
C	-2.49586	0.36618	-3.84802
C	-1.12801	1.86645	3.44254
C	-1.59070	2.75924	2.45028
C	-2.42713	3.82668	2.81031
C	-2.78417	4.02132	4.15448
C	-2.30404	3.14667	5.14438
C	-1.47986	2.06724	4.79276
C	0.89812	-0.15015	4.28766
C	2.29469	0.04233	4.22635
C	3.11394	-0.41897	5.26853
C	2.54384	-1.07525	6.37205
C	1.15311	-1.27277	6.43532

C	0.32881	-0.81421	5.39727
C	1.91945	1.03095	-0.98835
H	-1.60119	6.62653	0.01898
H	-3.52326	5.16675	-0.68075
H	-3.10189	2.83751	-1.46779
H	1.17272	3.43817	-0.95731
H	0.74395	5.74938	-0.12097
H	3.18659	-1.43855	7.18770
H	-2.17895	-6.83690	-0.45755
H	-4.34168	-6.21214	-1.56507
H	-4.66296	-3.87527	-2.43232
H	-2.85160	-2.18359	-2.15337
H	-0.35486	-5.16591	-0.22843
H	4.20207	-0.26570	5.21776
H	3.65830	-1.67835	-4.15083
H	-2.78472	4.51387	2.03101
H	2.23329	-1.61920	-6.21725
H	-0.26176	-1.83292	-6.01036
H	-1.30337	-2.16873	-3.78527
H	2.61313	-1.92731	-1.91235
H	-3.43128	4.86563	4.43533
H	-2.57114	3.30639	6.19956
H	-1.10030	1.39255	5.57333
H	-1.28932	2.62372	1.39994
H	4.98909	1.21008	-2.55232
H	3.52314	1.41068	-4.58010
H	3.98197	0.95039	-0.29428
H	1.04212	1.33777	-4.33226
H	4.12023	-4.65284	1.92416
H	3.01556	-2.56123	2.79396
H	3.35738	-5.64668	-0.24932
H	1.51011	-4.58417	-1.53653
H	1.17124	-1.50616	1.49304
H	0.70815	-1.79044	7.29803
H	-0.75688	-0.98889	5.44229
H	-3.34516	1.47723	-6.97679
H	-3.89608	-0.34789	-5.34692
H	-1.68069	3.24695	-6.35967
H	-0.54939	3.18481	-4.13408
H	2.73163	0.55102	3.35189
H	-2.73666	-0.41313	-3.11003
H	-2.83685	0.47484	1.78976
H	-4.18017	-1.32904	0.66471
C	-2.46800	-0.56044	1.77534
C	-3.26302	-1.59162	1.21192
C	-1.30214	-0.89710	2.52823
C	-2.93888	-2.94447	1.44816
H	-3.55697	-3.74068	1.01050
C	-1.00790	-2.24828	2.76651
C	-1.83608	-3.26313	2.24494
H	-0.12130	-2.52508	3.35248
H	-1.59070	-4.31555	2.44717
H	-2.62159	0.88696	-0.41067

ZPE(BP86/def2-SVP) = 0.8040717 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9935136 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.98558921506 Hartree (single point)

Cartesian coordinates in Å:

Au	-2.04894	-1.24386	0.47652
Pt	0.45389	-0.36011	0.17485
C	-0.63438	2.93421	1.53479
P	0.09514	2.08195	0.08148
P	0.13675	-0.85121	-2.17570
C	-1.79290	2.37037	2.10624
C	-2.45122	3.02323	3.15537
P	-0.40590	-0.98649	2.27521
C	-1.95517	4.24351	3.64404
C	-0.81363	4.81857	3.06363
C	-0.15737	4.17397	2.00302
C	-1.03430	2.71928	-1.21890
C	-0.81015	3.93718	-1.89392
C	-1.73213	4.38092	-2.85403
C	-2.88905	3.63052	-3.13152
C	-3.14226	2.44766	-2.41737
C	-2.22100	2.00127	-1.45918
C	1.73521	2.82450	-0.21259
C	2.62162	2.98981	0.87462
C	3.94150	3.40309	0.65241
C	4.39347	3.65103	-0.65475
C	3.52497	3.46172	-1.74060
C	2.20537	3.03679	-1.52557
C	-1.66812	-1.01272	-2.52773
C	-2.07523	-0.93450	-3.87961
C	-3.42489	-1.08462	-4.22776
C	-4.37847	-1.32082	-3.22569
C	-3.97761	-1.40886	-1.88139
C	0.83675	-2.51787	-2.51915
C	0.15180	-3.42868	-3.34909
C	0.70636	-4.69137	-3.61174
C	1.94478	-5.05135	-3.05644
C	2.62838	-4.14618	-2.22748
C	2.07600	-2.88676	-1.95125
C	0.83337	0.23303	-3.47835
C	2.14287	-0.00488	-3.95222
C	2.74575	0.89933	-4.83959
C	2.04459	2.03583	-5.27675
C	0.73035	2.25792	-4.83199
C	0.12523	1.36744	-3.93289
C	0.31630	-2.53584	2.90494
C	0.26793	-3.69521	2.09592
C	0.85789	-4.88480	2.53738
C	1.50082	-4.93267	3.78873
C	1.54523	-3.78666	4.59835
C	0.95402	-2.58966	4.16369
C	-0.43028	0.13253	3.70741
C	-1.44962	-0.00137	4.67314
C	-1.49047	0.87589	5.76656
C	-0.52263	1.88686	5.89558
C	0.49780	2.01467	4.93853

C	0.54762	1.13755	3.84647
C	-2.62712	-1.25837	-1.50107
H	2.37499	-6.04239	-3.26432
H	3.59594	-4.42229	-1.78268
H	2.61296	-2.19452	-1.28657
H	-0.82400	-3.16235	-3.77841
H	0.16048	-5.40003	-4.25217
H	-0.56485	2.58072	6.74811
H	4.62393	3.52312	1.50611
H	5.42963	3.97837	-0.82574
H	3.87429	3.63080	-2.76979
H	1.55245	2.85131	-2.38797
H	2.28330	2.78343	1.89952
H	-2.28650	0.77441	6.51911
H	-4.05053	1.85773	-2.60877
H	0.81425	-5.78260	1.90329
H	-3.60164	3.97961	-3.89354
H	-1.54721	5.32553	-3.38714
H	0.08321	4.53898	-1.67753
H	-2.42142	1.07562	-0.90568
H	1.96486	-5.86873	4.13318
H	2.04424	-3.82161	5.57822
H	0.98843	-1.69479	4.80212
H	-0.23132	-3.66065	1.11441
H	-5.44063	-1.43796	-3.48953
H	-3.72739	-1.01913	-5.28331
H	-4.74185	-1.59242	-1.11037
H	-1.33267	-0.75476	-4.67079
H	-2.46533	4.75088	4.47608
H	-3.34836	2.57080	3.60142
H	-0.43249	5.78260	3.43213
H	0.72229	4.64242	1.53984
H	-2.17877	1.40932	1.73062
H	1.25358	2.80719	5.03867
H	1.33856	1.23019	3.08821
H	2.51686	2.73985	-5.97788
H	0.16525	3.13488	-5.18013
H	3.76584	0.70462	-5.20245
H	2.68894	-0.90595	-3.63717
H	-2.21308	-0.78717	4.56402
H	-0.90052	1.55460	-3.59293
H	2.47506	-0.82955	2.50422
H	4.92218	-0.56853	2.79164
C	3.07911	-0.48419	1.65446
C	4.47111	-0.34868	1.81193
C	2.49228	-0.20145	0.40925
C	5.27579	0.04671	0.73282
H	6.36360	0.14807	0.86069
C	3.29317	0.17463	-0.67765
C	4.68311	0.30178	-0.51324
H	2.84799	0.40251	-1.65387
H	5.29727	0.61132	-1.37191
H	0.85008	-1.89746	0.19032

## 23

ZPE(BP86/def2-SVP) = 0.8063079 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0159454 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.02341331332 Hartree (single point)

Cartesian coordinates in Å:

Au	-2.17247	-2.13874	0.07355
Pt	-0.55168	-0.08916	-0.21939
C	0.69858	2.78900	1.30278
P	0.41493	1.94501	-0.29554
P	-0.73951	-0.62533	-2.50282
C	-0.30014	2.66484	2.28969
C	-0.22948	3.44111	3.45506
P	-0.75365	-1.17637	1.82452
C	0.83761	4.33763	3.63997
C	1.83722	4.45405	2.65946
C	1.77063	3.68567	1.48727
C	-0.75621	3.09949	-1.10250
C	-0.31482	4.31420	-1.66424
C	-1.24805	5.20351	-2.21800
C	-2.62027	4.90036	-2.18647
C	-3.06383	3.70646	-1.59214
C	-2.13446	2.80454	-1.05372
C	1.98477	1.96187	-1.21413
C	3.14030	1.48570	-0.55281
C	4.33751	1.33026	-1.26325
C	4.39057	1.64187	-2.63409
C	3.24221	2.11347	-3.29112
C	2.03687	2.27254	-2.58962
C	-2.28490	-1.55271	-2.86833
C	-2.77958	-1.55295	-4.19066
C	-3.91855	-2.30576	-4.51125
C	-4.55880	-3.06010	-3.51501
C	-4.06389	-3.06149	-2.19879
C	0.61197	-1.86592	-2.52520
C	0.34107	-3.24484	-2.63332
C	1.39192	-4.17130	-2.53660
C	2.71070	-3.73052	-2.33721
C	2.98209	-2.35487	-2.22431
C	1.93859	-1.42422	-2.30854
C	-0.44402	0.49483	-3.91103
C	0.60435	0.28505	-4.82984
C	0.83079	1.21815	-5.85398
C	0.02058	2.36050	-5.96402
C	-1.04251	2.55688	-5.06396
C	-1.27959	1.62507	-4.04498
C	0.60681	-2.31777	2.21204
C	1.40827	-2.75805	1.13168
C	2.42094	-3.69986	1.34687
C	2.65235	-4.20799	2.63748
C	1.85049	-3.78334	3.70919
C	0.82374	-2.85010	3.50150
C	-1.41019	-0.42817	3.33767
C	-2.78685	-0.10807	3.37331
C	-3.31835	0.58850	4.46765
C	-2.48413	0.96685	5.53510
C	-1.11396	0.65582	5.49977

C	-0.57118	-0.03139	4.40459
C	-2.92457	-2.31047	-1.84308
H	3.53016	-4.46180	-2.26948
H	4.01042	-1.99973	-2.06189
H	2.15365	-0.35349	-2.20240
H	-0.69103	-3.59131	-2.78438
H	1.17597	-5.24658	-2.62031
H	-2.90499	1.50571	6.39704
H	5.23126	0.96099	-0.73876
H	5.33071	1.51714	-3.19171
H	3.27532	2.35444	-4.36328
H	1.14037	2.62152	-3.11888
H	3.10257	1.22004	0.51334
H	-4.39131	0.82994	4.49282
H	-4.13794	3.47190	-1.55479
H	3.03494	-4.03233	0.49763
H	-3.34814	5.60385	-2.61745
H	-0.90097	6.14471	-2.66954
H	0.75494	4.56942	-1.67073
H	-2.46622	1.85228	-0.60752
H	3.45363	-4.94243	2.80648
H	2.01883	-4.18739	4.71839
H	0.18598	-2.54736	4.34359
H	1.24001	-2.35193	0.12213
H	-5.45265	-3.65265	-3.76326
H	-4.30219	-2.30519	-5.54224
H	-4.58356	-3.66101	-1.43533
H	-2.27083	-0.96959	-4.97251
H	0.89234	4.94602	4.55492
H	-1.01230	3.33906	4.21989
H	2.67713	5.14893	2.80584
H	2.54984	3.78884	0.71889
H	-1.13718	1.96710	2.14071
H	-0.45624	0.95858	6.32809
H	0.50697	-0.24087	4.37261
H	0.20887	3.09416	-6.76196
H	-1.69136	3.44037	-5.15262
H	1.64768	1.04935	-6.57147
H	1.24744	-0.60163	-4.74190
H	-3.43675	-0.40643	2.53538
H	-2.11188	1.78095	-3.34606
H	1.70928	0.09477	2.20630
H	1.92369	1.85330	3.96837
C	2.67635	0.25684	2.70389
C	2.79760	1.24804	3.69096
C	3.79021	-0.51918	2.34037
C	4.03760	1.46897	4.31299
H	4.13426	2.24683	5.08551
C	5.03074	-0.29533	2.96023
C	5.15480	0.69942	3.94612
H	5.90431	-0.90339	2.67978
H	6.12639	0.87286	4.43300
H	3.68416	-1.29977	1.57395

## 24

ZPE(BP86/def2-SVP) = 0.8062475 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0291675 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.03188384679 Hartree (single point)

Cartesian coordinates in Å:

C	-2.10449	1.48675	-2.22499
P	-1.88742	-0.24853	-1.69104
P	1.60159	-0.21357	-1.04558
C	-2.24711	2.46689	-1.21779
C	-2.44562	3.80776	-1.56705
P	-1.78966	-0.14186	1.91884
C	-2.48730	4.18453	-2.92105
C	-2.34957	3.21129	-3.92373
C	-2.16850	1.86124	-3.58201
C	-3.55310	-0.84206	-1.22815
C	-4.71292	-0.14223	-1.61484
C	-5.97262	-0.61326	-1.21036
C	-6.07727	-1.77220	-0.42212
C	-4.91928	-2.47713	-0.04664
C	-3.65985	-2.01454	-0.45153
C	-1.42425	-1.21958	-3.16628
C	-0.35903	-0.77556	-3.97985
C	0.08557	-1.56154	-5.04958
C	-0.52072	-2.80092	-5.31249
C	-1.58803	-3.24149	-4.51265
C	-2.04425	-2.45592	-3.44307
C	2.97652	-0.06818	0.14413
C	3.75278	1.09793	0.26505
C	4.77202	1.15410	1.22850
C	5.01537	0.05482	2.06538
C	4.23779	-1.11058	1.94358
C	1.70319	1.26391	-2.12048
C	1.08097	2.43017	-1.62189
C	1.05231	3.59938	-2.39383
C	1.63169	3.61007	-3.67344
C	2.25404	2.45334	-4.17225
C	2.29772	1.28293	-3.39811
C	2.00699	-1.72675	-1.98208
C	3.23673	-1.86748	-2.65989
C	3.51127	-3.04777	-3.36641
C	2.57827	-4.09968	-3.37378
C	1.37596	-3.98047	-2.65764
C	1.09123	-2.79762	-1.96169
C	-2.53515	-1.65161	2.57671
C	-1.86629	-2.87115	2.31348
C	-2.40478	-4.08022	2.76837
C	-3.60663	-4.08363	3.50210
C	-4.25690	-2.87199	3.79101
C	-3.72490	-1.65610	3.33574
C	-2.98844	1.21643	2.00416
C	-4.30857	1.04330	1.52869
C	-5.15707	2.15255	1.41092
C	-4.70331	3.43448	1.76764
C	-3.39545	3.60762	2.25328
C	-2.53649	2.50481	2.37043
C	3.21572	-1.17397	0.99182

H	1.59665	4.52307	-4.28609
H	2.70972	2.46021	-5.17356
H	2.77094	0.37767	-3.80312
H	0.60160	2.40639	-0.63028
H	0.55871	4.49929	-2.00040
H	-5.37374	4.30142	1.67133
H	0.91927	-1.20772	-5.67344
H	-0.16354	-3.42350	-6.14591
H	-2.07531	-4.20481	-4.72433
H	-2.88414	-2.80566	-2.82638
H	0.12891	0.18547	-3.77351
H	-6.17940	2.01361	1.02924
H	-4.99140	-3.37986	0.57742
H	-1.88454	-5.02628	2.55701
H	-7.06624	-2.12770	-0.09689
H	-6.87872	-0.06376	-1.50580
H	-4.63027	0.77641	-2.21315
H	-2.75228	-2.55079	-0.14029
H	-4.02859	-5.03402	3.86122
H	-5.18574	-2.87195	4.38055
H	-4.23459	-0.71089	3.57054
H	-0.92490	-2.85649	1.73940
H	5.80834	0.10966	2.82417
H	5.37652	2.06632	1.32950
H	4.42454	-1.96981	2.60423
H	3.56099	1.96204	-0.38719
H	-2.63246	5.23993	-3.19601
H	-2.56344	4.55963	-0.77295
H	-2.39026	3.50075	-4.98418
H	-2.08108	1.10438	-4.37353
H	-2.20398	2.17896	-0.15895
H	-3.04215	4.60725	2.54717
H	-1.50562	2.63430	2.73658
H	2.80009	-5.02480	-3.92643
H	0.65478	-4.81033	-2.64280
H	4.46681	-3.15446	-3.90115
H	3.98979	-1.06655	-2.61450
H	-4.66423	0.04784	1.23011
H	0.15268	-2.68901	-1.39745
H	2.57152	-0.39198	4.73333
H	4.50645	0.70684	5.84232
C	2.85106	0.63017	4.43449
C	3.94760	1.24584	5.06144
C	2.10497	1.30304	3.43566
C	4.33093	2.54644	4.69423
H	5.18904	3.02991	5.18559
C	2.51225	2.61214	3.07787
C	3.61145	3.22821	3.69768
H	1.96543	3.16225	2.29562
H	3.90841	4.24734	3.40431
H	2.60242	-2.08355	0.89681
Pt	-0.46218	-0.26262	0.07211
Au	0.41067	0.48931	2.62937

## 25

ZPE(BP86/def2-SVP) = 0.8018371 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9840108 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.98614360642 Hartree (single point)

Cartesian coordinates in Å:

C	0.19449	-3.26874	1.71560
P	0.37492	-1.44167	1.64911
P	-0.09199	-1.94878	-1.88666
C	-0.88373	-3.87224	2.39349
C	-1.06393	-5.26247	2.32439
P	-1.05070	1.62514	0.74669
C	-0.17765	-6.05735	1.57869
C	0.90224	-5.45967	0.90939
C	1.08904	-4.07236	0.97904
C	-0.21843	-0.84957	3.27473
C	0.63730	-0.55350	4.35077
C	0.09432	-0.14588	5.57952
C	-1.29607	-0.04008	5.74206
C	-2.15151	-0.31268	4.66126
C	-1.61514	-0.70556	3.42740
C	2.17652	-1.16596	1.51862
C	3.08721	-1.82497	2.37335
C	4.46440	-1.59579	2.23608
C	4.93984	-0.71964	1.24388
C	4.03791	-0.08011	0.37855
C	2.66125	-0.30616	0.51132
C	1.63662	-1.77025	-2.42384
C	2.01457	-0.58925	-3.09986
C	3.36963	-0.33232	-3.35647
C	4.35357	-1.24878	-2.94814
C	3.97831	-2.43298	-2.29163
C	-1.17859	-0.90190	-2.91446
C	-1.69047	-1.03084	-4.20688
C	-2.66154	-0.09891	-4.62794
C	-3.13296	0.88997	-3.74793
C	-2.64139	0.98758	-2.42917
C	-1.62711	0.09990	-1.99548
C	-0.59061	-3.69065	-1.95728
C	-1.63560	-4.08699	-1.09609
C	-2.08283	-5.41388	-1.10916
C	-1.48349	-6.34858	-1.97114
C	-0.44211	-5.95438	-2.82855
C	0.00542	-4.62409	-2.83048
C	1.18597	3.50094	-0.96768
C	2.55201	3.23928	-1.16908
C	3.50706	4.11414	-0.62009
C	3.09877	5.24869	0.09934
C	1.73011	5.51607	0.26289
C	0.76506	4.64121	-0.26609
C	-0.11131	2.20444	2.18849
C	1.29652	2.27267	2.09993
C	2.05409	2.67978	3.20474
C	1.41558	3.03927	4.40346
C	0.01465	2.98134	4.49301
C	-0.74996	2.56252	3.39513
C	-2.78249	2.12642	0.97420

C	-4.45240	3.86594	1.33926
C	-5.47787	2.91409	1.19297
C	-5.15814	1.57040	0.93699
C	-3.81587	1.17433	0.83157
C	2.62673	-2.69470	-2.02674
H	-3.90864	1.59263	-4.08797
H	-3.06279	1.74302	-1.74802
H	0.41997	2.13988	-2.99992
H	-1.35801	-1.84051	-4.87397
H	-3.06904	-0.15950	-5.64818
H	2.00966	3.36893	5.26881
H	5.17206	-2.10797	2.90483
H	6.02118	-0.54501	1.13993
H	4.40323	0.59193	-0.41048
H	1.94891	0.17302	-0.17704
H	2.72115	-2.53224	3.13284
H	3.14943	2.72979	3.11889
H	-3.24054	-0.20536	4.77372
H	4.57816	3.90728	-0.76759
H	-1.71458	0.27561	6.70920
H	0.76751	0.09786	6.41444
H	1.72730	-0.61567	4.22749
H	-2.27878	-0.87939	2.56592
H	3.84849	5.93118	0.52593
H	1.40235	6.40710	0.81942
H	-0.30355	4.84546	-0.11073
H	2.87599	2.35738	-1.74069
H	5.41537	-1.04546	-3.15160
H	3.65474	0.58705	-3.88969
H	4.74383	-3.15851	-1.97980
H	1.24845	0.13188	-3.41868
H	-0.32510	-7.14591	1.52466
H	-1.90249	-5.72816	2.86334
H	1.60361	-6.07713	0.32915
H	1.94321	-3.60449	0.47111
H	-1.57700	-3.26006	2.98819
H	-0.49053	3.25593	5.43078
H	-1.84386	2.50201	3.47926
H	-1.82915	-7.39307	-1.97410
H	0.02177	-6.68671	-3.50599
H	-2.89322	-5.72376	-0.43392
H	-2.07525	-3.35026	-0.40547
H	1.80281	2.02611	1.15959
H	-3.55266	0.12540	0.62397
H	-6.53022	3.22287	1.27951
H	0.81629	-4.31434	-3.50626
H	-5.95852	0.82414	0.82311
H	2.33972	-3.62425	-1.51673
C	-3.10992	3.47853	1.22663
H	-4.70176	4.91915	1.53682
H	-2.30898	4.22527	1.33765
Pt	-0.72016	-0.49817	-0.14765
Au	-0.14074	2.04828	-1.48267

## 26

ZPE(BP86/def2-SVP) = 0.8021899 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9675860 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.96887333463 Hartree (single point)

Cartesian coordinates in Å:

C	-1.41751	-3.00690	2.01000
P	-0.27774	-1.58234	1.89722
P	-0.02915	-1.89339	-1.65531
C	-2.69766	-2.85747	2.58184
C	-3.59481	-3.93679	2.58332
P	-0.06758	1.80458	0.63975
C	-3.22061	-5.16992	2.02522
C	-1.94505	-5.32289	1.45704
C	-1.05152	-4.24511	1.43922
C	-0.59194	-0.55300	3.38748
C	0.26597	-0.58758	4.50426
C	0.04541	0.28836	5.58052
C	-1.02335	1.19933	5.54828
C	-1.88633	1.22898	4.43815
C	-1.67022	0.35628	3.36356
C	1.41242	-2.23440	2.13377
C	1.67231	-3.36871	2.93193
C	2.99779	-3.77819	3.14683
C	4.06262	-3.05318	2.58485
C	3.80331	-1.91746	1.80028
C	2.48360	-1.51233	1.56882
C	1.68168	-2.53553	-1.57099
C	2.71207	-1.73085	-2.10346
C	4.05242	-2.11097	-1.94320
C	4.37567	-3.29399	-1.25682
C	3.35308	-4.09518	-0.72409
C	-0.17672	-1.07952	-3.28336
C	-0.35652	-1.90225	-4.41679
C	-0.46833	-1.34313	-5.69361
C	-0.40008	0.05084	-5.83107
C	-0.21489	0.86590	-4.70388
C	-0.09807	0.33798	-3.38931
C	-1.19691	-3.29370	-1.67453
C	-2.49709	-3.02612	-1.19326
C	-3.47992	-4.02252	-1.22982
C	-3.16768	-5.29696	-1.73339
C	-1.87366	-5.57037	-2.20688
C	-0.88752	-4.57079	-2.18588
C	0.13503	3.88197	-1.21992
C	1.27034	4.57721	-0.77891
C	1.15118	5.92120	-0.37641
C	-0.09234	6.56977	-0.42723
C	-1.22057	5.87648	-0.89765
C	-1.10864	4.53494	-1.29638
C	1.55371	2.01339	1.41716
C	2.72363	1.85294	0.64090
C	3.97583	1.78721	1.26581
C	4.06801	1.86082	2.66714
C	2.90475	2.00467	3.44122
C	1.64721	2.08433	2.82461
C	-1.25453	2.95273	1.35983

C	-1.83625	4.98382	2.55580
C	-3.19899	4.72187	2.33461
C	-3.59241	3.58005	1.61171
C	-2.62318	2.69692	1.12130
C	2.01179	-3.71499	-0.87261
H	-0.48911	0.51556	-6.82481
H	-0.16597	1.95246	-4.86139
H	0.49830	2.74779	-3.08648
H	-0.42684	-2.99310	-4.29224
H	-0.61249	-1.98967	-6.57166
H	5.05084	1.80128	3.15748
H	3.19944	-4.66573	3.76499
H	5.09921	-3.37849	2.75862
H	4.62975	-1.34764	1.35279
H	2.27539	-0.63561	0.93998
H	0.84307	-3.92946	3.38752
H	4.88439	1.67290	0.65623
H	-2.71753	1.94822	4.39529
H	2.04375	6.46051	-0.02398
H	-1.18241	1.89221	6.38781
H	0.72413	0.26486	6.44612
H	1.12040	-1.27852	4.52461
H	-2.32040	0.40771	2.47870
H	-0.18173	7.61899	-0.10895
H	-2.19730	6.37969	-0.95546
H	-2.00314	3.99980	-1.65034
H	2.25188	4.08634	-0.72820
H	5.42772	-3.59267	-1.13788
H	4.85031	-1.48336	-2.36767
H	3.59883	-5.01940	-0.18133
H	2.45775	-0.80898	-2.64847
H	-3.92450	-6.01515	2.03467
H	-4.58976	-3.81485	3.03660
H	-1.64558	-6.28388	1.01514
H	-0.05843	-4.36778	0.98915
H	-2.99144	-1.90353	3.04246
H	2.97179	2.04781	4.53828
H	0.73933	2.17062	3.43890
H	-3.93683	-6.08329	-1.75408
H	-1.63062	-6.56723	-2.60408
H	-4.48952	-3.80949	-0.85015
H	-2.72307	-2.03074	-0.77817
H	2.64369	1.75699	-0.45362
H	-2.91522	1.80521	0.54275
H	-3.96079	5.41698	2.71787
H	0.12074	-4.78713	-2.56912
H	-4.65883	3.38304	1.42729
H	1.21986	-4.34505	-0.44684
C	-0.85898	4.10611	2.06656
H	-1.53018	5.88767	3.10270
H	0.20726	4.32944	2.20848
Pt	-0.33464	-0.31049	-0.00359
Au	0.10728	1.81548	-1.84835

ZPE(BP86/def2-SVP) = 0.8060397 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0395984 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.04299986816 Hartree (single point)

Cartesian coordinates in Å:

C	-1.38712	-2.94206	2.03460
P	-0.27154	-1.49443	1.96664
P	-0.14117	-1.79326	-1.61183
C	-2.68395	-2.81463	2.57364
C	-3.56201	-3.90892	2.55197
P	0.04861	1.97081	0.72529
C	-3.15295	-5.13438	2.00108
C	-1.86176	-5.26487	1.46403
C	-0.98564	-4.17247	1.47218
C	-0.64923	-0.50607	3.46366
C	0.13043	-0.60120	4.63340
C	-0.14767	0.23912	5.72367
C	-1.19713	1.17139	5.65220
C	-1.98312	1.25827	4.49003
C	-1.70869	0.42258	3.39900
C	1.42923	-2.11890	2.19862
C	1.70494	-3.24425	3.00492
C	3.03452	-3.64735	3.20468
C	4.08777	-2.92728	2.61504
C	3.81291	-1.80318	1.81939
C	2.48890	-1.40113	1.60586
C	1.57960	-2.41642	-1.56131
C	2.59606	-1.58023	-2.07229
C	3.94281	-1.93987	-1.92018
C	4.28788	-3.13286	-1.26245
C	3.27968	-3.96621	-0.75239
C	-0.30011	-0.95511	-3.24767
C	-0.48998	-1.76413	-4.38864
C	-0.55359	-1.18681	-5.66341
C	-0.42752	0.20511	-5.80035
C	-0.24860	1.00968	-4.66356
C	-0.18462	0.46100	-3.36343
C	-1.29282	-3.20415	-1.64033
C	-2.58377	-2.96501	-1.12135
C	-3.55354	-3.97421	-1.15862
C	-3.23699	-5.23201	-1.70019
C	-1.95150	-5.47669	-2.21081
C	-0.97844	-4.46452	-2.18928
C	0.79306	4.05014	-2.62593
C	1.50283	4.60543	-1.53711
C	0.81173	5.26578	-0.50970
C	-0.58951	5.37375	-0.55657
C	-1.30524	4.81287	-1.62513
C	-0.62019	4.15572	-2.66616
C	1.66391	2.06928	1.54959
C	2.83088	2.08664	0.75444
C	4.09231	1.94707	1.35207
C	4.19812	1.78698	2.74444
C	3.03871	1.77039	3.53899
C	1.77445	1.90963	2.94969
C	-1.13513	3.03878	1.57981

C	-1.72991	4.82637	3.12383
C	-3.08145	4.69456	2.76314
C	-3.46112	3.73883	1.80080
C	-2.49430	2.91677	1.20975
C	1.93163	-3.60781	-0.89443
H	-0.47431	0.66809	-6.79794
H	-0.15942	2.09890	-4.80236
H	1.34005	3.60632	-3.47206
H	-0.59529	-2.85412	-4.28232
H	-0.70159	-1.82351	-6.54816
H	5.18720	1.67257	3.21217
H	3.24850	-4.52738	3.82938
H	5.12792	-3.24818	2.77554
H	4.62991	-1.23746	1.35036
H	2.26881	-0.53379	0.96737
H	0.88405	-3.80572	3.47494
H	4.99790	1.96290	0.72727
H	-2.79687	1.99484	4.41903
H	1.36898	5.69930	0.33361
H	-1.40023	1.83686	6.50435
H	0.46875	0.17163	6.63249
H	0.97017	-1.30881	4.68314
H	-2.29424	0.51739	2.47291
H	-1.12818	5.88838	0.25189
H	-2.40112	4.89428	-1.65844
H	-1.17869	3.76793	-3.53130
H	2.60008	4.53705	-1.50883
H	5.34520	-3.41412	-1.14805
H	4.72914	-1.28623	-2.32647
H	3.54202	-4.89947	-0.23319
H	2.32572	-0.64773	-2.59054
H	-3.84249	-5.99137	1.99148
H	-4.56993	-3.80496	2.98041
H	-1.53621	-6.21993	1.02751
H	0.02282	-4.27704	1.05279
H	-3.00486	-1.86543	3.02625
H	3.11661	1.63543	4.62801
H	0.87212	1.86675	3.57524
H	-3.99627	-6.02789	-1.72173
H	-1.70514	-6.46054	-2.63732
H	-4.55663	-3.78400	-0.75070
H	-2.81227	-1.98320	-0.67719
H	2.73729	2.19082	-0.33724
H	-2.78234	2.17150	0.45044
H	-3.84168	5.34018	3.22731
H	0.02331	-4.65750	-2.60092
H	-4.51764	3.63856	1.51043
H	1.15059	-4.26519	-0.49071
C	-0.75599	4.00576	2.53379
H	-1.42931	5.57768	3.86933
H	0.30130	4.12214	2.81079
Pt	-0.33628	-0.22322	0.09518
Au	0.00929	1.65963	-1.68207

**28**

ZPE(BP86/def2-SVP) = 0.8033490 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0050467 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.01159585632 Hartree (single point)

Cartesian coordinates in Å:

Au	-0.19337	-1.17431	-0.90847
Pt	1.73094	0.41363	0.76354
C	0.02547	1.84272	3.61880
P	0.28230	2.04679	1.80095
P	0.57800	0.19889	-2.63634
C	-0.94505	0.90802	4.05125
C	-1.11059	0.63604	5.41666
P	-0.62822	-2.65960	0.83605
C	-0.31408	1.28881	6.37145
C	0.63964	2.22878	5.95099
C	0.80944	2.50605	4.58449
C	-1.45342	2.18602	1.20509
C	-2.44282	2.82819	1.98236
C	-3.75894	2.92075	1.50701
C	-4.10030	2.38401	0.25154
C	-3.11601	1.76430	-0.53429
C	-1.79993	1.67138	-0.05516
C	0.96574	3.73124	1.56027
C	2.25605	4.02715	2.05339
C	2.84398	5.27394	1.79908
C	2.16992	6.22134	1.01091
C	0.90255	5.91902	0.48849
C	0.29627	4.68402	0.76772
C	1.56046	1.61707	-2.07105
C	1.84314	2.63140	-3.02231
C	2.75071	3.65270	-2.72592
C	3.41774	3.63356	-1.48940
C	3.13784	2.63353	-0.54922
C	-0.70704	0.85917	-3.76275
C	-1.33573	2.08569	-3.45544
C	-2.38873	2.55312	-4.25545
C	-2.82085	1.80506	-5.36362
C	-2.19073	0.58864	-5.67516
C	-1.13718	0.11365	-4.87940
C	1.68271	-0.84817	-3.65636
C	2.89888	-0.36185	-4.17378
C	3.71207	-1.20430	-4.94853
C	3.31748	-2.52625	-5.21206
C	2.10819	-3.01612	-4.68932
C	1.29673	-2.18452	-3.90404
C	-0.78697	-4.42088	0.41217
C	-0.03914	-4.89163	-0.69025
C	-0.08742	-6.24941	-1.03662
C	-0.89560	-7.13415	-0.30164
C	-1.65517	-6.66122	0.78142
C	-1.60206	-5.30648	1.14488
C	-1.95914	-2.15203	1.96801
C	-2.93861	-1.25381	1.49695
C	-3.94311	-0.79567	2.36269
C	-3.98026	-1.24536	3.69311
C	-3.00672	-2.14545	4.16382

C	-1.98743	-2.59145	3.30982
C	2.16573	1.63285	-0.78605
H	-3.64473	2.17545	-5.99154
H	-2.51685	0.00578	-6.54934
H	-0.64186	-0.83418	-5.13569
H	-0.99246	2.68258	-2.59832
H	-2.86996	3.51248	-4.01322
H	-4.76824	-0.88696	4.37202
H	3.84422	5.49765	2.19916
H	2.63751	7.19396	0.79733
H	0.37530	6.65301	-0.13893
H	-0.69945	4.45857	0.36007
H	2.82085	3.26464	2.61074
H	-4.68981	-0.07793	1.99440
H	-3.36376	1.35149	-1.52339
H	0.49956	-6.61710	-1.89122
H	-5.13507	2.45728	-0.11573
H	-4.52493	3.41840	2.12047
H	-2.18344	3.24957	2.96457
H	-1.02621	1.17357	-0.65672
H	-0.94081	-8.19720	-0.58106
H	-2.29700	-7.35167	1.34835
H	-2.20343	-4.93891	1.98908
H	0.57296	-4.18817	-1.27800
H	4.16016	4.40898	-1.24792
H	2.95335	4.44324	-3.46301
H	3.67996	2.63618	0.40442
H	1.34746	2.60893	-4.00474
H	-0.44537	1.07458	7.44240
H	-1.87553	-0.08796	5.73116
H	1.25383	2.76239	6.69163
H	1.54121	3.26505	4.27869
H	-1.60035	0.41039	3.32074
H	-3.03672	-2.49598	5.20623
H	-1.20394	-3.26521	3.68897
H	3.95908	-3.18110	-5.82026
H	1.79995	-4.05367	-4.88691
H	4.66419	-0.82325	-5.34665
H	3.21572	0.66922	-3.96117
H	-2.89771	-0.89752	0.45716
H	0.35964	-2.57188	-3.47125
H	1.93815	-4.24992	1.11293
H	4.14691	-3.56722	2.07388
C	2.03201	-3.29154	1.64501
C	3.28214	-2.89501	2.17396
C	0.92403	-2.45173	1.78412
C	3.43436	-1.65232	2.79169
H	4.41561	-1.34129	3.17770
C	1.04887	-1.20905	2.47411
C	2.31230	-0.79599	2.95560
H	0.14268	-0.67518	2.78302
H	2.38581	0.10783	3.57902
H	2.75376	-0.58158	0.02520

ZPE(BP86/def2-SVP) = 0.8035879 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9874535 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.98427589369 Hartree (single point)

Cartesian coordinates in Å:

Au	-0.76295	-1.17372	-1.29423
Pt	1.09995	-0.31739	0.47236
C	-0.02298	1.55711	3.37901
P	-0.07507	1.54131	1.55242
P	0.17334	0.20915	-2.94992
C	0.34315	0.39917	4.09102
C	0.36045	0.40915	5.49336
P	-0.61765	-1.94006	0.96977
C	0.01006	1.57410	6.19399
C	-0.35823	2.73380	5.48942
C	-0.37397	2.72938	4.08707
C	-1.85857	1.70129	1.12988
C	-2.84533	1.89764	2.11555
C	-4.18999	2.04876	1.74196
C	-4.56507	2.00325	0.39012
C	-3.58812	1.78692	-0.59567
C	-2.24622	1.63103	-0.22457
C	0.69290	3.13027	1.03477
C	1.68097	3.75306	1.82635
C	2.41015	4.84186	1.32173
C	2.16332	5.31924	0.02586
C	1.16547	4.71578	-0.75713
C	0.43454	3.63049	-0.25813
C	1.62807	1.07146	-2.22171
C	2.31084	1.90643	-3.14413
C	3.43221	2.64306	-2.75429
C	3.91055	2.50697	-1.44225
C	3.27075	1.64256	-0.54332
C	-1.02450	1.46101	-3.53632
C	-0.77987	2.84779	-3.50472
C	-1.78065	3.74506	-3.91183
C	-3.01851	3.26607	-4.36884
C	-3.26231	1.88152	-4.41327
C	-2.27600	0.98134	-3.98656
C	0.81901	-0.63772	-4.43087
C	0.46510	-0.25565	-5.73912
C	1.01231	-0.94590	-6.83356
C	1.90611	-2.00820	-6.62455
C	2.25814	-2.38771	-5.31638
C	1.71501	-1.70821	-4.21841
C	-0.21287	-3.70759	1.14743
C	0.93836	-4.20775	0.49573
C	1.28283	-5.56061	0.61253
C	0.48709	-6.42712	1.38310
C	-0.65961	-5.93524	2.02805
C	-1.01523	-4.58259	1.91144
C	-2.12582	-1.63623	1.94482
C	-3.34648	-1.38707	1.28299
C	-4.51125	-1.14196	2.02308
C	-4.46568	-1.13386	3.42695
C	-3.25261	-1.37990	4.09178

C	-2.08664	-1.63688	3.35608
C	2.10936	0.92500	-0.88743
H	-3.79800	3.97258	-4.69010
H	-4.23018	1.50127	-4.77240
H	-2.47643	-0.10205	-3.99914
H	0.19104	3.22496	-3.15635
H	-1.58767	4.82738	-3.87467
H	-5.38000	-0.93713	4.00639
H	3.17575	5.31949	1.95109
H	2.74064	6.16730	-0.37068
H	0.95495	5.09575	-1.76800
H	-0.34230	3.17335	-0.88355
H	1.87779	3.39742	2.84737
H	-5.45841	-0.95063	1.49856
H	-3.85943	1.74072	-1.66012
H	2.17905	-5.94138	0.10045
H	-5.62032	2.12736	0.10486
H	-4.95188	2.19465	2.52173
H	-2.57235	1.91397	3.17882
H	-1.49834	1.45079	-1.00662
H	0.76098	-7.48826	1.47815
H	-1.28804	-6.61113	2.62706
H	-1.91947	-4.20636	2.41125
H	1.55934	-3.52835	-0.11016
H	4.80450	3.06048	-1.11787
H	3.94272	3.29599	-3.47712
H	3.70242	1.52219	0.45748
H	1.96286	1.96316	-4.18762
H	0.02936	1.58290	7.29406
H	0.66144	-0.49735	6.03881
H	-0.63238	3.64899	6.03489
H	-0.65738	3.64092	3.53983
H	0.63975	-0.50403	3.54333
H	-3.21268	-1.37698	5.19112
H	-1.14655	-1.85132	3.88160
H	2.33158	-2.54550	-7.48502
H	2.95866	-3.21982	-5.15227
H	0.73870	-0.64747	-7.85647
H	-0.23223	0.57889	-5.90430
H	-3.37659	-1.38047	0.18266
H	1.99022	-1.99973	-3.19213
H	2.41787	-2.66921	1.93199
H	3.91867	-2.93009	3.88240
C	2.84302	-1.77164	2.40214
C	3.68910	-1.91762	3.51649
C	2.53465	-0.48381	1.93019
C	4.23561	-0.79166	4.15320
H	4.89656	-0.91279	5.02400
C	3.08738	0.64305	2.55326
C	3.93499	0.48775	3.66514
H	2.84361	1.65514	2.20880
H	4.34873	1.38318	4.15339
H	1.96185	-1.45716	-0.24684

## 30

ZPE(BP86/def2-SVP) = 0.8056750 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0180367 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.01581095979 Hartree (single point)

Cartesian coordinates in Å:

Au	-1.01257	-1.05001	-0.84860
Pt	0.98266	0.28227	0.58047
C	0.29067	2.19371	3.29387
P	0.01640	2.12295	1.48739
P	-0.05551	-0.10166	-2.77983
C	1.00716	1.16444	3.93638
C	1.24078	1.22709	5.31863
P	-0.69312	-1.23333	1.49435
C	0.75973	2.31570	6.06484
C	0.06751	3.35729	5.42251
C	-0.15646	3.30721	4.03858
C	-1.77958	2.22589	1.14291
C	-2.73901	2.57644	2.11040
C	-4.09135	2.66717	1.74810
C	-4.49649	2.40916	0.42827
C	-3.54330	2.04891	-0.53783
C	-2.19118	1.95806	-0.18042
C	0.68609	3.71986	0.88922
C	1.82384	4.26517	1.52143
C	2.43240	5.41584	0.99921
C	1.91970	6.02015	-0.16061
C	0.78492	5.47996	-0.78860
C	0.16468	4.33745	-0.26525
C	1.08294	1.27637	-2.30271
C	1.48478	2.13557	-3.35717
C	2.50294	3.07829	-3.16918
C	3.14905	3.15448	-1.92573
C	2.73333	2.32778	-0.87196
C	-1.07344	0.54890	-4.15081
C	-1.80253	1.74250	-3.95113
C	-2.65189	2.22174	-4.95740
C	-2.78547	1.51278	-6.16485
C	-2.06073	0.32714	-6.36476
C	-1.20449	-0.15782	-5.36239
C	1.03812	-1.38299	-3.50504
C	2.31447	-1.08038	-4.02163
C	3.12459	-2.10930	-4.52709
C	2.66605	-3.43744	-4.52796
C	1.39203	-3.74178	-4.01859
C	0.58307	-2.71987	-3.49956
C	-0.42413	-2.92089	2.15001
C	-0.74353	-4.04804	1.36701
C	-0.53244	-5.34084	1.87159
C	-0.00304	-5.51557	3.16175
C	0.31104	-4.39339	3.94859
C	0.10503	-3.10063	3.44480
C	-2.15760	-0.68685	2.46013
C	-3.43569	-0.74651	1.86663
C	-4.57616	-0.40505	2.60755
C	-4.45357	-0.00130	3.94739
C	-3.18331	0.06266	4.54341

C	-2.04001	-0.28041	3.80627
C	1.68298	1.39818	-1.01461
H	-3.45308	1.89010	-6.95349
H	-2.15630	-0.22525	-7.31133
H	-0.63328	-1.08352	-5.52575
H	-1.68766	2.31037	-3.01574
H	-3.21048	3.15659	-4.80057
H	-5.34981	0.26305	4.52835
H	3.31508	5.84043	1.50020
H	2.40222	6.91876	-0.57282
H	0.37626	5.95335	-1.69334
H	-0.72496	3.92571	-0.76037
H	2.23741	3.78488	2.42066
H	-5.56748	-0.45445	2.13322
H	-3.84829	1.82841	-1.57179
H	-0.78680	-6.21691	1.25630
H	-5.56011	2.47614	0.15579
H	-4.83712	2.92744	2.51293
H	-2.44461	2.74377	3.15427
H	-1.44130	1.66516	-0.92876
H	0.16041	-6.52879	3.55794
H	0.72125	-4.52783	4.96085
H	0.36695	-2.22484	4.05736
H	-1.15833	-3.90147	0.35714
H	3.96645	3.87334	-1.76661
H	2.79814	3.73919	-3.99732
H	3.22266	2.43921	0.10665
H	0.99901	2.05213	-4.34127
H	0.93812	2.36247	7.14946
H	1.80269	0.42194	5.81516
H	-0.29091	4.22126	6.00157
H	-0.66211	4.14476	3.53569
H	1.37170	0.31536	3.33710
H	-3.07851	0.37820	5.59232
H	-1.05367	-0.22456	4.28454
H	3.30650	-4.23998	-4.92296
H	1.03054	-4.78083	-4.01595
H	4.12357	-1.87075	-4.92124
H	2.68101	-0.04351	-4.01436
H	-3.52895	-1.06124	0.81573
H	-0.40714	-2.95527	-3.07622
H	1.78899	-3.28909	-0.96313
H	2.14032	-4.41711	1.25409
C	2.23959	-2.74568	-0.12008
C	2.44248	-3.37082	1.10855
C	2.64621	-1.39829	-0.30909
C	3.02324	-2.65609	2.18255
H	3.17530	-3.16271	3.14628
C	3.24160	-0.68003	0.77025
C	3.41091	-1.32480	2.02484
H	3.73357	0.28381	0.58248
H	3.89028	-0.78047	2.85164
H	2.66419	-0.97859	-1.32447

## 31

ZPE(BP86/def2-SVP) = 0.8025018 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9777357 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.98611038497 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.68772	1.20604	-1.40299
Au	0.67584	-0.44108	0.73250
C	-1.83571	-2.16772	2.48850
P	-0.29396	-1.22081	2.75011
P	0.12798	-0.66835	-2.63409
C	-2.97793	-1.99085	3.29614
C	-4.12560	-2.76555	3.06164
P	0.37127	2.01964	0.73882
C	-4.13585	-3.72612	2.03740
C	-2.98884	-3.92009	1.24760
C	-1.84352	-3.14300	1.46659
C	-0.63197	0.03783	4.03056
C	0.22273	0.16323	5.14669
C	-0.01645	1.16195	6.10296
C	-1.10859	2.03353	5.95875
C	-1.96263	1.90736	4.84990
C	-1.72503	0.92092	3.88186
C	0.90117	-2.37791	3.49974
C	0.47536	-3.55417	4.14695
C	1.42776	-4.42115	4.70554
C	2.79672	-4.11467	4.62544
C	3.22132	-2.93772	3.98371
C	2.27707	-2.07091	3.41573
C	-1.69666	-0.65090	-2.47777
C	-2.33268	-1.48926	-1.54033
C	-3.70625	-1.34894	-1.28640
C	-4.45150	-0.37938	-1.97657
C	-3.81944	0.45528	-2.91698
C	0.68773	-2.20785	-1.76940
C	0.79996	-3.38695	-2.53890
C	1.23975	-4.58133	-1.94966
C	1.57404	-4.60196	-0.58728
C	1.44481	-3.43565	0.18852
C	0.98845	-2.23242	-0.37950
C	0.53770	-0.89246	-4.39273
C	1.88155	-0.68320	-4.77249
C	2.26102	-0.83887	-6.11221
C	1.30142	-1.19289	-7.07795
C	-0.03562	-1.39867	-6.70097
C	-0.42230	-1.25228	-5.35874
C	-0.04804	2.55426	-2.75220
C	0.42595	2.57302	-4.08161
C	-0.15635	3.42638	-5.03568
C	-1.23011	4.25853	-4.67874
C	-1.70346	4.24888	-3.35600
C	-1.11180	3.41183	-2.39460
C	1.47507	2.96113	1.82319
C	2.64341	3.52215	1.26269
C	3.57103	4.17253	2.09030
C	3.33966	4.26270	3.47370
C	2.17809	3.70040	4.03303

C	1.24589	3.04758	3.21561
C	-1.35675	2.45033	1.08924
C	-3.07554	3.91180	2.00524
C	-4.07354	3.04859	1.52365
C	-3.71367	1.89469	0.80131
C	-2.36489	1.59996	0.57407
C	-2.44621	0.33058	-3.16518
H	1.93889	-5.52943	-0.12010
H	1.70329	-3.47554	1.25659
H	1.75848	0.07592	-0.60856
H	0.55753	-3.36478	-3.61221
H	1.33444	-5.49064	-2.56136
H	4.06826	4.77479	4.11979
H	1.09735	-5.34367	5.20542
H	3.53888	-4.79963	5.06162
H	4.29291	-2.69953	3.91549
H	2.60650	-1.15811	2.89324
H	-0.59622	-3.79538	4.20465
H	4.47732	4.61585	1.65183
H	-2.81847	2.58574	4.72533
H	0.22616	3.42729	-6.06798
H	-1.29636	2.81197	6.71294
H	0.65382	1.25280	6.97038
H	1.07361	-0.52088	5.27269
H	-2.39227	0.84425	3.01344
H	-1.69423	4.91621	-5.42900
H	-2.53939	4.90295	-3.06294
H	-1.50490	3.41669	-1.36783
H	1.24416	1.90677	-4.39182
H	-5.52951	-0.27132	-1.78354
H	-4.18647	-2.00133	-0.54195
H	-4.39748	1.22155	-3.45393
H	-1.74969	-2.24726	-1.00203
H	-5.03655	-4.33256	1.86015
H	-5.01483	-2.62091	3.69287
H	-2.98431	-4.67993	0.45216
H	-0.94573	-3.30093	0.85216
H	-2.97370	-1.25753	4.11408
H	1.99604	3.76654	5.11609
H	0.34467	2.60207	3.65621
H	1.59863	-1.30592	-8.13114
H	-0.78565	-1.67598	-7.45656
H	3.30808	-0.67569	-6.40733
H	2.62501	-0.39215	-4.01320
H	2.81276	3.44756	0.17697
H	-2.09156	0.70447	-0.00571
H	-5.13451	3.28110	1.69862
H	-1.46897	-1.41608	-5.06372
H	-4.48527	1.22015	0.40397
H	-1.95262	1.01103	-3.87378
C	-1.71890	3.61764	1.79219
H	-3.35295	4.82500	2.55289
H	-0.94207	4.29446	2.17582

## 32

ZPE(BP86/def2-SVP) = 0.8059660 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0150266 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.02459250619 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.66445	0.89044	-1.69227
Au	0.23233	-0.29073	0.60032
C	-1.69632	-1.70591	3.16153
P	-0.27871	-0.59321	2.88948
P	-0.09547	-1.13878	-2.51789
C	-2.29553	-1.77528	4.43929
C	-3.38607	-2.63059	4.65007
P	0.50846	2.06220	0.29016
C	-3.88950	-3.40561	3.58966
C	-3.30460	-3.32220	2.31579
C	-2.20907	-2.47362	2.09590
C	-0.71376	0.94198	3.77792
C	-0.00334	1.39139	4.90788
C	-0.36841	2.60232	5.51992
C	-1.42379	3.36941	5.00013
C	-2.13866	2.91447	3.87635
C	-1.79102	1.70042	3.27194
C	1.18700	-1.26219	3.73644
C	1.13843	-2.40680	4.55587
C	2.31831	-2.88223	5.15158
C	3.53711	-2.21817	4.93565
C	3.58319	-1.07553	4.11666
C	2.41457	-0.59943	3.50869
C	-1.91604	-1.13361	-2.23417
C	-2.57673	-2.28061	-1.74818
C	-3.95278	-2.23430	-1.47465
C	-4.67835	-1.04949	-1.68526
C	-4.02491	0.09172	-2.18057
C	0.47338	-2.52807	-1.45784
C	0.74058	-3.81251	-1.97249
C	1.12077	-4.84679	-1.10215
C	1.22809	-4.59517	0.27464
C	0.94611	-3.31505	0.78538
C	0.55920	-2.26199	-0.06460
C	0.13581	-1.70181	-4.24056
C	1.44727	-1.99415	-4.67517
C	1.67938	-2.36925	-6.00513
C	0.60871	-2.43368	-6.91630
C	-0.69462	-2.13271	-6.48850
C	-0.93495	-1.77129	-5.15205
C	1.80147	2.13518	-3.46533
C	1.93696	1.31183	-4.61455
C	0.85547	1.12220	-5.47681
C	-0.38700	1.73525	-5.20364
C	-0.53960	2.56028	-4.08556
C	0.55566	2.78585	-3.20774
C	1.85366	2.59177	1.38843
C	3.16677	2.20925	1.02652
C	4.22797	2.40371	1.92195
C	3.98847	2.97902	3.18305
C	2.68462	3.35953	3.54502

C	1.61639	3.16775	2.65701
C	-0.91191	3.17585	0.45676
C	-1.94952	5.32505	0.94474
C	-3.20852	4.79887	0.60938
C	-3.31862	3.46361	0.17730
C	-2.17783	2.65620	0.09663
C	-2.64822	0.05247	-2.44940
H	1.53072	-5.40141	0.96039
H	1.03791	-3.14550	1.86894
H	2.69245	2.40628	-2.87883
H	0.65480	-4.00537	-3.05210
H	1.33354	-5.84926	-1.50246
H	4.82116	3.13139	3.88565
H	2.28331	-3.77832	5.78877
H	4.45801	-2.59573	5.40437
H	4.53593	-0.55456	3.94158
H	2.45567	0.28686	2.85660
H	0.18416	-2.92836	4.72121
H	5.24742	2.10618	1.63457
H	-2.96522	3.50992	3.46189
H	0.96430	0.47945	-6.36172
H	-1.69564	4.32392	5.47475
H	0.18294	2.95076	6.40599
H	0.83740	0.80337	5.30273
H	-2.35228	1.34362	2.39637
H	-1.23541	1.57041	-5.88390
H	-1.49260	3.07606	-3.89665
H	0.48952	3.57950	-2.45021
H	2.90440	0.83431	-4.82526
H	-5.75583	-1.01699	-1.46503
H	-4.46392	-3.13201	-1.09578
H	-4.58865	1.02078	-2.35439
H	-2.00929	-3.20665	-1.57434
H	-4.74846	-4.07217	3.75838
H	-3.85106	-2.68777	5.64543
H	-3.70381	-3.91968	1.48317
H	-1.75171	-2.40213	1.09835
H	-1.91429	-1.15207	5.26262
H	2.49181	3.80066	4.53408
H	0.59650	3.44057	2.96118
H	0.79280	-2.72147	-7.96206
H	-1.53385	-2.18537	-7.19811
H	2.70115	-2.60719	-6.33681
H	2.28725	-1.92451	-3.96648
H	3.33857	1.74104	0.04400
H	-2.25859	1.61007	-0.24048
H	-4.10550	5.43238	0.67654
H	-1.95702	-1.54148	-4.81696
H	-4.30087	3.04824	-0.09367
H	-2.12407	0.94627	-2.81643
C	-0.80091	4.52174	0.86531
H	-1.85886	6.37270	1.26841
H	0.18166	4.94421	1.12098

### 33

ZPE(BP86/def2-SVP) = 1.2451918 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -5322.3798317 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -5320.80944253395 Hartree (single point)

Cartesian coordinates in Å:

Au	-0.06675	-0.00222	0.97770
Pt	-3.00270	2.11792	0.60324
Pt	-1.07574	1.63133	-1.15763
P	1.87083	-0.87865	0.03626
P	-4.43037	3.12995	1.99926
P	-0.30278	3.68635	-1.80783
P	-1.47097	1.39243	2.23755
P	-2.58370	0.01985	-1.72457
C	2.65017	-2.13363	1.10944
C	1.79791	-2.96361	1.86896
C	2.34170	-3.97031	2.68009
C	3.73503	-4.14300	2.74629
C	4.58537	-3.30663	2.00297
C	4.04756	-2.30151	1.18394
C	1.78013	-1.61872	-1.62978
C	2.33907	-2.87818	-1.92761
C	2.24787	-3.38625	-3.23418
C	1.61597	-2.63719	-4.24057
C	1.05689	-1.38300	-3.94138
C	1.12205	-0.88166	-2.63675
C	3.05360	0.51069	-0.12788
C	4.12888	0.44763	-1.03917
C	5.00350	1.53870	-1.16334
C	4.80523	2.69446	-0.38768
C	3.73487	2.75890	0.52042
C	2.85909	1.67178	0.65262
C	-4.46891	4.91396	1.55246
C	-3.93951	5.32656	0.31134
C	-3.93624	6.68455	-0.04019
C	-4.45774	7.63946	0.84874
C	-4.97820	7.23490	2.09083
C	-4.98072	5.87750	2.44829
C	-6.13636	2.47022	1.92187
C	-7.27681	3.29097	2.00136
C	-8.55467	2.71656	1.90871
C	-8.69560	1.32822	1.74636
C	-7.55551	0.50885	1.67517
C	-6.27744	1.07735	1.75438
C	-4.04702	3.18178	3.78713
C	-4.86296	2.54354	4.73939
C	-4.55293	2.65150	6.10463
C	-3.43058	3.38472	6.52043
C	-2.60481	4.00731	5.56694
C	-2.91235	3.91017	4.20420
C	0.78263	3.19498	-3.21047
C	1.93842	2.43044	-2.93571
C	2.69884	1.90135	-3.98747
C	2.30723	2.11325	-5.31976
C	1.15815	2.87235	-5.59709
C	0.39779	3.41586	-4.54980
C	0.58950	4.99331	-0.87021

C	1.96946	5.23320	-1.00219
C	2.56806	6.29322	-0.29894
C	1.79456	7.12409	0.52691
C	0.41532	6.88027	0.66739
C	-0.18254	5.81419	-0.01700
C	-1.62826	4.68303	-2.61336
C	-1.40538	6.02936	-2.97806
C	-2.41209	6.75189	-3.63640
C	-3.64574	6.14235	-3.93142
C	-3.86568	4.80180	-3.57755
C	-2.85715	4.07415	-2.92727
C	-0.13504	2.38141	3.01026
C	0.11269	3.67540	2.51397
C	1.24041	4.39572	2.93775
C	2.12748	3.83242	3.86930
C	1.89051	2.53716	4.36481
C	0.77342	1.80948	3.93149
C	-2.29755	0.42116	3.54634
C	-2.11945	0.62472	4.92725
C	-2.84459	-0.14697	5.84941
C	-3.75663	-1.11761	5.40639
C	-3.93433	-1.32513	4.02626
C	-3.20388	-0.56841	3.10267
C	-2.86900	-1.49383	-0.74047
C	-1.77869	-2.35146	-0.47325
C	-1.95124	-3.46353	0.36347
C	-3.20695	-3.72592	0.94014
C	-4.29521	-2.88261	0.66204
C	-4.12937	-1.76476	-0.17279
C	-2.24901	-0.54526	-3.43875
C	-2.38343	-1.88588	-3.84528
C	-2.15819	-2.23623	-5.18765
C	-1.80897	-1.25307	-6.12758
C	-1.66924	0.08722	-5.72130
C	-1.87916	0.43978	-4.38198
C	-4.19281	0.88466	-1.84004
C	-5.12167	0.55931	-2.84949
C	-6.29242	1.31824	-2.98841
C	-6.50677	2.40849	-2.12849
C	-5.57515	2.72271	-1.12565
C	-4.39793	1.96562	-0.93229
H	-1.26432	5.63871	0.08592
H	-0.20035	7.52441	1.31294
H	2.26390	7.96410	1.06042
H	3.64593	6.48181	-0.41618
H	2.57710	4.61027	-1.67309
H	-0.50386	4.00409	-4.77226
H	0.85034	3.04694	-6.63917
H	2.89743	1.68395	-6.14295
H	3.59145	1.30240	-3.75895
H	2.22516	2.22246	-1.89528
H	-3.02717	3.03084	-2.63283
H	-0.44555	6.51358	-2.74690
H	-2.23269	7.80010	-3.91943
H	-4.43533	6.71706	-4.43848
H	-4.82659	4.31210	-3.79198
H	-5.78717	3.59174	-0.48827
H	2.00943	1.73448	1.34931
H	3.56117	3.66146	1.12288
H	5.48669	3.55131	-0.49783
H	5.83913	1.49097	-1.87745
H	4.26318	-0.44485	-1.66944

H	4.71551	-1.64085	0.61163
H	5.67639	-3.43433	2.06457
H	4.16159	-4.92745	3.38913
H	1.67567	-4.61466	3.27304
H	0.70843	-2.80156	1.83126
H	-7.17009	4.37986	2.11314
H	-9.44611	3.35947	1.95901
H	-9.69897	0.88338	1.66932
H	-7.66377	-0.57804	1.54291
H	-5.37561	0.45366	1.66854
H	-3.32208	-0.74500	2.02329
H	-4.63770	-2.09052	3.66526
H	-4.32548	-1.71550	6.13407
H	-2.70327	0.02574	6.92684
H	-1.43839	1.40690	5.28788
H	-2.27505	4.41011	3.46145
H	-5.73903	1.96408	4.41627
H	-5.19381	2.15318	6.84664
H	-3.19307	3.46754	7.59157
H	-1.71717	4.57427	5.88441
H	-3.51980	4.57394	-0.37318
H	-3.51942	6.98724	-1.01209
H	-4.45446	8.70570	0.57659
H	-5.37797	7.98300	2.79170
H	-5.36096	5.56920	3.43386
H	-1.74688	1.48218	-4.05350
H	-1.38272	0.86156	-6.44822
H	-1.63917	-1.53121	-7.17850
H	-2.26227	-3.28607	-5.50002
H	-2.66524	-2.65755	-3.11416
H	0.64871	0.08660	-2.39150
H	0.55239	-0.79637	-4.72011
H	1.54817	-3.03595	-5.26369
H	2.67823	-4.37210	-3.46566
H	2.84417	-3.45754	-1.14073
H	-0.80142	-2.15752	-0.94092
H	-1.10013	-4.13223	0.56156
H	-3.33791	-4.59440	1.60242
H	-5.28214	-3.09328	1.10092
H	-4.97431	-1.09280	-0.38494
H	-7.41175	3.02611	-2.23758
H	-7.02400	1.06963	-3.77157
H	-4.91632	-0.27600	-3.53646
H	-0.57484	4.10096	1.76830
H	1.42566	5.39785	2.52722
H	3.01086	4.39738	4.20277
H	2.59198	2.08289	5.08075
H	0.62116	0.77807	4.28243

## 34

ZPE(BP86/def2-SVP) = 1.2445309 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -5322.3551336 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -5320.78473814401 Hartree (single point)

Cartesian coordinates in Å:

Pt	-0.98201	2.05998	-1.39597
P	1.15754	-0.62334	0.03866
P	-4.24524	3.07666	2.35478
P	-0.45578	3.92141	-2.45338
P	-1.42615	0.63805	2.35593
P	-2.20892	-0.01706	-1.92722
C	1.73317	-1.35956	1.61489
C	0.84330	-2.21990	2.29537
C	1.17178	-2.71112	3.56556
C	2.38984	-2.34219	4.16645
C	3.27896	-1.49175	3.48862
C	2.95429	-0.99714	2.21409
C	1.51225	-1.80955	-1.29860
C	1.78589	-3.16881	-1.05354
C	1.86400	-4.06554	-2.13284
C	1.67404	-3.60894	-3.44811
C	1.41831	-2.24711	-3.69220
C	1.33375	-1.34836	-2.62213
C	2.27285	0.78927	-0.28975
C	3.48824	0.62413	-0.98545
C	4.32962	1.73118	-1.19006
C	3.97016	2.99512	-0.68995
C	2.76469	3.15724	0.01253
C	1.91087	2.06176	0.19685
C	-3.96160	4.78374	1.77343
C	-3.62179	4.97916	0.41551
C	-3.43876	6.27877	-0.08091
C	-3.57525	7.38360	0.77478
C	-3.90291	7.19288	2.12931
C	-4.10033	5.89760	2.63155
C	-6.04604	2.77043	2.35394
C	-6.98828	3.81449	2.43432
C	-8.35964	3.51558	2.41323
C	-8.79167	2.18152	2.32069
C	-7.85160	1.13957	2.24128
C	-6.48029	1.43101	2.24829
C	-3.75354	3.01852	4.11626
C	-4.47667	2.22634	5.03297
C	-4.03405	2.10631	6.35900
C	-2.86504	2.76166	6.77956
C	-2.13799	3.54498	5.86652
C	-2.58033	3.67817	4.54301
C	0.63564	3.56795	-3.88760
C	1.73304	2.70715	-3.65294
C	2.55874	2.31666	-4.71382
C	2.28745	2.76517	-6.02059
C	1.19109	3.60993	-6.25781
C	0.36443	4.01501	-5.19395
C	0.48683	5.14601	-1.45532
C	1.68976	5.73126	-1.89356
C	2.35178	6.66680	-1.07975

C	1.80831	7.03475	0.16229
C	0.59993	6.45758	0.59609
C	-0.04853	5.50417	-0.20026
C	-1.84746	4.93172	-3.09561
C	-1.67665	6.29236	-3.43032
C	-2.77420	7.04603	-3.87452
C	-4.04316	6.44786	-3.98062
C	-4.21317	5.09366	-3.64754
C	-3.11893	4.33423	-3.20478
C	-0.16212	1.70464	3.08936
C	-0.07202	3.04566	2.65589
C	0.98311	3.85560	3.09507
C	1.96272	3.32976	3.95570
C	1.88778	1.98912	4.37018
C	0.83085	1.17339	3.94030
C	-2.01059	-0.52671	3.60902
C	-1.97743	-0.24313	4.99007
C	-2.49365	-1.17571	5.90215
C	-3.05062	-2.38273	5.44543
C	-3.09899	-2.65829	4.06584
C	-2.58062	-1.73618	3.14837
C	-2.72925	-1.65169	-1.17374
C	-1.78220	-2.70737	-1.11366
C	-2.06969	-3.88048	-0.39956
C	-3.30223	-4.02039	0.26141
C	-4.25043	-2.98390	0.19603
C	-3.96776	-1.80378	-0.50930
C	-1.72822	-0.48020	-3.63712
C	-2.13716	-1.69652	-4.22184
C	-1.77358	-1.99153	-5.54557
C	-1.00885	-1.07861	-6.29235
C	-0.60865	0.13892	-5.71392
C	-0.96816	0.43454	-4.39212
C	-3.79921	0.89229	-2.03210
C	-4.51835	0.92165	-3.24247
C	-5.71533	1.65153	-3.32510
C	-6.18144	2.34376	-2.19769
C	-5.45488	2.30763	-0.99256
C	-4.24975	1.58670	-0.87452
H	-0.98370	5.03605	0.14056
H	0.15583	6.75840	1.55732
H	2.32353	7.77581	0.79161
H	3.29538	7.11709	-1.42311
H	2.11400	5.44792	-2.86793
H	-0.49866	4.67030	-5.38311
H	0.97319	3.95744	-7.27894
H	2.92996	2.44943	-6.85630
H	3.41093	1.64809	-4.52022
H	1.91743	2.33064	-2.63575
H	-3.24151	3.27854	-2.91976
H	-0.68821	6.76505	-3.32628
H	-2.64083	8.10755	-4.13217
H	-4.90375	7.04407	-4.31951
H	-5.20253	4.62009	-3.71945
H	-5.85304	2.86337	-0.13168
H	0.95786	2.18672	0.72470
H	2.47546	4.14183	0.40463
H	4.62998	3.85998	-0.85392
H	5.27328	1.60324	-1.74121
H	3.77207	-0.36501	-1.37419
H	3.63826	-0.30911	1.69624
H	4.22967	-1.19971	3.95940

H	2.64307	-2.71574	5.16998
H	0.46486	-3.36652	4.09541
H	-0.12484	-2.47250	1.83552
H	-6.65064	4.85951	2.49785
H	-9.09601	4.33120	2.46770
H	-9.86772	1.95306	2.30205
H	-8.18896	0.09581	2.15789
H	-5.73650	0.62427	2.14813
H	-2.61148	-1.94510	2.06697
H	-3.53799	-3.59941	3.70224
H	-3.45171	-3.11074	6.16645
H	-2.46641	-0.95347	6.97943
H	-1.56142	0.70934	5.34791
H	-2.01356	4.30534	3.84316
H	-5.39146	1.70724	4.71289
H	-4.60958	1.49232	7.06730
H	-2.52045	2.66415	7.81980
H	-1.21907	4.06017	6.18326
H	-3.48773	4.11528	-0.25359
H	-3.17365	6.42098	-1.13786
H	-3.42141	8.40089	0.38496
H	-4.00857	8.05904	2.79968
H	-4.35406	5.74963	3.69204
H	-0.65597	1.37568	-3.91548
H	-0.01014	0.86486	-6.28364
H	-0.72590	-1.31733	-7.32877
H	-2.09282	-2.94294	-5.99686
H	-2.73887	-2.41405	-3.64650
H	1.10367	-0.28794	-2.80612
H	1.26039	-1.88258	-4.71745
H	1.72587	-4.31729	-4.28828
H	2.07460	-5.12883	-1.94345
H	1.92585	-3.52503	-0.02208
H	-0.82708	-2.61585	-1.64760
H	-1.32315	-4.68806	-0.36745
H	-3.52835	-4.94133	0.81953
H	-5.22092	-3.09265	0.70321
H	-4.70524	-0.98955	-0.54393
H	-7.11755	2.92095	-2.24982
H	-6.27797	1.67790	-4.27028
H	-4.13733	0.38334	-4.12291
H	-0.81930	3.43301	1.94438
H	1.05368	4.89512	2.74603
H	2.79614	3.96435	4.29179
H	2.66499	1.56787	5.02496
H	0.79021	0.11736	4.24525
Au	-3.11977	1.52895	0.91245
Pt	-1.04135	-0.03049	0.22408

## TS-2a/15

Imaginary frequency: 168.91 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8039719 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9989388 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.01565280857 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.44278	0.62951	1.31573
Au	0.75260	0.98951	-1.48024
C	1.70409	-2.02259	-2.82499
P	0.80174	-0.50059	-3.27145
P	-0.08585	-1.47901	2.03278
C	1.17519	-2.82327	-1.78924
C	1.86750	-3.96581	-1.37029
P	0.67866	2.67210	0.30531
C	3.09242	-4.30797	-1.96943
C	3.62182	-3.50682	-2.99461
C	2.93151	-2.36239	-3.42745
C	1.61333	0.15995	-4.76628
C	1.36795	-0.41104	-6.03262
C	2.03887	0.08441	-7.16016
C	2.95223	1.14533	-7.02938
C	3.19362	1.71772	-5.76932
C	2.52263	1.22975	-4.63784
C	-0.87102	-1.02249	-3.78472
C	-1.13645	-2.33513	-4.22315
C	-2.42741	-2.67578	-4.65702
C	-3.45153	-1.71386	-4.65291
C	-3.18803	-0.40547	-4.20853
C	-1.90157	-0.05878	-3.77092
C	1.37177	-2.54374	2.33173
C	2.49136	-2.37787	1.48965
C	3.60812	-3.21238	1.63914
C	3.61572	-4.20561	2.63371
C	2.50716	-4.36116	3.48408
C	-1.09966	-2.41725	0.82398
C	-1.06476	-3.82511	0.75610
C	-1.80573	-4.49667	-0.23011
C	-2.58345	-3.76903	-1.14670
C	-2.62859	-2.36648	-1.07532
C	-1.88669	-1.69153	-0.09640
C	-1.03440	-1.47367	3.59778
C	-0.63230	-0.55881	4.59560
C	-1.31257	-0.52012	5.82006
C	-2.40104	-1.38062	6.04988
C	-2.80862	-2.28227	5.05292
C	-2.12796	-2.33234	3.82510
C	0.60115	2.39608	2.47227
C	-0.57614	2.83422	3.12030
C	-0.50927	3.31454	4.43719
C	0.72313	3.37327	5.11022
C	1.89994	2.96202	4.45786
C	1.84918	2.49354	3.13784
C	-0.82722	3.64094	0.00515
C	-2.06168	2.95526	0.08181
C	-3.25745	3.63344	-0.18775

C	-3.23105	4.99337	-0.54578
C	-2.00365	5.66984	-0.63812
C	-0.79998	5.00021	-0.36548
C	2.14379	3.74452	0.27217
C	3.37423	5.69113	1.06088
C	4.46219	5.33273	0.24448
C	4.39655	4.17701	-0.55064
C	3.23838	3.38455	-0.54060
C	1.38410	-3.53113	3.33783
H	-3.15179	-4.29564	-1.92729
H	-3.22387	-1.79558	-1.80163
H	-1.88079	-0.59072	-0.05434
H	-0.44007	-4.39425	1.46098
H	-1.76814	-5.59478	-0.28767
H	-4.17023	5.52568	-0.75721
H	-2.63381	-3.70029	-5.00074
H	-4.46190	-1.98510	-4.99346
H	-3.99029	0.34713	-4.19899
H	-1.69262	0.96132	-3.41056
H	-0.33805	-3.09165	-4.21353
H	-4.21609	3.09789	-0.11879
H	3.90117	2.55391	-5.66817
H	-1.43143	3.64246	4.94006
H	3.47346	1.53285	-7.91737
H	1.84475	-0.35782	-8.14856
H	0.64763	-1.23631	-6.13714
H	2.69360	1.68228	-3.64815
H	0.76975	3.75130	6.14234
H	2.86821	3.01305	4.97820
H	2.77290	2.19346	2.62182
H	-1.54311	2.79196	2.60000
H	4.49529	-4.85548	2.75534
H	4.47769	-3.08346	0.97785
H	2.51891	-5.13029	4.27074
H	2.47639	-1.59014	0.71970
H	3.63752	-5.20243	-1.63318
H	1.45140	-4.58241	-0.56114
H	4.57914	-3.77445	-3.46618
H	3.34516	-1.73717	-4.23234
H	0.22472	-2.54978	-1.31128
H	-1.97952	6.73120	-0.92672
H	0.15737	5.53362	-0.45165
H	-2.93896	-1.34300	7.00900
H	-3.66492	-2.95028	5.22930
H	-0.99705	0.19391	6.59513
H	0.20462	0.13009	4.40095
H	-2.06596	1.88667	0.35496
H	3.17660	2.47275	-1.15641
H	5.36882	5.95593	0.23431
H	-2.45293	-3.03322	3.04182
H	5.25062	3.89032	-1.18184
H	0.51962	-3.64247	4.01003
C	2.21985	4.89691	1.08678
H	3.43100	6.59038	1.69201
H	1.38243	5.15977	1.74957

## TS-2a/20

Imaginary frequency: 291.27 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8003731 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9977810 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.99969856223 Hartree (single point)

Cartesian coordinates in Å:

Pt	-0.57260	0.72273	-1.57173
Au	0.63378	-0.72323	0.80730
C	-2.53778	-0.93006	2.17276
P	-0.77326	-1.14525	2.57511
P	-0.17211	-1.39459	-2.45699
C	-3.50571	-0.78060	3.19030
C	-4.86301	-0.68750	2.85009
P	-0.41189	2.74946	-0.50120
C	-5.25859	-0.74233	1.50093
C	-4.29371	-0.88283	0.49040
C	-2.93439	-0.97418	0.82316
C	-0.45003	-0.08859	4.02851
C	0.47385	-0.48958	5.01447
C	0.81725	0.39526	6.04858
C	0.24413	1.67737	6.10165
C	-0.68110	2.07345	5.12111
C	-1.02929	1.19804	4.08256
C	-0.56395	-2.88389	3.10776
C	-1.64745	-3.65381	3.57400
C	-1.44661	-4.99625	3.93073
C	-0.16925	-5.57310	3.82806
C	0.91352	-4.80597	3.36390
C	0.71699	-3.46646	2.99668
C	-1.05506	-2.76874	-1.62792
C	-0.45024	-3.52643	-0.60399
C	-1.21894	-4.43120	0.14678
C	-2.58561	-4.59176	-0.12762
C	-3.18482	-3.86038	-1.16889
C	1.61224	-1.57291	-2.01150
C	2.55549	-2.25091	-2.79501
C	3.92189	-2.15430	-2.46630
C	4.33964	-1.36953	-1.37785
C	3.39487	-0.69324	-0.58423
C	2.01926	-0.81129	-0.87372
C	-0.29576	-1.73334	-4.24291
C	-0.25713	-0.63796	-5.13046
C	-0.29239	-0.85930	-6.51511
C	-0.37133	-2.17051	-7.01501
C	-0.41747	-3.26297	-6.13140
C	-0.38045	-3.04941	-4.74498
C	-0.36220	4.19954	-1.61996
C	0.10260	3.98021	-2.93515
C	0.21944	5.05620	-3.82789
C	-0.14451	6.35002	-3.41878
C	-0.62584	6.56672	-2.11621
C	-0.73350	5.49692	-1.21450
C	1.20536	2.75594	0.37675
C	2.38374	3.12076	-0.30300
C	3.63256	2.93784	0.31216

C	3.71609	2.38361	1.60189
C	2.54238	2.01879	2.28289
C	1.29167	2.20211	1.67211
C	-1.63636	3.10829	0.80970
C	-2.35830	4.29584	2.81138
C	-3.57829	3.59619	2.78678
C	-3.82903	2.65471	1.77477
C	-2.86280	2.41492	0.78591
C	-2.42626	-2.94703	-1.91422
H	5.41241	-1.27681	-1.14995
H	3.72358	-0.07124	0.26151
H	0.97790	0.28556	-0.95145
H	2.23639	-2.82415	-3.67890
H	4.66760	-2.67533	-3.08526
H	4.69776	2.24420	2.07896
H	-2.29623	-5.59769	4.28663
H	-0.01787	-6.62718	4.10434
H	1.91305	-5.25659	3.27452
H	1.55326	-2.87094	2.59556
H	-2.65306	-3.21422	3.63657
H	4.54856	3.23099	-0.22198
H	-1.13855	3.07246	5.15850
H	0.58536	4.88205	-4.85074
H	0.51531	2.36784	6.91396
H	1.53387	0.07822	6.82074
H	0.92050	-1.49435	4.97707
H	-1.75384	1.51568	3.31832
H	-0.06225	7.19284	-4.12118
H	-0.92284	7.57763	-1.79949
H	-1.11949	5.67365	-0.20034
H	0.35907	2.95388	-3.24702
H	-3.18643	-5.29446	0.46819
H	-0.74376	-5.01016	0.95163
H	-4.25340	-3.99479	-1.39326
H	0.62209	-3.40923	-0.39087
H	-6.32485	-0.66997	1.23889
H	-5.61708	-0.56982	3.64245
H	-4.59546	-0.91774	-0.56664
H	-2.17277	-1.05671	0.03305
H	-3.19771	-0.72715	4.24529
H	2.58743	1.59196	3.29602
H	0.38058	1.93602	2.22333
H	-0.40405	-2.34267	-8.10123
H	-0.48597	-4.28810	-6.52504
H	-0.26533	-0.00517	-7.20790
H	-0.20626	0.38411	-4.72135
H	2.32625	3.54831	-1.31518
H	-3.04717	1.67436	-0.00616
H	-4.33530	3.78523	3.56244
H	-0.42667	-3.90229	-4.05079
H	-4.77593	2.09719	1.75496
H	-2.90118	-2.35738	-2.71435
C	-1.38365	4.04854	1.83299
H	-2.16361	5.03832	3.59986
H	-0.41773	4.57373	1.87492

## TS-2a/2b

Imaginary frequency: 62.38 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8049561 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0082847 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.02538316941 Hartree (single point)

Cartesian coordinates in Å:

Pt	-0.18010	0.77812	0.19148
Au	-2.68872	-0.12966	0.13353
C	-2.17525	2.84818	2.27573
P	-1.97784	2.38790	0.52632
P	0.71900	-1.25009	0.48722
C	-1.34486	2.22301	3.23283
C	-1.48785	2.53125	4.59235
P	-4.28235	-1.72000	-0.33657
C	-2.46696	3.45216	5.00596
C	-3.29631	4.06987	4.05500
C	-3.15421	3.77418	2.68995
C	-0.37599	3.10016	-0.06775
C	0.59298	3.65006	0.81880
C	1.81065	4.12916	0.31624
C	2.09418	4.06168	-1.05967
C	1.15809	3.49852	-1.94289
C	-0.06741	3.01083	-1.46200
C	-3.28184	3.27357	-0.39998
C	-3.03737	4.52031	-1.01096
C	-4.08466	5.19718	-1.65586
C	-5.37579	4.64332	-1.68142
C	-5.62259	3.40599	-1.06165
C	-4.57886	2.71686	-0.42930
C	2.55006	-1.34342	0.40043
C	3.28589	-0.21391	0.81359
C	4.68781	-0.25043	0.80950
C	5.36019	-1.40791	0.38039
C	4.62900	-2.52885	-0.04776
C	0.30170	-2.00833	2.11330
C	0.96277	-3.17153	2.56071
C	0.64319	-3.72537	3.80931
C	-0.32374	-3.11520	4.62851
C	-0.98152	-1.95468	4.18916
C	-0.67298	-1.40805	2.93381
C	0.15289	-2.46725	-0.76610
C	-0.67552	-3.55692	-0.43930
C	-1.08823	-4.44764	-1.44502
C	-0.67091	-4.26132	-2.77096
C	0.15102	-3.16785	-3.10034
C	0.55157	-2.26481	-2.10647
C	-3.98413	-3.28670	0.55439
C	-3.38729	-3.22882	1.83021
C	-3.10107	-4.41134	2.52682
C	-3.41030	-5.65573	1.95160
C	-4.01339	-5.71492	0.68305
C	-4.30013	-4.53421	-0.01950
C	-5.99108	-1.21188	0.06598
C	-6.66643	-1.73433	1.18608
C	-7.95175	-1.26680	1.50584

C	-8.56640	-0.28662	0.71050
C	-7.89385	0.23084	-0.41140
C	-6.60667	-0.22150	-0.73217
C	-4.29173	-2.11240	-2.11733
C	-5.40542	-2.95342	-4.11154
C	-4.22614	-2.75139	-4.85039
C	-3.08182	-2.23206	-4.22352
C	-3.10916	-1.91303	-2.85816
C	3.22545	-2.50083	-0.03938
H	-0.55711	-3.54282	5.61534
H	-1.73652	-1.46810	4.82501
H	-1.18594	-0.50381	2.57295
H	1.73905	-3.64093	1.93868
H	1.16330	-4.63229	4.15195
H	-9.57583	0.07207	0.96042
H	-3.89102	6.16808	-2.13568
H	-6.19351	5.17934	-2.18579
H	-6.63270	2.97105	-1.07029
H	-4.77005	1.74387	0.05204
H	-2.03089	4.96258	-0.98003
H	-8.47832	-1.67848	2.37963
H	1.37939	3.43430	-3.01836
H	-2.61462	-4.35531	3.51111
H	3.05220	4.44204	-1.44321
H	2.54528	4.56443	1.00980
H	0.37019	3.71774	1.89301
H	-0.81155	2.60009	-2.16152
H	-3.17601	-6.58491	2.49203
H	-4.25503	-6.68906	0.23225
H	-4.74823	-4.58421	-1.02252
H	-3.11700	-2.25496	2.26394
H	6.46011	-1.43293	0.36947
H	5.25966	0.63225	1.13258
H	5.15487	-3.43055	-0.39577
H	2.74469	0.69601	1.12162
H	-2.58319	3.68968	6.07386
H	-0.83312	2.04719	5.33230
H	-4.06108	4.79233	4.37675
H	-3.80454	4.26063	1.94864
H	-0.58219	1.50292	2.89265
H	-8.38149	0.98658	-1.04560
H	-6.08239	0.18301	-1.61179
H	-0.99161	-4.96456	-3.55347
H	0.48134	-3.01775	-4.13924
H	-1.73653	-5.29457	-1.17992
H	-0.99823	-3.71531	0.59868
H	-6.19053	-2.51006	1.80399
H	-2.21115	-1.51074	-2.36242
H	-4.20314	-2.99534	-5.92304
H	1.18879	-1.40398	-2.36262
H	-2.15874	-2.07145	-4.79877
H	2.65557	-3.37396	-0.39186
C	-5.44393	-2.63251	-2.74668
H	-6.30306	-3.35716	-4.60305
H	-6.37188	-2.77363	-2.17230

## TS-2a/2c

Imaginary frequency: 68.60 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8051994 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9988024 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.99635714085 Hartree (single point)

Cartesian coordinates in Å:

C	-2.62223	1.65372	-1.31496
P	-1.74098	0.06912	-1.57537
P	2.45911	-0.95269	-0.71940
C	-1.82190	2.80276	-1.12784
C	-2.42134	4.05658	-0.95014
P	-1.13920	0.37532	2.23379
C	-3.82260	4.17068	-0.94690
C	-4.61731	3.02668	-1.11646
C	-4.02292	1.76747	-1.30171
C	-3.00777	-1.24669	-1.73119
C	-3.88350	-1.28594	-2.83676
C	-4.83936	-2.30823	-2.93571
C	-4.91751	-3.30140	-1.94323
C	-4.03508	-3.27499	-0.84985
C	-3.08169	-2.25060	-0.74481
C	-1.12895	0.21477	-3.30835
C	-1.26867	1.39084	-4.07112
C	-0.80337	1.42865	-5.39587
C	-0.19383	0.30019	-5.96743
C	-0.05566	-0.87533	-5.20846
C	-0.51970	-0.91863	-3.88724
C	4.27016	-1.19576	-0.73530
C	5.14627	-0.14357	-1.07069
C	6.53354	-0.35991	-1.04676
C	7.04864	-1.61596	-0.68824
C	6.17374	-2.66423	-0.34852
C	2.18560	0.62557	-1.58937
C	2.02739	1.79443	-0.80997
C	1.85372	3.03339	-1.44217
C	1.83081	3.11256	-2.84576
C	1.99951	1.95141	-3.61758
C	2.18280	0.70709	-2.99635
C	1.80315	-2.35524	-1.68199
C	2.46477	-2.81726	-2.84094
C	1.88640	-3.83896	-3.60851
C	0.66891	-4.42295	-3.21041
C	0.02853	-3.99154	-2.03714
C	0.59765	-2.96232	-1.27138
C	-1.30814	-0.81469	3.62179
C	-0.55602	-2.00481	3.65097
C	-0.64377	-2.87641	4.74867
C	-1.49620	-2.56647	5.81975
C	-2.26573	-1.38907	5.78871
C	-2.18225	-0.51941	4.69227
C	-2.86407	0.98293	2.05888
C	-3.86353	0.02701	1.77419
C	-5.20556	0.41596	1.68398
C	-5.56159	1.76270	1.87291
C	-4.56771	2.71694	2.13874

C	-3.21975	2.33356	2.23144
C	4.78843	-2.45715	-0.36407
H	1.68693	4.08454	-3.34028
H	1.98703	2.00862	-4.71468
H	2.31043	-0.19566	-3.60796
H	2.03859	1.73090	0.28959
H	1.73815	3.94173	-0.83240
H	-6.61631	2.06870	1.80756
H	-0.92460	2.34925	-5.98646
H	0.16581	0.33316	-7.00678
H	0.41204	-1.76954	-5.64682
H	-0.42106	-1.84316	-3.30458
H	-1.74874	2.27850	-3.63722
H	-5.97725	-0.33789	1.46823
H	-4.08792	-4.05695	-0.07738
H	-0.05262	-3.80405	4.75999
H	-5.66526	-4.10415	-2.02787
H	-5.52372	-2.33470	-3.79681
H	-3.80923	-0.52102	-3.62466
H	-2.37092	-2.21309	0.09712
H	-1.57012	-3.24861	6.67987
H	-2.93632	-1.14664	6.62658
H	-2.79002	0.39751	4.66870
H	0.09382	-2.25277	2.79152
H	8.13614	-1.78063	-0.67131
H	7.21554	0.46082	-1.31438
H	6.57490	-3.64920	-0.06706
H	4.74527	0.83975	-1.35658
H	-4.29534	5.15397	-0.80565
H	-1.79289	4.94962	-0.81402
H	-5.71383	3.11047	-1.10139
H	-4.65110	0.87463	-1.42718
H	-0.72531	2.70557	-1.14597
H	-4.83981	3.77327	2.27965
H	-2.45053	3.08607	2.45360
H	0.22316	-5.22600	-3.81610
H	-0.92109	-4.44607	-1.71961
H	2.39030	-4.18512	-4.52317
H	3.42715	-2.37630	-3.14148
H	-3.59090	-1.02896	1.63878
H	0.09740	-2.60179	-0.35187
H	0.11995	0.97220	4.89606
H	1.55181	2.87354	5.65225
C	0.33749	1.80229	4.20854
C	1.14508	2.87123	4.62992
C	-0.18048	1.79020	2.89824
C	1.42936	3.93475	3.75736
H	2.06078	4.77029	4.09390
C	0.10914	2.85781	2.02003
C	0.90293	3.92871	2.45358
H	-0.29003	2.83660	0.99577
H	1.11616	4.76400	1.76930
H	4.10506	-3.27811	-0.09598
Pt	-0.36464	-0.27871	0.19433
Au	1.79827	-0.82575	1.61014

## TS-2b/11

Imaginary frequency: 202.99 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8036987 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9846743 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.99498393994 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.33067	-0.85827	-2.31549
Au	0.02613	-0.28861	0.46151
C	-0.93364	0.63494	3.76572
P	0.08096	1.18160	2.34898
P	0.10908	-2.69101	0.70376
C	-1.60647	1.54713	4.60404
C	-2.37273	1.06821	5.67909
P	-0.00199	1.20265	-1.59060
C	-2.46554	-0.31242	5.92438
C	-1.78850	-1.22239	5.09341
C	-1.02979	-0.75096	4.01421
C	-0.30122	2.94904	2.09833
C	0.61681	3.97123	2.41025
C	0.29252	5.30833	2.12921
C	-0.93876	5.62969	1.53357
C	-1.86223	4.61101	1.23554
C	-1.54581	3.27578	1.51828
C	1.81905	1.11286	2.91251
C	2.17151	0.76219	4.23042
C	3.52711	0.62836	4.57597
C	4.52862	0.84863	3.61537
C	4.17572	1.20554	2.30124
C	2.82684	1.33077	1.94583
C	1.69643	-3.30324	1.35207
C	2.18551	-4.57963	0.99984
C	3.40635	-5.02600	1.52811
C	4.13882	-4.20479	2.40409
C	3.65487	-2.93192	2.75058
C	-0.06754	-3.37611	-0.98917
C	-1.22544	-3.96842	-1.46685
C	-1.45380	-4.05439	-2.87734
C	-0.54765	-3.51818	-3.77803
C	0.68644	-2.93306	-3.32184
C	0.94745	-2.89578	-1.91004
C	-1.21849	-3.41236	1.72541
C	-2.51394	-2.86481	1.59013
C	-3.56135	-3.33285	2.39423
C	-3.31850	-4.33459	3.35097
C	-2.02782	-4.86946	3.49792
C	-0.97557	-4.41395	2.68611
C	0.02020	0.73664	-3.77200
C	1.12092	1.19820	-4.52626
C	0.94564	1.58664	-5.86390
C	-0.32557	1.52219	-6.45900
C	-1.42820	1.07377	-5.71048
C	-1.26235	0.69850	-4.37011
C	1.39453	2.33842	-1.40943
C	2.68957	1.81089	-1.62642
C	3.82066	2.59890	-1.37541

C	3.67198	3.90857	-0.88426
C	2.38751	4.42102	-0.63994
C	1.24720	3.64478	-0.89830
C	-1.58423	2.08322	-1.63137
C	-2.98506	3.94806	-2.31677
C	-4.09822	3.33288	-1.71603
C	-3.96013	2.08056	-1.09279
C	-2.70439	1.45713	-1.04688
C	2.43799	-2.47644	2.22230
H	-0.74680	-3.56313	-4.85866
H	1.50559	-2.77651	-4.03854
H	1.97741	-2.75066	-1.54021
H	-1.99826	-4.31587	-0.76502
H	-2.37708	-4.52751	-3.24261
H	4.55967	4.52589	-0.68228
H	3.80075	0.35308	5.60552
H	5.58836	0.74185	3.89133
H	4.95388	1.37942	1.54340
H	2.55384	1.59175	0.91253
H	1.38802	0.58630	4.98198
H	4.82410	2.18523	-1.55558
H	-2.83001	4.85270	0.77259
H	1.81019	1.94345	-6.44397
H	-1.18361	6.67808	1.30703
H	1.00981	6.10498	2.37730
H	1.58742	3.72125	2.86212
H	-2.26597	2.48159	1.27747
H	-0.45925	1.82965	-7.50696
H	-2.42668	1.02481	-6.17078
H	-2.13341	0.37621	-3.78025
H	2.11911	1.26289	-4.07098
H	5.09685	-4.55888	2.81321
H	3.78978	-6.02001	1.25358
H	4.22726	-2.27983	3.42626
H	1.61112	-5.21706	0.30960
H	-3.07087	-0.68083	6.76603
H	-2.90021	1.78062	6.33085
H	-1.86026	-2.30523	5.27199
H	-0.51395	-1.46249	3.35422
H	-1.53239	2.62811	4.41411
H	2.26445	5.43605	-0.23540
H	0.25061	4.04857	-0.67259
H	-4.13877	-4.69418	3.98981
H	-1.83629	-5.65014	4.24920
H	-4.56886	-2.90493	2.28609
H	-2.69031	-2.05592	0.86295
H	2.79419	0.76605	-1.96222
H	-2.57725	0.48085	-0.55122
H	-5.08139	3.82572	-1.74681
H	0.03584	-4.82971	2.80476
H	-4.83330	1.59036	-0.63723
H	2.06884	-1.47250	2.47881
C	-1.73163	3.32103	-2.29064
H	-3.09846	4.91747	-2.82429
H	-0.87171	3.78290	-2.79678

## TS-2b/28

Imaginary frequency: 345.80 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8014158 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9917493 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.99354795214 Hartree (single point)

Cartesian coordinates in Å:

Au	0.16609	-1.30849	-0.86915
Pt	1.55103	0.61577	0.77028
C	-0.30218	2.09232	3.26437
P	-0.15946	2.06041	1.43403
P	1.06501	0.02971	-2.58674
C	-1.14104	1.16461	3.92039
C	-1.12040	1.06601	5.31965
P	-0.33923	-2.64518	0.98418
C	-0.26574	1.88727	6.07388
C	0.56684	2.81442	5.42319
C	0.55299	2.91705	4.02332
C	-1.89141	1.82972	0.85871
C	-2.98748	2.34593	1.58509
C	-4.28512	2.25963	1.05790
C	-4.50250	1.66660	-0.19844
C	-3.41709	1.14484	-0.92029
C	-2.12187	1.22277	-0.38887
C	0.22427	3.79670	0.94929
C	1.55887	4.12609	0.63634
C	1.89060	5.43012	0.23810
C	0.89193	6.41380	0.14961
C	-0.43951	6.08956	0.46412
C	-0.77625	4.78604	0.85999
C	2.57624	0.90278	-2.06377
C	3.29653	1.64678	-3.02868
C	4.41846	2.39993	-2.66381
C	4.82600	2.42026	-1.31734
C	4.09476	1.72878	-0.34385
C	-0.05424	1.39829	-3.07928
C	0.07596	2.62917	-2.39973
C	-0.86278	3.64901	-2.60954
C	-1.93018	3.45149	-3.49987
C	-2.05160	2.23267	-4.18959
C	-1.12145	1.20272	-3.97880
C	1.39879	-1.02071	-4.04922
C	2.64127	-1.07590	-4.71197
C	2.81632	-1.94690	-5.79983
C	1.76072	-2.76362	-6.23443
C	0.52793	-2.73129	-5.56002
C	0.35175	-1.87784	-4.46238
C	-0.38789	-4.44100	0.67852
C	0.17845	-4.92883	-0.51800
C	0.21598	-6.31062	-0.76003
C	-0.32202	-7.20289	0.18214
C	-0.89785	-6.71573	1.36888
C	-0.93092	-5.33688	1.62258
C	-1.80234	-2.16353	1.95855
C	-2.89162	-1.56152	1.29806
C	-4.01992	-1.16105	2.02869

C	-4.06686	-1.36599	3.41763
C	-2.98645	-1.97757	4.07792
C	-1.85118	-2.37211	3.35476
C	2.92022	1.00699	-0.68484
H	-2.66824	4.25076	-3.66258
H	-2.87717	2.08101	-4.90098
H	-1.22456	0.25377	-4.52452
H	0.90261	2.78744	-1.69407
H	-0.75467	4.59748	-2.06402
H	-4.94997	-1.04651	3.99060
H	2.93382	5.67368	-0.01220
H	1.14935	7.43507	-0.16866
H	-1.22532	6.85661	0.39417
H	-1.82398	4.53768	1.07965
H	2.33039	3.34362	0.68389
H	-4.85863	-0.67803	1.50864
H	-3.57049	0.67608	-1.90315
H	0.65956	-6.69063	-1.69215
H	-5.52067	1.61043	-0.61208
H	-5.13271	2.66317	1.63188
H	-2.82900	2.81394	2.56762
H	-1.27516	0.80444	-0.94823
H	-0.29953	-8.28563	-0.01172
H	-1.32655	-7.41539	2.10156
H	-1.38808	-4.95890	2.54884
H	0.58159	-4.21836	-1.25840
H	5.71947	2.98984	-1.01959
H	4.97341	2.96580	-3.42575
H	4.41369	1.76117	0.70796
H	2.95254	1.65929	-4.07390
H	-0.25182	1.80934	7.17112
H	-1.78000	0.34188	5.82035
H	1.23110	3.46591	6.01049
H	1.20751	3.64180	3.51578
H	-1.81738	0.51974	3.34003
H	-3.02548	-2.14432	5.16467
H	-0.99374	-2.82037	3.87848
H	1.90334	-3.44048	-7.08982
H	-0.29562	-3.38723	-5.87906
H	3.79083	-1.98713	-6.30874
H	3.48196	-0.45659	-4.37242
H	-2.84763	-1.39291	0.21271
H	-0.59585	-1.89732	-3.90026
H	2.20730	-4.10952	1.50776
H	4.24865	-3.45207	2.79529
C	2.21895	-3.17084	2.08168
C	3.36631	-2.79504	2.80177
C	1.08635	-2.33743	2.09466
C	3.39372	-1.59037	3.52578
H	4.29769	-1.30491	4.08349
C	1.11083	-1.12215	2.82451
C	2.26209	-0.75721	3.54703
H	0.19842	-0.51819	2.92509
H	2.25437	0.17775	4.12651
H	2.82725	-0.29408	0.24758

## TS-2b/2b'

Imaginary frequency: 21.94 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8052115 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3363.0094971 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3362.01270660561 Hartree (single point)

Cartesian coordinates in Å:

Pt	-0.19488	-0.76704	-1.80130
Au	-1.16140	1.13013	0.32122
C	1.88395	2.58787	-0.30607
P	0.18024	2.55848	-0.95109
P	1.88310	-1.61385	-1.70479
C	2.24431	1.64817	0.68163
C	3.55240	1.62223	1.18492
P	-2.51870	-0.70069	0.78154
C	4.50244	2.54098	0.70707
C	4.14009	3.49371	-0.26244
C	2.83167	3.52441	-0.76895
C	0.17861	1.75605	-2.60096
C	1.26523	1.89509	-3.49533
C	1.21722	1.29001	-4.75710
C	0.08919	0.54140	-5.14813
C	-1.02653	0.44801	-4.30307
C	-1.00574	1.05572	-3.02112
C	-0.27578	4.30389	-1.21953
C	-0.62508	4.78649	-2.49624
C	-0.98951	6.13402	-2.65337
C	-1.00765	6.99462	-1.54430
C	-0.66390	6.51012	-0.26878
C	-0.30295	5.16682	-0.10190
C	3.15862	-0.77316	-2.73895
C	3.78818	0.38368	-2.23271
C	4.70117	1.09981	-3.01971
C	4.98982	0.68061	-4.32904
C	4.36952	-0.47288	-4.83699
C	2.67390	-1.73032	-0.05189
C	4.07075	-1.86211	0.09434
C	4.63545	-1.97445	1.37420
C	3.81090	-1.96341	2.51296
C	2.41782	-1.84237	2.36921
C	1.85063	-1.72388	1.09170
C	1.88366	-3.34180	-2.32999
C	2.42088	-4.41760	-1.59591
C	2.36394	-5.72156	-2.11576
C	1.78583	-5.96021	-3.37300
C	1.24503	-4.89057	-4.10826
C	1.27775	-3.59043	-3.58352
C	-1.89352	-1.92436	1.97563
C	-2.14706	-3.30543	1.83632
C	-1.68932	-4.19896	2.81706
C	-0.99740	-3.71996	3.94208
C	-0.75698	-2.34290	4.08841
C	-1.19342	-1.44550	3.10288
C	-4.23724	-0.31034	1.25409
C	-5.15054	-1.33759	1.57154
C	-6.47616	-1.01297	1.89024

C	-6.89427	0.33032	1.89098
C	-5.98552	1.35331	1.57602
C	-4.65490	1.03573	1.25994
C	-2.60641	-1.49616	-0.86578
C	-1.78252	-3.07505	-2.55719
C	-2.82645	-2.70621	-3.40421
C	-3.77796	-1.73894	-2.99890
C	-3.66986	-1.14692	-1.73858
C	3.46302	-1.19841	-4.04798
H	4.25597	-2.05145	3.51550
H	1.76535	-1.83924	3.25349
H	0.76201	-1.60968	0.96668
H	4.71761	-1.87142	-0.79527
H	5.72596	-2.07299	1.48306
H	-7.93576	0.57955	2.14314
H	-1.25898	6.51221	-3.65066
H	-1.29307	8.04941	-1.67177
H	-0.67994	7.18411	0.60057
H	-0.03636	4.78549	0.89659
H	-0.60692	4.11247	-3.36548
H	-7.18867	-1.81248	2.14171
H	-1.93397	-0.08580	-4.61954
H	-1.87956	-5.27650	2.70382
H	0.07213	0.04899	-6.13143
H	2.07996	1.38417	-5.43122
H	2.16428	2.44456	-3.18813
H	-1.94797	1.15366	-2.45816
H	-0.64553	-4.42394	4.71067
H	-0.22669	-1.96612	4.97580
H	-0.99572	-0.36638	3.20266
H	-2.69710	-3.68361	0.96192
H	5.70530	1.24304	-4.94726
H	5.18832	1.99223	-2.59986
H	4.60021	-0.82121	-5.85504
H	3.57001	0.72147	-1.21320
H	5.53043	2.52159	1.09828
H	3.82636	0.87300	1.94131
H	4.88099	4.22339	-0.62172
H	2.54291	4.28326	-1.51194
H	1.49952	0.92338	1.04207
H	-6.31102	2.40402	1.58071
H	-3.93068	1.83083	1.01802
H	1.75124	-6.98189	-3.77953
H	0.78349	-5.07283	-5.09054
H	2.78164	-6.55695	-1.53397
H	2.88463	-4.23787	-0.61541
H	-4.82625	-2.38884	1.57468
H	-4.42261	-0.41636	-1.40617
H	-2.93055	-3.19945	-4.38224
H	0.81328	-2.75690	-4.13370
H	-4.61575	-1.47238	-3.65935
H	3.00304	-2.10754	-4.45725
C	-1.59531	-2.44529	-1.27920
H	-1.09034	-3.87664	-2.84569
H	-0.99273	-2.97433	-0.52668

## TS-2c/24

Imaginary frequency: 210.52 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8040368 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9806755 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.98809544872 Hartree (single point)

Cartesian coordinates in Å:

C	-3.96128	-0.98651	-2.08101
P	-2.76335	-2.36438	-1.93167
P	0.26922	-0.45635	-3.32712
C	-3.90020	0.03424	-1.10813
C	-4.80290	1.10475	-1.15449
P	-0.23801	-1.86312	0.76831
C	-5.76383	1.17120	-2.17986
C	-5.82241	0.15812	-3.15136
C	-4.92834	-0.92399	-3.10209
C	-3.49216	-3.44326	-0.63864
C	-4.71866	-3.15017	-0.01024
C	-5.16242	-3.94210	1.06206
C	-4.39101	-5.02646	1.51195
C	-3.17679	-5.33535	0.87170
C	-2.73175	-4.54719	-0.19721
C	-2.90132	-3.29696	-3.50288
C	-2.51305	-2.63539	-4.69015
C	-2.54443	-3.31125	-5.91628
C	-2.94982	-4.65698	-5.96945
C	-3.33926	-5.31637	-4.79230
C	-3.32269	-4.64011	-3.56051
C	1.48013	0.77334	-2.64618
C	1.19843	2.12147	-2.48175
C	1.94026	2.90289	-1.54103
C	2.94714	2.33368	-0.77461
C	3.31552	0.96425	-0.98206
C	-0.89029	0.53200	-4.34059
C	-1.91595	1.21645	-3.65203
C	-2.89198	1.92396	-4.36635
C	-2.86141	1.93598	-5.77162
C	-1.84493	1.25197	-6.45963
C	-0.85479	0.55362	-5.74954
C	1.23654	-1.47627	-4.48847
C	2.27373	-0.93137	-5.27531
C	2.96934	-1.75189	-6.17632
C	2.63074	-3.11169	-6.29649
C	1.60271	-3.65680	-5.50859
C	0.90939	-2.84426	-4.59907
C	-0.01831	-3.54160	1.41640
C	0.45775	-4.51710	0.51717
C	0.65825	-5.83345	0.95972
C	0.36956	-6.17576	2.29195
C	-0.09550	-5.19703	3.18970
C	-0.27346	-3.87492	2.76151
C	-1.53534	-0.94708	1.64239
C	-2.64512	-1.62474	2.18821
C	-3.73222	-0.88649	2.68185
C	-3.72121	0.51686	2.63781
C	-2.62228	1.19161	2.07615

C	-1.53779	0.46442	1.56670
C	2.59111	0.18801	-1.92993
H	-3.63752	2.47608	-6.33407
H	-1.82236	1.25996	-7.55966
H	-0.06571	0.01039	-6.28985
H	-1.96341	1.16519	-2.55389
H	-3.69146	2.44532	-3.82095
H	-4.57533	1.08723	3.03143
H	-2.24372	-2.78405	-6.83386
H	-2.96667	-5.19069	-6.93139
H	-3.66701	-6.36605	-4.83065
H	-3.64232	-5.15816	-2.64477
H	-2.19227	-1.58447	-4.65403
H	-4.59908	-1.42097	3.09706
H	-2.56453	-6.18268	1.21403
H	1.03435	-6.59582	0.26156
H	-4.73816	-5.63643	2.35921
H	-6.11908	-3.70564	1.55183
H	-5.31929	-2.29353	-0.34720
H	-1.77403	-4.77605	-0.68453
H	0.51737	-7.21000	2.63703
H	-0.30606	-5.46442	4.23575
H	-0.59396	-3.09945	3.47215
H	0.65481	-4.23154	-0.52941
H	3.49431	2.93337	-0.03339
H	1.68381	3.96453	-1.40840
H	4.23667	0.56539	-0.53189
H	0.35661	2.57643	-3.02462
H	-6.46965	2.01442	-2.22084
H	-4.75194	1.89169	-0.38716
H	-6.57324	0.20660	-3.95407
H	-4.98127	-1.71741	-3.86127
H	-3.13863	-0.01400	-0.31680
H	-2.61469	2.29048	2.02391
H	-0.69947	0.98746	1.07928
H	3.17751	-3.75103	-7.00568
H	1.34124	-4.72146	-5.59880
H	3.77893	-1.32887	-6.78970
H	2.53506	0.13444	-5.18069
H	-2.68040	-2.72326	2.20036
H	0.10852	-3.25959	-3.96807
H	2.66040	-2.94746	1.71453
H	4.03866	-2.84878	3.79131
C	2.50576	-2.12538	2.43202
C	3.27245	-2.08041	3.60695
C	1.52131	-1.14379	2.18943
C	3.04981	-1.06170	4.55040
H	3.64054	-1.03306	5.47830
C	1.30914	-0.11877	3.12964
C	2.07005	-0.08317	4.31189
H	0.53789	0.64736	2.96368
H	1.89223	0.71263	5.05141
H	2.98933	-0.78386	-2.26989
Pt	-0.64395	-1.58911	-1.48928
Au	1.55135	-0.62197	-0.09233

## TS-11/12

Imaginary frequency: 223.60 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.7999327 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9719053 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.97894401713 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.06539	-0.57876	-2.27154
Au	-0.27546	0.00275	0.40817
C	-1.12644	0.40730	3.91409
P	-0.18449	1.15030	2.53800
P	-0.14395	-2.35756	0.56840
C	-2.32069	0.98592	4.38639
C	-3.05322	0.34540	5.39996
P	0.02288	1.60812	-1.38831
C	-2.59220	-0.85994	5.95240
C	-1.39940	-1.43716	5.48203
C	-0.67583	-0.81693	4.45697
C	-0.73449	2.88462	2.36980
C	-0.04258	3.95355	2.97399
C	-0.43116	5.27486	2.70159
C	-1.50526	5.53350	1.83165
C	-2.20703	4.46808	1.24146
C	-1.82043	3.14748	1.50837
C	1.55052	1.22523	3.10882
C	1.87823	1.30263	4.47963
C	3.22376	1.37379	4.87246
C	4.24404	1.37060	3.90484
C	3.91893	1.29483	2.54016
C	2.57733	1.22009	2.14079
C	1.60314	-2.81011	0.84425
C	2.26728	-3.73277	0.01128
C	3.62600	-4.01416	0.22986
C	4.32251	-3.38032	1.27237
C	3.66054	-2.45814	2.10235
C	-0.65707	-3.22710	-0.95179
C	-1.24325	-4.50735	-0.89188
C	-1.58659	-5.17524	-2.07719
C	-1.33724	-4.56563	-3.31734
C	-0.75374	-3.28803	-3.38236
C	-0.43545	-2.58501	-2.20207
C	-1.11403	-3.07502	1.93540
C	-2.40871	-2.55813	2.15629
C	-3.21341	-3.09672	3.16765
C	-2.72479	-4.14252	3.97008
C	-1.42954	-4.64575	3.76369
C	-0.61937	-4.11569	2.74598
C	0.25837	-0.28585	-4.28068
C	1.17845	-0.97532	-5.09666
C	1.17375	-0.77157	-6.48775
C	0.25019	0.10944	-7.07402
C	-0.66481	0.79878	-6.26210
C	-0.65216	0.61778	-4.86781
C	1.54275	2.52588	-1.01779
C	2.77941	2.01713	-1.47070
C	3.97638	2.62171	-1.05568

C	3.94525	3.73360	-0.19650
C	2.71308	4.24468	0.24823
C	1.51250	3.64542	-0.15465
C	-1.30763	2.77313	-1.78395
C	-2.14406	4.93958	-2.51710
C	-3.46331	4.46030	-2.44806
C	-3.70707	3.12977	-2.06016
C	-2.63593	2.28926	-1.73025
C	2.30675	-2.16966	1.88691
H	-1.60016	-5.08723	-4.25018
H	-0.56802	-2.82321	-4.36100
H	1.32756	-1.47787	-2.35078
H	-1.43409	-4.97600	0.08559
H	-2.04482	-6.17415	-2.03078
H	4.88480	4.20569	0.12680
H	3.47681	1.43271	5.94153
H	5.29740	1.42493	4.21822
H	4.70987	1.28821	1.77660
H	2.32977	1.14920	1.07142
H	1.08129	1.29866	5.23799
H	4.93872	2.22697	-1.41433
H	-3.03962	4.66173	0.54950
H	1.89453	-1.31590	-7.11721
H	-1.79409	6.57145	1.60926
H	0.11539	6.10970	3.16513
H	0.81521	3.75341	3.63253
H	-2.34316	2.31375	1.01618
H	0.24637	0.26157	-8.16353
H	-1.38702	1.49859	-6.70982
H	-1.35882	1.19096	-4.24619
H	1.89467	-1.68735	-4.65943
H	5.38730	-3.60311	1.43664
H	4.14316	-4.73520	-0.42055
H	4.20037	-1.94873	2.91398
H	1.72219	-4.22676	-0.80653
H	-3.16307	-1.35228	6.75357
H	-3.98360	0.80209	5.76916
H	-1.03535	-2.38304	5.90718
H	0.24634	-1.28492	4.08258
H	-2.67207	1.94207	3.97066
H	2.68428	5.11100	0.92541
H	0.55343	4.03369	0.21491
H	-3.35489	-4.56104	4.76890
H	-1.04679	-5.46052	4.39642
H	-4.21967	-2.68935	3.34230
H	-2.77811	-1.72500	1.53724
H	2.79091	1.14917	-2.14766
H	-2.82375	1.24866	-1.41679
H	-4.30430	5.12178	-2.70364
H	0.39494	-4.50881	2.57977
H	-4.73769	2.74771	-2.01290
H	1.80096	-1.42837	2.52199
C	-1.06613	4.10208	-2.19226
H	-1.95026	5.97561	-2.83266
H	-0.03595	4.48057	-2.25784

## TS-12/13

Imaginary frequency: 367.63 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8006352 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9747433 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.98249518895 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.16952	1.67947	-1.62335
Au	-0.33253	-0.41715	0.06210
C	-1.50080	-3.06686	2.35158
P	-0.32379	-1.69211	2.11849
P	-0.18144	-1.73321	-1.89917
C	-2.30953	-3.16236	3.50245
C	-3.19192	-4.24536	3.64524
P	0.15668	1.84532	0.67849
C	-3.26442	-5.23556	2.65145
C	-2.45600	-5.14217	1.50508
C	-1.58317	-4.05719	1.34931
C	-0.52106	-0.59988	3.57243
C	0.34184	-0.67199	4.68392
C	0.18656	0.23614	5.74400
C	-0.81833	1.21791	5.69553
C	-1.68591	1.28459	4.59035
C	-1.53901	0.37538	3.53406
C	1.34509	-2.41887	2.29363
C	1.54804	-3.72408	2.78441
C	2.85557	-4.21973	2.92001
C	3.95661	-3.41735	2.57559
C	3.75193	-2.11685	2.08367
C	2.45158	-1.61942	1.93591
C	1.52684	-2.37434	-1.85762
C	2.52745	-1.76172	-2.63858
C	3.86125	-2.18175	-2.51249
C	4.19800	-3.21203	-1.61893
C	3.19964	-3.82210	-0.83978
C	-0.38598	-0.77625	-3.43315
C	-0.71198	-1.46567	-4.62191
C	-0.84654	-0.76186	-5.82424
C	-0.65369	0.62974	-5.82967
C	-0.32492	1.30720	-4.64520
C	-0.18569	0.63578	-3.40357
C	-1.31607	-3.15659	-2.00894
C	-2.66489	-2.93061	-1.65893
C	-3.59503	-3.97466	-1.74033
C	-3.18254	-5.25155	-2.16068
C	-1.83978	-5.48041	-2.50474
C	-0.90352	-4.43498	-2.43565
C	0.14360	3.77615	-1.42134
C	1.21903	4.53556	-0.92425
C	1.01283	5.87910	-0.56657
C	-0.25683	6.46296	-0.70200
C	-1.32016	5.70537	-1.22085
C	-1.12419	4.36415	-1.58898
C	1.72525	1.89994	1.57934
C	2.92074	1.74437	0.84028
C	4.14598	1.62559	1.51130

C	4.18437	1.65186	2.91708
C	2.99538	1.80248	3.65133
C	1.76508	1.92885	2.99038
C	-1.05529	2.93184	1.45895
C	-1.65796	4.94317	2.68398
C	-3.01713	4.68860	2.43570
C	-3.39762	3.56211	1.68331
C	-2.42058	2.68896	1.18977
C	1.86939	-3.39713	-0.94627
H	-0.76136	1.19600	-6.76750
H	-0.18681	2.39857	-4.68824
H	0.72204	2.72637	-2.69010
H	-0.87088	-2.55471	-4.60070
H	-1.10429	-1.29541	-6.75092
H	5.14574	1.55346	3.44269
H	3.01351	-5.23843	3.30459
H	4.97830	-3.81046	2.68589
H	4.60633	-1.48502	1.80158
H	2.29902	-0.60496	1.54183
H	0.68715	-4.34999	3.06170
H	5.07549	1.51096	0.93409
H	-2.46742	2.05691	4.53824
H	1.85450	6.46684	-0.16957
H	-0.92524	1.93621	6.52189
H	0.86241	0.18155	6.61044
H	1.14334	-1.42431	4.71087
H	-2.20639	0.43754	2.66235
H	-0.41721	7.51129	-0.41019
H	-2.31544	6.15843	-1.34296
H	-1.96197	3.77272	-1.98692
H	2.21079	4.07998	-0.79385
H	5.24353	-3.54245	-1.52899
H	4.64100	-1.70493	-3.12491
H	3.45698	-4.62421	-0.13385
H	2.25817	-0.95836	-3.34028
H	-3.95527	-6.08351	2.76998
H	-3.82294	-4.31743	4.54352
H	-2.51003	-5.90902	0.71920
H	-0.96989	-3.97948	0.44076
H	-2.24580	-2.39380	4.28653
H	3.02190	1.81396	4.75090
H	0.83613	2.02779	3.56937
H	-3.91216	-6.07299	-2.21883
H	-1.51738	-6.47837	-2.83740
H	-4.64452	-3.79575	-1.46442
H	-2.97907	-1.93309	-1.31299
H	2.87143	1.69598	-0.25964
H	-2.70674	1.81451	0.58306
H	-3.78457	5.37611	2.82130
H	0.14604	-4.61407	-2.71157
H	-4.46071	3.36892	1.47667
H	1.10015	-3.86019	-0.31148
C	-0.67351	4.07078	2.19676
H	-1.35938	5.83471	3.25510
H	0.39012	4.28404	2.37364

## TS-15/16

Imaginary frequency: 57.35 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8043922 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9921388 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.99200845673 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.04446	0.51813	1.17303
Au	0.70752	1.38794	-1.40700
C	0.23162	-2.82290	-2.64461
P	0.03861	-1.02908	-2.30467
P	0.69035	-1.70450	1.40884
C	-0.83770	-3.61177	-3.11591
C	-0.65366	-4.98634	-3.33179
P	-0.17565	2.63887	0.36087
C	0.58539	-5.58981	-3.06595
C	1.64276	-4.81344	-2.56395
C	1.46682	-3.44067	-2.34315
C	1.06206	-0.14906	-3.58694
C	2.38783	-0.55531	-3.87820
C	3.22183	0.25179	-4.66239
C	2.77100	1.49302	-5.15257
C	1.46498	1.91409	-4.87323
C	0.60470	1.10562	-4.10028
C	-1.66782	-0.54884	-2.77105
C	-2.18426	-0.74982	-4.07056
C	-3.46638	-0.28182	-4.39569
C	-4.23483	0.40131	-3.43544
C	-3.72066	0.61854	-2.14709
C	-2.44303	0.14398	-1.81653
C	2.32718	-2.04706	0.65299
C	2.95292	-1.06534	-0.14186
C	4.17565	-1.33264	-0.77581
C	4.78877	-2.58663	-0.61474
C	4.19175	-3.55750	0.20913
C	-0.53927	-2.84713	0.67020
C	-0.27430	-4.20999	0.42551
C	-1.28426	-5.03688	-0.08370
C	-2.56015	-4.51379	-0.35799
C	-2.82686	-3.15667	-0.12374
C	-1.81987	-2.32838	0.39379
C	0.85769	-2.23665	3.14607
C	2.06587	-2.01435	3.83795
C	2.12610	-2.22910	5.22299
C	0.98051	-2.64291	5.92223
C	-0.22512	-2.85619	5.23328
C	-0.28989	-2.65924	3.84717
C	-0.67977	0.53273	3.04489
C	-2.04350	0.25825	3.26246
C	-2.54562	0.21677	4.57652
C	-1.69436	0.44536	5.66867
C	-0.33695	0.72720	5.44354
C	0.17412	0.77465	4.13531
C	-1.79503	3.26186	-0.18979
C	-2.89260	3.09885	0.68341
C	-4.16845	3.52716	0.28282

C	-4.35276	4.10545	-0.98503
C	-3.26111	4.25828	-1.85784
C	-1.98249	3.83833	-1.46380
C	0.82902	4.02735	0.94018
C	1.21858	6.40065	1.29095
C	2.44167	6.10558	1.91594
C	2.85889	4.76889	2.05808
C	2.05586	3.72878	1.57567
C	2.97291	-3.28772	0.84956
H	-3.34592	-5.16813	-0.76387
H	-3.81854	-2.73583	-0.34554
H	-2.01272	-1.26399	0.58999
H	0.71996	-4.63156	0.62058
H	-1.06963	-6.09735	-0.27799
H	-5.35463	4.43627	-1.29701
H	-3.86506	-0.44159	-5.40870
H	-5.23574	0.77465	-3.69906
H	-4.30320	1.17380	-1.39806
H	-2.02809	0.33169	-0.81349
H	-1.57391	-1.25563	-4.83403
H	-5.02304	3.40743	0.96533
H	1.09083	2.86864	-5.27173
H	-3.61204	-0.00226	4.74116
H	3.43746	2.12182	-5.76059
H	4.24063	-0.09222	-4.89611
H	2.76150	-1.51674	-3.50093
H	-0.44752	1.40240	-3.96978
H	-2.08809	0.40450	6.69497
H	0.33892	0.90696	6.29326
H	1.24191	0.98067	3.97248
H	-2.71938	0.06264	2.41630
H	5.74526	-2.80206	-1.11396
H	4.64873	-0.55573	-1.39424
H	4.68440	-4.52904	0.36283
H	2.47084	-0.08085	-0.26159
H	0.72375	-6.66734	-3.23942
H	-1.49304	-5.59058	-3.70722
H	2.61295	-5.27701	-2.33136
H	2.29136	-2.85494	-1.91734
H	-1.81957	-3.15858	-3.30664
H	-3.40832	4.70443	-2.85250
H	-1.12501	3.94606	-2.14569
H	1.02677	-2.79867	7.01025
H	-1.12489	-3.17432	5.77969
H	3.07190	-2.06361	5.76016
H	2.95783	-1.66638	3.29533
H	-2.74160	2.63496	1.67056
H	2.36509	2.67706	1.68900
H	3.07295	6.92097	2.29916
H	-1.23659	-2.81699	3.31087
H	3.81375	4.53879	2.55359
H	2.53415	-4.03864	1.52264
C	0.40765	5.36610	0.79964
H	0.89062	7.44550	1.18612
H	-0.55254	5.59579	0.31457

## TS-15/29

Imaginary frequency: 730.12 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8003212 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9656540 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.96260432206 Hartree (single point)

Cartesian coordinates in Å:

Au	2.31773	5.43209	5.25018
Pt	5.01673	5.80432	5.22091
C	6.48424	8.02164	7.74506
P	5.32457	7.95137	6.34075
P	2.06413	6.39536	3.11393
C	6.85481	6.81896	8.37676
C	7.69550	6.84511	9.49860
P	3.88463	4.47167	6.78081
C	8.17549	8.06933	9.99025
C	7.81153	9.27329	9.36053
C	6.96684	9.25408	8.24116
C	3.74763	8.64430	6.98595
C	3.62519	9.16847	8.28773
C	2.37469	9.61051	8.75141
C	1.23814	9.53352	7.92919
C	1.35493	9.02010	6.62582
C	2.60182	8.57771	6.16632
C	5.92468	9.18595	5.11951
C	7.29965	9.48510	4.99738
C	7.76020	10.28095	3.93567
C	6.86015	10.78584	2.98426
C	5.49005	10.50267	3.10897
C	5.02573	9.71010	4.16623
C	3.73915	6.86474	2.49380
C	3.76493	7.59124	1.28067
C	4.97741	7.98174	0.69861
C	6.18705	7.60939	1.30831
C	6.17678	6.84281	2.47950
C	1.00226	7.88196	3.09067
C	1.49616	9.18861	2.90744
C	0.63442	10.28977	3.03792
C	-0.72205	10.09445	3.34030
C	-1.22025	8.79086	3.51942
C	-0.36274	7.68829	3.40598
C	1.39013	5.24271	1.87173
C	0.61236	5.68944	0.78426
C	0.17080	4.76706	-0.17690
C	0.50474	3.40734	-0.05783
C	1.27808	2.96247	1.02843
C	1.71873	3.87559	1.99675
C	3.84998	2.65746	6.62952
C	4.23701	2.08760	5.39416
C	4.16806	0.70066	5.20518
C	3.71818	-0.12990	6.24663
C	3.33044	0.43212	7.47540
C	3.39102	1.81991	7.67074
C	3.94150	4.88449	8.54451
C	3.18676	5.97062	9.03314
C	3.36676	6.40853	10.35342

C	4.29418	5.76818	11.19122
C	5.04302	4.68001	10.70901
C	4.87396	4.23822	9.38999
C	4.96870	6.47509	3.11347
H	-1.39482	10.95900	3.43938
H	-2.28267	8.63249	3.75649
H	-0.75292	6.67047	3.56377
H	2.55568	9.34764	2.66683
H	1.02981	11.30693	2.90098
H	4.43323	6.11543	12.22566
H	8.83330	10.51140	3.85824
H	7.22469	11.40616	2.15229
H	4.77509	10.90291	2.37456
H	3.95206	9.50578	4.25507
H	8.01448	9.10834	5.74265
H	2.77450	7.25587	10.72798
H	0.48044	8.95764	5.96152
H	4.47692	0.26395	4.24371
H	0.26189	9.87590	8.30310
H	2.28893	10.01510	9.77121
H	4.50026	9.21049	8.95061
H	2.67918	8.16298	5.15449
H	3.67140	-1.21934	6.10107
H	2.97294	-0.21622	8.28930
H	3.07357	2.25526	8.62960
H	4.59949	2.74827	4.58927
H	7.14705	7.90225	0.85838
H	4.97560	8.55763	-0.23816
H	7.12799	6.51327	2.92003
H	2.82020	7.85024	0.77845
H	8.84026	8.08877	10.86684
H	7.97975	5.90091	9.98502
H	8.18728	10.23331	9.74482
H	6.67990	10.19721	7.75199
H	6.48844	5.86347	7.98110
H	5.76870	4.17564	11.36438
H	5.47815	3.40162	9.00720
H	0.15458	2.68839	-0.81325
H	1.53213	1.89679	1.12681
H	-0.43948	5.11330	-1.02418
H	0.34416	6.75278	0.69407
H	2.46424	6.47539	8.37422
H	2.31562	3.52951	2.85616
H	6.45659	3.16411	6.07857
H	8.80696	2.51433	6.49529
C	7.25069	3.90424	5.91253
C	8.58885	3.53550	6.14642
C	6.95731	5.20689	5.47153
C	9.63173	4.45200	5.94119
H	10.67458	4.15803	6.13067
C	7.99749	6.12248	5.25042
C	9.33171	5.74437	5.48585
H	7.78332	7.14080	4.90155
H	10.13584	6.47587	5.31235
H	4.96698	5.12381	3.66075

## TS-15/31

Imaginary frequency: 449.74 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8003822 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9600964 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.96634686493 Hartree (single point)

Cartesian coordinates in Å:

Pt	2.91240	5.34564	4.05689
Au	5.07726	6.77993	4.94514
C	8.32508	8.16295	5.70704
P	7.06140	6.93610	6.20542
P	3.57560	5.73142	1.88951
C	7.89907	9.50800	5.64366
C	8.80218	10.51556	5.28127
P	3.81601	4.97294	6.12945
C	10.13524	10.18755	4.97585
C	10.56322	8.85269	5.04932
C	9.66422	7.83762	5.41765
C	7.85200	5.29526	6.21435
C	7.80199	4.44838	7.33896
C	8.35762	3.16185	7.27102
C	8.96980	2.71873	6.08874
C	9.00005	3.55212	4.95787
C	8.42774	4.82946	5.01055
C	6.64091	7.42487	7.91188
C	7.60724	7.36253	8.93927
C	7.28269	7.81567	10.22582
C	6.01092	8.35852	10.48430
C	5.05847	8.44541	9.45736
C	5.36837	7.97136	8.17485
C	4.82243	4.42621	1.59690
C	6.19897	4.72933	1.63688
C	7.14500	3.69582	1.53790
C	6.72278	2.36398	1.39685
C	5.34918	2.06151	1.36612
C	4.51070	7.32264	1.83297
C	4.77995	7.94510	0.59819
C	5.39864	9.20422	0.56986
C	5.73433	9.84867	1.77279
C	5.47603	9.22901	3.00725
C	4.89277	7.94872	3.04577
C	2.45542	5.76828	0.45602
C	1.32696	6.61182	0.55029
C	0.42040	6.68737	-0.51483
C	0.62909	5.91443	-1.67150
C	1.74978	5.07370	-1.76462
C	2.66781	4.99868	-0.70417
C	1.67093	3.80802	3.55982
C	0.49332	4.03491	2.81956
C	-0.31625	2.95325	2.42840
C	0.04942	1.63825	2.75752
C	1.22493	1.40954	3.49208
C	2.03310	2.48651	3.89670
C	3.33584	5.38249	7.83042
C	2.14976	6.12182	8.03024
C	1.78931	6.53178	9.32257

C	2.60307	6.20142	10.42045
C	3.78863	5.47243	10.22345
C	4.16205	5.07130	8.93444
C	4.71269	3.39109	6.14669
C	5.03953	1.13323	7.01067
C	5.86215	0.82799	5.91489
C	6.10311	1.80197	4.93039
C	5.53423	3.07506	5.04074
C	4.39785	3.08444	1.47300
H	6.20409	10.84368	1.75270
H	5.75513	9.74341	3.93652
H	3.75345	7.23059	3.92101
H	4.47591	7.45564	-0.33984
H	5.59852	9.69431	-0.39441
H	2.31243	6.51498	11.43415
H	8.03229	7.75965	11.02908
H	5.76513	8.72083	11.49359
H	4.06322	8.86743	9.65513
H	4.61583	8.01968	7.37273
H	8.61430	6.97050	8.73090
H	0.85945	7.09951	9.47573
H	9.45808	3.19807	4.02275
H	-1.23392	3.14547	1.85144
H	9.41025	1.71211	6.04232
H	8.30846	2.50149	8.14872
H	7.32984	4.79555	8.26868
H	8.42170	5.46560	4.11221
H	-0.58064	0.79303	2.44249
H	1.51916	0.38305	3.76090
H	2.95286	2.28635	4.46620
H	0.20167	5.05528	2.53120
H	7.46573	1.55694	1.30984
H	8.21852	3.93652	1.55664
H	5.01431	1.01834	1.26882
H	6.52863	5.77337	1.74312
H	10.84407	10.97802	4.68811
H	8.46698	11.56263	5.24094
H	11.60935	8.59565	4.82592
H	10.01256	6.79753	5.48977
H	6.86079	9.76640	5.90689
H	4.43410	5.22572	11.07917
H	5.10160	4.52256	8.77945
H	-0.08846	5.96740	-2.50371
H	1.91362	4.47050	-2.66991
H	-0.45787	7.34562	-0.44096
H	1.16374	7.20681	1.46330
H	1.50977	6.36097	7.16603
H	5.71255	3.82359	4.25444
H	6.30997	-0.17270	5.82324
H	3.54668	4.34217	-0.78046
H	6.73806	1.57338	4.06403
H	3.32565	2.83993	1.48350
C	4.45918	2.40597	7.12744
H	4.83206	0.37087	7.77645
H	3.78781	2.62284	7.97031

## TS-16/17

Imaginary frequency: 208.19 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8042592 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9846031 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.97891548500 Hartree (single point)

Cartesian coordinates in Å:

Pt	-2.31174	-2.94415	-0.40763
Au	-0.93003	-0.62766	-2.30634
C	-0.18820	-4.37985	-3.01246
P	-1.43220	-3.08722	-2.70093
P	-2.03711	-5.22732	0.07226
C	-0.18424	-5.28477	-4.09188
C	0.83395	-6.24391	-4.18780
P	-2.50361	-0.56348	-0.57405
C	1.84542	-6.31514	-3.21501
C	1.83625	-5.42285	-2.12957
C	0.82768	-4.45685	-2.03321
C	-0.06036	-1.57665	-4.01045
C	-0.63966	-1.10235	-5.20938
C	0.16814	-0.89235	-6.33797
C	1.54531	-1.16838	-6.27546
C	2.12478	-1.63832	-5.08254
C	1.32400	-1.85227	-3.95207
C	-2.79275	-3.13690	-3.91051
C	-2.65393	-3.41106	-5.28955
C	-3.78700	-3.44155	-6.11437
C	-5.06111	-3.17163	-5.58196
C	-5.20269	-2.86913	-4.21755
C	-4.07572	-2.85516	-3.38516
C	-0.45079	-5.50785	0.93628
C	0.38306	-4.40374	1.20726
C	1.59635	-4.58424	1.88793
C	1.97956	-5.86928	2.30747
C	1.13528	-6.96838	2.07017
C	-2.13280	-6.31258	-1.40170
C	-1.24980	-7.37585	-1.66466
C	-1.42553	-8.15943	-2.81563
C	-2.47286	-7.88735	-3.71152
C	-3.34759	-6.81735	-3.46012
C	-3.17843	-6.03400	-2.30988
C	-3.27244	-5.92390	1.23463
C	-3.06261	-5.76290	2.62088
C	-4.05926	-6.14373	3.52795
C	-5.26613	-6.69287	3.06336
C	-5.46994	-6.86872	1.68549
C	-4.47815	-6.48413	0.76953
C	-3.22115	-2.80167	1.42504
C	-4.59517	-3.09762	1.54508
C	-5.24442	-2.99348	2.78656
C	-4.52431	-2.60811	3.92973
C	-3.15168	-2.33480	3.82302
C	-2.50419	-2.43059	2.57884
C	-4.12812	-0.11108	-1.28188
C	-5.31977	-0.58540	-0.68768
C	-6.55555	-0.35480	-1.31042

C	-6.61520	0.33814	-2.53252
C	-5.43426	0.81442	-3.12498
C	-4.19629	0.59689	-2.50109
C	-2.24213	0.29403	1.00422
C	-3.06000	1.29895	3.06061
C	-1.75108	1.33393	3.56850
C	-0.68191	0.86206	2.78662
C	-0.92444	0.34510	1.50694
C	-0.08348	-6.78981	1.39860
H	-2.60145	-8.50545	-4.61250
H	-4.16153	-6.58349	-4.16217
H	-3.85453	-5.18740	-2.12064
H	-0.40654	-7.57855	-0.99110
H	-0.72750	-8.98490	-3.01891
H	-7.58570	0.51166	-3.02118
H	-3.67355	-3.66438	-7.18573
H	-5.94406	-3.18636	-6.23830
H	-6.19004	-2.63599	-3.79378
H	-4.17924	-2.63329	-2.31032
H	-1.66098	-3.57484	-5.72759
H	-7.47857	-0.72514	-0.83939
H	3.20387	-1.84706	-5.03548
H	-6.31666	-3.23013	2.86163
H	2.17397	-1.01738	-7.16585
H	-0.28022	-0.51330	-7.26851
H	-1.71907	-0.89471	-5.26014
H	1.77714	-2.24865	-3.03170
H	-5.03162	-2.52925	4.90285
H	-2.57519	-2.03682	4.71191
H	-1.43181	-2.19731	2.51640
H	-5.16457	-3.44063	0.66753
H	2.93123	-6.01342	2.84049
H	2.24063	-3.71795	2.09957
H	1.42196	-7.97007	2.42342
H	0.05458	-3.40175	0.88309
H	2.63544	-7.07619	-3.29716
H	0.82510	-6.95661	-5.02553
H	2.60830	-5.48186	-1.34828
H	0.81416	-3.76083	-1.18320
H	-0.99187	-5.27681	-4.83294
H	-5.47601	1.36370	-4.07726
H	-3.26927	0.97284	-2.96132
H	-6.04841	-6.98855	3.77813
H	-6.40732	-7.31169	1.31721
H	-3.89330	-6.00150	4.60565
H	-2.12996	-5.31574	2.99047
H	-5.27285	-1.15657	0.25064
H	-0.09140	-0.02680	0.88850
H	-1.56103	1.73897	4.57351
H	-4.64635	-6.62880	-0.30700
H	0.34674	0.90294	3.17503
H	-0.76140	-7.64442	1.25660
C	-3.31065	0.78289	1.78051
H	-3.89758	1.67344	3.66741
H	-4.33893	0.75024	1.39439

## TS-17/18

Imaginary frequency: 16.51 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8036620 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9868532 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.98790102011 Hartree (single point)

Cartesian coordinates in Å:

Pt	-2.67053	-3.50935	-0.13971
Au	-0.96159	-1.55145	-2.74401
C	-0.84651	-4.71321	-3.16334
P	-2.16648	-3.69257	-2.45440
P	-2.41708	-5.72919	0.49561
C	-0.97041	-5.40756	-4.38627
C	0.08797	-6.20801	-4.83952
P	-2.60099	-1.34155	-0.99416
C	1.26730	-6.32360	-4.08505
C	1.39077	-5.63909	-2.86244
C	0.34200	-4.83584	-2.40321
C	0.49601	-0.34710	-3.55064
C	0.29756	0.28924	-4.80400
C	1.30331	1.07982	-5.38017
C	2.52542	1.26023	-4.70872
C	2.73897	0.64731	-3.46046
C	1.73413	-0.14538	-2.88748
C	-3.49432	-3.45666	-3.66700
C	-3.22653	-3.04227	-4.99347
C	-4.28720	-2.73484	-5.85581
C	-5.61531	-2.82052	-5.40095
C	-5.88497	-3.21556	-4.08001
C	-4.83002	-3.53382	-3.21412
C	-0.79511	-5.97030	1.29604
C	0.17964	-4.95649	1.20100
C	1.44526	-5.14022	1.77685
C	1.73856	-6.33604	2.45402
C	0.76415	-7.34411	2.56173
C	-2.42980	-6.78193	-1.00096
C	-1.35193	-7.61764	-1.34684
C	-1.38597	-8.33619	-2.55271
C	-2.48883	-8.22511	-3.41406
C	-3.56212	-7.38275	-3.07725
C	-3.52971	-6.65647	-1.87937
C	-3.63172	-6.44459	1.65732
C	-3.62302	-5.98256	2.99292
C	-4.56758	-6.47263	3.90416
C	-5.52418	-7.41734	3.49440
C	-5.52924	-7.88111	2.16894
C	-4.58530	-7.39870	1.24811
C	-3.14970	-3.00479	1.79010
C	-4.51235	-3.00826	2.16116
C	-4.90375	-2.69001	3.47289
C	-3.93617	-2.37557	4.44112
C	-2.57722	-2.37562	4.08540
C	-2.18758	-2.68411	2.76947
C	-4.12329	-0.73728	-1.78010
C	-5.33648	-0.95655	-1.09035
C	-6.54600	-0.54504	-1.66783

C	-6.55082	0.05820	-2.93713
C	-5.34340	0.27005	-3.62490
C	-4.12672	-0.11758	-3.04712
C	-1.84066	0.02256	-0.08612
C	-1.68639	2.36138	0.54860
C	-0.55944	2.06811	1.33638
C	-0.06940	0.75095	1.41396
C	-0.70662	-0.27267	0.70543
C	-0.50360	-7.16420	1.98825
H	-2.50720	-8.78805	-4.35894
H	-4.42340	-7.28090	-3.75386
H	-4.36002	-5.98075	-1.62533
H	-0.48026	-7.69783	-0.68213
H	-0.53715	-8.98052	-2.82382
H	-7.50297	0.36542	-3.39479
H	-4.07663	-2.41392	-6.88680
H	-6.44444	-2.56948	-6.07897
H	-6.92224	-3.26926	-3.71924
H	-5.02902	-3.81957	-2.17013
H	-2.18716	-2.94177	-5.34074
H	-7.49073	-0.70472	-1.12725
H	3.69421	0.79348	-2.93303
H	-5.97122	-2.70203	3.74176
H	3.31293	1.88474	-5.15729
H	1.13524	1.56131	-6.35579
H	-0.65504	0.16268	-5.34281
H	1.91344	-0.61022	-1.90537
H	-4.23963	-2.13298	5.47049
H	-1.81020	-2.13592	4.83809
H	-1.11589	-2.69591	2.52224
H	-5.28298	-3.29582	1.42761
H	2.72933	-6.48043	2.91008
H	2.20234	-4.34511	1.70571
H	0.99199	-8.27530	3.10134
H	-0.08255	-4.01913	0.68292
H	2.09386	-6.95113	-4.44999
H	-0.01399	-6.75334	-5.78949
H	2.30935	-5.73110	-2.26464
H	0.43279	-4.30299	-1.44589
H	-1.89973	-5.34121	-4.96807
H	-5.34900	0.73920	-4.61953
H	-3.17811	0.04154	-3.58156
H	-6.26550	-7.79759	4.21298
H	-6.26795	-8.63029	1.84745
H	-4.55699	-6.10638	4.94115
H	-2.88120	-5.24018	3.32008
H	-5.32294	-1.44685	-0.10502
H	-0.33345	-1.30681	0.75286
H	-0.05780	2.87242	1.89464
H	-4.58540	-7.77759	0.21619
H	0.81157	0.52541	2.03264
H	-1.27161	-7.94676	2.08348
C	-2.32943	1.34411	-0.17012
H	-2.06656	3.39202	0.49263
H	-3.20972	1.56806	-0.78991

## TS-18/19

Imaginary frequency: 196.08 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8041600 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9865169 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.98254183580 Hartree (single point)

Cartesian coordinates in Å:

Pt	-1.40746	-3.00272	-0.35361
Au	-0.63503	-0.76594	-2.61462
C	1.72085	-3.39811	-2.17144
P	-0.04930	-3.03954	-2.40936
P	-0.75527	-5.12459	0.32796
C	2.19250	-4.72397	-2.04935
C	3.52983	-4.97032	-1.71021
P	-2.11609	-0.75240	-0.60623
C	4.41001	-3.90061	-1.47903
C	3.95089	-2.57880	-1.60641
C	2.61613	-2.32737	-1.95689
C	-1.86524	0.95047	-2.25090
C	-2.95068	1.01976	-3.15626
C	-3.42438	2.26769	-3.58009
C	-2.84005	3.44614	-3.07942
C	-1.77167	3.37975	-2.16803
C	-1.28466	2.13248	-1.74538
C	-0.69956	-3.99948	-3.81538
C	0.09280	-4.81471	-4.64585
C	-0.49912	-5.51545	-5.70974
C	-1.87358	-5.39318	-5.96613
C	-2.66566	-4.56545	-5.14819
C	-2.08508	-3.88008	-4.07536
C	0.91639	-5.03772	1.05322
C	1.60287	-3.80640	1.04198
C	2.89247	-3.71523	1.58194
C	3.50240	-4.85147	2.13769
C	2.81099	-6.07488	2.17730
C	-0.78037	-6.34270	-1.03794
C	0.19668	-7.34394	-1.20835
C	0.08452	-8.25686	-2.26830
C	-1.01005	-8.19140	-3.14684
C	-1.99184	-7.20409	-2.97166
C	-1.87069	-6.27327	-1.93071
C	-1.79049	-5.88604	1.63139
C	-1.53890	-5.56574	2.98179
C	-2.40981	-6.02036	3.98002
C	-3.52779	-6.80124	3.64178
C	-3.76933	-7.13480	2.29965
C	-2.90533	-6.67812	1.29266
C	-2.37986	-2.83227	1.47673
C	-3.69032	-3.30634	1.68639
C	-4.28184	-3.24556	2.95853
C	-3.56907	-2.71166	4.04543
C	-2.25924	-2.24639	3.85129
C	-1.66991	-2.30701	2.57660
C	-3.91068	-0.49932	-0.64588
C	-4.69438	-1.61874	-0.99530
C	-6.08732	-1.49164	-1.09992

C	-6.69702	-0.25106	-0.85229
C	-5.91355	0.87011	-0.51870
C	-4.52122	0.75550	-0.42897
C	-1.33617	0.21294	0.71648
C	-1.38387	1.36182	2.85643
C	0.01947	1.39976	2.87211
C	0.75056	0.83160	1.81272
C	0.07736	0.23424	0.73962
C	1.51518	-6.16951	1.64819
H	-1.09424	-8.90965	-3.97565
H	-2.84174	-7.13808	-3.66491
H	-2.61501	-5.47072	-1.81400
H	1.05691	-7.40099	-0.52720
H	0.85750	-9.02754	-2.40576
H	-7.78998	-0.15152	-0.92909
H	0.12603	-6.15543	-6.35016
H	-2.32948	-5.93758	-6.80632
H	-3.74256	-4.45905	-5.34826
H	-2.70400	-3.24214	-3.42251
H	1.17432	-4.89917	-4.46989
H	-6.69867	-2.36469	-1.37159
H	-1.31742	4.30308	-1.77869
H	-5.30449	-3.62608	3.10198
H	-3.22665	4.42590	-3.39784
H	-4.26047	2.32263	-4.29282
H	-3.43475	0.09878	-3.51588
H	-0.46350	2.08292	-1.01562
H	-4.03258	-2.66579	5.04236
H	-1.68675	-1.83210	4.69550
H	-0.64163	-1.93724	2.44483
H	-4.25835	-3.75322	0.85745
H	4.51757	-4.78221	2.55618
H	3.42388	-2.75319	1.56307
H	3.27904	-6.95889	2.63536
H	1.11007	-2.92564	0.60233
H	5.45758	-4.09698	-1.20691
H	3.88341	-6.00764	-1.61434
H	4.64058	-1.73669	-1.44543
H	2.25667	-1.29301	-2.07962
H	1.50666	-5.56640	-2.20439
H	-6.39298	1.84413	-0.34169
H	-3.90661	1.64286	-0.21833
H	-4.21049	-7.15497	4.42862
H	-4.63558	-7.75800	2.03186
H	-2.21558	-5.75680	5.02981
H	-0.67327	-4.94479	3.24956
H	-4.19464	-2.58339	-1.17885
H	0.64564	-0.23298	-0.08172
H	0.54815	1.86551	3.71689
H	-3.09906	-6.94512	0.24398
H	1.85029	0.84963	1.82647
H	0.96039	-7.11691	1.72048
C	-2.06709	0.76808	1.78386
H	-1.95694	1.78357	3.69515
H	-3.16281	0.69802	1.80424

## TS-20/31

Imaginary frequency: 221.85 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8005835 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9457930 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.94830902724 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.94016	0.39093	-1.82588
Au	0.96168	-0.70101	0.70203
C	-1.63681	-0.99274	2.96131
P	0.13310	-0.55203	2.91899
P	0.17651	-1.65387	-2.60085
C	-2.55565	-0.37517	3.83318
C	-3.90583	-0.75883	3.80833
P	0.57899	1.81779	-0.08829
C	-4.33863	-1.76941	2.93418
C	-3.41699	-2.40121	2.08089
C	-2.07180	-2.01026	2.08339
C	0.34798	1.04137	3.78507
C	1.43865	1.23910	4.65822
C	1.67431	2.51042	5.20479
C	0.83163	3.58770	4.88571
C	-0.26127	3.38807	4.02620
C	-0.50538	2.12266	3.47717
C	0.99809	-1.78380	3.95414
C	0.33440	-2.45887	4.99742
C	1.03762	-3.38468	5.78364
C	2.39888	-3.63271	5.53717
C	3.06244	-2.95856	4.49746
C	2.36280	-2.03940	3.70151
C	-1.64478	-1.44692	-2.52544
C	-2.45178	-2.19893	-1.64944
C	-3.82872	-1.93004	-1.56391
C	-4.40216	-0.91374	-2.34345
C	-3.59735	-0.16285	-3.21985
C	0.55003	-2.98556	-1.36686
C	0.39002	-4.32364	-1.79506
C	0.60565	-5.38880	-0.90951
C	0.98086	-5.12337	0.41638
C	1.13848	-3.79597	0.85079
C	0.93051	-2.71024	-0.02241
C	0.52549	-2.37097	-4.24155
C	1.85646	-2.32323	-4.70743
C	2.18192	-2.88506	-5.94957
C	1.18084	-3.48351	-6.73536
C	-0.14661	-3.52166	-6.27752
C	-0.47900	-2.96858	-5.03049
C	0.52058	2.47565	-2.26262
C	1.65237	3.20192	-2.70599
C	1.49671	4.25062	-3.62318
C	0.21270	4.60607	-4.07585
C	-0.91733	3.90787	-3.61485
C	-0.76813	2.85074	-2.70411
C	1.50599	3.22345	0.59999
C	1.34399	4.56220	0.17726
C	2.06069	5.58266	0.81821

C	2.94446	5.27686	1.86896
C	3.11921	3.94524	2.27800
C	2.40399	2.91882	1.64478
C	-1.19629	2.05937	0.25396
C	-3.07868	3.39747	1.02669
C	-3.91226	2.26631	0.96947
C	-3.39313	1.03650	0.53250
C	-2.04484	0.93351	0.16653
C	-2.22440	-0.42359	-3.30983
H	1.15838	-5.95198	1.11900
H	1.43245	-3.61012	1.89415
H	1.84093	-0.70243	-0.86529
H	0.10133	-4.53377	-2.83639
H	0.48601	-6.42471	-1.25982
H	3.50627	6.08280	2.36433
H	0.51797	-3.91757	6.59370
H	2.944494	-4.36076	6.15529
H	4.12571	-3.15760	4.29796
H	2.86998	-1.52766	2.86712
H	-0.73227	-2.26744	5.18713
H	1.93490	6.62504	0.48939
H	-0.93110	4.22375	3.77554
H	2.38031	4.80203	-3.97821
H	1.02437	4.58349	5.31095
H	2.52350	2.65715	5.88875
H	2.10199	0.40009	4.91427
H	-1.36221	1.97648	2.80889
H	0.09211	5.43966	-4.78387
H	-1.92218	4.19240	-3.96219
H	-1.65343	2.31467	-2.33114
H	2.65469	2.94673	-2.32883
H	-5.47973	-0.70454	-2.27066
H	-4.45865	-2.52243	-0.88434
H	-4.04401	0.63317	-3.83404
H	-2.00081	-2.99620	-1.04120
H	-5.39656	-2.07132	2.92345
H	-4.62229	-0.26919	4.48441
H	-3.74751	-3.20706	1.40947
H	-1.35141	-2.49499	1.40682
H	-2.22041	0.40711	4.52875
H	3.81391	3.70134	3.09449
H	2.52707	1.87342	1.96629
H	1.43685	-3.91695	-7.71364
H	-0.93033	-3.98538	-6.89501
H	3.22004	-2.84868	-6.31182
H	2.63267	-1.83822	-4.09437
H	0.67092	4.80135	-0.65798
H	-1.64917	-0.03273	-0.17981
H	-4.96914	2.34547	1.26418
H	-1.51842	-2.99779	-4.67087
H	-4.03080	0.14333	0.48360
H	-1.58821	0.17248	-3.98204
C	-1.72470	3.29851	0.67324
H	-3.48325	4.36508	1.35924
H	-1.07254	4.17829	0.75574

## TS-21/22

Imaginary frequency: 175.00 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8031552 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9708600 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.96695146302 Hartree (single point)

Cartesian coordinates in Å:

Au	-0.92127	-0.80346	-0.71868
Pt	1.17231	0.53093	0.77765
C	-1.68441	2.66912	1.91360
P	-0.05158	2.62723	1.07717
P	1.78591	0.80526	-1.50213
C	-2.42116	1.48226	2.07013
C	-3.69089	1.50653	2.66587
P	-0.16558	-1.41957	1.47280
C	-4.23711	2.72591	3.09529
C	-3.51864	3.92182	2.91221
C	-2.24973	3.89938	2.31660
C	-0.42765	3.68737	-0.36893
C	0.01963	5.01858	-0.47563
C	-0.34189	5.78364	-1.59627
C	-1.13531	5.22247	-2.61160
C	-1.60149	3.90104	-2.49089
C	-1.26080	3.13909	-1.36519
C	1.12078	3.60290	2.09355
C	0.83668	4.05849	3.39454
C	1.83273	4.70597	4.14414
C	3.11294	4.90223	3.60262
C	3.40101	4.44417	2.30513
C	2.41487	3.78979	1.55536
C	0.44415	0.83683	-2.76661
C	0.68755	1.48999	-3.99528
C	-0.28848	1.47192	-5.00138
C	-1.49648	0.78718	-4.78893
C	-1.71897	0.10279	-3.58162
C	2.83731	-0.61971	-2.02842
C	2.59241	-1.26391	-3.25766
C	3.38717	-2.35335	-3.65368
C	4.43929	-2.79812	-2.83904
C	4.68569	-2.16114	-1.61022
C	3.88114	-1.08927	-1.20191
C	2.82847	2.29850	-1.74596
C	4.18565	2.26783	-1.35552
C	4.95345	3.44065	-1.37703
C	4.37824	4.65499	-1.79054
C	3.03338	4.68654	-2.18941
C	2.25646	3.51813	-2.16483
C	0.88699	-2.90958	1.42705
C	1.56523	-3.18458	0.21697
C	2.35175	-4.33724	0.09789
C	2.46749	-5.22576	1.18106
C	1.78481	-4.96262	2.38116
C	0.99379	-3.81142	2.50738
C	-1.37112	-1.71067	2.82412
C	-2.69036	-1.94760	2.37691
C	-3.70066	-2.27142	3.29585

C	-3.40277	-2.34842	4.66572
C	-2.09045	-2.11493	5.11395
C	-1.07465	-1.79951	4.20072
C	-0.76060	0.10852	-2.54535
H	5.06194	-3.64843	-3.15491
H	5.49739	-2.51242	-0.95624
H	4.04863	-0.63502	-0.21312
H	1.77047	-0.92588	-3.90285
H	3.17626	-2.85623	-4.60906
H	-4.19570	-2.59039	5.38893
H	1.60336	5.05984	5.16035
H	3.88911	5.41080	4.19358
H	4.40143	4.58902	1.87145
H	2.65313	3.42406	0.54634
H	-0.16034	3.90524	3.83083
H	-4.72405	-2.45776	2.93788
H	-2.23045	3.45570	-3.27514
H	2.87148	-4.53845	-0.84959
H	-1.40230	5.82150	-3.49493
H	0.00500	6.82462	-1.67900
H	0.66076	5.45158	0.30534
H	-1.63465	2.11051	-1.26467
H	3.08461	-6.13175	1.08709
H	1.86366	-5.66221	3.22642
H	0.45354	-3.62206	3.44431
H	1.47193	-2.49567	-0.63528
H	-2.26594	0.77396	-5.57628
H	-0.09878	1.98684	-5.95479
H	-2.66191	-0.44660	-3.44240
H	1.64199	2.00385	-4.17776
H	-5.23205	2.74987	3.56425
H	-4.24709	0.56651	2.79301
H	-3.95472	4.88086	3.22915
H	-1.70439	4.84050	2.15056
H	-1.99977	0.53498	1.71189
H	-1.85479	-2.17877	6.18659
H	-0.05463	-1.61964	4.56397
H	4.98191	5.57445	-1.80762
H	2.57265	5.62894	-2.51907
H	6.01024	3.40312	-1.07370
H	4.64983	1.32601	-1.03375
H	-2.91997	-1.87168	1.30092
H	1.20477	3.56237	-2.47131
H	2.82435	-1.48019	2.57328
H	3.70569	-1.24441	4.89036
C	2.33449	-0.78787	3.27331
C	2.82451	-0.66258	4.58161
C	1.21314	-0.03135	2.85176
C	2.18806	0.19895	5.49223
H	2.57267	0.29628	6.51849
C	0.54176	0.77799	3.79767
C	1.04495	0.91558	5.09744
H	-0.38250	1.30247	3.52525
H	0.53017	1.57708	5.80969
H	2.28712	-0.58375	0.65989

## TS-22/23

Imaginary frequency: 345.05 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8019764 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9821009 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.97214676400 Hartree (single point)

Cartesian coordinates in Å:

Au	-0.93070	-0.91117	-1.12155
Pt	0.79468	0.28776	0.60093
C	-2.07382	2.14983	1.94125
P	-0.46180	2.28368	1.08571
P	1.87959	0.92313	-1.46496
C	-3.01316	1.23836	1.41768
C	-4.28786	1.13579	1.98856
P	-0.62441	-1.47554	1.21994
C	-4.62977	1.93782	3.08995
C	-3.70272	2.85997	3.60245
C	-2.42892	2.97768	3.02494
C	-0.85011	3.47594	-0.24965
C	-0.70676	4.87165	-0.10113
C	-1.01377	5.71982	-1.17608
C	-1.48280	5.18769	-2.39085
C	-1.67846	3.80261	-2.51993
C	-1.36865	2.95114	-1.44978
C	0.71790	3.09399	2.21748
C	0.75979	2.71307	3.57776
C	1.75750	3.21775	4.42203
C	2.72870	4.10080	3.92139
C	2.71662	4.45089	2.56215
C	1.72998	3.93765	1.70835
C	0.69586	0.91760	-2.87780
C	1.01944	1.67783	-4.02278
C	0.17755	1.65934	-5.14382
C	-0.98446	0.87175	-5.12887
C	-1.29677	0.09718	-3.99774
C	2.99641	-0.49454	-1.83971
C	2.79332	-1.26677	-3.00196
C	3.56424	-2.41985	-3.22566
C	4.54579	-2.80842	-2.30098
C	4.75702	-2.03749	-1.14427
C	3.98387	-0.89253	-0.90938
C	2.85192	2.46547	-1.59937
C	4.24737	2.47831	-1.39208
C	4.93907	3.69953	-1.34588
C	4.25047	4.91152	-1.51850
C	2.86407	4.89962	-1.75180
C	2.16334	3.68620	-1.78713
C	0.37506	-2.96579	1.52097
C	1.33392	-3.33692	0.54594
C	2.17890	-4.42839	0.77406
C	2.07086	-5.16813	1.96673
C	1.11010	-4.81447	2.92877
C	0.26235	-3.71705	2.71191
C	-1.81902	-1.38981	2.58637
C	-3.01610	-2.13270	2.52456
C	-3.95710	-2.02061	3.55911

C	-3.71133	-1.16473	4.64635
C	-2.51619	-0.42847	4.71060
C	-1.56834	-0.54266	3.68487
C	-0.47139	0.09845	-2.85324
H	5.14633	-3.71276	-2.47964
H	5.52163	-2.33373	-0.41103
H	4.14206	-0.32678	0.01942
H	2.02028	-0.97825	-3.72672
H	3.39019	-3.01823	-4.13223
H	-4.45812	-1.06909	5.44839
H	1.77814	2.91485	5.47889
H	3.50543	4.50117	4.58942
H	3.48854	5.11895	2.15231
H	1.75949	4.18769	0.63999
H	0.00613	2.02170	3.97935
H	-4.89210	-2.59850	3.51220
H	-2.06031	3.37386	-3.45778
H	2.92389	-4.70401	0.01336
H	-1.71091	5.85820	-3.23270
H	-0.89043	6.80725	-1.06197
H	-0.34962	5.29780	0.84668
H	-1.51301	1.86843	-1.55576
H	2.73532	-6.02689	2.14363
H	1.02109	-5.39549	3.85875
H	-0.48559	-3.43677	3.46833
H	1.42278	-2.76083	-0.38875
H	-1.65000	0.85367	-6.00553
H	0.43557	2.25712	-6.03047
H	-2.20878	-0.51911	-4.00939
H	1.93632	2.28426	-4.04530
H	-5.62621	1.84761	3.54711
H	-5.01202	0.41631	1.58059
H	-3.97454	3.50046	4.45469
H	-1.71492	3.71535	3.41815
H	-2.73877	0.59974	0.56291
H	-2.32602	0.24414	5.55960
H	-0.63200	0.03365	3.71579
H	4.79706	5.86568	-1.48667
H	2.31666	5.84133	-1.90548
H	6.02760	3.70017	-1.18652
H	4.80043	1.53469	-1.28140
H	-3.21347	-2.78986	1.66355
H	1.08039	3.68819	-1.96685
H	1.45999	-1.34760	3.28632
H	3.00935	-0.94370	5.18612
C	2.23258	-0.57217	3.19921
C	3.11946	-0.35142	4.26526
C	2.36005	0.18182	2.01419
C	4.14099	0.60534	4.15455
H	4.83501	0.77350	4.99105
C	3.39732	1.12905	1.89329
C	4.27704	1.34038	2.96586
H	3.50488	1.72999	0.97990
H	5.06919	2.09701	2.86675
H	2.07654	-0.74176	0.81765

## TS-24/25

Imaginary frequency: 657.49 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8004699 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9587981 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.96462878816 Hartree (single point)

Cartesian coordinates in Å:

C	-1.09381	-3.24283	1.97973
P	-0.35012	-1.57837	2.02972
P	-0.28653	-1.78430	-1.69212
C	-2.35737	-3.49999	2.54655
C	-2.89967	-4.79370	2.48022
P	-0.01420	1.79728	0.80837
C	-2.18400	-5.82826	1.85694
C	-0.92615	-5.57020	1.28391
C	-0.38561	-4.28048	1.33308
C	-1.19895	-0.66762	3.37519
C	-0.71199	-0.65617	4.69731
C	-1.33217	0.15798	5.65908
C	-2.43176	0.95992	5.30788
C	-2.92873	0.93680	3.99280
C	-2.31553	0.12348	3.03040
C	1.36440	-1.86958	2.59929
C	1.64613	-2.88302	3.54215
C	2.95655	-3.05048	4.01446
C	3.98862	-2.21697	3.54822
C	3.71193	-1.21775	2.60070
C	2.40462	-1.04518	2.12447
C	1.44035	-2.03702	-2.21813
C	1.82876	-1.88613	-3.56459
C	3.17694	-2.04841	-3.92199
C	4.13519	-2.35938	-2.94225
C	3.74843	-2.50701	-1.59827
C	-1.11331	-0.82294	-3.00973
C	-2.07353	-1.38903	-3.86817
C	-2.83735	-0.56998	-4.71763
C	-2.64506	0.81870	-4.70007
C	-1.66289	1.38888	-3.86833
C	-0.88964	0.58129	-3.01297
C	-1.11451	-3.40524	-1.68805
C	-2.40187	-3.47095	-1.11161
C	-3.11353	-4.67583	-1.13264
C	-2.53718	-5.82185	-1.71035
C	-1.24861	-5.76181	-2.26517
C	-0.53329	-4.55264	-2.25964
C	1.69947	3.34912	-1.53797
C	3.01597	3.23885	-2.03350
C	3.92933	4.29897	-1.88315
C	3.53341	5.48841	-1.25036
C	2.21770	5.61621	-0.77421
C	1.30936	4.55308	-0.91312
C	1.32897	2.15415	1.97111
C	2.64557	2.39691	1.52685
C	3.68648	2.48195	2.46409
C	3.42465	2.31770	3.83459
C	2.11135	2.07955	4.27611

C	1.06159	1.99970	3.35192
C	-1.43757	2.83227	1.22138
C	-2.52132	4.64237	2.43343
C	-3.74458	4.32181	1.82062
C	-3.81347	3.26645	0.89097
C	-2.66547	2.52610	0.58671
C	2.40557	-2.34061	-1.23352
H	-3.24258	1.46984	-5.35566
H	-1.48457	2.47491	-3.90370
H	0.56270	1.36762	-3.18785
H	-2.25398	-2.47401	-3.83798
H	-3.58998	-1.01920	-5.38193
H	4.24633	2.37907	4.56363
H	3.17399	-3.84026	4.74887
H	5.01445	-2.35365	3.92184
H	4.51361	-0.56464	2.22694
H	2.18675	-0.27283	1.37452
H	0.84346	-3.54588	3.89831
H	4.71050	2.68350	2.11612
H	-3.78104	1.57028	3.70641
H	4.95470	4.19582	-2.27138
H	-2.90077	1.60966	6.06161
H	-0.94305	0.17613	6.68800
H	0.17018	-1.25304	4.96890
H	-2.67610	0.12888	1.99073
H	4.24730	6.31763	-1.13353
H	1.89782	6.54724	-0.28085
H	0.28982	4.66679	-0.51066
H	3.34566	2.31564	-2.53519
H	5.19092	-2.48119	-3.22689
H	3.48100	-1.92796	-4.97241
H	4.49734	-2.74122	-0.82718
H	1.07730	-1.63372	-4.32798
H	-2.60838	-6.84222	1.81453
H	-3.88269	-4.99557	2.93108
H	-0.36845	-6.37627	0.78638
H	0.59627	-4.08020	0.87916
H	-2.90773	-2.69450	3.05486
H	1.90089	1.94871	5.34790
H	0.03866	1.79881	3.70024
H	-3.09495	-6.77008	-1.72055
H	-0.79811	-6.66035	-2.71262
H	-4.11617	-4.72739	-0.68442
H	-2.83549	-2.57330	-0.64318
H	2.84935	2.52503	0.45496
H	-2.70587	1.69821	-0.14054
H	-4.64761	4.90326	2.05900
H	0.47298	-4.49804	-2.70159
H	-4.76765	3.02471	0.39969
H	2.10748	-2.42550	-0.17775
C	-1.36514	3.90554	2.13464
H	-2.46506	5.47656	3.14840
H	-0.40749	4.15991	2.61115
Pt	-0.34730	-0.33610	0.12531
Au	0.38098	1.70160	-1.59827

## TS-25/26

Imaginary frequency: 11.04 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8022435 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9660882 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.96999032869 Hartree (single point)

Cartesian coordinates in Å:

C	-0.06844	-0.02399	0.00295
P	1.51844	-0.15640	0.90073
P	1.05559	-3.74012	1.19927
C	-0.11321	0.46665	-1.31774
C	-1.33611	0.51583	-2.00483
P	4.82053	-1.55407	0.90220
C	-2.51687	0.08408	-1.37947
C	-2.47461	-0.40890	-0.06444
C	-1.25588	-0.47326	0.62133
C	2.56187	1.23162	0.30121
C	2.71262	2.42490	1.03403
C	3.59340	3.41855	0.57486
C	4.32877	3.22621	-0.60622
C	4.17644	2.03706	-1.34166
C	3.29610	1.04536	-0.88946
C	1.12269	0.23640	2.64018
C	0.17720	1.23506	2.96581
C	-0.05921	1.55603	4.31044
C	0.64619	0.89216	5.33111
C	1.58389	-0.10040	5.00699
C	1.81770	-0.43261	3.66556
C	0.75309	-3.86472	2.99416
C	1.53114	-4.75149	3.76823
C	1.40576	-4.75203	5.16588
C	0.50360	-3.87766	5.79647
C	-0.27293	-2.99549	5.02645
C	1.80137	-5.30709	0.64110
C	0.95903	-6.35767	0.21636
C	1.50413	-7.53190	-0.31514
C	2.89780	-7.64505	-0.42762
C	3.73375	-6.60819	0.01880
C	3.21824	-5.40874	0.57062
C	-0.54771	-3.63641	0.34052
C	-0.51109	-3.19451	-1.00002
C	-1.68459	-3.17168	-1.76216
C	-2.90310	-3.57351	-1.18653
C	-2.94438	-4.00222	0.15005
C	-1.76745	-4.04227	0.91619
C	6.80887	-3.53188	1.55924
C	7.34710	-3.38492	2.84841
C	8.71728	-3.11365	3.01209
C	9.55791	-3.00736	1.89238
C	9.02558	-3.18861	0.60598
C	7.65500	-3.45201	0.43863
C	5.21712	-0.58347	2.37390
C	5.09791	-1.17796	3.64881
C	5.20725	-0.39093	4.80191
C	5.41574	0.99509	4.69150
C	5.51291	1.59188	3.42373

C	5.41574	0.81056	2.26287
C	5.85272	-1.04626	-0.48349
C	7.83663	-0.01938	-1.43997
C	7.39577	-0.36939	-2.72798
C	6.19193	-1.07938	-2.89533
C	5.42160	-1.42032	-1.77661
C	-0.14262	-2.98018	3.63092
H	3.34698	-8.55482	-0.85433
H	4.82108	-6.74851	-0.06708
H	5.43862	-5.40685	1.60878
H	-0.13301	-6.23672	0.27606
H	0.84525	-8.34609	-0.65086
H	5.49742	1.61292	5.59792
H	-0.79742	2.33136	4.56390
H	0.45683	1.14948	6.38404
H	2.12867	-0.63262	5.79962
H	2.53175	-1.22532	3.40215
H	-0.37598	1.75569	2.17003
H	5.12612	-0.86054	5.79339
H	4.75961	1.86915	-2.25906
H	9.12797	-2.99375	4.02628
H	5.02760	4.00195	-0.95273
H	3.71488	4.34503	1.15560
H	2.16679	2.56996	1.97652
H	3.20521	0.09978	-1.44342
H	10.62965	-2.79627	2.02365
H	9.67588	-3.12198	-0.27946
H	7.25265	-3.57576	-0.57840
H	6.71379	-3.48832	3.74031
H	0.40301	-3.88646	6.89204
H	2.01068	-5.44820	5.76581
H	-0.97661	-2.30527	5.51414
H	2.23167	-5.43983	3.27188
H	-3.47458	0.13207	-1.91845
H	-1.36659	0.90829	-3.03210
H	-3.39449	-0.75385	0.42861
H	-1.22902	-0.85953	1.64932
H	0.80261	0.83096	-1.80525
H	5.65996	2.67821	3.33292
H	5.46777	1.28857	1.27431
H	-3.82689	-3.54860	-1.78351
H	-3.89766	-4.31939	0.59867
H	-1.65300	-2.82654	-2.80555
H	0.44551	-2.86492	-1.43570
H	4.89651	-2.25610	3.72865
H	4.47992	-1.98196	-1.89159
H	7.99963	-0.09954	-3.60716
H	-1.79736	-4.39725	1.95690
H	5.85656	-1.36941	-3.90204
H	-0.73462	-2.27048	3.03622
C	7.07554	-0.36423	-0.31420
H	8.78953	0.51434	-1.30939
H	7.43873	-0.12209	0.69432
Pt	2.66328	-2.12415	0.80102
Au	4.75785	-4.02694	1.17633

## TS-26/27

Imaginary frequency: 132.20 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8014429 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9674867 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.96906054769 Hartree (single point)

Cartesian coordinates in Å:

C	-1.44159	-3.04025	2.00276
P	-0.28009	-1.63331	1.89119
P	-0.15345	-1.83724	-1.67996
C	-2.69886	-2.88303	2.62134
C	-3.61754	-3.94411	2.62121
P	-0.03758	1.78819	0.72854
C	-3.28750	-5.16692	2.01463
C	-2.03475	-5.32765	1.39974
C	-1.12015	-4.26763	1.38394
C	-0.53017	-0.63814	3.41689
C	0.35382	-0.72631	4.51003
C	0.18413	0.12528	5.61476
C	-0.86022	1.06450	5.63454
C	-1.74958	1.14754	4.54808
C	-1.58382	0.29950	3.44509
C	1.40552	-2.31839	2.05811
C	1.67092	-3.48292	2.80931
C	2.99555	-3.91925	2.97038
C	4.05467	-3.19157	2.40129
C	3.79038	-2.02592	1.66354
C	2.47107	-1.59327	1.48587
C	1.54591	-2.51525	-1.66319
C	2.57758	-1.71577	-2.20101
C	3.91385	-2.12615	-2.08830
C	4.23167	-3.33412	-1.44421
C	3.20789	-4.13041	-0.90642
C	-0.32463	-0.97395	-3.28124
C	-0.53592	-1.75949	-4.43522
C	-0.64779	-1.15989	-5.69385
C	-0.54530	0.23554	-5.79297
C	-0.33216	1.01356	-4.64461
C	-0.21820	0.44384	-3.34793
C	-1.34864	-3.21391	-1.70213
C	-2.62551	-2.93925	-1.16565
C	-3.62707	-3.91705	-1.19692
C	-3.35650	-5.18021	-1.75049
C	-2.08553	-5.46091	-2.27894
C	-1.08114	-4.47960	-2.26313
C	0.11026	3.93316	-1.16311
C	1.27507	4.59250	-0.74525
C	1.19218	5.92005	-0.28441
C	-0.04282	6.58659	-0.25760
C	-1.20019	5.92805	-0.70590
C	-1.12597	4.60245	-1.16374
C	1.61023	1.95824	1.45766
C	2.75266	1.80921	0.63947
C	4.02350	1.71135	1.22157
C	4.16119	1.74273	2.62066
C	3.02508	1.87668	3.43605

C	1.74956	1.98727	2.86304
C	-1.17668	2.95371	1.49578
C	-1.67467	4.98646	2.72709
C	-3.04875	4.76498	2.53463
C	-3.49011	3.64287	1.80851
C	-2.55731	2.73942	1.28559
C	1.87099	-3.72040	-1.00765
H	-0.63155	0.72962	-6.77271
H	-0.25926	2.10320	-4.76960
H	0.34126	2.90415	-2.92018
H	-0.62765	-2.85194	-4.34246
H	-0.81655	-1.77689	-6.58865
H	5.15845	1.65811	3.07708
H	3.20118	-4.83033	3.55190
H	5.09065	-3.53803	2.53270
H	4.61222	-1.45360	1.21071
H	2.25860	-0.69238	0.89342
H	0.84668	-4.04662	3.27028
H	4.91085	1.60505	0.58010
H	-2.56209	1.88904	4.54622
H	2.10640	6.43253	0.05212
H	-0.97963	1.73773	6.49636
H	0.88336	0.06014	6.46169
H	1.18931	-1.44003	4.48970
H	-2.25418	0.39206	2.57875
H	-0.10277	7.62371	0.10411
H	-2.17065	6.44637	-0.70238
H	-2.04020	4.09382	-1.50529
H	2.24952	4.08505	-0.75678
H	5.28036	-3.65610	-1.36218
H	4.71249	-1.50216	-2.51667
H	3.44958	-5.07432	-0.39672
H	2.32718	-0.77397	-2.71269
H	-4.00803	-5.99803	2.02259
H	-4.59425	-3.81643	3.11115
H	-1.76998	-6.28053	0.91973
H	-0.14523	-4.39607	0.89727
H	-2.95758	-1.93748	3.11897
H	3.12807	1.88715	4.53114
H	0.86238	2.06460	3.50818
H	-4.14015	-5.95220	-1.76719
H	-1.87507	-6.44900	-2.71477
H	-4.61822	-3.69885	-0.77404
H	-2.81791	-1.95389	-0.71169
H	2.63636	1.74568	-0.45406
H	-2.88741	1.86378	0.70300
H	-3.78196	5.47616	2.94331
H	-0.09097	-4.70144	-2.68817
H	-4.56555	3.47735	1.64681
H	1.07803	-4.34715	-0.57899
C	-0.73359	4.08720	2.20650
H	-1.33101	5.87499	3.27679
H	0.34143	4.27797	2.32872
Pt	-0.36825	-0.30449	0.02998
Au	0.02688	1.84854	-1.75196

## TS-28/29

Imaginary frequency: 136.27 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8031078 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9635948 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.96021586691 Hartree (single point)

Cartesian coordinates in Å:

Au	-1.39633	-0.59558	-0.73990
Pt	1.13498	0.15627	0.46140
C	0.07531	2.80846	3.15541
P	0.18840	2.29485	1.38168
P	-0.48336	-0.03619	-2.82446
C	-0.58771	1.96723	4.07672
C	-0.72524	2.34369	5.42024
P	-0.47964	-1.36728	1.33843
C	-0.20207	3.56846	5.86571
C	0.44311	4.41820	4.95358
C	0.57783	4.04711	3.60571
C	-1.54581	2.52236	0.79843
C	-2.61699	2.72511	1.69137
C	-3.94036	2.73953	1.22061
C	-4.21124	2.55959	-0.14437
C	-3.14769	2.39561	-1.04755
C	-1.82374	2.37608	-0.58065
C	1.17811	3.64899	0.64211
C	2.51832	3.76350	1.07510
C	3.35725	4.74053	0.52371
C	2.87740	5.58669	-0.49080
C	1.54984	5.46769	-0.92998
C	0.69490	4.51197	-0.35668
C	0.93709	1.09426	-2.53740
C	1.39465	1.83912	-3.65365
C	2.56781	2.59786	-3.58063
C	3.31915	2.58532	-2.39558
C	2.87139	1.84915	-1.29039
C	-1.42051	0.64650	-4.23976
C	-1.78676	2.01200	-4.23210
C	-2.58007	2.53483	-5.26271
C	-3.01866	1.70305	-6.30777
C	-2.64902	0.34885	-6.32328
C	-1.85208	-0.18130	-5.29588
C	0.26654	-1.60930	-3.38897
C	1.63834	-1.70226	-3.69553
C	2.18500	-2.94079	-4.07044
C	1.36815	-4.08039	-4.15405
C	-0.00023	-3.98973	-3.84229
C	-0.54763	-2.76241	-3.44360
C	-0.23512	-3.15892	1.07280
C	0.34596	-3.57701	-0.14618
C	0.52766	-4.94143	-0.40487
C	0.11744	-5.90061	0.53757
C	-0.48156	-5.48769	1.73851
C	-0.65668	-4.12182	2.01176
C	-1.45479	-1.15381	2.86206
C	-2.70984	-0.52497	2.70748
C	-3.52578	-0.29748	3.82577

C	-3.09419	-0.69865	5.10050
C	-1.84972	-1.33687	5.25677
C	-1.02741	-1.56595	4.14461
C	1.65868	1.12508	-1.30647
H	-3.64139	2.11476	-7.11562
H	-2.97657	-0.30363	-7.14621
H	-1.55728	-1.23997	-5.32468
H	-1.42437	2.67803	-3.43542
H	-2.85183	3.60095	-5.25277
H	-3.73027	-0.51470	5.97920
H	4.39569	4.83083	0.87565
H	3.53995	6.34306	-0.93702
H	1.16846	6.13225	-1.71931
H	-0.35042	4.44705	-0.68820
H	2.90480	3.07973	1.84787
H	-4.49686	0.20272	3.69914
H	-3.34760	2.27217	-2.12181
H	0.98668	-5.25091	-1.35472
H	-5.24885	2.56112	-0.50944
H	-4.76508	2.89540	1.93208
H	-2.42524	2.86419	2.76315
H	-0.98895	2.26650	-1.28754
H	0.25818	-6.97210	0.33192
H	-0.81758	-6.23399	2.47366
H	-1.13344	-3.81242	2.95172
H	0.66078	-2.83249	-0.89275
H	4.26200	3.14815	-2.32855
H	2.90572	3.17232	-4.45557
H	3.48627	1.83926	-0.38092
H	0.83264	1.80564	-4.59815
H	-0.30335	3.86383	6.92060
H	-1.24646	1.67017	6.11605
H	0.84333	5.38666	5.28877
H	1.07103	4.73331	2.90483
H	-1.01413	1.01571	3.74168
H	-1.51498	-1.65562	6.25509
H	-0.04943	-2.04832	4.27411
H	1.80074	-5.04600	-4.45599
H	-0.64094	-4.88249	-3.89208
H	3.25797	-3.01264	-4.30241
H	2.27800	-0.81040	-3.63110
H	-3.02983	-0.19477	1.70611
H	-1.60824	-2.70049	-3.15213
H	2.34543	-2.77378	1.12955
H	4.02061	-3.39688	2.84291
C	2.43202	-2.16625	2.03957
C	3.37587	-2.52170	3.01241
C	1.60019	-1.03680	2.22797
C	3.49859	-1.76776	4.19246
H	4.23794	-2.05275	4.95577
C	1.71312	-0.30142	3.42739
C	2.66711	-0.65488	4.39391
H	1.06568	0.55918	3.61859
H	2.74830	-0.05376	5.31204
H	1.84350	-0.99654	-0.37967

## TS-29/30

Imaginary frequency: 644.34 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8010553 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9709369 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.96780761296 Hartree (single point)

Cartesian coordinates in Å:

Au	2.44922	5.27937	5.04889
Pt	5.15592	5.76942	5.05742
C	6.52870	7.81373	7.51933
P	5.18787	7.82307	6.27229
P	2.24217	6.37237	2.99197
C	7.19572	6.62021	7.85366
C	8.23927	6.63466	8.79249
P	3.93242	4.60905	6.78630
C	8.61835	7.83917	9.40513
C	7.96048	9.03632	9.06916
C	6.92530	9.02895	8.12380
C	3.66907	8.36238	7.14367
C	3.67163	8.75706	8.49571
C	2.47723	9.16984	9.10543
C	1.27604	9.19332	8.37867
C	1.26570	8.78485	7.03522
C	2.45497	8.36478	6.42416
C	5.66063	9.19750	5.15459
C	7.02784	9.41317	4.88039
C	7.41124	10.33414	3.89414
C	6.43720	11.03197	3.16266
C	5.07593	10.82067	3.43759
C	4.68601	9.91225	4.43198
C	3.92242	6.89123	2.44715
C	3.92530	7.49134	1.16084
C	5.09757	8.01349	0.60855
C	6.29046	7.90998	1.33780
C	6.29699	7.27534	2.58776
C	1.21912	7.88183	3.14651
C	1.67992	9.16467	2.79139
C	0.85944	10.28490	3.00270
C	-0.42388	10.13111	3.55062
C	-0.89053	8.85004	3.89646
C	-0.06899	7.72979	3.70865
C	1.56022	5.41513	1.59602
C	0.47864	5.87117	0.81834
C	0.01053	5.08401	-0.24711
C	0.61763	3.85173	-0.53617
C	1.69866	3.39831	0.24162
C	2.16930	4.17417	1.30871
C	4.06308	2.80132	6.97207
C	3.96802	2.00851	5.80346
C	4.12002	0.61790	5.87890
C	4.36745	0.00335	7.11965
C	4.45426	0.78568	8.28334
C	4.30132	2.17940	8.21564
C	3.55122	5.26994	8.44280
C	2.22190	5.62459	8.75570
C	1.90750	6.11799	10.02935

C	2.91464	6.26559	10.99790
C	4.24058	5.92067	10.68946
C	4.56045	5.42188	9.41757
C	5.13510	6.75336	3.18716
H	-1.06352	11.01150	3.71123
H	-1.89625	8.72453	4.32444
H	-0.42392	6.72937	4.00385
H	2.68332	9.28732	2.36115
H	1.22620	11.28628	2.73221
H	2.66513	6.65439	11.99642
H	8.47974	10.50228	3.69273
H	6.73852	11.74708	2.38316
H	4.30883	11.37673	2.87802
H	3.61850	9.76644	4.64572
H	7.79522	8.86058	5.44230
H	0.86924	6.39385	10.26463
H	0.33447	8.78965	6.45088
H	4.04012	0.00884	4.96624
H	0.34445	9.52119	8.86339
H	2.48775	9.46752	10.16409
H	4.59890	8.72184	9.08269
H	2.43123	8.03764	5.37680
H	4.48536	-1.08871	7.17947
H	4.63911	0.30664	9.25646
H	4.36118	2.78428	9.13202
H	3.77365	2.49283	4.83276
H	7.22998	8.30994	0.92809
H	5.07966	8.48446	-0.38502
H	7.25855	7.19549	3.10606
H	2.98779	7.54197	0.58485
H	9.43679	7.85049	10.14042
H	8.76095	5.69761	9.03657
H	8.26164	9.98367	9.54050
H	6.43079	9.97140	7.84440
H	6.90625	5.68015	7.36623
H	5.03396	6.03797	11.44257
H	5.59844	5.15092	9.18506
H	0.24765	3.23939	-1.37181
H	2.17568	2.43334	0.01476
H	-0.83324	5.44035	-0.85652
H	0.00463	6.83869	1.04035
H	1.43682	5.51726	7.99178
H	3.01803	3.82449	1.91810
H	6.25897	2.76453	5.75598
H	8.48999	1.93855	6.43017
C	7.13264	3.41316	5.61541
C	8.40120	2.94681	5.99831
C	6.99151	4.70383	5.06893
C	9.53934	3.75002	5.82547
H	10.53137	3.38174	6.12563
C	8.13628	5.49960	4.86663
C	9.39986	5.02545	5.25711
H	8.05551	6.51883	4.47264
H	10.27845	5.67460	5.12403
H	5.68662	4.50986	4.13673

## TS-31/32

Imaginary frequency: 318.17 cm<sup>-1</sup>

ZPE(BP86/def2-SVP) = 0.8002657 Hartree (optimized geometry)  
E(BP86/def2-SVP) = -3362.9632883 Hartree (optimized geometry)  
E(PBE0/def2-TZVPP) = -3361.96948886662 Hartree (single point)

Cartesian coordinates in Å:

Pt	2.98461	5.09759	3.96770
Au	5.24624	6.29168	4.79649
C	8.81067	6.84895	5.26389
P	7.22112	6.68077	6.14548
P	3.55596	6.04381	1.90921
C	10.03309	6.68650	5.95147
C	11.24544	6.83018	5.26081
P	4.06001	4.55214	5.96884
C	11.24449	7.13025	3.88707
C	10.02857	7.28474	3.20034
C	8.81153	7.14095	3.88401
C	7.52979	5.41149	7.42425
C	7.62627	5.71793	8.79600
C	7.81432	4.68340	9.72798
C	7.89296	3.34779	9.29897
C	7.80673	3.04276	7.92777
C	7.63244	4.07160	6.99354
C	6.91225	8.23101	7.05270
C	7.81427	9.31270	7.03821
C	7.48651	10.49931	7.71525
C	6.26910	10.60566	8.40760
C	5.36899	9.52457	8.42191
C	5.68046	8.34170	7.73936
C	4.72352	4.67392	1.56366
C	6.11965	4.87104	1.64632
C	6.98570	3.77141	1.56079
C	6.46757	2.47435	1.39155
C	5.07898	2.27384	1.31096
C	4.50824	7.58785	2.09950
C	4.49841	8.56391	1.08012
C	5.18862	9.77037	1.26839
C	5.87855	9.99571	2.47071
C	5.90252	9.00920	3.47317
C	5.23158	7.77973	3.31180
C	2.44499	6.23759	0.48542
C	1.33330	7.09602	0.64093
C	0.43294	7.27130	-0.41814
C	0.63085	6.58501	-1.63015
C	1.73499	5.73122	-1.78467
C	2.64651	5.55581	-0.73090
C	1.44612	3.80766	3.50606
C	0.50162	4.06694	2.48650
C	-0.39311	3.06956	2.06776
C	-0.35509	1.79332	2.65723
C	0.57089	1.52487	3.67839
C	1.45428	2.52745	4.11450
C	3.59221	5.08656	7.63379
C	2.51794	5.99274	7.78042
C	2.27315	6.59259	9.02408

C	3.09232	6.29049	10.12654
C	4.15491	5.38156	9.98411
C	4.41144	4.77978	8.74420
C	4.72203	2.86801	5.99822
C	4.90957	0.62969	6.93611
C	5.73704	0.24778	5.86642
C	6.04262	1.17177	4.84972
C	5.53795	2.47568	4.91113
C	4.20278	3.36550	1.40404
H	6.40608	10.94850	2.63136
H	6.45518	9.21155	4.40426
H	2.44985	6.44536	4.49633
H	3.94017	8.38592	0.14860
H	5.17752	10.53757	0.48019
H	2.89816	6.76178	11.10142
H	8.19001	11.34508	7.70316
H	6.01791	11.53699	8.93662
H	4.41350	9.60402	8.96105
H	4.96948	7.50049	7.74405
H	8.76902	9.22632	6.49839
H	1.43357	7.29470	9.13515
H	7.86305	1.99971	7.58320
H	-1.12076	3.28923	1.27136
H	8.02532	2.54055	10.03452
H	7.89335	4.92427	10.79865
H	7.54308	6.76047	9.13546
H	7.56122	3.83239	5.92280
H	-1.05376	1.01064	2.32517
H	0.60051	0.53107	4.15137
H	2.16458	2.29813	4.92322
H	0.46723	5.05262	2.00080
H	7.15190	1.61570	1.31962
H	8.07246	3.93031	1.62326
H	4.67053	1.26063	1.18511
H	6.51890	5.88620	1.77918
H	12.19796	7.23983	3.34904
H	12.19757	6.70407	5.79743
H	10.02612	7.51718	2.12496
H	7.85645	7.26159	3.35263
H	10.03279	6.44095	7.02420
H	4.80010	5.14386	10.84266
H	5.25994	4.09039	8.63422
H	-0.08117	6.71750	-2.45819
H	1.89172	5.19802	-2.73405
H	-0.43129	7.94083	-0.29656
H	1.17486	7.62347	1.59506
H	1.87848	6.22373	6.91473
H	5.78280	3.20204	4.11904
H	6.13940	-0.77505	5.82006
H	3.51372	4.89126	-0.85570
H	6.68101	0.87565	4.00471
H	3.11502	3.20394	1.36041
C	4.39442	1.93359	7.00345
H	4.65925	-0.09489	7.72526
H	3.74025	2.22516	7.83803