SUPPORTING INFORMATION

Monoaurated vs. Diaurated Intermediates: Causality or Independence?

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1. Preparation of reaction mixtures

Table S1. Composition of stock solutions for experiments with 1-phenylpropyne and 3-hexyne

Solution	Catalyst	Quantity	Solvent	Quantity
I	[Au(IPr)(CH_3CN)]BF_4 (5.4 mol%)	9.3 mg	Acetone	1 ml
II	[Au(IPr)(CH_3CN)]BF_4 (2.7 mol%)	4.7 mg	Acetone	1 ml
III	[Au(IPr)(CH_3CN)]BF_4 (10.8 mol%)	18.6 mg	Acetone	1 ml
IV	[Au_2(IPr)$_2$(OH)]BF_4 (5.4 mol%)	16.5 mg	Acetone	1 ml
V	[Au(IPr)Cl] (5.4 mol%)	8 mg	Acetone	0.5 ml
	$AgSbF_6$ (6.5 mol%)	5 mg	Acetone	0.5 ml
VI	[Au(IPr)Cl] (5.4 mol%)	8 mg	Acetone	0.5 ml
	$AgBF_4$ (6.5 mol%)	3 mg	Acetone	0.5 ml
VII	[Au(IPr)Cl] (5.4 mol%)	8 mg	Acetone	0.9 ml
	$AgPF_6$ (6.5 mol%)	4 mg	Water	0.1 ml
VIII	[Au(IPr)(CH_3CN)]BF_4 (5.4 mol%)	9.3 mg	Acetone	0.5 ml
	TsOH (10.8 mol%)	5 mg	Acetone	0.5 ml
IX	$PhCCCH_3$	10 µl	Acetone	1 ml
X	$PhCCCD_3$	10.2 µl	Acetone	1 ml
XI	D_5-$PhCCCH_3$	10.4 µl	Acetone	1 ml
XII	EtCCEt	8 µl	THF	1 ml
XIII	D_{10}-EtCCEt	8 µl	THF	1 ml
XIV	PhCCPh	12.39 mg	THF	1 ml

1.1 Reaction mixtures for Delayed Reactant Labelling experiments

Experiments with PhCCCD$_3$ /D$_5$-PhCCCH$_3$ or with EtCCEt/D$_{10}$-EtCCEt: Reaction mixtures were prepared by mixing 80 µl of the stock solution **I - VIII**, 120 µl of **IX** or **XII** (see Table S1) and 100 µl of H_2O (or D_2O) in 200 µl of acetone and left to react for a time delay. After a time delay elapsed, 120 µl of solution **X** (event. **XI**) or **XIII**, respectively, was added. Reaction mixture was immediately monitored by ESI-MS. For the sheath liquid: 30 mg of $NaSbF_6$ was dissolved in 3 ml of acetone.

Labelling by D_2O – experiment without a time delay: Reaction mixtures were prepared by mixing 80 µl of the stock solution **I - VII**, 240 µl of **IX**, 100 µl of mixture of H_2O and D_2O (the ratio was 1: 0.5, 1, 2, 3, 4, 5, 6, 7, 10, 20) in 200 µl of acetone (for composition of the stock solutions see Table S1). After mixing, reaction mixture was immediately monitored by ESI-MS. For the sheath liquid: 30 mg of $NaSbF_6$ was dissolved in 3 ml of acetone.

2. Results on NMR experiments

2.1 Results for experiments with 1-phenylpropyne

The NMR experiments were recorded using a Bruker AVANCE III (600 MHz) and the δ scale was referenced to the solvent residual peak at δ = 3.31 ppm. The solutions of a catalyst and reactants were mixed and immediately probed by the NMR instrument.

Reaction mixtures were prepared by mixing 80 µl of the stock solution **I**, 240 µl of **IX** and 100 µl of H_2O in 200 µl of D_6-acetone (see Table S1, we used D_6-acetone instead of acetone). Reaction mixture was immediately monitored by NMR spectroscopy.

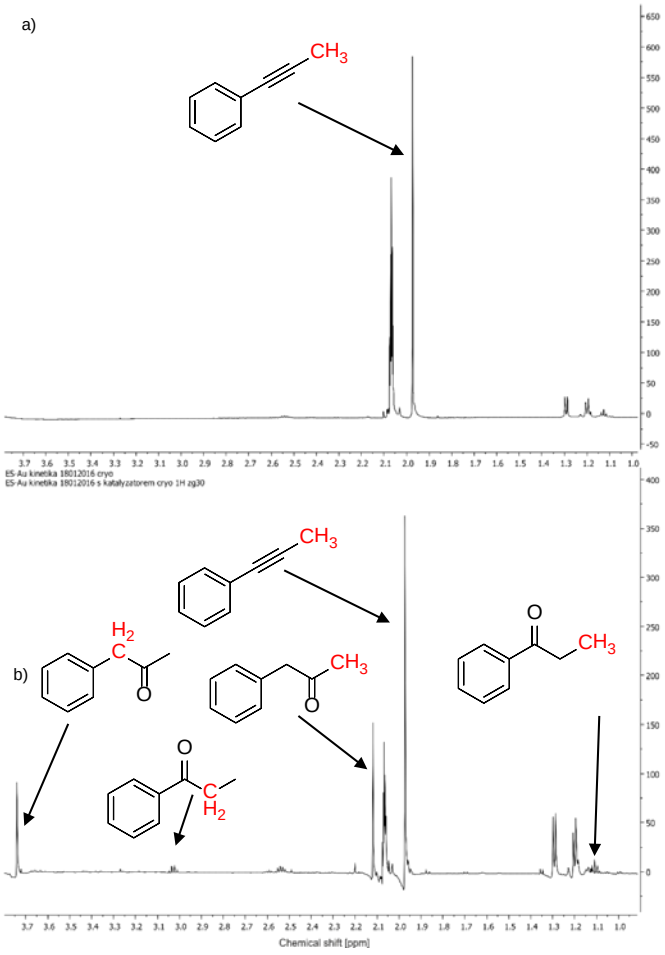


Figure S1. ^{1}H NMR spectrum of the reaction mixture of 5.4 mol% [Au(IPr)(CH_3CN)(BF_4)] in acetone/water (5:1) a) 3 and b) 200 minutes after the addition of $PhCCCH_3$.

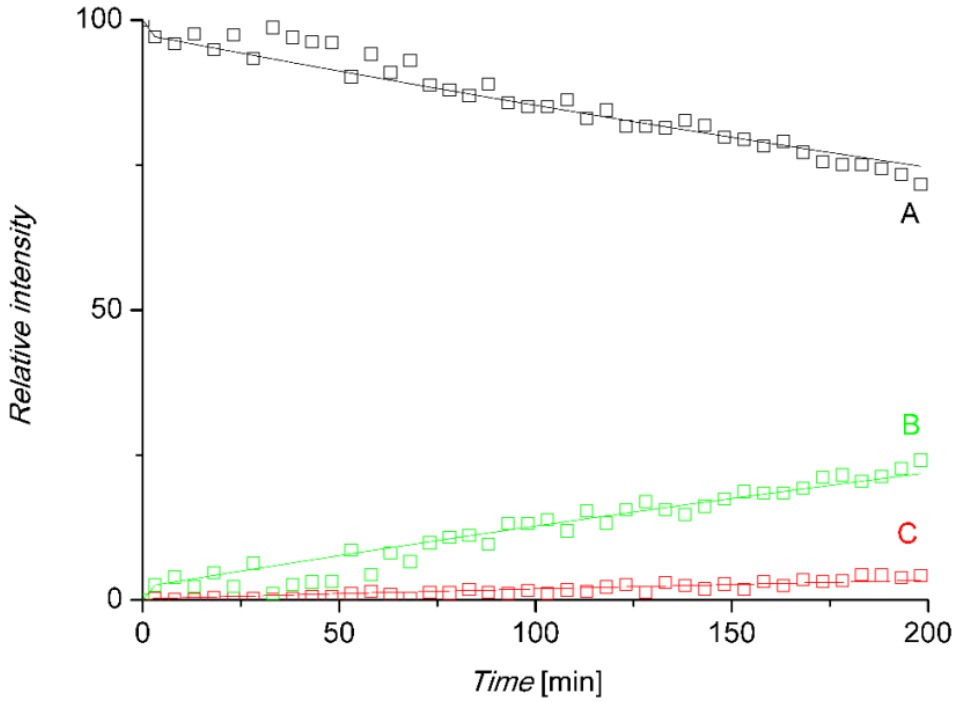
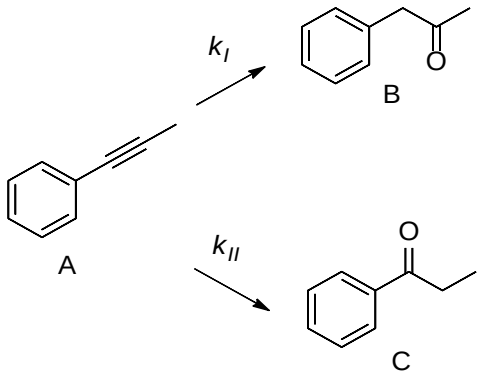


Figure S2. Relative ratio of 1-phenylpropyne (A), phenylacetone (B) and propiophenone (C). Full curves represents fits obtained in GNU Octave.



Scheme S1. Addition of water to phenylpropyne.

We have assumed pseudo-first order kinetics based on Scheme S1:

$$\frac{d[A]}{dt} = -k_I[A] - k_{II}[A], \quad \text{(S1)}$$

$$\frac{d[B]}{dt} = k_I[A], \quad \text{(S2)}$$

$$\frac{d[C]}{dt} = k_{II}[A]. \quad \text{(S3)}$$

These equations were used as a kinetic model for the fitting of experimental data with mathematic software GNU Octave. Rate constants k_I and k_{II} were free fit parameters and equations were solved numerically. We used the least squares method for the fitting of experimental data. Obtained rate constants are shown in Table S2.

Table S2. Rate constants obtained by NMR spectroscopy.

k_I^{NMR} [min^{-1}]	k_{II}^{NMR} [min^{-1}]
$12 \cdot 10^{-4}$	$1{,}86 \cdot 10^{-4}$

2.2 Results for experiments with 3-hexyne

The NMR experiments were recorded using a Bruker AVANCE (400 MHz) and the δ scale was referenced to the solvent residual peak at δ = 1.73 ppm (D_8-THF). The solutions of the catalyst and the reactants were mixed and immediately probed by the NMR instrument, before and after the addition of water.

Reaction mixtures were prepared by mixing 80 µl of the stock solution **I**, 240 µl of **XII** and 100 µl of H_2O in 200 µl of D_8-THF (see Table S1, we used D_8-THF instead of THF). Reaction mixture was immediately monitored by NMR spectroscopy.

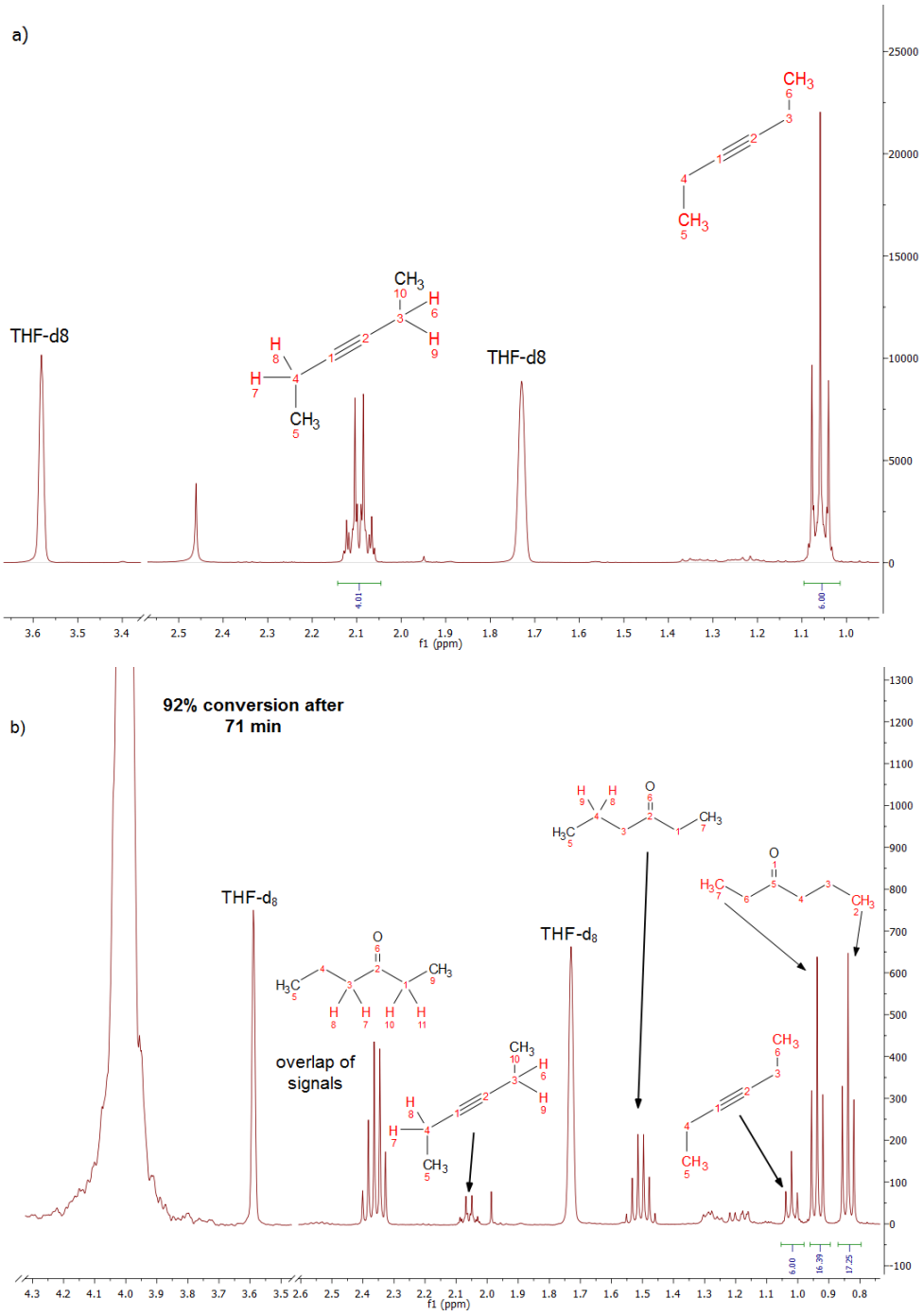


Figure S3. ^{1}H NMR spectrum of the reaction mixture of 6 mol% [Au(IPr)(CH_3CN)(BF_4)] in THF/water (5:1) and 3-hexyne a) 0 and b) 71 minutes after the addition of water.

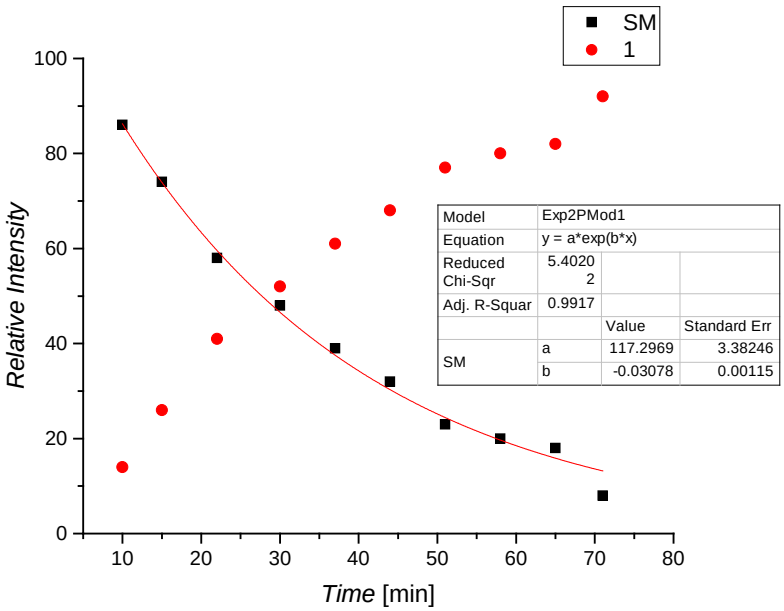


Figure S4. Evolution of concentrations of 3-hexyne (SM) and 3-hexanone (1) in time determined from NMR experiments.

3. Mass spectrometry experiments

3.1 Experimental details

The experiments were performed with a TSQ 7000 mass spectrometer[1] with a quadrupole-octopole-quadrupole configuration. The ions were generated by electrospray ionization (ESI) from the reaction mixtures of an alkyne with 5.4 mol% [Au(IPr)(CH_3CN)(BF_4)] in acetone/water (5:1) at soft ionization (low potentials on the entrance ion optics and the temperature of the capillary was 200 °C). The collision-induced dissociation experiments were performed with mass-selected ions, which were collided with xenon ($p_{Xe} \cong 0.2$ mTorr). The ionic products were analyzed by the second quadropole.

3.2 Isotopic correction for carbon-13 for experiments with 1-phenylpropyne

The isotopic correction for carbon-13 was performed based on experimentally determined isotopic pattern. Hence, we recorded the mass spectra of the reaction mixture of 1-phenylpropyne

with 5.4 mol% [Au(IPr)(CH_3CN)(BF_4)] in acetone/water (5:1) in four independent measurements (0.12 mmol solution of $NaSbF_6$ in 3 ml of acetone was infused as a sheath liquid with the reaction mixture in order to trap neutral complexes by sodium cations). From the MS spectra, we have determined the percentage of carbon-13 from the ratio of peaks corresponding to the ions M, M+1, and M+2, where

M = [Au(IPr)($PhCCCH_3$,OH)]H^+ (**1**H^+), [Au(acetone)(IPr)($PhCCCH_3$,OH)]Na^+ (**1**(acetone)Na^+), $[Au_2(IPr)_2(OH)]^+$, and $[Au_2(IPr)_2(PhCCCH_3,HO)]^+$ (**2**$^+$) (Table S3).

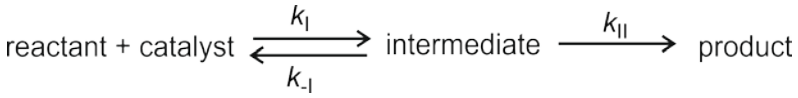
This experimentally determined ratio was used for the carbon-13 correction in determination of the abundance of [Au(IPr)($PhCCCH_3$,OD)]H^+ (*m*/*z* 720), [Au(IPr)($PhCCCH_3$,OD)]D^+ (*m*/*z* 721), [Au(acetone)(IPr)($PhCCCH_3$,OD)]Na^+ (*m*/*z* 800), $[Au_2(IPr)_2(OD)]^+$ (*m*/*z* 1188), and $[Au_2(IPr)_2(PhCCCH_3,DO)]^+$ (*m*/*z* 1304).

Table S3. Isotopic correction for carbon-13

M	M+1 (%)	M+2 (%)
1H^+	40.9 ± 1.5	8.9 ± 2.2
1(acetone)Na^+	41.1 ± 1.4	9.3 ± 0.8
$[Au_2(IPr)_2(OH)]^+$	60.5 ± 0.5	19.4 ± 1.3
2$^+$	69.3 ± 0.5	24.4 ± 0.6

3.3 Kinetic model for Delayed Reactant Labelling experiments

The delayed reactant labelling method is based on monitoring of a reaction mixture containing one of the reactants as a mixture of isotopically labelled and unlabelled molecules with different reaction times.[2] All signals of ions containing the labelled/unlabelled reactant (reactant complexes, intermediates, product complexes) appear as a couple of MS peaks in the spectrum (isotopically labelled and unlabelled). The key trick is the time delay (t_D) for the addition of the labelled reactant to the reaction mixture. This allows us to follow the kinetics of all ions that contain this particular reactant. We assume that labelling does not affect effectivity of ion ionization. We evaluate the signals only relative to each other, thus overall intensity is not important.



Scheme S2. Model reaction for a kinetic model derivation

Kinetic model for mathematic description of the experimental data was derived from a model shown in Scheme S2. Here we assume first-order kinetics for the reaction between a reactant (React) and a catalyst (Cat) yielding an intermediate (Int), which then converts to a product (Prod). If formation and degradation of the intermediate (Int) can be described using steady-state approximation, then we can assemble the following equation:

$$k_I[\text{React}][\text{Cat}] = (k_{-I} + k_{II})[\text{Int}]_{eq} \quad \text{(S4)},$$

where $[\text{Int}]_{eq}$ is the equilibrium concentration of the intermediate.

The reaction mixture is first prepared with unlabelled reactants and allowed to react for the t_D. During this time a certain steady-state concentration of intermediate $[\text{Int}]_{eq}$ is achieved. With a time delay a labelled reactant (React^{label}) is added and system is deflected out of steady-state conditions. Immediately, the reaction mixture is being monitored by ESI-MS.

The evolution of the intensity of the signals that corresponds to the reaction intermediate (Int) and to the labelled intermediate (Int^{label}) in time reflects reestablishment of the steady-state conditions and can be described by following equation:

$$\frac{d[\text{Int}]}{dt} = (k_{-I} + k_{II})[\text{Int}]_{eq} - (k_{-I} + k_{II})[\text{Int}] = k'([\text{Int}]_{eq} - [\text{Int}]), \quad \text{(S5)},$$

where $k_{deg} = k_{-I} + k_{II}$.

At the mixing time t_0 no labelled intermediate is present in the reaction mixture ($[\text{Int}^{label}] = 0$). If we normalize a sum of concentration of the labelled and unlabelled intermediate to one ($[\text{Int}^{label}] + [\text{Int}] = 1$), their time dependence can be described by following equations:

$$[\text{Int}]_t = e^{-k_{deg}'t} + [\text{Int}]_{eq}\,(1 - e^{-k_{deg}\ t}) \quad \text{(S6a)}$$

$$[\text{Int}^{label}]_t = [\text{Int}^{label}]_{eq}\left(1 - e^{-k_{deg}\ t}\right). \quad \text{(S6b)}$$

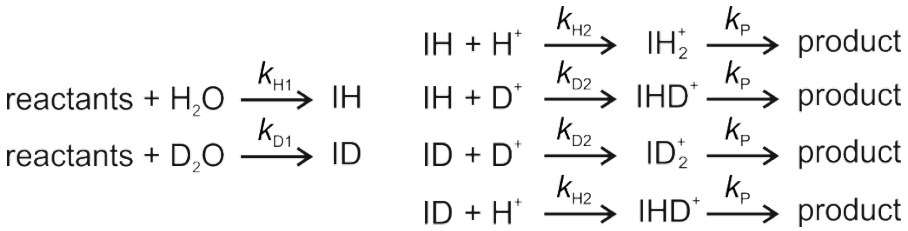
In the real experiment a precise ratio of the labelled and unlabelled intermediates is obtain by fitting experimental data.

For the half-life of the intermediates the following equation can be used:

$$t_{1/2} = \frac{\ln 2}{k_{deg}}. \quad \text{(S7)}$$

The intermediates formation rate (k_1) does not influence a shape of the curves if we assume that the rate constant for the formation of labelled and unlabelled intermediates is the same. Further we assume that labelled and unlabelled intermediates react with the same rate constant.

3.4 Kinetic model for the experiments without the delay



Scheme S3. Kinetic model for the distribution of H and D in the monoaurated complex in the experiments without the delay

Kinetic model for mathematic description of the experimental data was derived from a model shown in Scheme S3. Here, we assume pseudo first-order kinetics for the reaction of reactants (R) with H_2O (OH) or D_2O (OD) yielding an intermediate (I), which then converts to a product. If the formation and the degradation of the intermediates can be described using the steady-state approximation, then we can assemble following equation:

$$d[IH]/dt = 0 = k_{H1}[R][OH]-k_{H2}[IH][H]-k_{D2}[IH][D] \quad \text{(S8)}$$

$$[IH] = k_{H1}[R][OH]/(k_{H2}[H]+k_{D2}[D]) \quad \text{(S9)}$$

$$d[ID]/dt = 0 = k_{D1}[R][OD]-k_{H2}[ID][H]-k_{D2}[ID][D] \quad \text{(S10)}$$

$$[ID] = k_{D1}[R][OD]/(k_{H2}[H]+k_{D2}[D]) \quad \text{(S11)}$$

$$[IH]/([IH]+[ID]) = (k_{H1}[R][OH]/(k_{H2}[H]+k_{D2}[D]))((k_{H2}[H]+k_{D2}[D])/[R](k_{H1}[OH]+k_{D1}[OD])) =$$
$$= k_{H1}[OH]/(k_{H1}[OH]+k_{D1}[OD]) = (k_{H1}[OH]/k_{D1}[OD])/((k_{H1}[OH]/k_{D1}[OD])+1) = ax/(ax+1),$$
where $a = k_{H1}/k_{D1}$ and $x = [OH]/[OD]$ (S12)

$$[ID]/([IH]+[ID]) = (k_{D1}[R][OD]/(k_{H2}[H]+k_{D2}[D]))((k_{H2}[H]+k_{D2}[D])/[R](k_{H1}[OH]+k_{D1}[OD])) =$$
$$= k_{D1}[OD]/(k_{H1}[OH]+k_{D1}[OD]) = 1/((k_{H1}[OH]/k_{D1}[OD])+1) = 1/(ax+1),$$
where $a = k_{H1}/k_{D1}$ and $x = [OH]/[OD]$ (S13)

$$d[IH_2]/dt = 0 = k_{H2}[IH][H]-k_P[IH_2] \quad \text{(S14)}$$
$$[IH_2] = k_{H2}[IH][H]/k_P = k_{H2}[H]k_{H1}[R][OH]/k_P(k_{H2}[H]+k_{D2}[D]) \quad \text{(S15)}$$

$$d[ID_2]/dt = 0 = k_{D2}[ID][D]-k_P[ID_2] \quad \text{(S16)}$$
$$[ID_2] = k_{D2}[ID][D]/k_P = k_{D2}[D]k_{D1}[R][OD]/k_P(k_{H2}[H]+k_{D2}[D]) \quad \text{(S17)}$$
$$d[IHD]/dt = 0 = k_{H2}[ID][H]+k_{D2}[IH][D]-k_P[IHD] \quad \text{(S18)}$$
$$[IHD] = (k_{H2}[ID][H]+k_{D2}[IH][D])/k_P = (k_{H2}[H]k_{D1}[R][OD]+k_{D2}[D]k_{H1}[R][OH])/k_P(k_{H2}[H]+k_{D2}[D])$$
(S16)

$$[IH_2]+[ID_2]+[IHD] =$$
$$((k_{H2}[H]k_{H1}[R][OH])+(k_{D2}[D]k_{D1}[R][OD])+(k_{H2}[H]k_{D1}[R][OD])+(k_{D2}[D]k_{H1}[R][OH]))/((k_{H2}[H]+$$
$$k_{D2}[D])k_P) \quad \text{(S19)}$$

$$[IH_2]/([IH_2]+[ID_2]+[IHD]) = k_{H2}[H]k_{H1}[OH]/$$
$$((k_{H2}[H]k_{H1}[OH])+(k_{D2}[D]k_{D1}[OD])+(k_{H2}[H]k_{D1}[OD])+(k_{D2}[D]k_{H1}[OH]))=$$
$$(k_{H2}[H]k_{H1}[OH]/k_{D2}[D]k_{D1}[OD])/(1+(k_{H2}[H]k_{H1}[OH]/k_{D2}[D]k_{D1}[OD])+(k_{H2}[H]/k_{D2}[D])+(k_{H1}[OH]/$$
$$k_{D1}[OD])) = abx^2/(abx^2+ax+bx+1),$$
where $a = k_{H1}/k_{D1}$, $b = k_{H2}/k_{D2}$, and $x = [OH]/[OD]$ (S20)

$$[ID_2]/([IH_2]+[ID_2]+[IHD]) = k_{D2}[D]k_{D1}[OD]/$$
$$((k_{H2}[H]k_{H1}[OH])+(k_{D2}[D]k_{D1}[OD])+(k_{H2}[H]k_{D1}[OD])+(k_{D2}[D]k_{H1}[OH]))=$$
$$1/(1+(k_{H2}[H]k_{H1}[OH]/k_{D2}[D]k_{D1}[OD])+(k_{H2}[H]/k_{D2}[D])+(k_{H1}[OH]/k_{D1}[OD])) =$$
$$1/(abx^2+ax+bx+1),$$
where $a = k_{H1}/k_{D1}$, $b = k_{H2}/k_{D2}$, and $x = [OH]/[OD]$ (S21)

$[IHD]/([IH_2]+[ID_2]+[IHD]) = (k_{H2}[H]k_{D1}[OD]+ k_{D2}[D]k_{H1}[OH])/((k_{H2}[H]k_{H1}[OH])+(k_{D2}[D]k_{D1}[OD])+(k_{H2}[H]k_{D1}[OD])+(k_{D2}[D]k_{H1}[OH]))= ((k_{H2}[H]/k_{D2}[D])+(k_{H1}[OH]/k_{D1}[OD]))/(1+(k_{H2}[H]k_{H1}[OH]/k_{D2}[D]k_{D1}[OD])+(k_{H2}[H]/k_{D2}[D])+(k_{H1}[OH]/k_{D1}[OD])) = (ax+bx)/(abx^2+ax+bx+1),$

where $a = k_{H1}/k_{D1}$, $b = k_{H2}/k_{D2}$, and $x = [OH]/[OD]$ (S22)

3.5 Results of ESI-MS experiments for reactions with 1-phenylpropyne

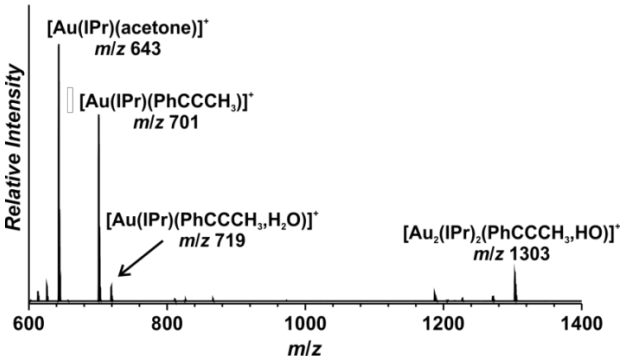


Figure S5. ESI-MS source spectrum of a solution of 1-phenylpropyne with 5.4 mol% $[Au(IPr)(CH_3CN)(BF_4)]$ in acetone/water (5:1).

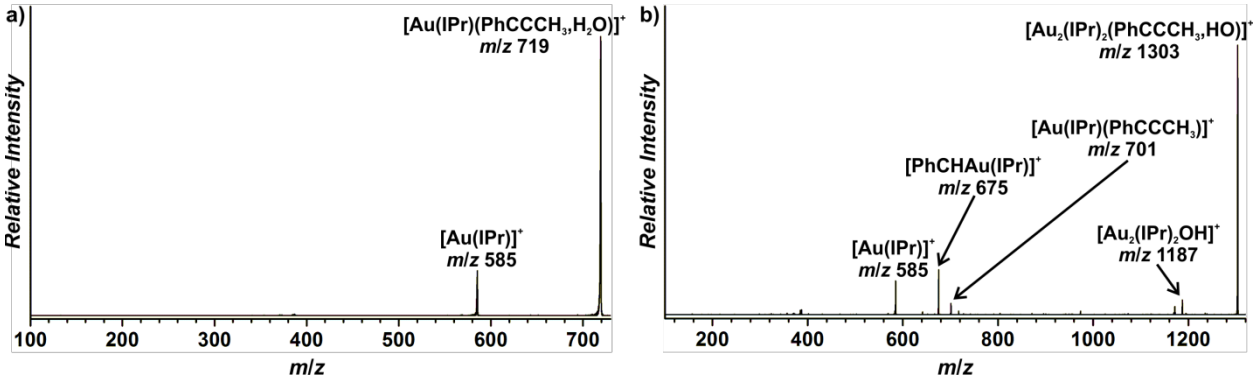


Figure S6. a) CID spectrum of the complex **1**H^+ $[Au(IPr)(PhCCCH_3,OH)]H^+$ (*m*/*z* 719) (E_{coll} = 4.6 eV, p_{Xe} = 0.2 mTorr). b) CID spectrum of the complex **2**$^+$ $[Au_2(IPr)_2(PhCCCH_3,HO)]^+$ (*m*/*z* 1303) (E_{coll} = 2.7 eV, p_{Xe} = 0.2 mTorr).

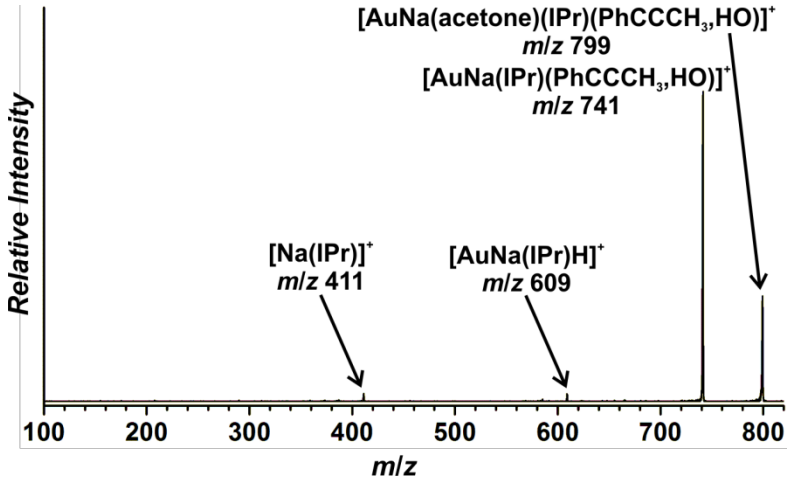


Figure S7. CID spectrum of the complex [Au(IPr)(acetone)(PhCCCH$_3$,OH)]Na$^+$ (*m*/*z* 799) (E_{coll} = 4.2 eV, p_{Xe} = 0.2 mTorr).

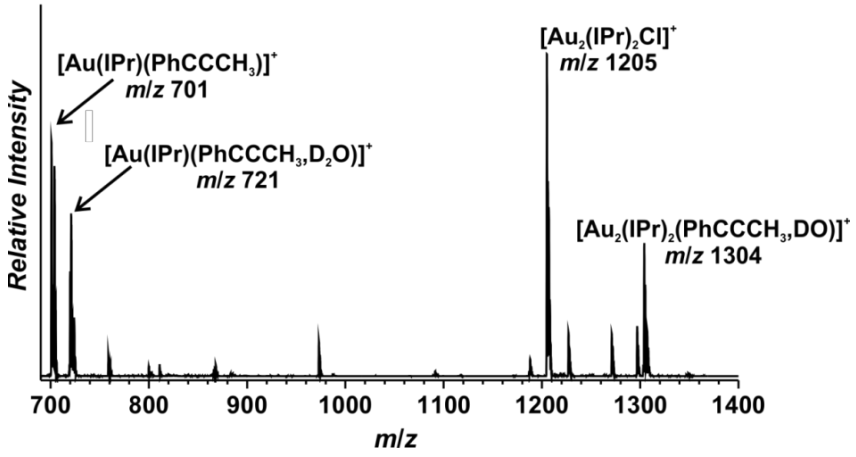


Figure S8. ESI-MS source spectrum of a solution of 1-phenylpropyne with 5.4 mol% [Au(IPr)(CH$_3$CN)(BF$_4$)] in acetone/D$_2$O (5:1).

3.5.1 Results of labelling experiments

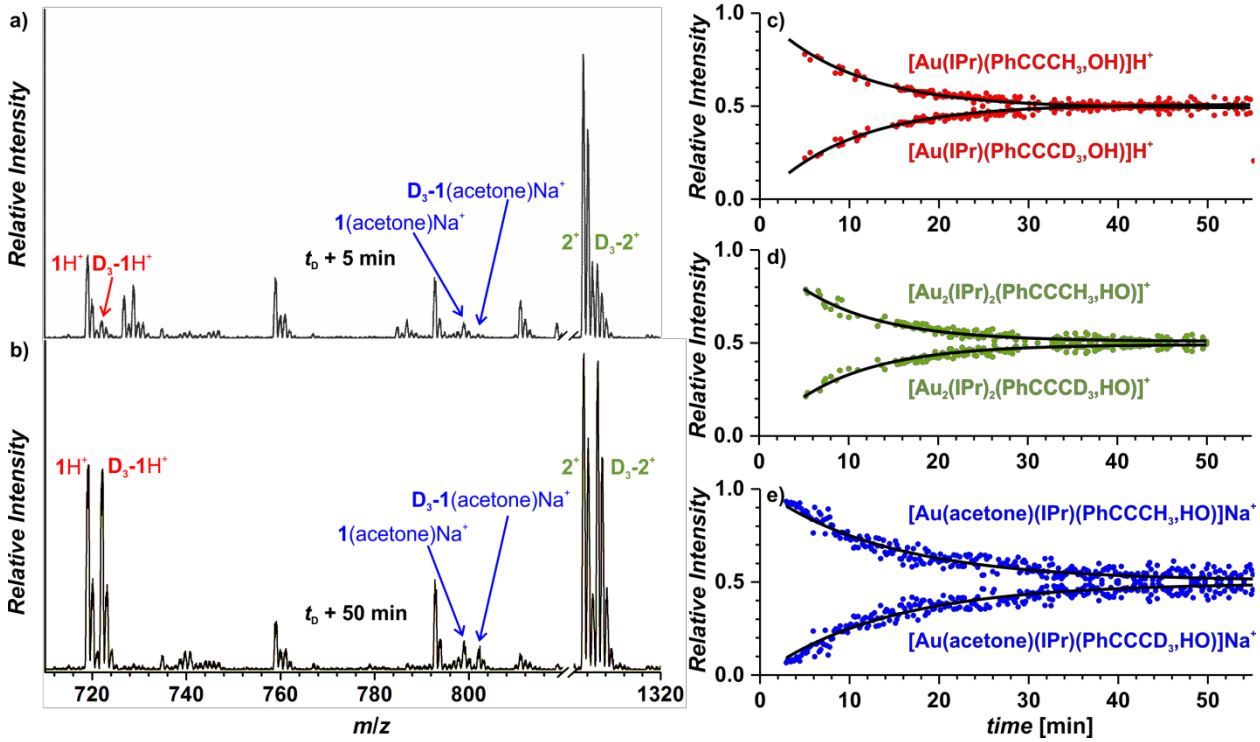


Figure S9. Delayed reactant labelling method. a) ESI-MS spectrum recorded 5 min after the solution of $PhCCCD_3$ in acetone is added to the reaction mixture of 1-phenylpropyne with 5.4 mol% [Au(IPr)(CH_3CN)(BF_4)] in acetone/water (5:1) (0.12 mmol solution of $NaSbF_6$ in 3 ml of acetone was infused as a sheath liquid with the reaction mixture in order to trap neutral complexes by sodium cations); time-delay was 30 min. b) The same as a), but the ESI-MS spectrum was recorded 50 minutes after the labelling of the reaction mixture. Mutual time evolution of c) the **1**H^+ and D_3-**1**H^+**,** d) the **2**$^+$ and D_3-**2**$^+$, and e) the **1**(acetone)Na^+ and D_3-**1**(acetone)Na^+ signals in the experiment described in a) (symbols). The dashed lines correspond to the data fits according to Eq. S6a and S6b.

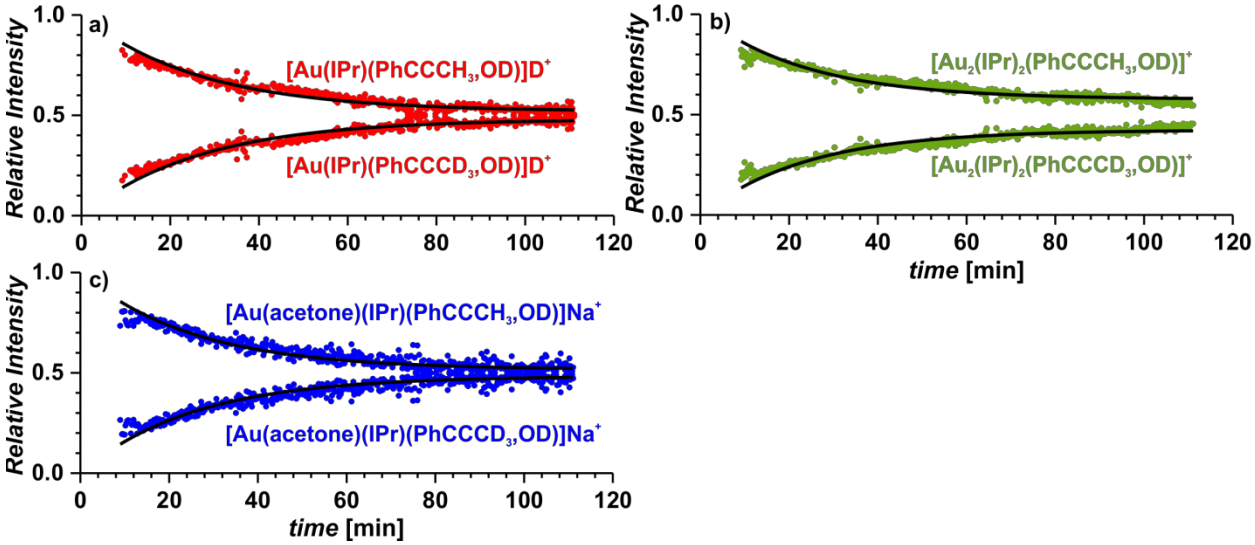


Figure S10. Mutual time evolution of a) **1**H^+ and D_3-**1**H^+, d) **2**$^+$ and D_3-**2**$^+$, and c) **1**(acetone)Na^+ and D_3-**1**(acetone)Na^+ (symbols) in the experiment, where the solution of $PhCCCD_3$ in acetone is added to the reaction mixture of 1-phenylpropyne with 5.4 mol% [Au(IPr)(CH_3CN)(BF_4)] in acetone/D_2O (5:1); time-delay was 30 min (0.12 mmol solution of $NaSbF_6$ in 3 ml of acetone was infused as a sheath liquid with the reaction mixture in order to trap neutral complexes by sodium cations). The dashed lines correspond to the data fits according to Eq. S6a and S6b.

Table S4. Relative intensities of the signals of complexes **1**X^+ ([Au(IPr)($PhCCCH_3$,X_2O)]$^+$), **2**$^+$ ([Au_2(IPr)$_2$($PhCCCH_3$,XO)]$^+$), **1**(acetone)Na^+ ([Au(IPr)(acetone)($PhCCCH_3$,XO)]Na^+), and [Au_2(IPr)$_2$(XO)]$^+$ (X = H or D).

Catalyst	$Au_2(IPr)_2(OX)$		**1**X^+			**2**$^+$		**1**(acetone)Na^+	
	H	D	HH	HD	DD	H	D	H	D
5.4 mol% Au(IPr)Cl/	0.50	0.50	0.42	0.52	0.07	0.82	0.18	-	-
6.5 mol% $AgBF_4$	0.69	0.31	0.69	0.30	0.01	0.86	0.14	-	-
5.4 mol% Au(IPr)Cl/ 6.5 mol% $AgPF_6$	0.65	0.35	0.67	0.31	0.02	0.85	0.15	-	-
5.4 mol% Au(IPr)Cl/	0.79	0.21	0.72	0.26	0.01	0.86	0.14	-	-
6.5 mol% $AgSbF_6$	0.64	0.36	0.66	0.32	0.02	0.84	0.16	-	-
5.4 mol% Au(IPr)(CH_3CN)BF_4	0.49	0.51	0.41	0.53	0.07	0.80	0.20	0.85	0.15
	0.32	0.68	0.22	0.59	0.19	0.68	0.32	0.73	0.27
	0.48	0.52	0.38	0.54	0.08	0.80	0.20	0.87	0.13
	0.32	0.68	0.23	0.59	0.17	0.67	0.33	0.75	0.25
	0.71	0.29	0.67	0.32	0.02	0.89	0.11	0.95	0.05
	0.49	0.51	0.40	0.52	0.08	0.76	0.24	0.73	0.27
	0.26	0.74	0.19	0.56	0.25	0.53	0.47	0.59	0.41
	0.20	0.80	0.13	0.55	0.32	0.52	0.48	-	-
	0.17	0.83	0.10	0.51	0.39	0.47	0.53	-	-
	0.18	0.82	0.10	0.53	0.37	0.47	0.53	-	-
	0.13	0.87	0.07	0.45	0.48	0.37	0.62	-	-
	0.09	0.91	0.03	0.38	0.59	0.31	0.69	-	-
	0.05	0.95	0.02	0.26	0.72	0.21	0.79	-	-
	0.49	0.51	0.39	0.53	0.08	0.79	0.21	-	-
Au(IPr)(CH_3CN)BF_4 10.8 mol%	0.49	0.51	0.39	0.56	0.05	0.82	0.18	0.87	0.13
	0.32	0.68	0.23	0.58	0.18	0.70	0.30	0.76	0.24
	0.66	0.34	0.60	0.37	0.03	0.91	0.09	1.00	0.00
Au(IPr)(CH_3CN)BF_4 2.7 mol%	0.47	0.53	0.37	0.56	0.07	0.81	0.19	0.89	0.11
	0.31	0.69	0.22	0.60	0.18	0.70	0.30	0.77	0.23
	0.37	0.63	0.26	0.57	0.17	0.73	0.27	0.78	0.22
5.4 mol% $Au_2(IPr)_2(OH)BF_4$	0.32	0.68	0.27	0.58	0.15	0.70	0.30	0.74	0.26

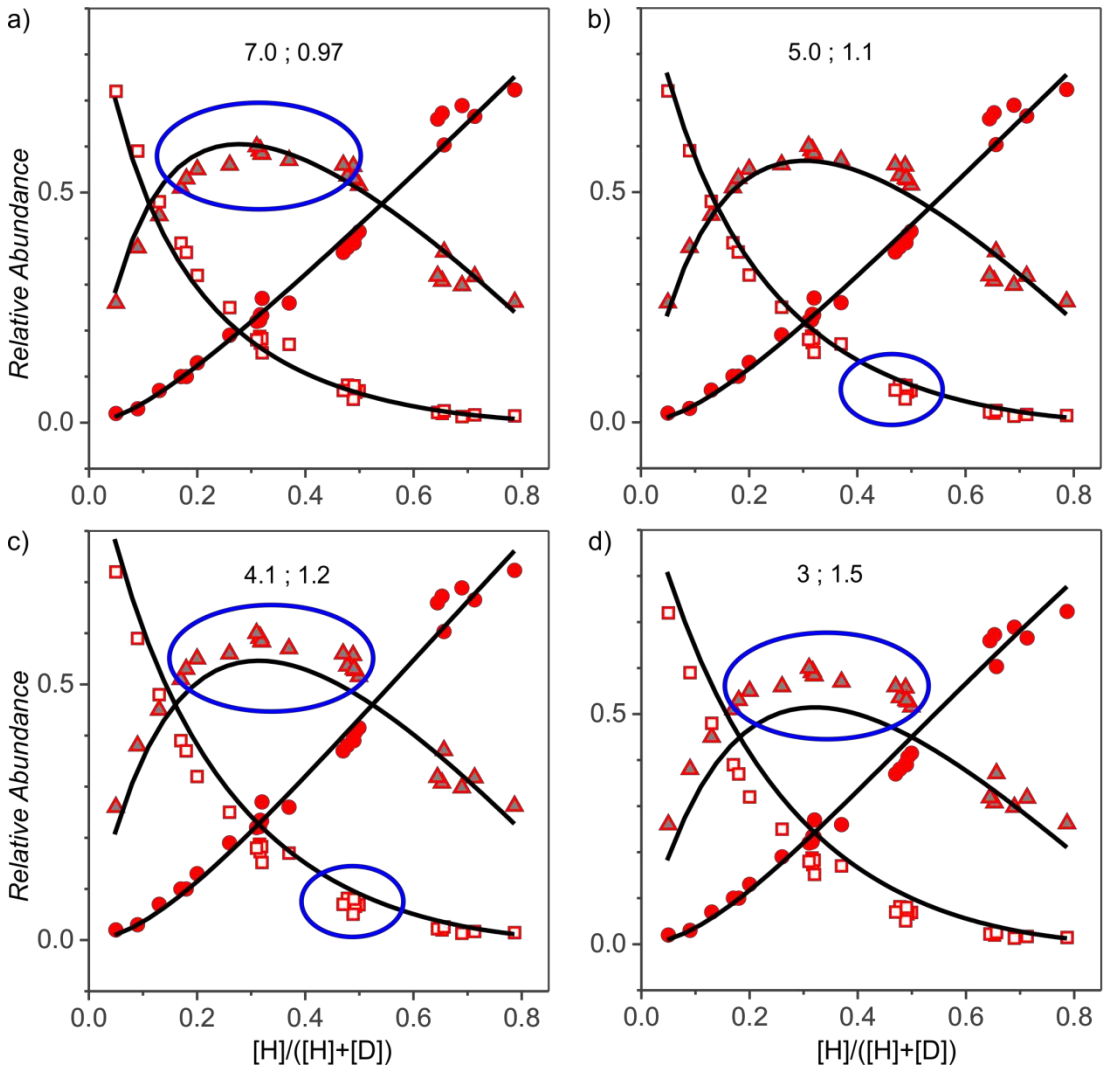


Figure S11. Formation of the monoaurated intermediates in the reaction of 1-phenylpropyne with a mixture of H_2O and D_2O with a variable H/D ratio (catalyst: 5.4 mol% [Au(IPr)(CH_3CN)(BF_4)]). The ratio of "acidic" H and D (x-axis) was determined from the ratio of $[Au_2(IPr)_2(OH)]^+$ and $[Au_2(IPr)_2(OD)]^+$ in each experiment. The graphs show the relative abundances of H-**1**H^+ (circles) vs. D-**1**H^+ + H-**1**D^+ (triangles), and vs. D-**1**D^+ (squares). The experimental results were fitted with kinetic equations S21 – S22, where the parameter "**a**" (KIE) was fixed as a) 7, b) 5, c) 4.1, and d) 3. Parameter "**b**" was fitted and is given in the figure as the second number.

The paper shows an unconstrained fit of the data. Here, we show robustness of the fit by testing constrained fits. The constrains of *KIE* = 3, 4.1, or 5 leads to a too slow decline of the D-**1**D^+ intensity. Conversely, KIE = 7 results in a too fast decline of the D-**1**D^+ intensity. Concomitant with these problems, the intensities of mixed ions D-**1**H^+ + H-**1**D^+ do not fit either.

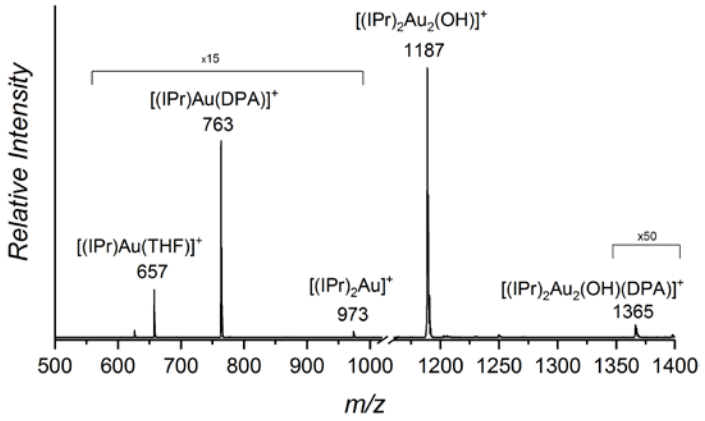


Figure S12. ESI-MS source spectrum of a solution of diphenylacetylene with 5.4 mol% [Au(IPr)(CH_3CN)(BF_4)] in THF/water (1:1).

3.6 Results of ESI-MS experiments for reactions with 3-hexyne

Standard reaction conditions for the following MS experiments:

6 mol % of [(IPr)Au(CH_3CN)(BF_4)] (0.18 mM) and 2.98 mM of 3-hexyne (in delayed reactant labelling 1.49 mM of 3-hexyne and 1.49 mM of D_{10}-3-hexyne) and THF/water (3.6:1)

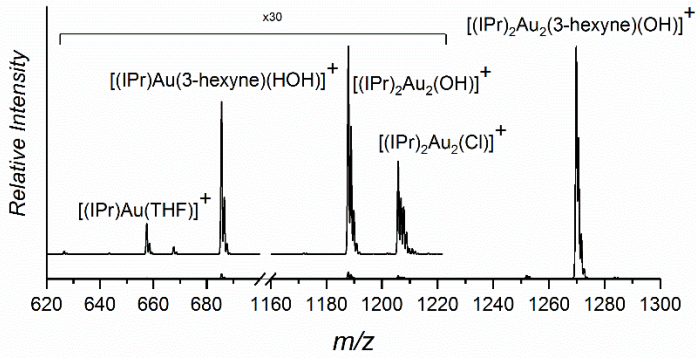


Figure S13. ESI-MS source spectrum of a solution of 3-hexyne with 6 mol% [Au(IPr)(CH_3CN)(BF_4)] in THF/water (5:1).

3.6.1 Delayed reactant labeling

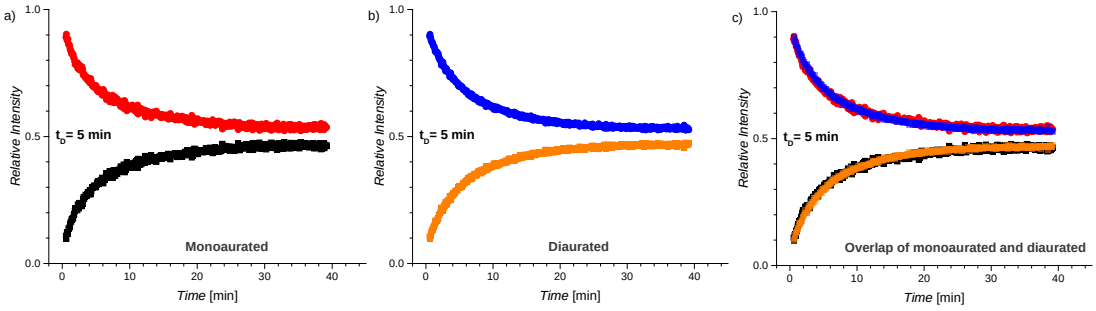


Figure S14: Relative evolution of MS signals of ions containing 3-hexyne and D_{10}-EtCCEt in time. The reaction was performed under the standard conditions with half amount of hexyne D_{10}-EtCCEt, the second half, D_0-EtCCEt, was added after t_d = 5 min. The graphs show the mutual time evolution of (a) the monoaurated signals [(IPr)Au(EtCCEt)OH_2] (black line) and [(IPr)Au(D_{10}-EtCCEt)OH_2] (red line), (b) the diaurated signals [$(IPr)_2Au_2$(EtCCEt)OH] (orange line) and [$(IPr)_2Au_2$(D_{10}-EtCCEt)OH] (blue line) and (c) the overlap of the time evolution of the signals of monoaurated and diaurated ions.

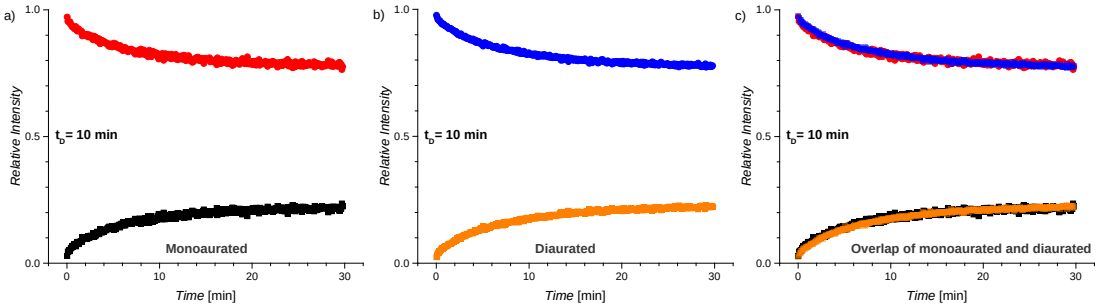


Figure S15. Relative evolution of MS signals of ions containing 3-hexyne and D_{10}-EtCCEt in time. The reaction was performed under the standard conditions with half amount of hexyne D_{10}-EtCCEt, the second half, D_0-EtCCEt, was added after t_d = 10 min. The graphs show the mutual time evolution of (a) the monoaurated signals [(IPr)Au(EtCCEt)OH_2] (black line) and [(IPr)Au(D_{10}-EtCCEt)OH_2] (red line) and (b) the diaurated signals [$(IPr)_2Au_2$(EtCCEt)OH] (orange line) and [$(IPr)_2Au_2$(D_{10}-EtCCEt)OH] (blue line) and (c) the overlap of the time evolution of the signals of monoaurated and diaurated ions.

3.6.2 Analysis of the kinetics revealed by delayed reactant labelling

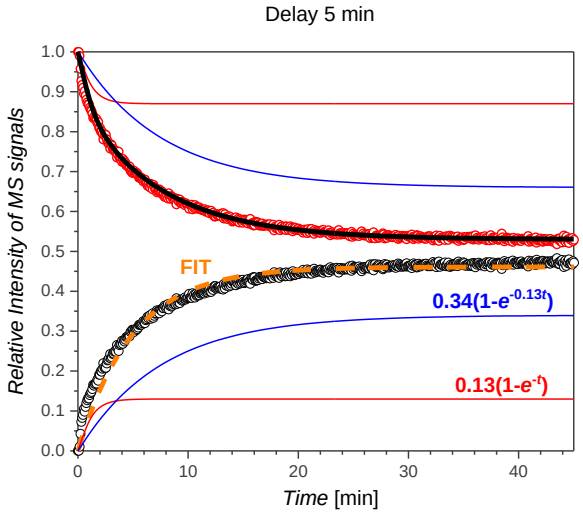


Figure S16. Fit (dashed orange line) of the evolution of the signals of [$(IPr)_2Au_2$(EtCCEt)OH] and [$(IPr)_2Au_2$(D_{10}-EtCCEt)OH] from the experiment shown in Figure S14. The fit shows that the time dependence does not correspond to a single process (see the difference between the black experimental data and the yellow fit). The evolution can be fitted by two processes, one fast (red) and one slower (blue). The sum of these fits is shown as a black line (upper half, see the agreement between the red experimental data and the black fit). The results suggest that we probably see a small portion of ions corresponding to the intermediates and a larger portion of the ions originating from the products. The fact that the results are identical for monoaurated and diaurated ions suggests that probably both types of ions originate from the same precursor in solution *(i.e.*, neutral α-gold-ketone).

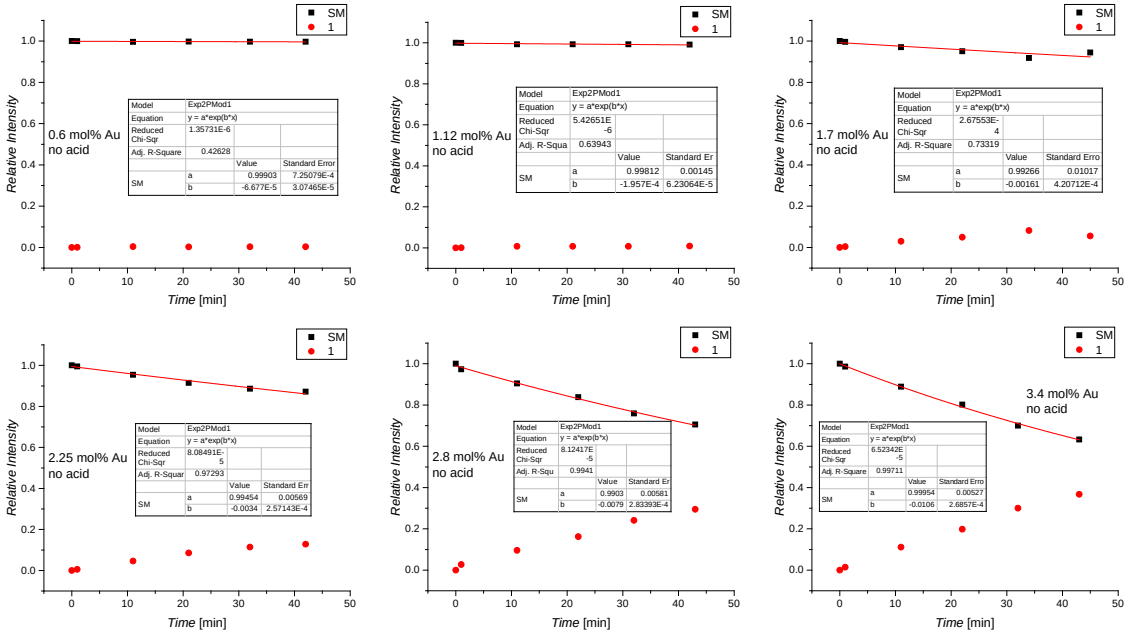
4. Reaction kinetics determined with gas chromatography

Standard conditions of the experiments: 6 mol% of [(IPr)Au(CH_3CN)(BF_4)] (1.67 mM) and 27.6 mM of 3-hexyne in THF/water (5:1).

Gold-concentration ([(IPr)Au(CH_3CN)(BF_4)]) dependence in presence of additives specified in the tables

Table S5: Concentrations of the reagents

Exp. No.	mol % of Au	[Au]	[acid]	[3-hexyne]
1	0.6	0.16 mM	-	27.6 mM
2	1.12	0.31 mM	-	27.6 mM
3	1.7	0.46 mM	-	27.6 mM
4	2.25	0.62 mM	-	27.6 mM
5	2.8	0.77 mM	-	27.6 mM
6	3.4	0.93 mM	-	27.6 mM
7	4.5	1.24 mM	-	27.6 mM
8	5.6	1.55 mM	-	27.6 mM
9	6.7	1.86 mM	-	27.6 mM
10	7.8	2.17 mM	-	27.6 mM
11	9	2.48 mM	-	27.6 mM



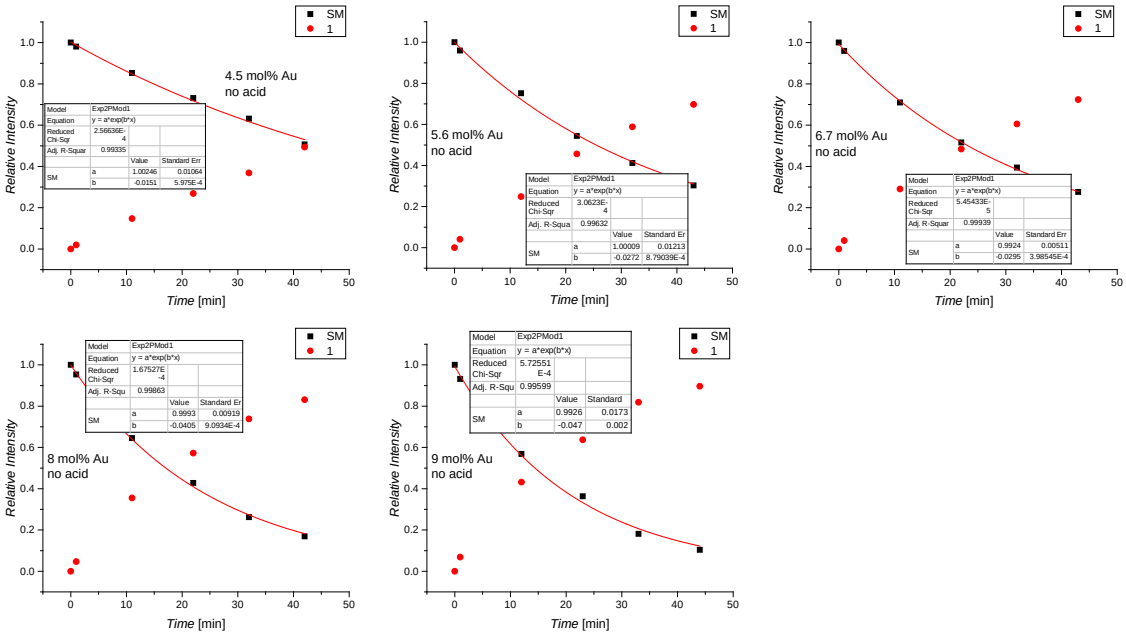


Figure S17: Results of the experiments (Table S5). **SM** is 3-hexyne and **1** is 3-hexanone. The relative concentrations of **SM** and **1** were obtained by GC measurements. The decrease of the **SM** concentration in time was fitted by an exponential function providing the rate constant for the given conditions.

Table S6. Concentrations of the reagents.

Exp. No.	[Au] mol%	[Au]	1 mol% of base	3-hexyne
1	1.12	0.31 mM	0.31 mM	27.6 mM
2	1.7	0.47 mM	0.31 mM	27.6 mM
3	2.25	0.62 mM	0.31 mM	27.6 mM
4	2.8	0.77 mM	0.31 mM	27.6 mM
5	3.4	0.93 mM	0.31 mM	27.6 mM
6	4	9.67 mM	0.31 mM	27.6 mM
7	4.5	1.08 mM	0.31 mM	27.6 mM
8	5.6	1.55 mM	0.31 mM	27.6 mM
9	6.7	1.86 mM	0.31 mM	27.6 mM
10	8	2.17 mM	0.31 mM	27.6 mM
11	9	2.48 mM	0.31 mM	27.6 mM

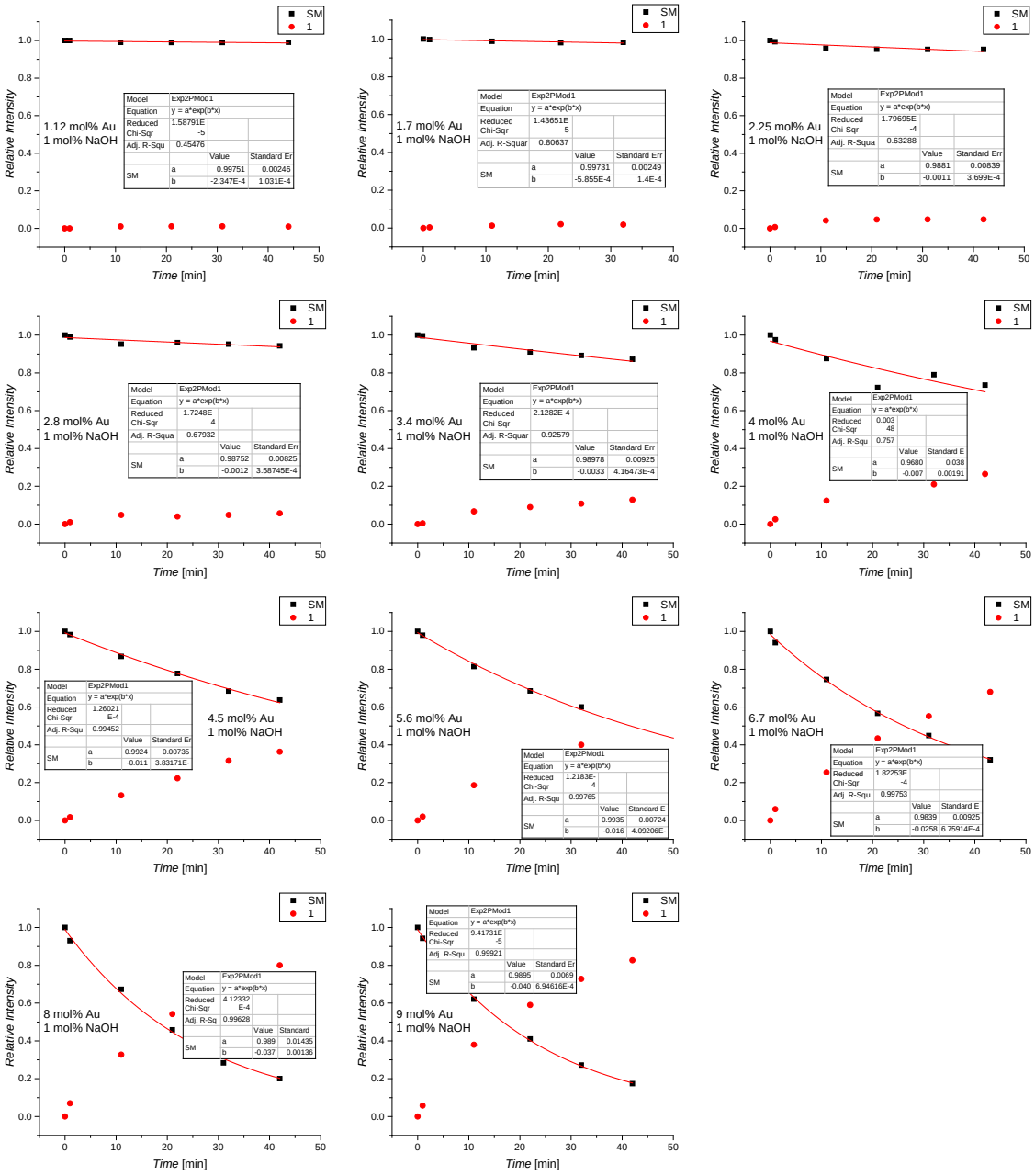
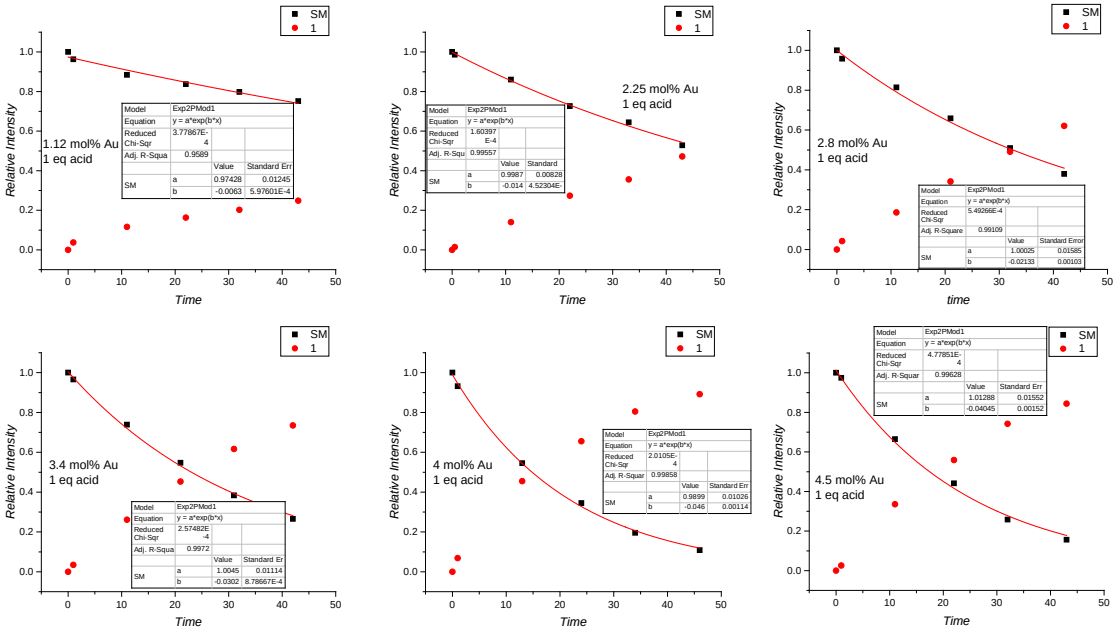


Figure S18: Results of the experiments (Table S6). **SM** is 3-hexyne and **1** is 3-hexanone. The relative concentrations of **SM** and **1** were obtained by GC measurements. The decrease of the **SM** concentration in time was fitted by an exponential function providing the rate constant for the given conditions.

Table S7. Concentrations of the reagents.

Exp. No.	mol % of Au	[Au]	Equivalents of acid	[acid]	[3-hexyne]
1	1.12	0.31 mM	1	0.31 mM	27.6 mM
2	2.25	0.62 mM	1	0.62 mM	27.6 mM
3	2.8	0.77 mM	1	0.77 mM	27.6 mM
4	3.4	0.93 mM	1	0.93 mM	27.6 mM
5	4	1.08 mM	1	1.08 mM	27.6 mM
6	4.5	1.24 mM	1	1.24 mM	27.6 mM
7	5.6	1.55 mM	1	1.55 mM	27.6 mM
8	6.7	1.86 mM	1	1.86 mM	27.6 mM
9	8	2.17 mM	1	2.17 mM	27.6 mM
10	9	2.48 mM	1	2.48 mM	27.6 mM



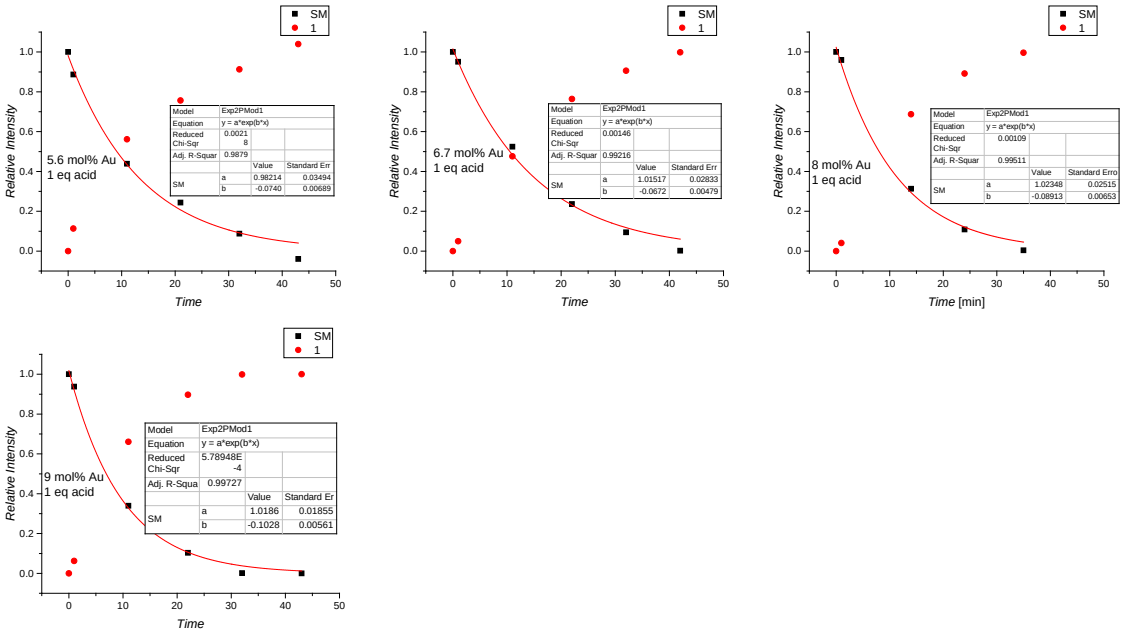


Figure S19: Results of the experiments (Table S7). **SM** is 3-hexyne and **1** is 3-hexanone. The relative concentrations of **SM** and **1** were obtained by GC measurements. The decrease of the **SM** concentration in time was fitted by an exponential function providing the rate constant for the given conditions.

Table S8. Concentrations of the reagents.

Exp. No.	mol % of Au	[Au]	Equivalents of acid	[acid]	[3-hexyne]
1	1.12	0.31 mM	4	1.24 mM	27.6 mM
2	3	0.84 mM	4	3.36 mM	27.6 mM
3	4.5	1.24 mM	4	4.96 mM	27.6 mM
4	6	1.67 mM	4	6.68 mM	27.6 mM
5	9	2.51 mM	4	10.04 mM	27.6 mM

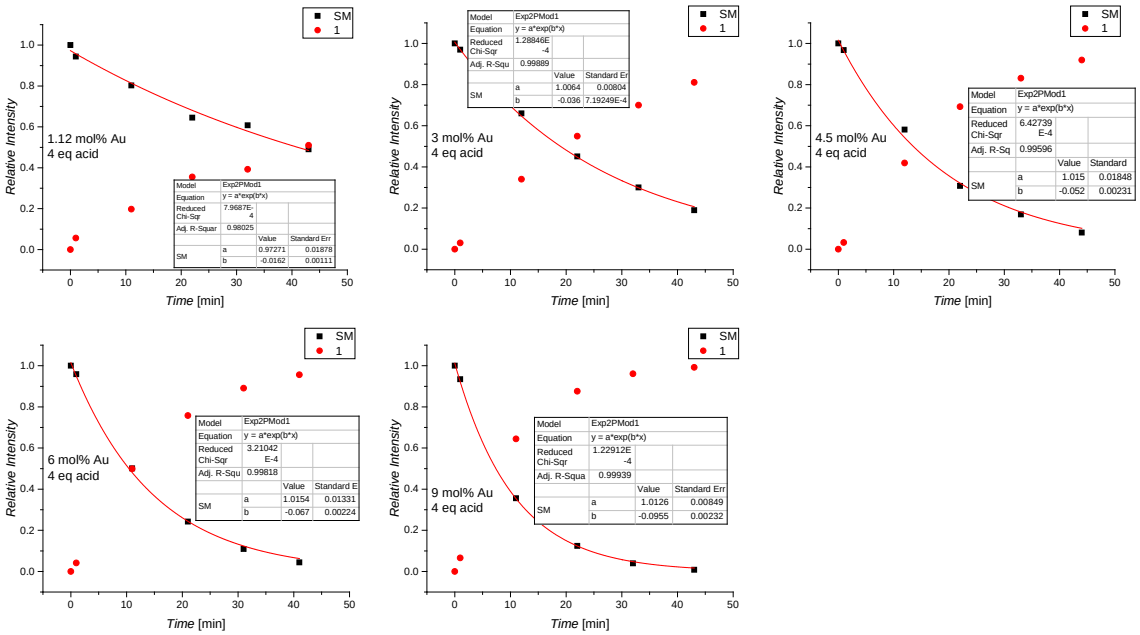


Figure S20: Results of the experiments (Table S8). **SM** is 3-hexyne and **1** is 3-hexanone. The relative concentrations of **SM** and **1** were obtained by GC measurements. The decrease of the **SM** concentration in time was fitted by an exponential function providing the rate constant for the given conditions.

Table S9. Concentrations of the reagents.

Exp. No.	mol % of Au	[Au]	Equivalents of acid	[acid]	[3-hexyne]
1	1.12	0.31 mM	8	2.48 mM	27.6 mM
2	3	0.84 mM	8	6.72 mM	27.6 mM
3	4.5	1.24 mM	8	9.92 mM	27.6 mM
4	6	1.67 mM	8	13.36 mM	27.6 mM
5	9	2.51 mM	8	20.08 mM	27.6 mM

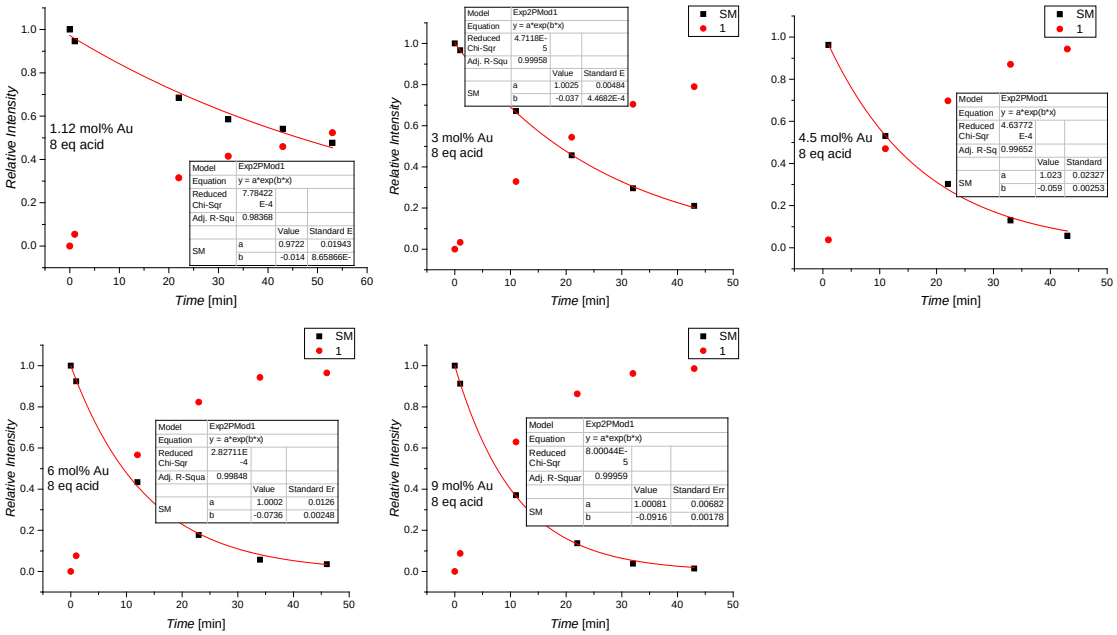


Figure S21: Results of the experiments (Table S9). **SM** is 3-hexyne and **1** is 3-hexanone. The relative concentrations of **SM** and **1** were obtained by GC measurements. The decrease of the **SM** concentration in time was fitted by an exponential function providing the rate constant for the given conditions.

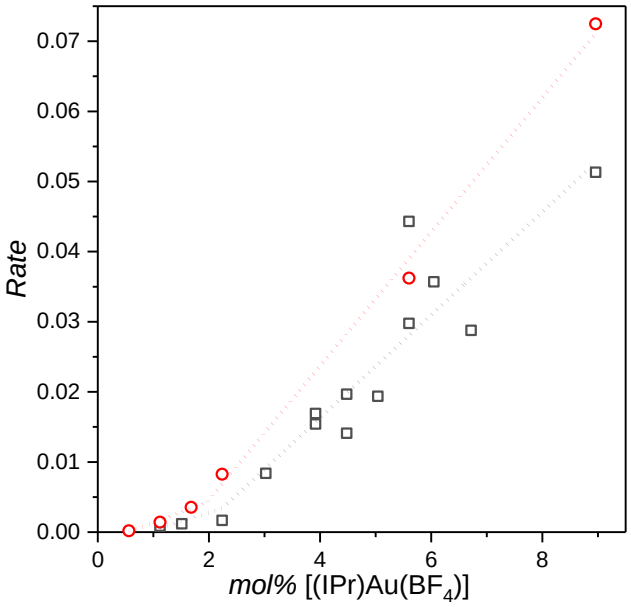


Figure S22. Rate of the ketone product formation in the reaction of 3-hexyne with water catalysed by [Au(IPr)(CH_3CN)(BF_4)]. Dependence of the reaction rate on the concentration of the catalyst under the standard conditions in a glass vial (in gray) and in a plastic vial (in red). The lines are bimodal linear fits of the data.

5. DFT calculations

The calculations were performed using the density functional theory method mPW1PW91[3] together with the LanL2DZ basis set for gold atom and cc-pVDZ for the remaining atoms as implemented in the Gaussian 09 suite[4]. Computation of the Hessian matrix was performed for all optimized structures at the same level of theory in order to ensure that the structures correspond to genuine minima as well as to calculate the thermochemical data and IR spectra. The optimized geometries as well as the calculated energies are listed in Table S10. We used two different scaling factors. The finger print region was scaled by a factor of 0.97. The region of C-H stretching vibrations was scaled by a factor of 0.945.

Table S10. Relative energies and geometry parameters corresponding to the heighted bonds and the angle in Figure 1 and 2 in the main document. The geometry optimization was performed with the mPW1PW91 DFT functional and the combination of the LanL2DZ basis set for the gold atoms and the cc-pVDZ for the rest of the atoms. The values in brackets correspond to the calculations performed at the B3LYP level with the LanL2DZ/6-31+G* basis set combination.

Structure	E_{rel} (kJ/mol)	α(Au-C-C)	R(C-C)	R(C-O)	R(Au-C)
M_C2a	0.0 (0.0)	88.4 (90.8)	1.403 (1.403)	1.320 (1.330)	2.209 (2.253)
M_C2b	12.5 (9.8)	83.0 (84.5)	1.392 (1.392)	1.339 (1.349)	2.238 (2.289)
M_C2c	12.8 (9.2)	82.4 (84.6)	1.392 (1.392)	1.340 (1.349)	2.245 (2.291)
M_C1a	11.8 (10.4)	89.3 (90.8)	1.404 (1.403)	1.330 (1.330)	2.200 (2.253)
M_C1b	26.8 (24.3)	84.8 (88.4)	1.392 (1.393)	1.343 (1.353)	2.231 (2.268)
M_C1c	31.7 (28.4)	86.3 (91.4)	1.400 (1.404)	1.339 (1.347)	2.224 (2.255)
N_C2a	0.0 (0.0)	102.2 (103.8)	1.484 (1.487)	1.226 (1.233)	2.122 (2.153)
N_C1a	7.9 (10.6)	104.3 (105.3)	1.480 (1.484)	1.229 (1.237)	2.109 (2.139)
N_C1b	23.5 (21.9)	106.1 (106.9)	1.488 (1.492)	1.227 (1.237)	2.102 (2.131)
D_C2a	0.0	99.9 (100.7)	1.434 (1.437)	1.270 (1.276)	2.162 (2.197)
D_C2b	1.0	101.0	1.435	1.269	2.162
D_C1a	14.4	99.1	1.431	1.272	2.154

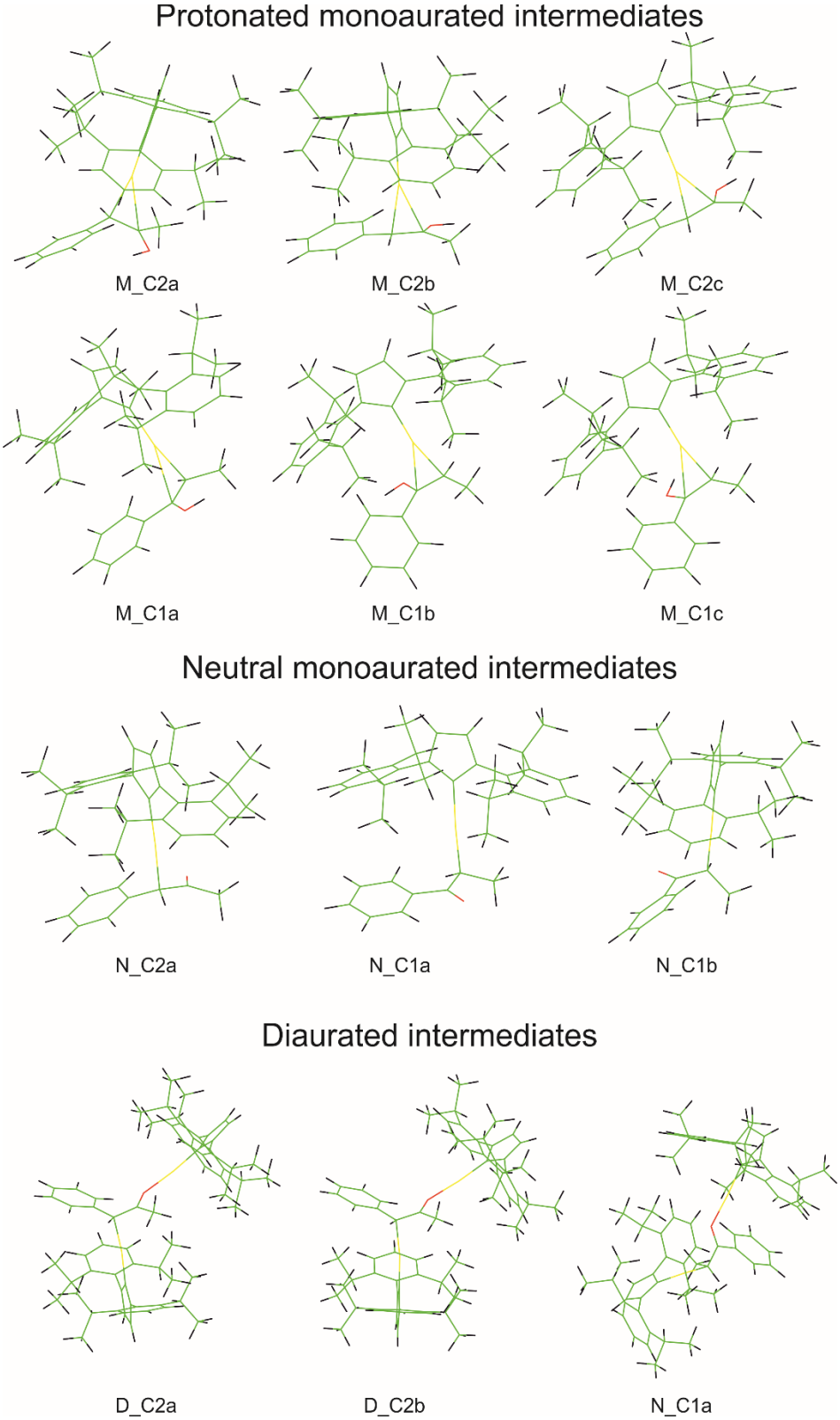


Figure S23. Selected calculated structures (mPW1PW91/LanL2DZ:cc-pVDZ). XYZ coordinates can be found in Table S11.

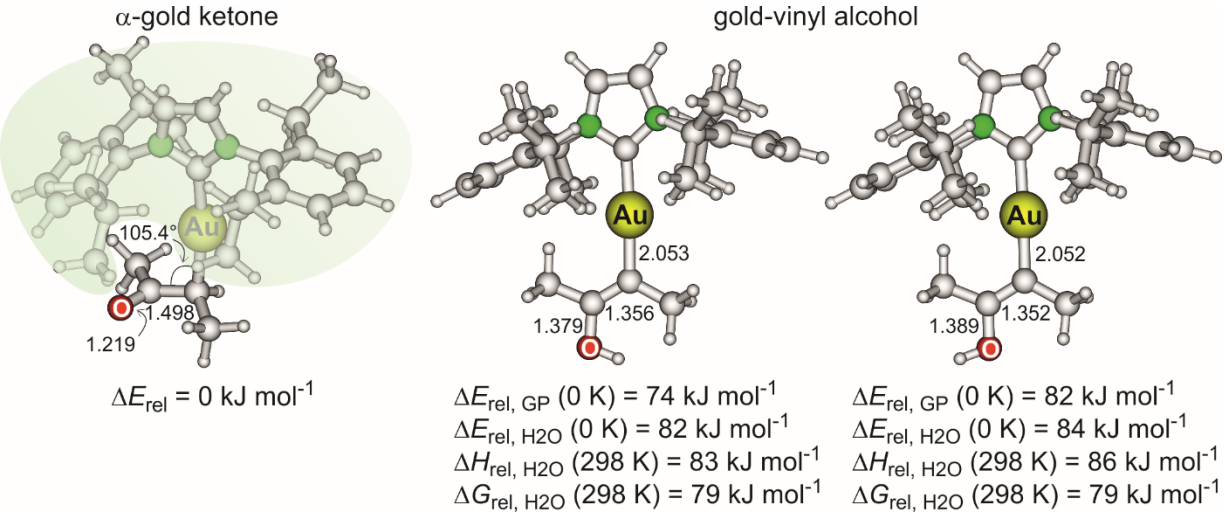


Figure S24. Calculated structures and energies (B3LYP-D3/def2SVP, for simulation of the solvent effect the SMD model and solvent=water was used) of possible tautomers of neutral monoaurated intermediates formed by the addition reaction to 2-butyne. The (IPr)Au unit is in a shade in the first structure to highlight the geometry of the keto intermediate. The bond distances and the angle are given for the geometries optimized in the gas phase.

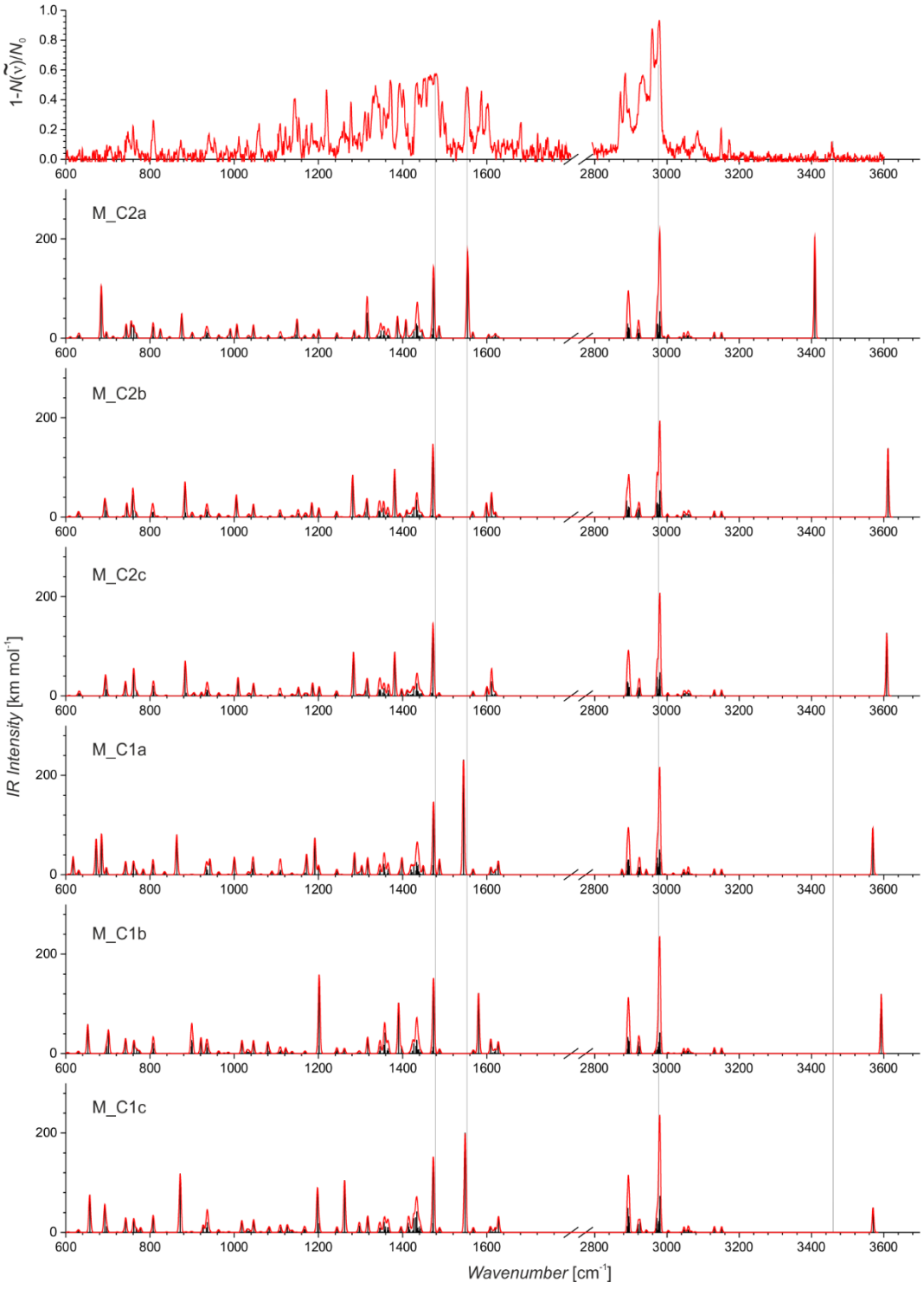


Figure S25. Comparison of the IRPD spectrum of [Au(IPr)($PhCCCH_3$,HO)]H^+ (upper panel) with theoretical IR spectra of protonated monoaurated intermediates calculated at the mPW1PW91/LanL2DZ:cc-pVDZ level of theory (see Figure S23 for the structures of the complexes). The theoretical frequencies were scaled by 0.97 in the finger print region and by 0.945 above 2000 cm^{-1}.

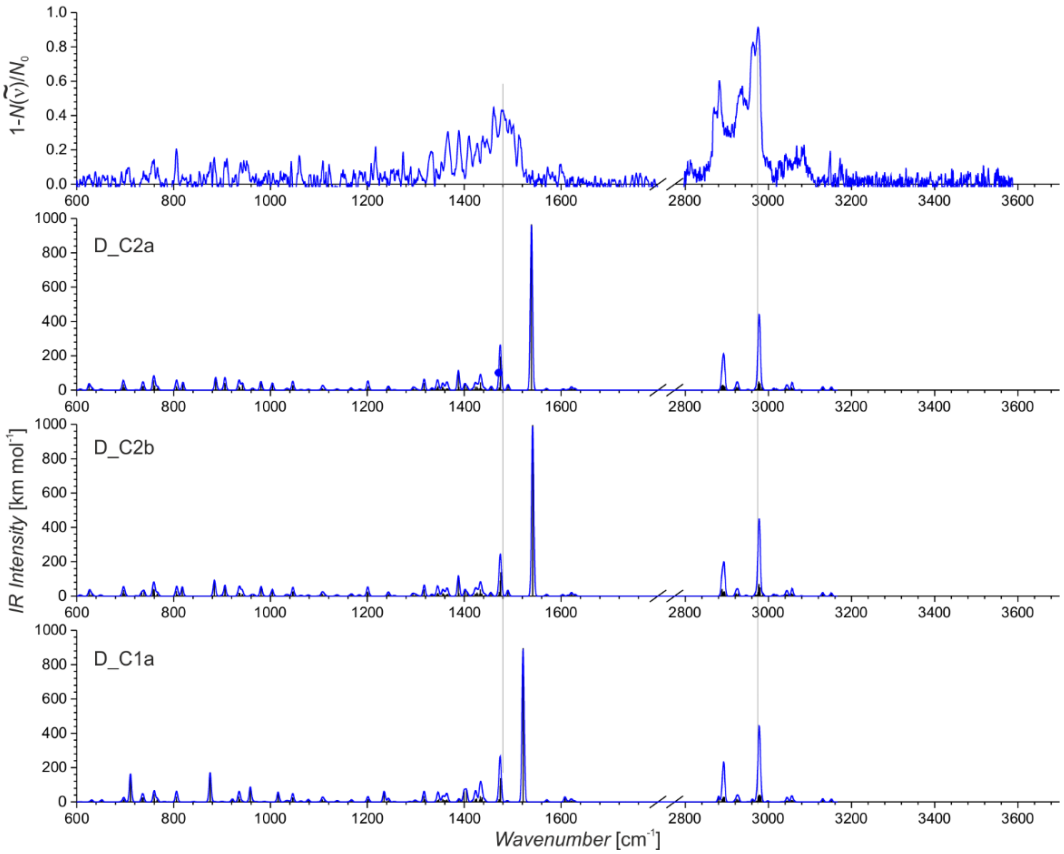
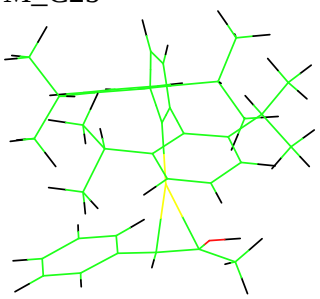


Figure S26. Comparison of the IRPD spectrum of $[Au_2(IPr)_2(PhCCCH_3,HO)]^+$ (upper panel) with theoretical IR spectra of diaurated intermediates calculated at the mPW1PW91/LanL2DZ:cc-pVDZ level of theory (see Figure S23 for the structures of the complexes). The theoretical frequencies were scaled by 0.97 in the finger print region and by 0.945 above 2000 cm^{-1}.

Table S11. Geometries and energetics for calculated structures optimized at the mPW1PW91/cc-pVDZ:LanL2DZ(Au) level of theory.

Name of the structure	Energetics and XYZ coordinates of the optimized structure

M_C2b



Charge = 1 Multiplicity = 1

Zero-point correction= 0.743068 (Hartree/Particle)
Thermal correction to Energy= 0.786249
Thermal correction to Enthalpy= 0.787193
Thermal correction to Gibbs Free Energy= 0.661203
Sum of electronic and zero-point Energies= -1718.620011
Sum of electronic and thermal Energies= -1718.576830
Sum of electronic and thermal Enthalpies= -1718.575886
Sum of electronic and thermal Free Energies= -1718.701876

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.156130	-2.271663	-1.739368
2	6	0	-0.505171	3.496175	-1.157607
3	6	0	0.730227	0.725369	0.569712
4	7	0	1.993919	0.736225	1.053108
5	6	0	2.172124	1.802800	1.911671
6	6	0	0.989094	2.468979	1.959495
7	7	0	0.116710	1.792067	1.131069
8	6	0	-1.257383	2.168700	0.911232
9	6	0	-2.226394	1.710430	1.820470
10	6	0	-3.546625	2.112015	1.598279
11	6	0	-3.878804	2.928588	0.524148
12	6	0	-2.895494	3.363048	-0.356878
13	6	0	-1.558295	2.995050	-0.185508
14	6	0	3.014939	-0.221125	0.709577
15	6	0	3.888041	0.088341	-0.347691
16	6	0	4.865432	-0.859055	-0.664776
17	6	0	4.966574	-2.051008	0.043123
18	6	0	4.095588	-2.319142	1.092392
19	6	0	3.098584	-1.409172	1.456005
20	6	0	-2.495263	-2.386726	-1.119383
21	1	0	-0.476153	-3.099047	-1.514815
22	6	0	-0.797708	-1.563623	-2.883124
23	8	0	-1.676324	-0.730920	-3.455817
24	79	0	-0.085165	-0.608871	-0.691762
25	6	0	2.182182	-1.717306	2.626586
26	6	0	2.970507	-1.782463	3.938429
27	6	0	3.809013	1.386451	-1.131919
28	6	0	3.470159	1.128158	-2.602383
29	6	0	-1.894097	0.820713	3.005100
30	6	0	-2.628033	-0.520463	2.920377
31	6	0	-0.360125	5.019066	-1.085116
32	6	0	-0.801787	3.035081	-2.587521
33	6	0	0.458673	-1.842438	-3.646030
34	6	0	1.381258	-3.000817	2.393823
35	6	0	5.097459	2.202219	-0.992599
36	6	0	-2.182253	1.530944	4.331054
37	1	0	-4.914936	3.233564	0.374018
38	1	0	5.738914	-2.774578	-0.219532
39	1	0	3.117677	1.989639	2.406634
40	1	0	0.690055	3.356326	2.504614
41	1	0	-4.328217	1.779338	2.281422
42	1	0	-3.170911	4.007414	-1.192143
43	1	0	4.195313	-3.252261	1.647269
44	1	0	5.563210	-0.656534	-1.477724
45	1	0	0.461018	3.058485	-0.868287
46	1	0	-0.816099	0.605114	2.975961
47	1	0	2.991543	1.989845	-0.712012
48	1	0	1.458661	-0.894612	2.718157
49	1	0	0.437633	5.362519	-1.759501
50	1	0	-1.289122	5.526248	-1.384481
51	1	0	-0.112403	5.353224	-0.067747

52	1	0	0.009901	3.340354	-3.264196
53	1	0	-0.906990	1.941260	-2.638569
54	1	0	-1.733252	3.477924	-2.970308
55	1	0	-1.885951	0.895539	5.177999
56	1	0	-1.635343	2.481304	4.410681
57	1	0	-3.253457	1.753845	4.443863
58	1	0	-2.326907	-1.171350	3.754122
59	1	0	-3.718302	-0.389792	2.983089
60	1	0	-2.410518	-1.043932	1.978591
61	1	0	5.002410	3.162962	-1.518756
62	1	0	5.329895	2.412966	0.060809
63	1	0	5.959928	1.672857	-1.423403
64	1	0	3.374589	2.078382	-3.147693
65	1	0	4.252716	0.537112	-3.100818
66	1	0	2.520823	0.580707	-2.696282
67	1	0	0.693121	-3.179359	3.232601
68	1	0	0.784666	-2.937435	1.471938
69	1	0	2.036875	-3.880312	2.312166
70	1	0	2.291150	-1.951099	4.786294
71	1	0	3.700661	-2.605071	3.929117
72	1	0	3.522598	-0.850370	4.124710
73	1	0	-1.269817	-0.296341	-4.217623
74	6	0	-2.738898	-3.519426	-0.326187
75	6	0	-3.975857	-3.716504	0.277552
76	6	0	-4.991899	-2.778079	0.107302
77	6	0	-4.757187	-1.642542	-0.666286
78	6	0	-3.522415	-1.441175	-1.274439
79	1	0	-1.949295	-4.260974	-0.190742
80	1	0	-4.147579	-4.608614	0.880242
81	1	0	-5.963883	-2.931287	0.576758
82	1	0	-5.545567	-0.901303	-0.799793
83	1	0	-3.355365	-0.545206	-1.867061
84	1	0	0.944747	-0.910807	-3.970309
85	1	0	1.175205	-2.420211	-3.052447
86	1	0	0.200760	-2.422710	-4.547429

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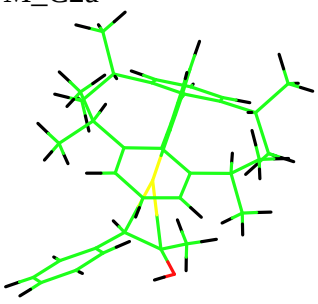


Charge = 1 Multiplicity = 1

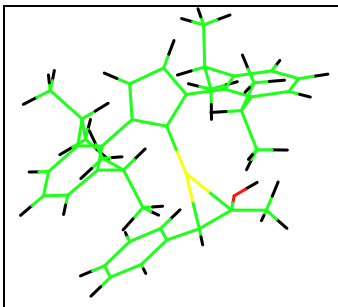
Zero-point correction= 0.743277 (Hartree/Particle)
Thermal correction to Energy= 0.786236
Thermal correction to Enthalpy= 0.787180
Thermal correction to Gibbs Free Energy= 0.662443
Sum of electronic and zero-point Energies= -1718.624768
Sum of electronic and thermal Energies= -1718.581809
Sum of electronic and thermal Enthalpies= -1718.580865
Sum of electronic and thermal Free Energies= -1718.705602

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.882035	0.122759	0.583652
2	6	0	-3.094063	0.137076	-0.580313
3	6	0	-3.224360	1.107705	-1.588511
4	6	0	-4.175348	2.111781	-1.384323
5	6	0	-4.959083	2.137654	-0.236879
6	6	0	-4.816364	1.151477	0.732235
7	7	0	-2.117316	-0.907800	-0.753717
8	6	0	-0.819630	-0.818824	-0.383259
9	7	0	-0.267982	-2.011257	-0.703768
10	6	0	-1.212717	-2.844205	-1.269789
11	6	0	-2.378627	-2.147674	-1.302731
12	79	0	0.130138	0.763713	0.418674
13	6	0	1.299939	2.549143	0.988550
14	6	0	1.002785	2.267094	2.330210
15	8	0	1.854632	1.663854	3.138483
16	1	0	2.705570	1.538391	2.672499
17	6	0	1.112699	-2.363803	-0.489830
18	6	0	1.478505	-2.910957	0.752989
19	6	0	2.820943	-3.262457	0.922750
20	6	0	3.746383	-3.080459	-0.098799

	21	6	0	3.350423	-2.536490	-1.315044
	22	6	0	2.022475	-2.163381	-1.542363
	23	6	0	0.486663	-3.142749	1.879073
	24	6	0	0.885579	-2.383788	3.147527
	25	6	0	1.619700	-1.577055	-2.884054
	26	6	0	1.799629	-2.599019	-4.010764
	27	6	0	-2.405144	1.087880	-2.866941
	28	6	0	-1.548792	2.348725	-3.008947
	29	6	0	-3.757386	-0.947487	1.654470
	30	6	0	-3.242842	-0.358302	2.970515
	31	6	0	2.700746	2.465587	0.487432
	32	6	0	3.286110	3.602662	-0.086760
	33	6	0	4.613314	3.584717	-0.502252
	34	6	0	5.385486	2.433317	-0.347572
	35	6	0	4.814468	1.292524	0.207969
	36	6	0	3.479701	1.302459	0.614028
	37	6	0	-0.235390	2.722042	3.020271
	38	6	0	0.310126	-4.638608	2.157805
	39	6	0	2.379519	-0.281293	-3.180776
	40	6	0	-3.301567	0.882669	-4.092115
	41	6	0	-5.078507	-1.694793	1.855994
	42	1	0	5.050855	4.479467	-0.945830
	43	1	0	2.695914	4.513322	-0.200617
	44	1	0	6.426711	2.424777	-0.669897
	45	1	0	5.400458	0.379247	0.312163
	46	1	0	3.030178	0.374178	0.978844
	47	1	0	-0.650164	1.920063	3.643521
	48	1	0	0.039929	3.548727	3.694294
	49	1	0	-0.991234	3.071311	2.309340
	50	1	0	-5.696803	2.929175	-0.101379
	51	1	0	4.786103	-3.372875	0.052672
	52	1	0	-0.971116	-3.849260	-1.594539
	53	1	0	-3.363829	-2.420010	-1.662171
	54	1	0	-4.310159	2.883881	-2.142242
	55	1	0	-5.447672	1.178198	1.620748
	56	1	0	4.086177	-2.402492	-2.108252
	57	1	0	3.144484	-3.696845	1.869039
	58	1	0	-3.014295	-1.684092	1.316840
	59	1	0	-1.717236	0.231468	-2.817575
	60	1	0	-0.488837	-2.749920	1.558255
	61	1	0	0.550702	-1.323994	-2.837137
	62	1	0	-4.950100	-2.508493	2.584113
	63	1	0	-5.866731	-1.030833	2.239819
	64	1	0	-5.441923	-2.133244	0.915839
	65	1	0	-3.136578	-1.146643	3.729835
	66	1	0	-2.260942	0.117231	2.832296
	67	1	0	-3.933241	0.398507	3.371556
	68	1	0	-2.692420	0.809995	-5.004590
	69	1	0	-3.898094	-0.036709	-4.007051
	70	1	0	-4.000562	1.721255	-4.226618
	71	1	0	-0.938087	2.295455	-3.921801
	72	1	0	-2.168408	3.254888	-3.078598
	73	1	0	-0.869569	2.469295	-2.152079
	74	1	0	-0.444621	-4.797212	2.941494
	75	1	0	-0.013869	-5.181822	1.258742
	76	1	0	1.248586	-5.097125	2.502817
	77	1	0	0.120591	-2.514536	3.926509
	78	1	0	1.836955	-2.751723	3.559545
	79	1	0	0.995844	-1.306092	2.956907
	80	1	0	2.032787	0.153446	-4.129419
	81	1	0	2.232154	0.464809	-2.386766
	82	1	0	3.460889	-0.458331	-3.276239
	83	1	0	1.455504	-2.179607	-4.967041
	84	1	0	2.855696	-2.881231	-4.133785
	85	1	0	1.230451	-3.519759	-3.818891
	86	1	0	0.679056	3.339435	0.553450

M_C2c	Charge = 1 Multiplicity = 1					
	Zero-point correction=			0.743557 (Hartree/Particle)		
	Thermal correction to Energy=			0.786534		



Thermal correction to Enthalpy= 0.787478
Thermal correction to Gibbs Free Energy= 0.663258
Sum of electronic and zero-point Energies= -1718.619881
Sum of electronic and thermal Energies= -1718.576904
Sum of electronic and thermal Enthalpies= -1718.575960
Sum of electronic and thermal Free Energies= -1718.700180

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.549507	-1.772841	1.769742
2	6	0	-2.467702	-2.448504	1.180962
3	6	0	-2.716457	-3.273380	0.071285
4	6	0	-4.011594	-3.418574	-0.416954
5	6	0	-5.076951	-2.746940	0.179805
6	6	0	-4.840389	-1.920839	1.276864
7	6	0	-1.139013	-2.250331	1.802175
8	6	0	0.045261	-2.945631	1.575435
9	6	0	1.200495	-2.919832	2.525941
10	79	0	-0.079645	-0.656713	0.627966
11	6	0	0.614491	0.906853	-0.425444
12	7	0	-0.076786	1.983367	-0.859967
13	6	0	0.751118	2.835903	-1.563957
14	6	0	1.986365	2.271540	-1.565320
15	7	0	1.882863	1.088373	-0.859732
16	6	0	-1.479064	2.216642	-0.620693
17	6	0	-2.403836	1.763863	-1.577503
18	6	0	-3.754207	2.021178	-1.326211
19	6	0	-4.156087	2.696631	-0.180117
20	6	0	-3.214484	3.133702	0.743851
21	6	0	-1.849690	2.906566	0.546652
22	6	0	-1.989989	1.047080	-2.850194
23	6	0	-2.667936	-0.318769	-2.981306
24	6	0	-0.842793	3.411164	1.565080
25	6	0	-0.852250	4.940921	1.642409
26	6	0	2.974414	0.182567	-0.608258
27	6	0	3.193639	-0.870598	-1.513462
28	6	0	4.266398	-1.726687	-1.246519
29	6	0	5.076960	-1.538052	-0.132691
30	6	0	4.834904	-0.483330	0.740173
31	6	0	3.779437	0.407512	0.522309
32	6	0	2.337916	-1.089470	-2.748331
33	6	0	3.140236	-0.827821	-4.026623
34	6	0	3.550114	1.561020	1.482748
35	6	0	3.194020	1.058008	2.884299
36	8	0	0.125593	-3.825434	0.567887
37	6	0	1.711273	-2.486072	-2.761028
38	6	0	4.756187	2.504119	1.518562
39	6	0	-1.075223	2.782476	2.941561
40	6	0	-2.256442	1.921084	-4.080140
41	1	0	-1.166364	-1.752981	2.776484
42	1	0	-5.215411	2.889107	-0.007400
43	1	0	5.913289	-2.213511	0.051092
44	1	0	2.922982	2.602004	-1.998329
45	1	0	0.387549	3.760920	-1.995240
46	1	0	-3.545095	3.667697	1.635040
47	1	0	-4.504432	1.688105	-2.043343
48	1	0	5.484721	-0.341620	1.604089
49	1	0	4.476534	-2.549252	-1.930669
50	1	0	-0.905764	0.868745	-2.800964
51	1	0	0.159901	3.105675	1.232775
52	1	0	1.512587	-0.363992	-2.721656
53	1	0	2.690819	2.141458	1.117752
54	1	0	-1.911330	1.415642	-4.993687
55	1	0	-3.330585	2.126707	-4.198956
56	1	0	-1.739754	2.889155	-4.011506
57	1	0	-2.297732	-0.840857	-3.875634
58	1	0	-2.472878	-0.953469	-2.105413
59	1	0	-3.758486	-0.223236	-3.087280

	60	1	0	-0.083901	5.295007	2.344770
	61	1	0	-0.652971	5.396433	0.662004
	62	1	0	-1.822778	5.320907	1.993849
	63	1	0	-0.306618	3.119893	3.651973
	64	1	0	-2.054000	3.065236	3.355988
	65	1	0	-1.036320	1.684326	2.890480
	66	1	0	2.499649	-0.944031	-4.912619
	67	1	0	3.558464	0.188581	-4.040751
	68	1	0	3.978322	-1.533316	-4.126750
	69	1	0	1.040292	-2.595995	-3.624973
	70	1	0	2.475662	-3.273627	-2.840051
	71	1	0	1.122889	-2.669892	-1.850324
	72	1	0	2.995329	1.905282	3.556324
	73	1	0	2.295914	0.423315	2.862609
	74	1	0	4.014220	0.472244	3.325281
	75	1	0	4.549578	3.364197	2.171448
	76	1	0	5.652756	2.000890	1.909228
	77	1	0	4.999661	2.887605	0.517619
	78	1	0	-3.373467	-1.126933	2.631869
	79	1	0	-5.665623	-1.393088	1.755399
	80	1	0	-6.088863	-2.870240	-0.206686
	81	1	0	-4.189543	-4.070330	-1.272824
	82	1	0	-1.900955	-3.810375	-0.405356
	83	1	0	2.150344	-2.764986	1.992928
	84	1	0	1.090269	-2.132514	3.279050
	85	1	0	1.250873	-3.891831	3.043814
	86	1	0	1.027263	-4.168414	0.503404

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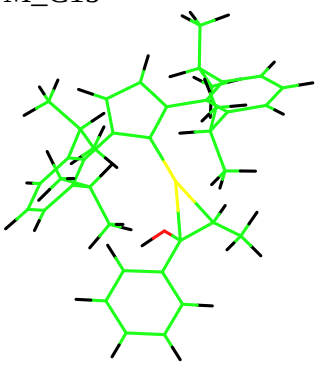

Charge = 1 Multiplicity = 1
Zero-point correction= 0.743504 (Hartree/Particle)
Thermal correction to Energy= 0.786430
Thermal correction to Enthalpy= 0.787375
Thermal correction to Gibbs Free Energy= 0.663634
Sum of electronic and zero-point Energies= -1718.614576
Sum of electronic and thermal Energies= -1718.571650
Sum of electronic and thermal Enthalpies= -1718.570706
Sum of electronic and thermal Free Energies= -1718.694446

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.718519	-1.009738	-0.528612
2	6	0	-3.020292	-2.132759	-0.999547
3	6	0	-3.514654	-3.415670	-0.735387
4	6	0	-4.689434	-3.571970	-0.004831
5	6	0	-5.372823	-2.455145	0.471304
6	6	0	-4.885097	-1.175127	0.210151
7	6	0	-1.832879	-1.944223	-1.867281
8	8	0	-2.016703	-1.156753	-2.940005
9	6	0	-0.595623	-2.566983	-1.734112
10	79	0	-0.020389	-0.728836	-0.608296
11	6	0	0.846702	0.802349	0.365796
12	7	0	2.153574	0.901951	0.697369
13	6	0	2.404922	2.111659	1.314959
14	6	0	1.222709	2.777756	1.366150
15	7	0	0.277677	1.957236	0.779423
16	6	0	3.140592	-0.118850	0.449878
17	6	0	3.355497	-1.089819	1.443471
18	6	0	4.314137	-2.071222	1.176331
19	6	0	5.023162	-2.076562	-0.019082
20	6	0	4.793863	-1.094288	-0.975185
21	6	0	3.846985	-0.087589	-0.765030
22	6	0	2.607509	-1.101885	2.765004
23	6	0	1.761803	-2.369052	2.916845
24	6	0	3.633424	0.984209	-1.819055
25	6	0	4.888418	1.846008	-1.988687
26	6	0	-1.118103	2.285692	0.646443
27	6	0	-1.976555	1.986693	1.718748
28	6	0	-3.321065	2.343233	1.576048
29	6	0	-3.781206	2.965960	0.421221

30	6	0	-2.905050	3.245414	-0.621949
31	6	0	-1.548788	2.916283	-0.534530
32	6	0	-1.502610	1.309772	2.992883
33	6	0	-1.710187	2.210031	4.214126
34	6	0	-0.608370	3.265844	-1.674162
35	6	0	-0.462777	4.784127	-1.817142
36	6	0	-2.173439	-0.053421	3.181737
37	6	0	-1.049756	2.622430	-2.991178
38	6	0	3.185255	0.383207	-3.153703
39	6	0	3.565820	-0.926670	3.946865
40	1	0	-4.832000	3.245913	0.336481
41	1	0	5.768769	-2.850387	-0.204377
42	1	0	3.395036	2.385483	1.659308
43	1	0	0.968096	3.752817	1.764013
44	1	0	-4.017816	2.136368	2.388850
45	1	0	-3.277978	3.744062	-1.516990
46	1	0	4.512706	-2.842801	1.920632
47	1	0	5.365408	-1.106533	-1.903515
48	1	0	0.384030	2.859714	-1.431643
49	1	0	-0.422537	1.128538	2.899390
50	1	0	2.825436	1.645178	-1.473542
51	1	0	1.916715	-0.246481	2.773860
52	1	0	0.257412	5.027239	-2.611478
53	1	0	-1.420801	5.256238	-2.080754
54	1	0	-0.109646	5.246999	-0.884691
55	1	0	-0.319429	2.838815	-3.784034
56	1	0	-1.134016	1.530015	-2.898294
57	1	0	-2.021508	3.012788	-3.329052
58	1	0	-1.310961	1.726439	5.117137
59	1	0	-1.203622	3.178274	4.094795
60	1	0	-2.776521	2.412562	4.392487
61	1	0	-1.778735	-0.550945	4.079403
62	1	0	-3.261484	0.045129	3.311161
63	1	0	-1.995202	-0.710917	2.318645
64	1	0	4.705544	2.652863	-2.712972
65	1	0	5.195546	2.305159	-1.038248
66	1	0	5.737113	1.252898	-2.360043
67	1	0	2.989405	1.180395	-3.885324
68	1	0	3.954925	-0.274828	-3.582937
69	1	0	2.264110	-0.206352	-3.038144
70	1	0	1.197511	-2.342539	3.860339
71	1	0	1.042127	-2.470279	2.091474
72	1	0	2.387480	-3.273687	2.931509
73	1	0	3.004895	-0.879731	4.891374
74	1	0	4.271629	-1.766763	4.022848
75	1	0	4.156228	-0.003967	3.855377
76	1	0	-3.000305	-4.292091	-1.126750
77	1	0	-5.075751	-4.573049	0.186489
78	1	0	-6.291004	-2.582348	1.045168
79	1	0	-5.413441	-0.299265	0.586092
80	1	0	-3.330301	-0.003995	-0.707666
81	1	0	0.034552	-2.479263	-2.627070
82	1	0	-2.914556	-0.795625	-2.912660
83	6	0	-0.308890	-3.747063	-0.837587
84	1	0	-0.543968	-4.689023	-1.358915
85	1	0	0.757945	-3.781136	-0.582051
86	1	0	-0.883494	-3.719871	0.096812

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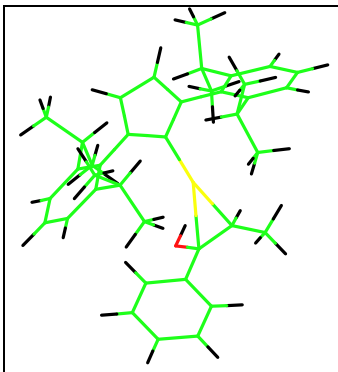
Charge = 1 Multiplicity = 1
Zero-point correction= 0.743757 (Hartree/Particle)
Thermal correction to Energy= 0.786572
Thermal correction to Enthalpy= 0.787517
Thermal correction to Gibbs Free Energy= 0.663508
Sum of electronic and zero-point Energies= -1718.612695
Sum of electronic and thermal Energies= -1718.569879
Sum of electronic and thermal Enthalpies= -1718.568935
Sum of electronic and thermal Free Energies= -1718.692944
Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)



Number	Number	Type	X	Y	Z
1	6	0	-1.571443	2.962957	-0.406414
2	6	0	-1.139901	2.254788	0.728735
3	6	0	-1.998323	1.881531	1.777383
4	6	0	-3.342401	2.247536	1.659866
5	6	0	-3.802113	2.950183	0.552139
6	6	0	-2.926682	3.299813	-0.469765
7	7	0	0.258762	1.927329	0.843243
8	6	0	0.838476	0.795015	0.384408
9	7	0	2.144213	0.891866	0.723424
10	6	0	2.383843	2.076927	1.391025
11	6	0	1.195519	2.729720	1.466364
12	79	0	-0.005240	-0.720203	-0.637211
13	6	0	-0.587641	-2.526669	-1.795993
14	6	0	-0.281443	-3.727161	-0.929530
15	6	0	3.139653	-0.112204	0.443914
16	6	0	3.362579	-1.112744	1.405836
17	6	0	4.330567	-2.076368	1.108739
18	6	0	5.040801	-2.037378	-0.085221
19	6	0	4.803571	-1.026895	-1.009659
20	6	0	3.847839	-0.035878	-0.768013
21	6	0	2.615862	-1.173040	2.726805
22	6	0	3.572261	-0.997979	3.910383
23	6	0	3.625794	1.068576	-1.785878
24	6	0	3.185743	0.507879	-3.140662
25	6	0	-1.526151	1.116492	3.000919
26	6	0	-2.210930	-0.249450	3.099024
27	6	0	-0.633592	3.377867	-1.525698
28	6	0	-1.085756	2.812094	-2.874376
29	6	0	-1.839942	-1.918331	-1.942058
30	8	0	-2.089272	-1.079812	-2.955705
31	6	0	-3.032567	-2.111085	-1.094882
32	6	0	-3.833944	-1.001792	-0.784473
33	6	0	-4.992833	-1.168684	-0.037442
34	6	0	-5.377703	-2.441548	0.384617
35	6	0	-4.598519	-3.549192	0.058415
36	6	0	-3.426380	-3.388349	-0.674386
37	6	0	1.803987	-2.464711	2.853956
38	6	0	4.872200	1.947828	-1.925926
39	6	0	-1.720627	1.934691	4.280647
40	6	0	-0.482474	4.900927	-1.584200
41	1	0	-4.852975	3.234664	0.486751
42	1	0	5.793698	-2.798004	-0.294137
43	1	0	3.370594	2.344765	1.749463
44	1	0	0.931167	3.684447	1.905085
45	1	0	-4.039832	1.981985	2.454659
46	1	0	-3.300830	3.855177	-1.330097
47	1	0	4.535113	-2.869123	1.828702
48	1	0	5.376643	-1.003592	-1.936879
49	1	0	0.358192	2.954647	-1.311458
50	1	0	-0.448157	0.931325	2.890997
51	1	0	2.810393	1.709010	-1.419876
52	1	0	1.902675	-0.336682	2.754246
53	1	0	0.233610	5.186743	-2.368087
54	1	0	-1.440410	5.390360	-1.814042
55	1	0	-0.121764	5.308916	-0.629369
56	1	0	-0.349734	3.050888	-3.655678
57	1	0	-1.202414	1.719690	-2.828348
58	1	0	-2.049630	3.236455	-3.191599
59	1	0	-1.324729	1.387999	5.148529
60	1	0	-1.204019	2.903458	4.224990
61	1	0	-2.784492	2.136021	4.474347
62	1	0	-1.812156	-0.816351	3.952757
63	1	0	-3.296162	-0.148710	3.247716
64	1	0	-2.052384	-0.842635	2.186882
65	1	0	4.682360	2.776084	-2.623800
66	1	0	5.173134	2.378800	-0.960564
67	1	0	5.727256	1.375369	-2.314595
68	1	0	2.978384	1.326689	-3.844811

	69	1	0	3.963615	-0.125172	-3.592138
	70	1	0	2.273673	-0.099344	-3.042152
	71	1	0	1.239201	-2.470365	3.797441
	72	1	0	1.086939	-2.569435	2.026820
	73	1	0	2.452453	-3.353233	2.852709
	74	1	0	3.013338	-0.988866	4.857148
	75	1	0	4.301738	-1.819404	3.964126
	76	1	0	4.136245	-0.057160	3.838947
	77	1	0	-2.845346	-4.265254	-0.952000
	78	1	0	-4.908136	-4.547414	0.367463
	79	1	0	-6.293842	-2.571553	0.961374
	80	1	0	-5.604158	-0.301169	0.210409
	81	1	0	-3.535264	-0.008917	-1.119175
	82	1	0	0.047532	-2.447820	-2.690095
	83	1	0	-1.291475	-0.969082	-3.495718
	84	1	0	-0.552532	-4.660862	-1.447936
	85	1	0	0.795506	-3.773474	-0.723350
	86	1	0	-0.809648	-3.701861	0.031435

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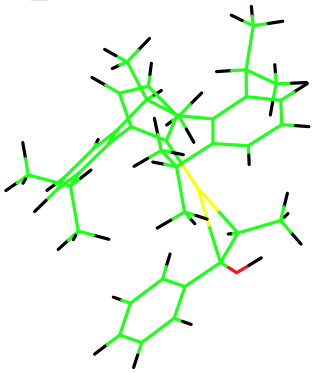

Charge = 1 Multiplicity = 1
Zero-point correction= 0.743332 (Hartree/Particle)
Thermal correction to Energy= 0.786416
Thermal correction to Enthalpy= 0.787360
Thermal correction to Gibbs Free Energy= 0.662280
Sum of electronic and zero-point Energies= -1718.620279
Sum of electronic and thermal Energies= -1718.577196
Sum of electronic and thermal Enthalpies= -1718.576251
Sum of electronic and thermal Free Energies= -1718.701332

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.889778	-1.474004	1.571770
2	6	0	2.931520	-0.307449	0.788393
3	6	0	3.881073	-0.093937	-0.226117
4	6	0	4.811626	-1.112367	-0.451697
5	6	0	4.795549	-2.280573	0.301237
6	6	0	3.846140	-2.456982	1.301022
7	7	0	1.968426	0.730940	1.053155
8	6	0	0.734445	0.799387	0.501914
9	7	0	0.172915	1.919984	1.009822
10	6	0	1.045841	2.548438	1.875976
11	6	0	2.177489	1.797844	1.904684
12	79	0	-0.060184	-0.496305	-0.819434
13	6	0	-0.720265	-1.784681	-2.476021
14	6	0	0.474870	-2.267880	-3.271114
15	6	0	-1.151586	2.393794	0.698255
16	6	0	-1.313959	3.243765	-0.409537
17	6	0	-2.608846	3.694593	-0.681158
18	6	0	-3.682587	3.320228	0.118257
19	6	0	-3.484888	2.485476	1.211783
20	6	0	-2.213143	2.001695	1.531784
21	6	0	-0.156493	3.692455	-1.284198
22	6	0	0.057207	5.205830	-1.182564
23	6	0	-2.026690	1.104539	2.742893
24	6	0	-2.819510	-0.197846	2.604754
25	6	0	3.932390	1.176092	-1.056951
26	6	0	3.701401	0.882973	-2.541797
27	6	0	1.881509	-1.686165	2.687095
28	6	0	1.036516	-2.941164	2.453267
29	6	0	-1.347299	-2.629689	-1.545946
30	8	0	-0.736987	-3.720394	-1.090968
31	6	0	-2.721274	-2.479716	-1.037537
32	6	0	-3.509996	-1.364036	-1.363091
33	6	0	-4.819485	-1.278081	-0.912915
34	6	0	-5.362222	-2.300063	-0.131696
35	6	0	-4.585203	-3.406681	0.202141
36	6	0	-3.271463	-3.498607	-0.245162
37	6	0	-0.345924	3.253731	-2.738625

	38	6	0	-2.386182	1.839886	4.037464
	39	6	0	5.245840	1.931895	-0.835912
	40	6	0	2.574705	-1.728487	4.052510
	41	1	0	5.535993	-3.058491	0.111990
	42	1	0	-4.682847	3.690913	-0.108421
	43	1	0	0.783687	3.465973	2.389166
	44	1	0	3.105698	1.925468	2.448855
	45	1	0	5.567165	-0.985653	-1.227488
	46	1	0	3.852816	-3.374202	1.890461
	47	1	0	-2.777297	4.358573	-1.529380
	48	1	0	-4.334898	2.207008	1.835107
	49	1	0	1.194307	-0.828046	2.692807
	50	1	0	3.115233	1.833024	-0.726206
	51	1	0	-0.963162	0.832744	2.805167
	52	1	0	0.757806	3.206190	-0.914473
	53	1	0	1.832635	-1.832620	4.857185
	54	1	0	3.266706	-2.580431	4.126033
	55	1	0	3.153915	-0.813231	4.240246
	56	1	0	0.276249	-3.041338	3.241388
	57	1	0	0.518060	-2.904814	1.484079
	58	1	0	1.650939	-3.853473	2.473637
	59	1	0	5.244095	2.876169	-1.399083
	60	1	0	5.402486	2.169148	0.225899
	61	1	0	6.111783	1.345216	-1.176171
	62	1	0	3.699785	1.817929	-3.120574
	63	1	0	4.491030	0.239334	-2.956816
	64	1	0	2.736424	0.380416	-2.702148
	65	1	0	-2.194991	1.196917	4.908631
	66	1	0	-1.797558	2.760390	4.158362
	67	1	0	-3.449597	2.120240	4.060074
	68	1	0	-2.629267	-0.852484	3.467723
	69	1	0	-3.902576	-0.009540	2.566995
	70	1	0	-2.543301	-0.744445	1.691816
	71	1	0	0.523847	3.548323	-3.343559
	72	1	0	-0.460807	2.162445	-2.815676
	73	1	0	-1.234057	3.718773	-3.191290
	74	1	0	0.931424	5.510666	-1.775679
	75	1	0	-0.812029	5.762143	-1.563168
	76	1	0	0.224506	5.521622	-0.143006
	77	1	0	-2.669825	-4.369412	0.006906
	78	1	0	-5.004975	-4.207911	0.810056
	79	1	0	-6.393334	-2.231458	0.216036
	80	1	0	-5.421472	-0.407329	-1.171504
	81	1	0	-3.100811	-0.547448	-1.956929
	82	1	0	-1.402262	-1.130029	-3.024388
	83	1	0	0.125943	-3.813282	-1.522136
	84	1	0	0.168065	-2.987765	-4.047762
	85	1	0	0.964653	-1.427437	-3.777474
	86	1	0	1.255597	-2.739272	-2.652028

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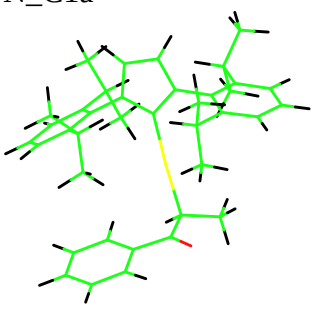

Charge = 0 Multiplicity = 1
Zero-point correction= 0.730057 (Hartree/Particle)
Thermal correction to Energy= 0.772721
Thermal correction to Enthalpy= 0.773665
Thermal correction to Gibbs Free Energy= 0.649398
Sum of electronic and zero-point Energies= -1718.219428
Sum of electronic and thermal Energies= -1718.176765
Sum of electronic and thermal Enthalpies= -1718.175820
Sum of electronic and thermal Free Energies= -1718.300087
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.124687	3.316677	-0.342905
2	6	0	-0.975205	2.434150	0.740094
3	6	0	-2.043769	2.054216	1.569523
4	6	0	-3.301211	2.591783	1.281138
5	6	0	-3.481393	3.467147	0.217290
6	6	0	-2.404033	3.824265	-0.584836

	7	7	0	0.331483	1.905686	1.021689
	8	6	0	0.842333	0.775515	0.468925
	9	7	0	2.073623	0.652121	1.028323
	10	6	0	2.325229	1.682322	1.916712
	11	6	0	1.225275	2.475989	1.911075
	12	79	0	-0.028273	-0.523067	-0.843618
	13	6	0	-0.834599	-1.941038	-2.180535
	14	6	0	0.264903	-2.730609	-2.885033
	15	6	0	2.998482	-0.410332	0.738093
	16	6	0	2.878161	-1.621013	1.441572
	17	6	0	3.810580	-2.621937	1.154668
	18	6	0	4.808635	-2.425769	0.208382
	19	6	0	4.894357	-1.220794	-0.478434
	20	6	0	3.990388	-0.184509	-0.231345
	21	6	0	1.803620	-1.864378	2.485922
	22	6	0	2.414377	-1.913935	3.890280
	23	6	0	4.077179	1.104820	-1.028471
	24	6	0	3.676556	0.863374	-2.487128
	25	6	0	-1.879429	1.094414	2.734279
	26	6	0	-2.684377	-0.189265	2.515960
	27	6	0	0.030864	3.711015	-1.244895
	28	6	0	-0.173753	3.174512	-2.664293
	29	6	0	-1.696583	-2.794279	-1.332166
	30	8	0	-1.323687	-3.878111	-0.889892
	31	6	0	-3.092782	-2.324880	-0.978460
	32	6	0	-3.621981	-1.086773	-1.362326
	33	6	0	-4.924636	-0.734287	-1.015374
	34	6	0	-5.717379	-1.614290	-0.279916
	35	6	0	-5.198274	-2.848921	0.110530
	36	6	0	-3.896967	-3.197565	-0.236598
	37	6	0	0.988263	-3.124246	2.185338
	38	6	0	5.458998	1.753991	-0.925326
	39	6	0	-2.240445	1.764158	4.063283
	40	6	0	0.257583	5.224979	-1.243361
	41	1	0	-4.472090	3.873586	0.009591
	42	1	0	5.522918	-3.222874	-0.001365
	43	1	0	3.256831	1.754874	2.464874
	44	1	0	0.996269	3.385301	2.453591
	45	1	0	-4.155645	2.311785	1.897744
	46	1	0	-2.558959	4.508794	-1.419492
	47	1	0	3.747507	-3.575745	1.678727
	48	1	0	5.674058	-1.085193	-1.228577
	49	1	0	0.942289	3.242463	-0.847791
	50	1	0	-0.819701	0.808660	2.789689
	51	1	0	3.351951	1.814010	-0.605055
	52	1	0	1.107532	-1.014526	2.456346
	53	1	0	1.134664	5.481481	-1.855743
	54	1	0	-0.604767	5.765815	-1.661320
	55	1	0	0.429075	5.606766	-0.226428
	56	1	0	0.691146	3.422881	-3.297359
	57	1	0	-0.293142	2.081552	-2.658696
	58	1	0	-1.067836	3.612083	-3.133935
	59	1	0	-2.062696	1.073042	4.900363
	60	1	0	-1.642425	2.670711	4.237713
	61	1	0	-3.301533	2.054074	4.094727
	62	1	0	-2.513912	-0.890828	3.346110
	63	1	0	-3.764697	0.012653	2.467737
	64	1	0	-2.398219	-0.688975	1.580431
	65	1	0	5.469201	2.716242	-1.458184
	66	1	0	5.740912	1.941038	0.121020
	67	1	0	6.241354	1.123706	-1.373799
	68	1	0	3.695875	1.806865	-3.053106
	69	1	0	4.367003	0.162160	-2.979807
	70	1	0	2.663760	0.441011	-2.552855
	71	1	0	0.177899	-3.231789	2.921334
	72	1	0	0.533505	-3.091090	1.185530
	73	1	0	1.605911	-4.032941	2.246011
	74	1	0	1.627692	-2.047659	4.647625
	75	1	0	3.118990	-2.753714	3.990027
	76	1	0	2.962375	-0.990236	4.128175

	77	1	0	-3.464134	-4.155737	0.051155
	78	1	0	-5.813816	-3.543004	0.685353
	79	1	0	-6.739049	-1.338893	-0.012579
	80	1	0	-5.321757	0.235137	-1.320406
	81	1	0	-3.009564	-0.382837	-1.925217
	82	1	0	-1.441692	-1.379075	-2.907436
	83	1	0	-0.158918	-3.487901	-3.567513
	84	1	0	0.912915	-2.068744	-3.477514
	85	1	0	0.894574	-3.269445	-2.164827

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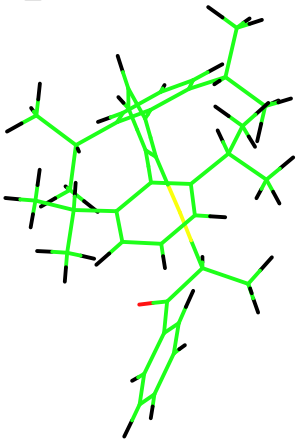

Charge = 0 Multiplicity = 1
Zero-point correction= 0.729988 (Hartree/Particle)
Thermal correction to Energy= 0.772662
Thermal correction to Enthalpy= 0.773606
Thermal correction to Gibbs Free Energy= 0.649369
Sum of electronic and zero-point Energies= -1718.213459
Sum of electronic and thermal Energies= -1718.170786
Sum of electronic and thermal Enthalpies= -1718.169842
Sum of electronic and thermal Free Energies= -1718.294079
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.766943	1.979836	-1.832957
2	6	0	-0.803565	2.370783	-0.887750
3	6	0	-1.084273	3.249667	0.172112
4	6	0	-2.387075	3.746783	0.265068
5	6	0	-3.361373	3.382051	-0.656617
6	6	0	-3.053572	2.507170	-1.691471
7	7	0	0.532466	1.857128	-1.018043
8	6	0	0.980168	0.717075	-0.432093
9	7	0	2.272347	0.614768	-0.837388
10	6	0	2.624177	1.668349	-1.661746
11	6	0	1.524624	2.454576	-1.775642
12	79	0	-0.041281	-0.622328	0.724183
13	6	0	-0.997233	-2.099234	1.874600
14	6	0	-1.499561	-1.647309	3.249689
15	6	0	3.165074	-0.447690	-0.458790
16	6	0	3.994768	-0.255412	0.659060
17	6	0	4.869746	-1.291439	0.995262
18	6	0	4.911949	-2.464079	0.250550
19	6	0	4.073585	-2.627022	-0.845092
20	6	0	3.177699	-1.624360	-1.226611
21	6	0	3.939291	0.998919	1.512297
22	6	0	5.303569	1.684806	1.613716
23	6	0	2.273005	-1.835713	-2.426804
24	6	0	1.383767	-3.069988	-2.253710
25	6	0	-0.045747	3.644768	1.206332
26	6	0	-0.402334	3.075487	2.582481
27	6	0	-1.462674	1.012627	-2.962692
28	6	0	-2.246391	-0.292574	-2.798904
29	6	0	-1.987231	-2.747194	0.972666
30	8	0	-1.717576	-3.750115	0.318420
31	6	0	-3.379805	-2.176639	0.826148
32	6	0	-3.684842	-0.818526	0.970996
33	6	0	-4.987840	-0.361473	0.780870
34	6	0	-6.005454	-1.257784	0.459068
35	6	0	-5.710106	-2.612920	0.306723
36	6	0	-4.405230	-3.063360	0.476391
37	6	0	3.362600	0.686417	2.896380
38	6	0	3.088291	-1.909354	-3.721541
39	6	0	0.154626	5.161259	1.259955
40	6	0	-1.715069	1.650691	-4.331322
41	1	0	-4.372425	3.781206	-0.565354
42	1	0	5.600761	-3.261793	0.531253
43	1	0	3.616728	1.760638	-2.086009
44	1	0	1.356653	3.375576	-2.320779
45	1	0	-2.643375	4.428526	1.076709
46	1	0	-3.829855	2.219265	-2.400799

47	1	0	5.523597	-1.180687	1.860847
48	1	0	4.108826	-3.555659	-1.415211
49	1	0	-0.393821	0.761570	-2.910556
50	1	0	0.912936	3.197802	0.908254
51	1	0	1.608025	-0.964306	-2.504326
52	1	0	3.253115	1.706645	1.026333
53	1	0	-1.430510	0.955364	-5.134641
54	1	0	-2.777622	1.899068	-4.473226
55	1	0	-1.135795	2.576582	-4.461205
56	1	0	-1.984314	-0.997692	-3.601609
57	1	0	-2.028099	-0.775280	-1.836340
58	1	0	-3.332035	-0.120383	-2.846625
59	1	0	0.953553	5.416282	1.971767
60	1	0	0.432405	5.567436	0.276559
61	1	0	-0.757239	5.681159	1.589947
62	1	0	0.378566	3.325756	3.316062
63	1	0	-1.353330	3.487182	2.953601
64	1	0	-0.498844	1.980935	2.543588
65	1	0	2.421157	-2.015965	-4.589723
66	1	0	3.698198	-1.005976	-3.869705
67	1	0	3.769295	-2.773985	-3.718265
68	1	0	0.702068	-3.167507	-3.111382
69	1	0	1.979360	-3.993897	-2.201538
70	1	0	0.772906	-3.010102	-1.342191
71	1	0	3.275008	1.606208	3.494137
72	1	0	2.364993	0.231910	2.814093
73	1	0	4.007655	-0.012440	3.450237
74	1	0	5.219119	2.621672	2.183896
75	1	0	6.040836	1.052164	2.130287
76	1	0	5.709838	1.926357	0.620775
77	1	0	-4.146098	-4.113017	0.337248
78	1	0	-6.501162	-3.318665	0.047843
79	1	0	-7.027338	-0.900249	0.321362
80	1	0	-5.207237	0.702348	0.883934
81	1	0	-2.889479	-0.108846	1.202513
82	1	0	-0.208077	-2.857869	2.009282
83	1	0	-1.971458	-2.478558	3.802806
84	1	0	-0.657749	-1.289251	3.860561
85	1	0	-2.235301	-0.833132	3.206061

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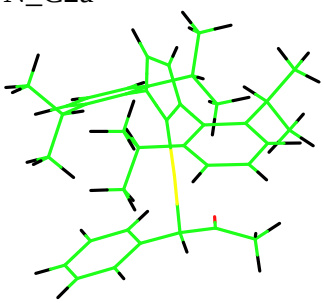

Charge = 0 Multiplicity = 1

Zero-point correction= 0.729588 (Hartree/Particle)
Thermal correction to Energy= 0.772470
Thermal correction to Enthalpy= 0.773414
Thermal correction to Gibbs Free Energy= 0.648773
Sum of electronic and zero-point Energies= -1718.222417
Sum of electronic and thermal Energies= -1718.179535
Sum of electronic and thermal Enthalpies= -1718.178591
Sum of electronic and thermal Free Energies= -1718.303231

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.590112	2.884978	-0.595679
2	6	0	-1.187354	2.299152	0.616667
3	6	0	-2.080027	2.018325	1.664466
4	6	0	-3.418972	2.370986	1.476956
5	6	0	-3.845237	2.969226	0.297850
6	6	0	-2.940876	3.217594	-0.727299
7	7	0	0.205069	1.983964	0.798970
8	6	0	0.785576	0.813556	0.432679
9	7	0	2.088103	0.951786	0.788563
10	6	0	2.317686	2.187514	1.367678
11	6	0	1.127721	2.839311	1.372820
12	79	0	-0.135538	-0.755658	-0.467688
13	6	0	-1.205803	-2.344771	-1.379041
14	6	0	-1.154464	-1.974643	-2.814862
15	8	0	-1.955558	-1.241080	-3.382313
16	6	0	3.099200	-0.049502	0.586858

17	6	0	3.845943	-0.019153	-0.602982
18	6	0	4.829657	-0.998245	-0.767599
19	6	0	5.054262	-1.961514	0.208389
20	6	0	4.298705	-1.964843	1.374541
21	6	0	3.303745	-1.008126	1.593320
22	6	0	3.605482	1.005425	-1.696721
23	6	0	3.072127	0.336904	-2.966559
24	6	0	2.484690	-1.044947	2.870857
25	6	0	3.370989	-0.915392	4.112446
26	6	0	-1.651611	1.333368	2.949368
27	6	0	-2.344851	-0.023092	3.105206
28	6	0	-0.627866	3.158712	-1.737083
29	6	0	-0.424602	4.664053	-1.934406
30	6	0	-2.530149	-2.456737	-0.692200
31	6	0	-3.623426	-1.619541	-0.975386
32	6	0	-4.830813	-1.769237	-0.297245
33	6	0	-4.985051	-2.744466	0.687039
34	6	0	-3.908772	-3.580528	0.981193
35	6	0	-2.703780	-3.437849	0.299232
36	6	0	-1.883968	2.228785	4.169265
37	6	0	-1.079262	2.479459	-3.032852
38	6	0	4.861204	1.833116	-1.982278
39	6	0	1.615100	-2.303954	2.930228
40	6	0	-0.003989	-2.577331	-3.604300
41	1	0	-0.604184	-3.248322	-1.199866
42	1	0	-4.895797	3.233525	0.171542
43	1	0	5.824850	-2.718608	0.057737
44	1	0	3.298499	2.485374	1.718133
45	1	0	0.853608	3.824929	1.729068
46	1	0	-4.142289	2.161212	2.265344
47	1	0	-3.290776	3.671391	-1.654775
48	1	0	4.482233	-2.728792	2.130711
49	1	0	5.425956	-1.009819	-1.680541
50	1	0	0.345442	2.725337	-1.466741
51	1	0	-0.571564	1.140241	2.885076
52	1	0	2.829392	1.699022	-1.344428
53	1	0	1.805903	-0.180731	2.861064
54	1	0	0.304575	4.852872	-2.736326
55	1	0	-1.365595	5.160180	-2.216981
56	1	0	-0.055878	5.148384	-1.018127
57	1	0	-0.322529	2.625995	-3.818024
58	1	0	-1.230248	1.399050	-2.900177
59	1	0	-2.022627	2.905305	-3.406812
60	1	0	-1.525826	1.732542	5.083459
61	1	0	-1.356150	3.189101	4.074278
62	1	0	-2.952723	2.449422	4.310609
63	1	0	-1.976458	-0.538073	4.005139
64	1	0	-3.434318	0.088963	3.208779
65	1	0	-2.160182	-0.669779	2.236185
66	1	0	4.646037	2.606287	-2.734406
67	1	0	5.230928	2.333893	-1.075666
68	1	0	5.678396	1.209930	-2.375777
69	1	0	2.854230	1.092912	-3.735517
70	1	0	3.805176	-0.367081	-3.388814
71	1	0	2.146423	-0.219037	-2.761826
72	1	0	0.995631	-2.299321	3.839380
73	1	0	0.945371	-2.363414	2.060370
74	1	0	2.230280	-3.216402	2.949576
75	1	0	2.752638	-0.883332	5.021539
76	1	0	4.058454	-1.768807	4.212193
77	1	0	3.979073	0.000367	4.081774
78	1	0	-1.871198	-4.105539	0.534388
79	1	0	-4.009353	-4.356282	1.742903
80	1	0	-5.933100	-2.855396	1.215543
81	1	0	-5.665164	-1.109396	-0.543869
82	1	0	-3.512472	-0.864082	-1.750018
83	1	0	0.229614	-1.944564	-4.469377
84	1	0	0.892562	-2.730317	-2.988237
85	1	0	-0.323677	-3.563332	-3.978730

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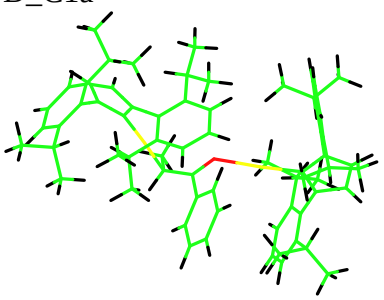

Charge = 1 Multiplicity = 1

Zero-point correction= 1.305707 (Hartree/Particle)
Thermal correction to Energy= 1.382707
Thermal correction to Enthalpy= 1.383651
Thermal correction to Gibbs Free Energy= 1.178236
Sum of electronic and zero-point Energies= -3012.912804
Sum of electronic and thermal Energies= -3012.835804
Sum of electronic and thermal Enthalpies= -3012.834860
Sum of electronic and thermal Free Energies= -3013.040275

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.093349	-1.735509	3.153334
2	6	0	-0.008213	-0.875351	2.052685
3	6	0	0.293107	0.476442	2.262484
4	6	0	0.489856	0.959902	3.552102
5	6	0	0.412365	0.095274	4.644028
6	6	0	0.126566	-1.253448	4.441626
7	6	0	-0.216740	-1.379243	0.662704
8	6	0	-1.319772	-2.244052	0.372502
9	6	0	-1.223654	-3.114516	-0.868012
10	8	0	0.576565	-1.011986	-0.261938
11	79	0	2.579780	-0.399658	-0.197853
12	6	0	4.496950	0.014297	-0.355487
13	7	0	5.076799	1.131372	-0.856868
14	6	0	6.453388	1.001251	-0.864761
15	6	0	6.733681	-0.224527	-0.354994
16	7	0	5.522949	-0.815609	-0.049158
17	6	0	4.372402	2.297893	-1.320793
18	6	0	3.934109	2.331906	-2.655695
19	6	0	3.271931	3.487726	-3.079568
20	6	0	3.065591	4.556535	-2.215450
21	6	0	3.518139	4.493255	-0.902759
22	6	0	4.183948	3.362212	-0.422433
23	6	0	4.162002	1.190577	-3.630552
24	6	0	2.837090	0.608395	-4.130228
25	6	0	4.673974	3.325281	1.014147
26	6	0	3.507028	3.413083	2.000886
27	6	0	5.380157	-2.133108	0.516228
28	6	0	5.246280	-3.226674	-0.356334
29	6	0	5.122106	-4.492041	0.224088
30	6	0	5.132922	-4.654448	1.604104
31	6	0	5.270515	-3.551551	2.438243
32	6	0	5.399445	-2.262164	1.915124
33	6	0	5.239457	-3.084402	-1.867723
34	6	0	3.925855	-3.590001	-2.469987
35	6	0	5.539996	-1.075264	2.851038
36	6	0	6.777053	-1.204901	3.743447
37	6	0	6.448545	-3.784137	-2.495562
38	6	0	4.267210	-0.876356	3.678310
39	6	0	5.713098	4.418459	1.277869
40	6	0	5.055655	1.628014	-4.795011
41	79	0	-2.867365	-0.761752	0.153358
42	6	0	-4.426262	0.493043	-0.160045
43	7	0	-5.631805	0.159589	-0.682254
44	6	0	-6.451943	1.268066	-0.777416
45	6	0	-5.738964	2.320840	-0.303735
46	7	0	-4.502229	1.826517	0.070058
47	6	0	-6.006351	-1.169111	-1.091152
48	6	0	-5.777992	-1.546447	-2.425652
49	6	0	-6.152717	-2.840938	-2.795871
50	6	0	-6.727752	-3.712346	-1.878707
51	6	0	-6.946383	-3.305645	-0.568044
52	6	0	-6.593567	-2.022207	-0.141347
53	6	0	-3.449893	2.633927	0.626965
54	6	0	-2.495613	3.186333	-0.244819
55	6	0	-1.511560	4.003168	0.319403
56	6	0	-1.486898	4.258472	1.685557

	57	6	0	-2.440918	3.690983	2.521676
	58	6	0	-3.444986	2.861682	2.013703
	59	6	0	-5.155188	-0.615470	-3.450563
	60	6	0	-3.829360	-1.171677	-3.976343
	61	6	0	-6.845940	-1.606461	1.296887
	62	6	0	-6.010891	-2.444076	2.269407
	63	6	0	-2.504665	2.936495	-1.741874
	64	6	0	-1.221197	2.236776	-2.197620
	65	6	0	-4.465504	2.244411	2.953035
	66	6	0	-5.298916	3.316890	3.659651
	67	6	0	-6.128847	-0.316737	-4.594215
	68	6	0	-8.336053	-1.666654	1.643926
	69	6	0	-2.743076	4.233054	-2.521000
	70	6	0	-3.792782	1.304941	3.957554
	71	1	0	2.554473	5.451776	-2.571667
	72	1	0	5.036043	-5.651921	2.034054
	73	1	0	7.676830	-0.728589	-0.181843
	74	1	0	7.100791	1.789210	-1.230280
	75	1	0	3.357163	5.341778	-0.237096
	76	1	0	2.917988	3.553231	-4.108674
	77	1	0	5.279148	-3.693386	3.519149
	78	1	0	5.016065	-5.366496	-0.418332
	79	1	0	4.688648	0.387583	-3.095903
	80	1	0	5.165556	2.356481	1.180775
	81	1	0	5.317000	-2.014686	-2.109764
	82	1	0	5.672973	-0.172403	2.237741
	83	1	0	5.259222	0.777943	-5.462120
	84	1	0	4.577385	2.414421	-5.397534
	85	1	0	6.019436	2.020411	-4.440331
	86	1	0	3.023126	-0.245216	-4.798259
	87	1	0	2.213826	0.258149	-3.294723
	88	1	0	2.257144	1.351831	-4.697309
	89	1	0	6.098926	4.341230	2.304660
	90	1	0	6.565494	4.341438	0.587929
	91	1	0	5.281417	5.423580	1.161245
	92	1	0	3.874508	3.341471	3.035086
	93	1	0	2.969212	4.368405	1.905346
	94	1	0	2.788203	2.598468	1.836186
	95	1	0	6.457800	-3.631084	-3.584512
	96	1	0	7.395011	-3.399087	-2.089741
	97	1	0	6.425719	-4.868847	-2.313531
	98	1	0	3.917224	-3.428093	-3.557788
	99	1	0	3.788910	-4.667590	-2.295884
	100	1	0	3.061063	-3.066106	-2.038207
	101	1	0	4.360477	0.013829	4.317662
	102	1	0	3.387453	-0.743281	3.032749
	103	1	0	4.074922	-1.737929	4.335027
	104	1	0	6.889971	-0.310204	4.372731
	105	1	0	6.704236	-2.072820	4.415320
	106	1	0	7.694907	-1.320814	3.149429
	107	1	0	-7.012586	-4.717959	-2.189950
	108	1	0	-0.717391	4.909387	2.102895
	109	1	0	-5.994849	3.368263	-0.198163
	110	1	0	-7.459734	1.205585	-1.170067
	111	1	0	-7.402251	-3.998672	0.139524
	112	1	0	-5.991639	-3.172689	-3.821957
	113	1	0	-2.407573	3.895698	3.592019
	114	1	0	-0.755266	4.451515	-0.325717
	115	1	0	-4.932896	0.338268	-2.951220
	116	1	0	-6.525133	-0.560952	1.408699
	117	1	0	-3.341128	2.260069	-1.965897
	118	1	0	-5.154534	1.635823	2.350653
	119	1	0	-5.683651	0.398682	-5.300930
	120	1	0	-6.380306	-1.226851	-5.158690
	121	1	0	-7.069740	0.113511	-4.222215
	122	1	0	-3.368191	-0.460902	-4.677861
	123	1	0	-3.120314	-1.353658	-3.156251
	124	1	0	-3.974213	-2.120165	-4.514777
	125	1	0	-8.504711	-1.309412	2.670210
	126	1	0	-8.935295	-1.044219	0.964147

127	1	0	-8.724810	-2.693948	1.584244
128	1	0	-6.165900	-2.099810	3.302520
129	1	0	-6.290463	-3.507487	2.228369
130	1	0	-4.938351	-2.366959	2.039095
131	1	0	-2.797245	4.027585	-3.600037
132	1	0	-3.682334	4.718931	-2.220337
133	1	0	-1.929119	4.956152	-2.361477
134	1	0	-1.274136	2.006733	-3.272097
135	1	0	-0.335964	2.870943	-2.039044
136	1	0	-1.062084	1.293798	-1.655032
137	1	0	-4.549618	0.816309	4.588652
138	1	0	-3.212251	0.523794	3.447029
139	1	0	-3.107963	1.849996	4.624100
140	1	0	-6.065113	2.849787	4.295127
141	1	0	-4.675892	3.952360	4.306547
142	1	0	-5.809001	3.973682	2.940440
143	1	0	-1.682181	-2.765378	1.269304
144	1	0	-2.175478	-3.624682	-1.065662
145	1	0	-0.963672	-2.522387	-1.754615
146	1	0	-0.445948	-3.888122	-0.750033
147	1	0	0.335602	1.154019	1.408864
148	1	0	0.697445	2.018951	3.707097
149	1	0	0.573500	0.473621	5.654151
150	1	0	0.073611	-1.935325	5.290871
151	1	0	-0.309699	-2.793113	3.000341

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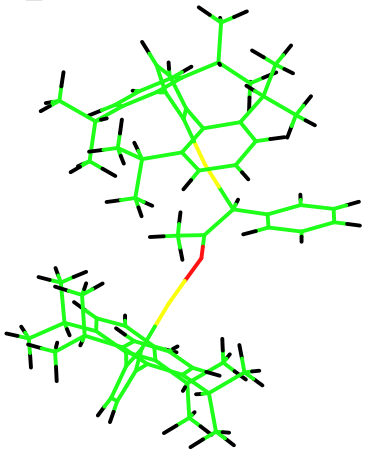

Charge = 1 Multiplicity = 1

Zero-point correction= 1.305699 (Hartree/Particle)

Thermal correction to Energy= 1.382627

Thermal correction to Enthalpy= 1.383571

Thermal correction to Gibbs Free Energy= 1.179024

Sum of electronic and zero-point Energies= -3012.918302

Sum of electronic and thermal Energies= -3012.841374

Sum of electronic and thermal Enthalpies= -3012.840430

Sum of electronic and thermal Free Energies= -3013.044977

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.030426	3.078732	-0.216159
2	6	0	-4.939871	2.054908	-1.174562
3	6	0	-4.502023	2.269901	-2.492537
4	6	0	-4.135366	3.573362	-2.837673
5	6	0	-4.208849	4.608378	-1.913033
6	6	0	-4.652112	4.362455	-0.619378
7	7	0	-5.337527	0.723046	-0.797221
8	6	0	-4.528398	-0.197148	-0.221913
9	7	0	-5.301670	-1.294473	-0.041755
10	6	0	-6.585114	-1.063490	-0.499305
11	6	0	-6.607636	0.207585	-0.974537
12	79	0	-2.653869	0.021805	0.340029
13	8	0	-0.722988	0.353983	1.065617
14	6	0	0.107801	-0.509589	1.485769
15	6	0	-0.166636	-1.967786	1.245498
16	6	0	-4.849782	-2.527967	0.547436
17	6	0	-4.944926	-2.679789	1.941537
18	6	0	-4.498088	-3.889438	2.481539
19	6	0	-3.988381	-4.895336	1.669019
20	6	0	-3.915535	-4.715279	0.292763
21	6	0	-4.345781	-3.526764	-0.303276
22	6	0	-5.510788	-1.606221	2.853643
23	6	0	-6.781707	-2.091913	3.556953
24	6	0	-4.261945	-3.360292	-1.810184
25	6	0	-2.812815	-3.428288	-2.299118
26	6	0	-4.397869	1.154550	-3.517700
27	6	0	-5.201304	1.465866	-4.782583
28	6	0	-5.528796	2.846023	1.198942
29	6	0	-6.861174	3.563542	1.436836
30	6	0	1.285379	-0.139158	2.215714

	31	79	0	2.740468	-0.173093	0.616735
	32	6	0	4.239017	-0.103890	-0.737052
	33	7	0	5.041594	-1.116923	-1.145426
	34	6	0	5.988117	-0.661979	-2.044546
	35	6	0	5.769205	0.668306	-2.199975
	36	7	0	4.695606	0.991110	-1.391785
	37	6	0	4.930608	-2.482959	-0.706556
	38	6	0	5.634397	-2.877056	0.444148
	39	6	0	5.511540	-4.211683	0.841466
	40	6	0	4.730084	-5.107278	0.121553
	41	6	0	4.054052	-4.687530	-1.018002
	42	6	0	4.139253	-3.365155	-1.461732
	43	6	0	4.146358	2.316518	-1.270156
	44	6	0	4.678822	3.177161	-0.295422
	45	6	0	4.150697	4.469527	-0.228642
	46	6	0	3.140655	4.879229	-1.090010
	47	6	0	2.630553	4.000731	-2.038337
	48	6	0	3.120842	2.697349	-2.152200
	49	6	0	6.505820	-1.925690	1.244554
	50	6	0	7.969311	-2.377176	1.241805
	51	6	0	3.390910	-2.934548	-2.710728
	52	6	0	3.847878	-3.723324	-3.940776
	53	6	0	5.782771	2.761269	0.659811
	54	6	0	7.069590	3.548001	0.393341
	55	6	0	2.541251	1.759222	-3.195554
	56	6	0	1.050017	1.512697	-2.951095
	57	6	0	1.406949	1.172673	2.915644
	58	6	0	0.982015	2.389764	2.359301
	59	6	0	1.127583	3.581010	3.065574
	60	6	0	1.704530	3.590989	4.334423
	61	6	0	2.140031	2.391214	4.893329
	62	6	0	1.993410	1.198786	4.190108
	63	6	0	5.977683	-1.750369	2.670859
	64	6	0	1.876570	-3.038428	-2.510801
	65	6	0	5.339557	2.892574	2.119366
	66	6	0	2.798927	2.272802	-4.614755
	67	6	0	-4.466638	-1.117574	3.861334
	68	6	0	-5.144144	-4.382394	-2.532774
	69	6	0	-2.932145	0.853533	-3.844121
	70	6	0	-4.482133	3.250927	2.239959
	71	1	0	2.335814	0.264249	4.639807
	72	1	0	2.594411	2.381076	5.885003
	73	1	0	1.816175	4.526842	4.882971
	74	1	0	0.789234	4.514821	2.613882
	75	1	0	0.539116	2.398489	1.365619
	76	1	0	-1.039285	-2.260594	1.851270
	77	1	0	-0.433655	-2.133704	0.192953
	78	1	0	0.684538	-2.605199	1.511272
	79	1	0	-3.921440	5.618974	-2.205132
	80	1	0	-3.649554	-5.832015	2.113016
	81	1	0	-7.358093	-1.820542	-0.444620
	82	1	0	-7.404304	0.790342	-1.421015
	83	1	0	-3.788229	3.781684	-3.849948
	84	1	0	-4.709232	5.185132	0.093640
	85	1	0	-3.518499	-5.514784	-0.333311
	86	1	0	-4.554510	-4.047555	3.558807
	87	1	0	-5.708597	1.768498	1.322672
	88	1	0	-4.826389	0.244007	-3.074823
	89	1	0	-5.788891	-0.743968	2.231102
	90	1	0	-4.642444	-2.360509	-2.062716
	91	1	0	-7.237425	3.348964	2.447591
	92	1	0	-6.751941	4.654691	1.348035
	93	1	0	-7.626953	3.246482	0.714389
	94	1	0	-4.844008	3.021092	3.252591
	95	1	0	-3.534124	2.715910	2.086418
	96	1	0	-4.269632	4.329580	2.204601
	97	1	0	-5.161642	0.615917	-5.479063
	98	1	0	-6.256938	1.667594	-4.551852
	99	1	0	-4.802452	2.343072	-5.312638
	100	1	0	-2.859366	0.013552	-4.550792

101	1	0	-2.439314	1.722249	-4.305896
102	1	0	-2.369465	0.590754	-2.936624
103	1	0	-7.211185	-1.286882	4.170568
104	1	0	-7.545732	-2.414296	2.835187
105	1	0	-6.574461	-2.941725	4.223939
106	1	0	-4.884774	-0.314267	4.485066
107	1	0	-4.144699	-1.924932	4.535721
108	1	0	-3.574494	-0.723109	3.353505
109	1	0	-2.767262	-3.268659	-3.386373
110	1	0	-2.194661	-2.658775	-1.814917
111	1	0	-2.360576	-4.409050	-2.088873
112	1	0	-5.117712	-4.212377	-3.618879
113	1	0	-4.802761	-5.412102	-2.350335
114	1	0	-6.191026	-4.316791	-2.203877
115	1	0	4.651985	-6.144671	0.448713
116	1	0	2.746419	5.893681	-1.020917
117	1	0	6.274473	1.409851	-2.806997
118	1	0	6.724219	-1.322337	-2.487068
119	1	0	3.449551	-5.402188	-1.577284
120	1	0	6.041367	-4.555958	1.730052
121	1	0	1.835422	4.333598	-2.706070
122	1	0	4.537814	5.166509	0.514707
123	1	0	6.465573	-0.940220	0.759499
124	1	0	3.621452	-1.876001	-2.896097
125	1	0	6.002532	1.699007	0.481076
126	1	0	3.049205	0.789233	-3.099127
127	1	0	8.595419	-1.648512	1.776775
128	1	0	8.094286	-3.349574	1.740830
129	1	0	8.360506	-2.475719	0.219094
130	1	0	6.599927	-1.030893	3.222812
131	1	0	4.943912	-1.375568	2.668640
132	1	0	5.994996	-2.699130	3.227616
133	1	0	3.337756	-3.355526	-4.842975
134	1	0	4.931324	-3.629532	-4.101202
135	1	0	3.617700	-4.794822	-3.844891
136	1	0	1.345948	-2.681211	-3.405876
137	1	0	1.564335	-4.078354	-2.331404
138	1	0	1.550373	-2.432966	-1.653054
139	1	0	7.872888	3.207995	1.063035
140	1	0	7.415449	3.423460	-0.642992
141	1	0	6.925342	4.624588	0.568324
142	1	0	6.128605	2.521016	2.789553
143	1	0	5.144517	3.940327	2.391168
144	1	0	4.421325	2.321939	2.317302
145	1	0	0.659214	0.784381	-3.677176
146	1	0	0.870245	1.121671	-1.939341
147	1	0	0.464257	2.437549	-3.061721
148	1	0	2.413999	1.559531	-5.358293
149	1	0	2.301252	3.237976	-4.791923
150	1	0	3.872490	2.414419	-4.804549
151	1	0	1.646128	-0.979677	2.823689

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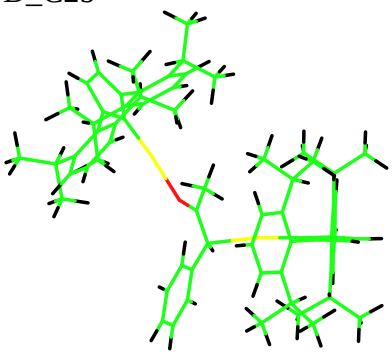

Charge = 1 Multiplicity = 1
Zero-point correction= 1.306117 (Hartree/Particle)
Thermal correction to Energy= 1.382788
Thermal correction to Enthalpy= 1.383732
Thermal correction to Gibbs Free Energy= 1.181333
Sum of electronic and zero-point Energies= -3012.917935
Sum of electronic and thermal Energies= -3012.841264
Sum of electronic and thermal Enthalpies= -3012.840320
Sum of electronic and thermal Free Energies= -3013.042719
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.391285	-2.801232	0.590103
2	6	0	5.226021	-2.046756	-0.584010
3	6	0	4.852421	-2.611157	-1.815539
4	6	0	4.635877	-3.991293	-1.845022

5	6	0	4.789253	-4.766690	-0.701899
6	6	0	5.162667	-4.177135	0.499582
7	7	0	5.473336	-0.628487	-0.529971
8	6	0	4.555915	0.310372	-0.197914
9	7	0	5.209912	1.494148	-0.269348
10	6	0	6.525842	1.299254	-0.644405
11	6	0	6.691628	-0.037821	-0.807456
12	79	0	2.686375	0.019086	0.343285
13	8	0	0.753954	-0.404654	1.008225
14	6	0	-0.109596	0.385890	1.497611
15	6	0	0.114651	1.868985	1.401630
16	6	0	4.621716	2.777135	0.014430
17	6	0	4.697259	3.271487	1.328076
18	6	0	4.122740	4.522328	1.571747
19	6	0	3.508728	5.241913	0.553476
20	6	0	3.457949	4.727043	-0.736410
21	6	0	4.015724	3.481802	-1.039452
22	6	0	5.361940	2.508595	2.460289
23	6	0	4.341871	2.100781	3.527073
24	6	0	3.949027	2.947030	-2.458910
25	6	0	4.678711	3.869427	-3.439356
26	6	0	4.664064	-1.786896	-3.076655
27	6	0	3.192745	-1.771300	-3.500921
28	6	0	5.806173	-2.189750	1.916183
29	6	0	4.742535	-2.417855	2.993637
30	6	0	-1.278544	-0.096900	2.175143
31	79	0	-2.756383	0.053753	0.604151
32	6	0	-4.279596	0.087865	-0.724598
33	7	0	-5.218245	1.053027	-0.881756
34	6	0	-6.132035	0.696137	-1.855716
35	6	0	-5.753025	-0.522618	-2.316722
36	7	0	-4.617980	-0.877995	-1.612564
37	6	0	-5.268583	2.281994	-0.134484
38	6	0	-5.982801	2.301573	1.075539
39	6	0	-6.019941	3.511650	1.774600
40	6	0	-5.381896	4.644808	1.284818
41	6	0	-4.692044	4.594251	0.079266
42	6	0	-4.619546	3.411535	-0.661631
43	6	0	-3.908040	-2.116709	-1.796651
44	6	0	-4.289442	-3.227714	-1.025406
45	6	0	-3.602183	-4.424184	-1.248075
46	6	0	-2.586828	-4.505244	-2.193030
47	6	0	-2.230786	-3.386073	-2.936196
48	6	0	-2.882236	-2.163137	-2.755816
49	6	0	-6.699770	1.083967	1.630604
50	6	0	-6.086506	0.635867	2.960112
51	6	0	-3.857337	3.383226	-1.974561
52	6	0	-2.360441	3.612321	-1.748591
53	6	0	-5.400410	-3.173582	0.007766
54	6	0	-4.893824	-3.558274	1.400078
55	6	0	-2.465910	-0.954288	-3.574105
56	6	0	-2.682048	-1.187688	-5.071687
57	6	0	-1.350448	-1.476992	2.737734
58	6	0	-1.951275	-1.659038	3.992781
59	6	0	-2.049674	-2.921785	4.570341
60	6	0	-1.548599	-4.037608	3.902813
61	6	0	-0.957071	-3.872902	2.651478
62	6	0	-0.861536	-2.611426	2.069740
63	6	0	-8.204306	1.335128	1.765223
64	6	0	-4.430420	4.384760	-2.980804
65	6	0	-6.588613	-4.042502	-0.415556
66	6	0	-1.018258	-0.557438	-3.271655
67	6	0	6.520768	3.303309	3.068533
68	6	0	2.500381	2.704166	-2.890921
69	6	0	5.570454	-2.269975	-4.211567
70	6	0	7.175222	-2.711739	2.362357
71	1	0	-2.342729	-0.791508	4.528525
72	1	0	-2.516669	-3.032622	5.549964
73	1	0	-1.621371	-5.027903	4.353594
74	1	0	-0.567391	-4.739469	2.114988

75	1	0	-0.406305	-2.499392	1.088283
76	1	0	0.968984	2.131287	2.045976
77	1	0	0.387762	2.148401	0.374624
78	1	0	-0.761144	2.446462	1.719370
79	1	0	4.618149	-5.842648	-0.748424
80	1	0	3.071006	6.217805	0.766382
81	1	0	7.217470	2.125263	-0.758364
82	1	0	7.558472	-0.621504	-1.093069
83	1	0	4.342336	-4.467002	-2.781045
84	1	0	5.281101	-4.797602	1.388138
85	1	0	2.978774	5.305511	-1.526771
86	1	0	4.160405	4.941920	2.577426
87	1	0	5.898876	-1.103265	1.775369
88	1	0	4.948410	-0.749109	-2.850794
89	1	0	5.783815	1.582657	2.044356
90	1	0	4.461135	1.974671	-2.480106
91	1	0	7.485453	-2.223100	3.297315
92	1	0	7.152361	-3.795963	2.547045
93	1	0	7.948652	-2.519659	1.604928
94	1	0	5.035426	-1.921078	3.930061
95	1	0	3.765823	-2.018739	2.684433
96	1	0	4.612628	-3.487436	3.215168
97	1	0	5.458808	-1.621852	-5.092813
98	1	0	6.628915	-2.261407	-3.914866
99	1	0	5.320808	-3.294843	-4.523200
100	1	0	3.054303	-1.133558	-4.386478
101	1	0	2.840028	-2.781405	-3.758171
102	1	0	2.552311	-1.385803	-2.694497
103	1	0	7.030318	2.706774	3.838855
104	1	0	7.263486	3.581612	2.307388
105	1	0	6.171358	4.229755	3.547497
106	1	0	4.830086	1.521089	4.323940
107	1	0	3.873926	2.979670	3.995207
108	1	0	3.543685	1.478753	3.096216
109	1	0	2.468683	2.280626	-3.905504
110	1	0	1.996988	2.001463	-2.211222
111	1	0	1.921230	3.639723	-2.902640
112	1	0	4.673145	3.435407	-4.449686
113	1	0	4.198248	4.857033	-3.501625
114	1	0	5.725403	4.027310	-3.142919
115	1	0	-5.427823	5.578912	1.845761
116	1	0	-2.067627	-5.451019	-2.352071
117	1	0	-6.183509	-1.165708	-3.074896
118	1	0	-6.961998	1.337371	-2.127228
119	1	0	-4.201592	5.492614	-0.296545
120	1	0	-6.562387	3.567620	2.718777
121	1	0	-1.430330	-3.462213	-3.672726
122	1	0	-3.868885	-5.308405	-0.669007
123	1	0	-6.568740	0.258072	0.917060
124	1	0	-3.970069	2.380064	-2.409760
125	1	0	-5.755386	-2.134792	0.067219
126	1	0	-3.102937	-0.109060	-3.277639
127	1	0	-8.713843	0.424604	2.112280
128	1	0	-8.419342	2.131194	2.493310
129	1	0	-8.652719	1.631300	0.806125
130	1	0	-6.592672	-0.267863	3.329553
131	1	0	-5.017310	0.405402	2.846884
132	1	0	-6.186917	1.412515	3.733049
133	1	0	-3.907537	4.301054	-3.944668
134	1	0	-5.501061	4.210481	-3.158864
135	1	0	-4.315769	5.422014	-2.632549
136	1	0	-1.814954	3.549872	-2.702014
137	1	0	-2.166313	4.606166	-1.317573
138	1	0	-1.944738	2.858516	-1.064642
139	1	0	-7.404968	-3.959361	0.316612
140	1	0	-6.981698	-3.743876	-1.398124
141	1	0	-6.306801	-5.104145	-0.479052
142	1	0	-5.700675	-3.449573	2.139510
143	1	0	-4.555989	-4.604451	1.435047
144	1	0	-4.051332	-2.926387	1.714340

	145	1	0	-0.748582	0.357055	-3.820825
	146	1	0	-0.872871	-0.371380	-2.197758
	147	1	0	-0.313482	-1.346409	-3.574188
	148	1	0	-2.423992	-0.284141	-5.643198
	149	1	0	-2.053552	-2.008476	-5.448163
	150	1	0	-3.728138	-1.442545	-5.293647
	151	1	0	-1.666782	0.663416	2.866693

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