Electronic Supplementary Information

Synthesis of a (N,C,C) Au(III) Pincer Complex via C_{sp3}-H Bond Activation: Increasing Catalyst Robustness by Rational Catalyst Design

Marte Sofie Martinsen Holmsen,[a] Ainara Nova,*[b] Knut Hylland,[a] David S. Wragg,[a] Sigurd Øien-Ødegaard,[a] Richard H. Heyn,[c] and Mats Tilset *[a,b]

[a] Department of Chemistry, University of Oslo, P.O. Box 1033 Blindern, N-0315 Oslo, Norway

[b] Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry, University of Oslo, P.O. Box 1033, Blindern, N-0315 Oslo, Norway.

[c] SINTEF Industry, P.O. Box 124 Blindern, N-0314 Oslo, Norway

*Corresponding authors: ainara.nova@kjemi.uio.no, mats.tilset@kjemi.uio.no

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Note added after first publication:

This Supplementary Information file replaces that originally published on 07 Sep 2018. There was an error on page S3, where the quantities of the reagents used in the preparation of compound L_1 were incorrectly swapped with each other. This has now been corrected, and the text now reads, "2-Bromopyridine (0.785 g, 4.96 mmol, 1.00 equiv.) and 3,5-(di-*tert*-butyl)phenylboronic acid (1.17 g, 5.02 mmol, 1.01 equiv.) were dissolved in *n*-PrOH (10 mL) in a 100 mL Schlenk flask."

General procedures

2-Bromopyridine, $Pd(OAc)_2$, and PPh_3 were purchased from Sigma Aldrich. 2-Bromo-6-(*tert*-butyl)pyridine and 3,5-(di-*tert*-butyl)phenylboronic acid were purchased from Fluorochem. 4-Methylphenylboronic acid was purchased from AK Scientific. $Au(OCOCH_3)_3$ was purchased from ABCR. All chemicals were used as received. Hexanes were distilled before use. CH_2Cl_2 used for **1** was purified using a MB SPS-800 solvent purifying system from MBraun. Distilled water was used in all reactions and work-ups. CD_2Cl_2 and $CDCl_3$ were dried over 3 Å molecular sieves. All other solvents were purchased from Sigma Aldrich or VWR and used as received. As a precaution, all reactions involving gold were performed in the absence of light. The ligand syntheses were performed under Argon, all other reactions and work-ups were carried out in air. Acetylene 2.6 was purchased from AGA and Praxiar and passed through a double cooling trap at -78 °C (dry ice/acetone) prior to use. Microwave reactions were performed with a Milestone MicroSYNTH microwave reactor with a SK-10 rotor. NMR spectra were recorded on Bruker Avance DPX200, DPX300, DRX500, AVII600, and AVIIIHD800 instruments at ambient temperature. ^1H and ^{13}C NMR spectra have been referenced relative to the residual solvent signals (CD_2Cl_2: $\delta(^1H)$ 5.34, $\delta(^{13}C)$ 53.84, $CDCl_3$: $\delta(^1H)$ 7.26, $\delta(^{13}C)$ 77.0, CF_3COOD: $\delta(^1H)$ 11.50). ^{19}F NMR has been referenced to $CFCl_3$ by using C_6F_6 (-164.9 ppm with respect to $CFCl_3$ at 0 ppm) as an internal standard. The peaks in the ^1H NMR spectrum were assigned by the aid of 2D NMR techniques such as HSQC, HMBC, COSY and NOESY according to the numbering scheme shown in Figure S 1. Mass spectra (ESI) were obtained on a Bruker maXis II ETD spectrometer by Osamu Sekiguchi. Elemental analysis was performed by Microanalytisches Laboratorium Kolbe, Mülheim an der Ruhr, Germany.

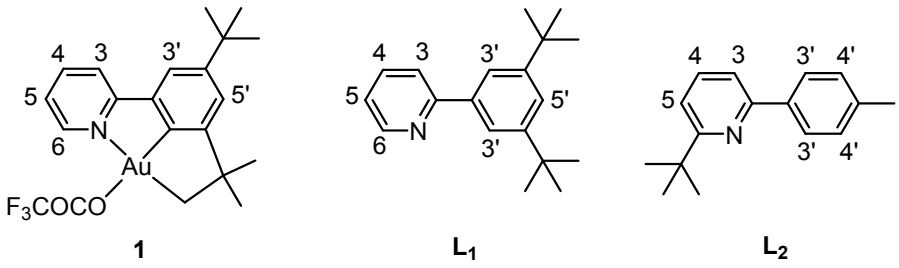
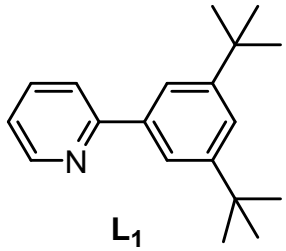


Figure S 1. Numbering scheme used for reporting the NMR data.

Synthesis of 2-(3,5-di-*tert*-butylphenyl)pyridine (L_1)



L_1
89-92%

2-Bromopyridine (0.785 g, 4.96 mmol, 1.00 equiv.) and 3,5-(di-*tert*-butyl)phenylboronic acid (1.17 g, 5.02 mmol, 1.01 equiv.) were dissolved in *n*-PrOH (10 mL) in a 100 mL Schlenk flask. 1 M K_3PO_4 (aq) (10 mL) was added and the biphasic mixture was degassed with Ar for 10 min. $Pd(OAc)_2$ (0.0220 g, 0.0980 mmol, 0.0197 equiv.) and PPh_3 (0.0782 g, 0.298 mmol, 0.0600 equiv.) were then added and the mixture was further degassed for 5 min and then heated at reflux for 3 hours under Ar. After cooling to room temperature, CH_2Cl_2 (50 mL) and H_2O (50 mL) was added, the phases were separated and the organic phase was washed with 2 M NaOH (2x 50 mL), H_2O (50 mL) and brine (50 mL), and dried with Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by flash chromatography (5% ethyl acetate in hexane) furnishing 2-(3,5-di-*tert*-butylphenyl)pyridine (**A**) as a thick colorless oil (1.22 g, 4.56 mmol, 92 %).

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.70 (d, *J* = 4.8 Hz, 1H, **H^6**), 7.80 (d, *J* = 1.8 Hz, 2H, **H$^{3'}$**), 7.70-7.75 (m, 2H, **H^3** and **H^4**) 7.50 (t, *J* = 1.8 Hz, 1H, **H$^{5'}$**) 7.21 (ddd, *J* = 7.2, 4.8, 1.4 Hz, 1H, **H^5**), 1.40 (s, 18H, (**C**H_3)$_3$).

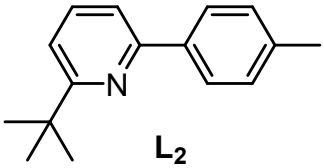
^{13}C NMR (151 MHz, $CDCl_3$): δ 158.7 (Ar-**C**), 151.1 (Ar-**C**), 149.6 (Ar-**C**), 138.9 (Ar-**C**), 136.5 (Ar-**C**), 123.2 (Ar-**C**), 121.7 (Ar-**C**), 121.4 (Ar-**C**), 120.9 (Ar-**C**), 35.0 (**C**$(CH_3)_3$), 31.5 (C(**C**H_3)$_3$).

MS (ESI, MeCN): *m/z* (rel. %): 268 ($[M+H]^+$, 100), 290 ($[M+Na]^+$, 9).

HRMS (ESI, MeCN): Found: 268.2059; calcd for $C_{19}H_{26}N$: 268.2060.

The NMR data is in agreement with that reported previously (**L_1** has previously been synthesized in 66% yield using the Kumada coupling).[1]

Synthesis of 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (L_2)



L_2
87-90%

The same procedure as for 2-(3,5-di-*tert*-butylphenyl)pyridine was used, but with a slight excess of the *p*-tolylboronic acid (1.1 equiv with respect to 2-bromo-6-*tert*-butylpyridine). The reaction was performed with 2 mmol 2-bromo-6-*tert*-butylpyridine. 2-*tert*-butyl-6-(*p*-tolyl)pyridine (**L_2**) was obtained as a colorless oil (0.406 g, 1.80 mmol, 90 %) after purification by flash chromatography (hexane to 5% ethyl acetate in hexane).

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.00 (d, *J* = 8.1 Hz, 2H, **H$^{3'}$**), 7.64 (t, *J* = 7.8 Hz, 1H, **H^4**), 7.52 (d, *J* = 7.8 Hz, 1H, **H^3**), 7.27 (d, *J* = 8.1 Hz, 2H, **H$^{4'}$**), 7.24 (d, *J* = 7.8 Hz, 1H, **H^5**), 2.41, (s, C**H**$_3$), 1.43 (s, 9H, (C**H**$_3$)$_3$).

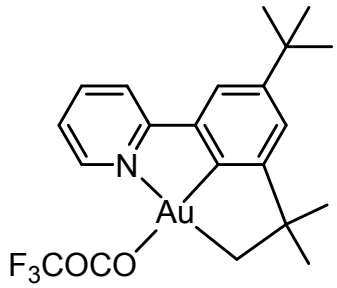
^{13}C NMR (151 MHz, $CDCl_3$): δ 168.8 (Ar-**C**), 155.4 (Ar-**C**), 138.5 (Ar-**C**), 137.2 (Ar-**C**), 136.6 (Ar-**C**), 129.3 (Ar-**C**), 126.7 (Ar-**C**), 117.0 (Ar-**C**), 116.5 (Ar-**C**), 37.7 (**C**(CH$_3$)$_3$), 30.2 (C(**C**H$_3$)$_3$), 21.3 (**C**H$_3$).

MS (ESI, MeCN): *m/z* (rel. %): 226 ([M+H]$^+$, 100), 248 ([M+Na]$^+$, 51).

HRMS (ESI, MeCN): Found: 226.1590; calcd for $C_{16}H_{20}N$: 226.1590.

The NMR data is in agreement with that reported previously (**L_2** has previously been synthesized from 4,4-Dimethyl-1-piperidinopentan-3-one hydrochloride in 37% yield over two steps).[2]

Microwave assisted synthesis of Au(III) complex 1



1
74-78%

$Au(OCOCH_3)_3$ (187 mg, 0.500 mmol, 1.00 equiv), a 1:1 mixture of CF_3COOH and H_2O (15 mL), and 2-(3,5-di-*tert*-butylphenyl)pyridine (**L_1**, 135 mg, 0.505 mmol, 1.01 equiv) were added to a microwave vessel. The reaction mixture was heated in a microwave oven at 120 °C for 30 min. After the reaction mixture had cooled down, CF_3COOH (*ca.* 20 mL) was added and the reaction mixture was stirred until all of the white precipitate was dissolved. The reaction mixture was filtered and placed in an ice bath. H_2O (25 mL) was added furnishing a white precipitate. The white precipitate was collected on a fine frit, washed with H_2O (3 x 5-10 mL), and dried under a stream of air for *ca*. 2 hours furnishing **1** (223 mg, 0.388 mmol, 78 %) as a white solid.

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.53 (d, 1H, *J* = 5.0 Hz, **H^6**), 8.04 (ddd, 1H, *J* = 7.8, 7.7, 1.6 Hz, **H^4**), 7.99 (d, 1H, *J* = 8.0 Hz, **H^3**), 7.52 – 7.54 (m, 2H, **H^5** + **$H^{3'}$**), 7.02 (d, 1H, *J* = 1.7 Hz, **$H^{5'}$**), 3.16 (s, 2H, AuCH_2), 1.40 (s, 6H, $C(CH_3)_2$), 1.39 (s, 9H, $C(CH_3)_3$).

^{13}C NMR (151 MHz, CD_2Cl_2): δ 163.4 (Ar-**C**), 162.0 (Ar-**C**), 161.3 (q, *J* = 36.3 Hz, O**C**OCF_3), 152.0 (Ar-**C**), 148.0 (Ar-**C**), 144.7 (Ar-**C**), 141.3 (Ar-**C**), 139.5 (Ar-**C**), 124.9 (Ar-**C**), 124.7 (Ar-**C**), 120.5 (Ar-**C**), 120.0 (Ar-**C**), 118.4 (q, *J* = 290.4 Hz, OCO**C**F_3), 51.3 (**C**$(CH_3)_2$), 49.1 (Au**C**H_2), 35.5 (**C**$(CH_3)_3$), 31.8 (C(**C**$H_3)_2$), 31.6 (C(**C**$H_3)_3$).

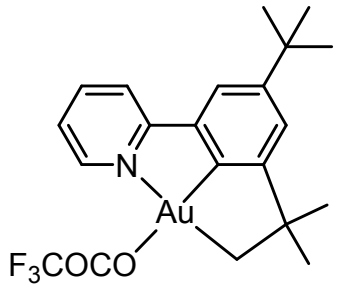
^{19}F NMR (188 MHz, CD_2Cl_2): δ -76.9 (OCOC**F_3**)

MS (ESI, MeCN): *m/z* (rel. %): 959 (22), 951 (14), 950 (32), 503 ([M-$OCOCF_3$+MeCN]$^+$, 100], 480 ([M-$OCOCF_3$+H_2O]$^+$, 45], 462 ([M-$OCOCF_3$]$^+$, 35).

HRMS (ESI, MeCN): Found: 503.1754; calcd for $C_{21}H_{26}AuN_2$: 503.1756. Found: 480.1594; calcd for $C_{19}H_{25}AuNO$: 480.1596. Found: 462.1490; calcd for $C_{19}H_{23}AuN$:462.1491.

Elemental analysis: Anal. Calcd. for $C_{21}H_{23}AuF_3NO_2$: C, 43.84; H, 4.03; N, 2.43. Found: C, 44.01; H, 3.91; N, 2.47.

Thermal synthesis of Au(III) complex 1



1
58-62%

$Au(OCOCH_3)_3$ (187 mg, 0.500 mmol, 1.00 equiv), a 1:1 mixture of CF_3COOH and H_2O (15 mL), and 2-(3,5-di-*tert*-butylphenyl)pyridine (**L_1**, 135 mg, 0.505 mmol, 1.01 equiv) were added to a round bottom flask. The reaction mixture was heated at 80 °C for 4 days. After the reaction mixture had cooled down, CF_3COOH (*ca.* 20 mL) was added and the reaction mixture was stirred until all of the white precipitate was dissolved. The reaction mixture was filtered and placed in an ice bath. H_2O (25 mL) was added furnishing a white precipitate. The precipitate was collected on a fine frit, washed with H_2O (3 x 5-10 mL), and dried under a stream of air for *ca*. 30 min furnishing a grey solid. The grey solid was dissolved in CH_2Cl_2 and the solution was filtered through Celite. CH_2Cl_2 was removed under reduced pressure furnishing **1** (179 mg, 0.311 mmol, 62%) as a white solid.

Miscellaneous experiments

Attempt at synthesis of 1 in CF_3COOD at lower temperature

$Au(OCOCH_3)_3$ (5.0 mg, 0.013 mmol, 1.0 equiv), 2-(3,5-di-*tert*-butylphenyl)pyridine (**L_1**, 3.6 mg, 0.013 mmol, 1.0 equiv), and CF_3COOD (0.5 – 0.7 mL) were added to a *J*-Young NMR tube and a reference ^1H NMR spectrum was recorded. After 1 d, no reaction was observed by ^1H NMR. The sample was then heated at 60 °C for 1 d and still no reaction could be observed by ^1H NMR. Following this, the sample was heated at 70 °C for 4 days. The sample was again investigated by ^1H NMR and this time small amounts (*ca.* 6%) of **1** has been formed. The sample was heated further at 70 °C for 18 days and then investigated by ^1H NMR again, and no significant change in the amount of **1** was observed. The reaction was not investigated further due to the low conversion into **1** under these conditions.

Reactivity of $Au(OCOCH_3)_3$ toward 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (L_2) in a CF_3COOD/H_2O mixture

$Au(OCOCH_3)_3$ (188 mg, 0.503 mmol, 1.00 equiv), a 1:1 mixture of CF_3COOH and H_2O (15 mL), and 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (**L_2**, 115 mg, 0.510 mmol, 1.01 equiv) were added to a microwave vessel. The reaction mixture was heated in a microwave oven at 120 °C for 30 min furnishing a yellow solution with a lot of black precipitate. The reaction mixture was filtered and a small portion of the reaction mixture was collected. The solvent were removed under reduced pressure and the remaining residue was investigated by ^1H NMR. Protonated ligand, [2-(*tert*-butyl)-6-(*p*-tolyl)pyridine]H^+ (**L_2H^+**), was recovered and no cyclometalated Au(III) complexes could be observed by ^1H NMR.

Reactivity of $Au(OCOCH_3)_3$ toward 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (L_2) in CF_3COOD

$Au(OCOCH_3)_3$ (5.0 mg, 0.013 mmol, 1.0 equiv), 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (**L_2**, 3.2 mg, 0.014 mmol, 1.1 equiv), and CF_3COOD (0.5-0.7 mL) were added to a *J*-Young NMR tube and a reference ^1H NMR spectrum was recorded. After 1 d, no reaction was observed by ^1H NMR. The sample was then heated at 60 °C for 1 d and still no reaction could be observed by ^1H NMR. Following this, the sample was heated at 70 °C for 4 days. The sample was again investigated by ^1H NMR and this time traces of two or more unknown products were observed. The sample was further heated at 70 °C for 18 days and then investigated by ^1H NMR again, and at this point there are only some small changes in the intensity of the resonances of the unknown products. The reaction was not investigated further due to the low reactivity observed under these conditions.

Reactivity of $HAuCl_4 \cdot 3H_2O$ toward 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (L_2) and $NaHCO_3$ in H_2O.

$HAuCl_4 \cdot 3H_2O$ (124 mg, 0.316 mmol, 1.00 equiv), 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (**L_2**, 71.5 mg, 0.317 mmol, 1.00 equiv), $NaHCO_3$ (81.5 mg, 0.917 mmol, 3.07 equiv) and H_2O (15 mL) were added to a microwave vessel. The reaction mixture was heated in a microwave oven at 120 ^oC for 30 min furnishing a brown solution with small amounts of a dark brown precipitate. The reaction mixture was filtered and diluted with H_2O to a total volume of 50 mL. It was not possible to precipitate or crystallize any organogold complexes from the reaction mixture and the reaction mixture was not subjected to further investigations.

Reactivity of $HAuCl_4 \cdot 3H_2O$ toward 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (L_2) and Na_2CO_3 in H_2O.

$HAuCl_4 \cdot 3H_2O$ (197 mg, 0.500 mmol, 1.00 equiv), 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (**L_2**, 113 mg, 0.504 mmol, 1.01 equiv), Na_2CO_3 (159 mg, 1.50 mmol, 3.00 equiv) and H_2O (15 mL) were added to a microwave vessel. The reaction mixture was heated in a microwave oven at 120 ^oC for 30 min furnishing a dark brown solution with a lot of black precipitate and some oily droplets. The reaction mixture was filtered and diluted with H_2O to a total volume of 50 mL. It was not possible to precipitate or crystallize any organogold complexes from the reaction mixture and the reaction mixture was not subjected to further investigations.

Reactivity of $HAuCl_4 \cdot 3H_2O$ toward 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (L_2) and Na_2CO_3 in a mixture of MeCN and H_2O.

$HAuCl_4 \cdot 3H_2O$ (200 mg, 0.508 mmol, 1.00 equiv), 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (**L_2**, 113 mg, 0.500 mmol, 0.98 equiv), Na_2CO_3 (159 mg, 1.50 mmol, 2.95 equiv) and a 1:1 mixture of MeCN and H_2O (15 mL) were added to a microwave vessel. The reaction mixture was heated in a microwave oven at 80 ^oC for 30 min furnishing a yellow solution with a red precipitate. The red precipitate was collected on a fine frit, washed with H_2O (3 x 5mL), and dried under a stream of air for *ca*. 1 hour furnishing a red solid (129 mg). The true identity of the red solid has not been assessed, but it is evident from ^1H NMR that no formation of any cyclometalated Au(III) complexes has occurred.

Preliminary catalytic testing of 1: Catalytic transformation of acetylene at 1 (and A)

The catalytic testing of **1** was performed by the same method as previously reported.[3] Complex **1** (5.0 mg, 0.0087 mmol) was dissolved in CF_3COOD (0.7 mL) and the solution was transferred to a NMR tube. 1,2-dichloroethane (1 µL) was added as an internal standard (ISTD). A reference ^{1}H NMR (500 MHz or 300 MHz) spectrum was recorded and the peaks of **1** were integrated against the ISTD. Acetylene was bubbled through the solution for 1 minute and the reaction was monitored by ^{1}H NMR (See Figure S 20). The turnover of (*E*)-vinyl trifluoroacetate-*d* (**8-*d***) per Au was determined by integration of the most upfield resonance of **8-*d*** against the resonance of the ISTD in the ^{1}H NMR spectrum. The turnover numbers (TONs) were measured after 5, 10, 15, and 30 minutes and after 1, 2, 3, 8, and 24 hours and the results are summarized in Table S 1 and Figure S 2.[i] After 8 hours reaction time, there are only small amounts of acetylene left in the solution and after 24 hours there are only traces of acetylene left in the solution. At this point, a maximum of *ca.* 10% decomposition of **1** was observed. Therefore, the potential turnover number for complex **1** should be significantly higher than that reported here and further work will be needed in order to properly determine the catalytic potential of **1**. The decomposition product(s) has not been characterized. The turnover numbers for complex **A** was measured by the same method (but with 0.0085 mmol of **A**) and some of these results have been previously reported.[3]

Table S 1. TONs for **1** and **A**.[i]

	Complex **1**			Complex **A**		
Reaction time	TON		Number of repetitions	TON		Number of repetitions
	Range	Average		Range	Average	
5 minutes	0.44-0.69	0.58	6	0.22-0.26	0.24	4
10 minutes	0.93-1.4	1.1	6	0.55-0.57	0.57	3
15 minutes	1.4-2.0	1.6	6	0.82-0.93	0.87	4
30 minutes	2.6-3.7	3.0	6	1.6-1.9	1.8	4
1 hour	4.4-6.3	5.0	8	2.6-3.5	3.1	7
2 hours	6.4-9.3	7.7	6	5.6-5.8	5.7	2
3 hours	7.3-11	8.9	6	7.1	7.1	2
8 hours	13-17	15	5	10-11	11	2
24 hours	16-22	18	7	13-15[3]	14	8

[i]It should be considered that the turnover numbers might be affected by sources of error such as the lack of full control of the bubbling rate of acetylene, rate of mixing, convection rates, evaporation of volatile components (during the addition of acetylene or later in the experiment), inaccurate integration of the ^{1}H NMR spectrum etc.

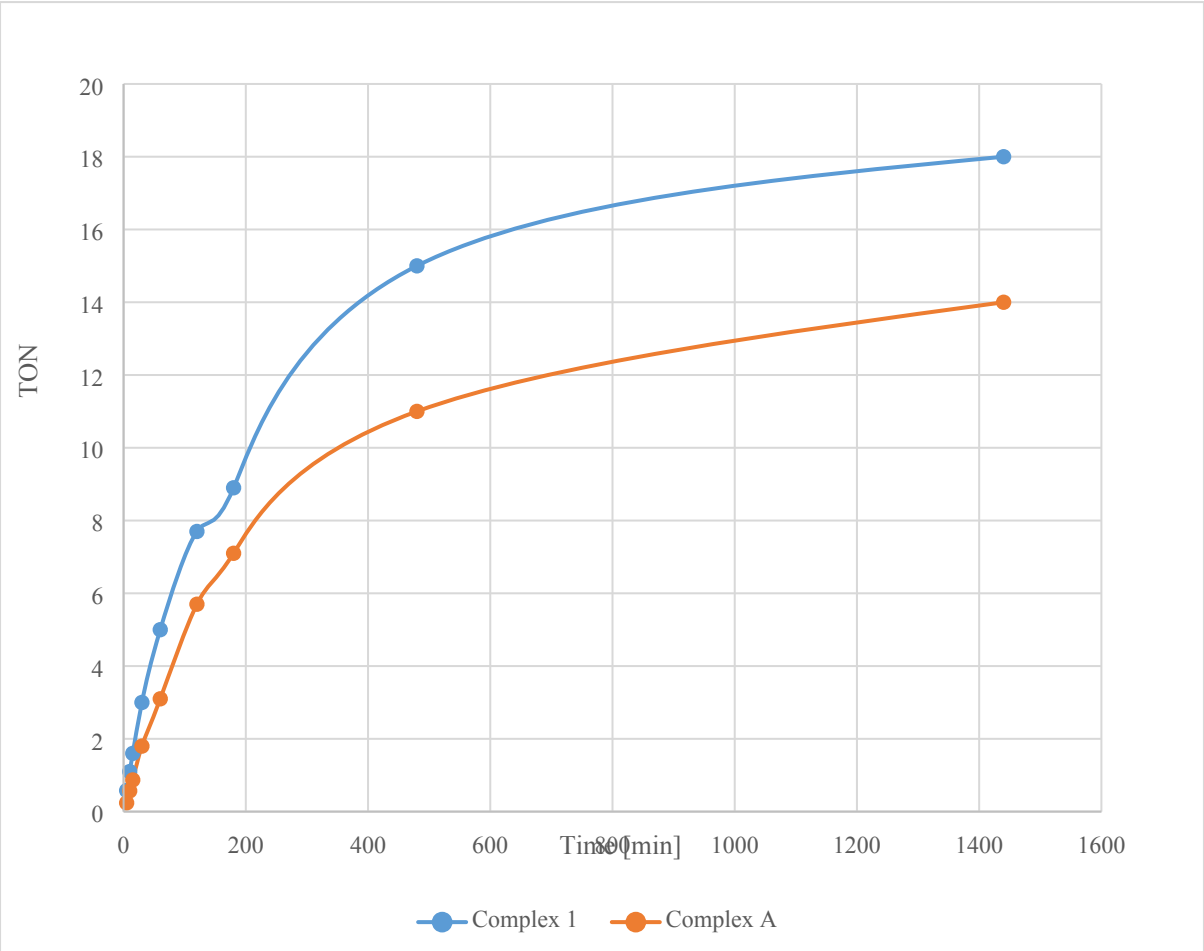
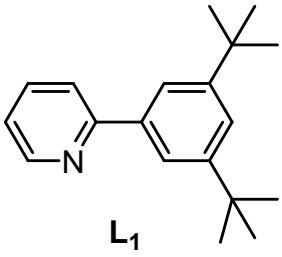


Figure S 2. Plots of the TONs (average values from Table S 1) for **1** and **A**.

Figure S 3. Photographs of the NMR tubes after 24 hours of catalysis visually illustrating the different degree of decomposition when using **1** (left tube) and **A** (right tube) as a (pre)catalyst for the acetylene trifluoroacetylation.

NMR spectra of 2-(3,5-di-*tert*-butylphenyl)pyridine (L_1)



L_1

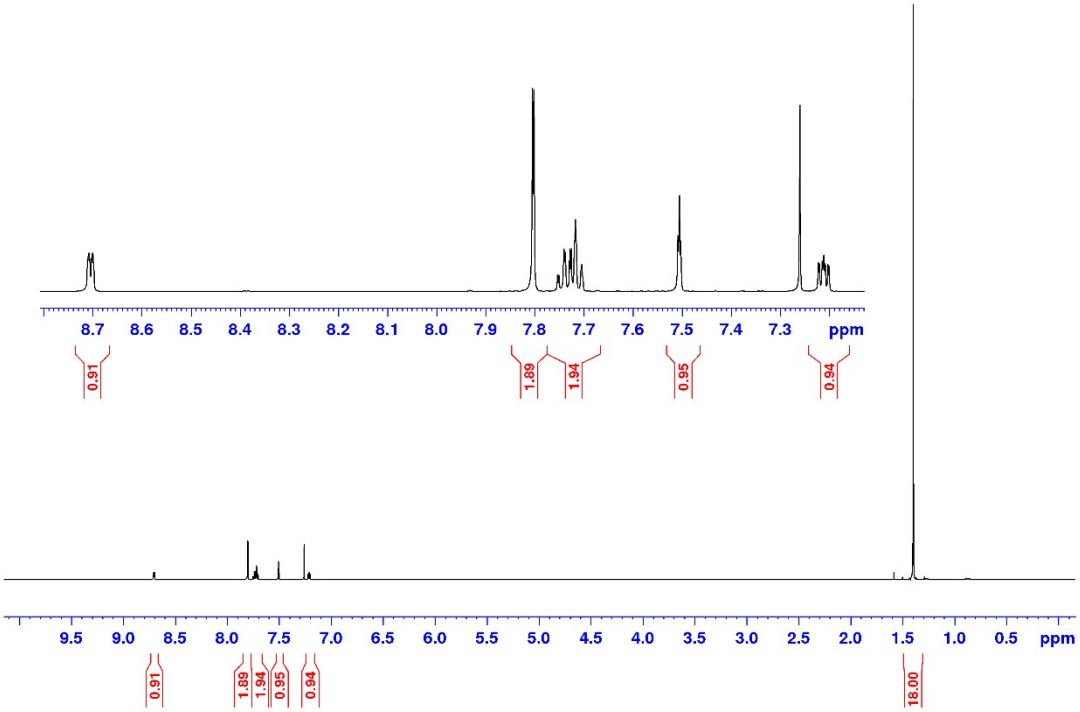


Figure S 4. ^{1}H NMR (600 MHz, $CDCl_3$) of 2-(3,5-di-*tert*-butylphenyl)pyridine (**L_1**).

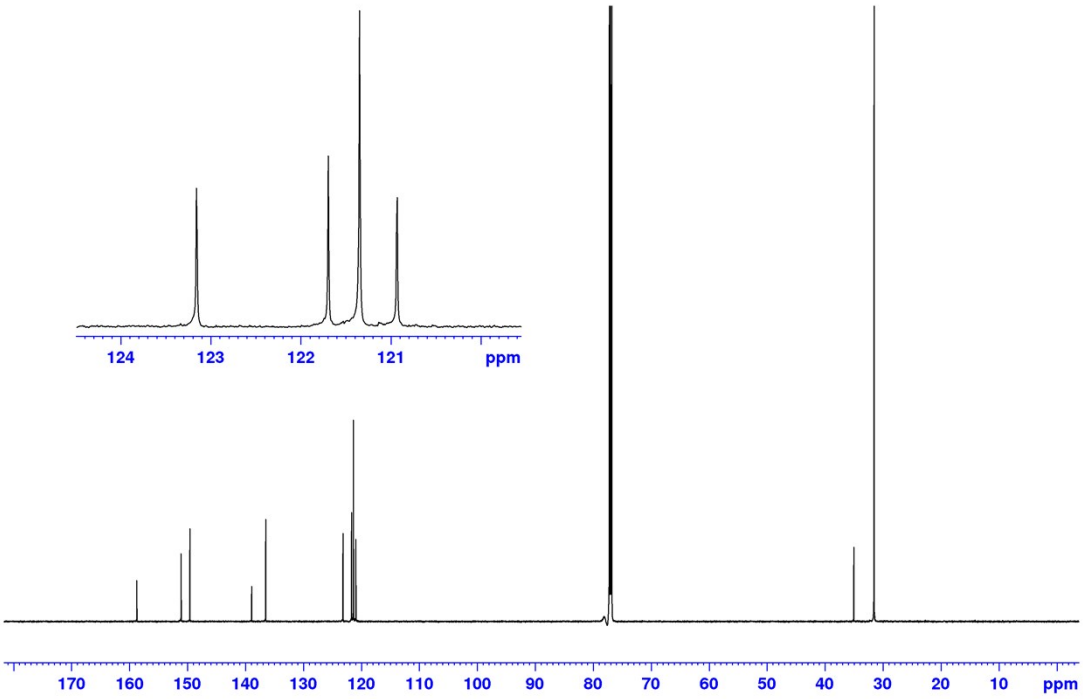
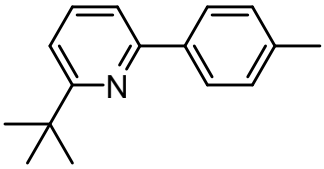


Figure S 5. ^{13}C NMR (151 MHz, $CDCl_3$) of 2-(3,5-di-*tert*-butylphenyl)pyridine (**L_1**).

NMR spectra of 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (L_2)



L_2

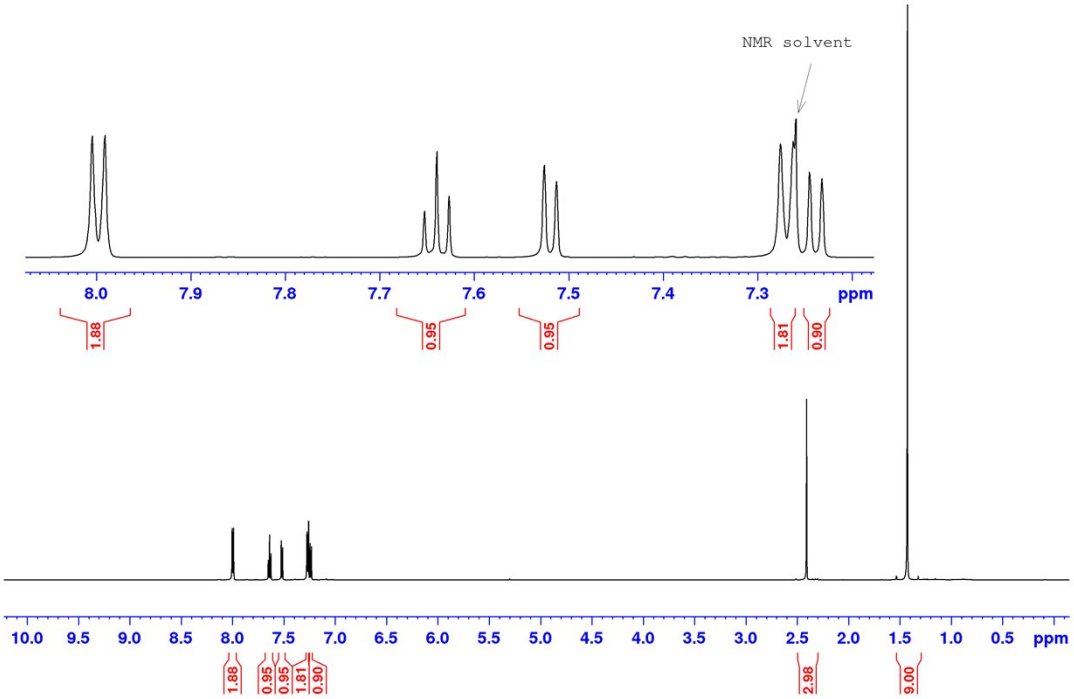


Figure S 6. ^{1}H NMR (600 MHz, $CDCl_3$) of 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (**L_2**).

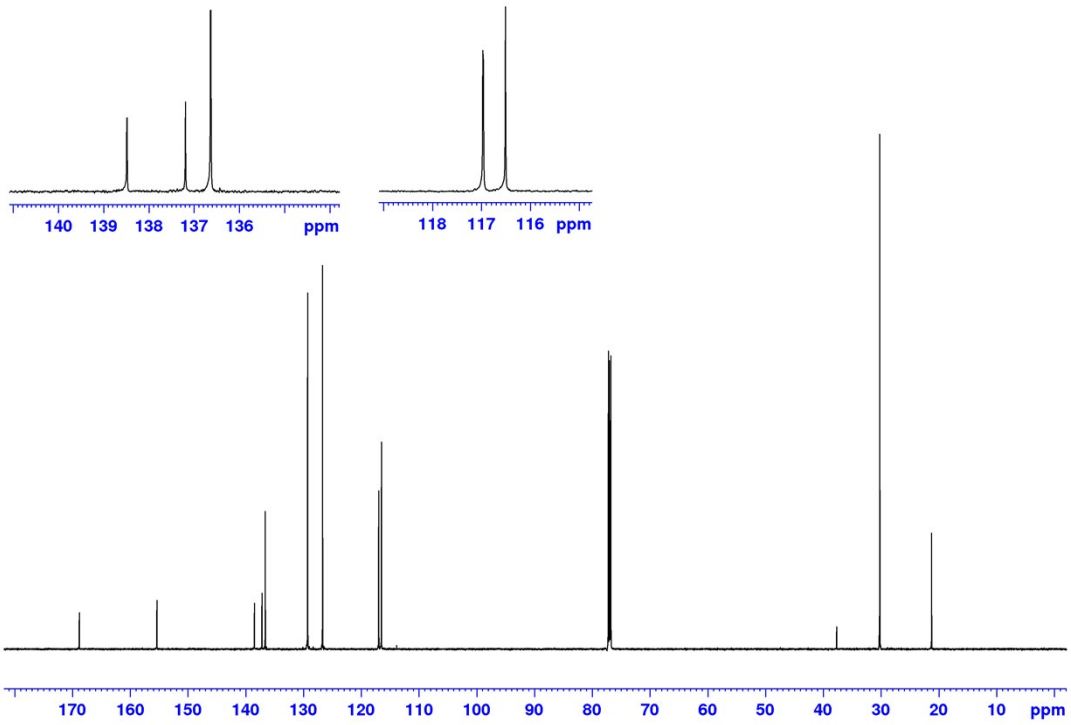
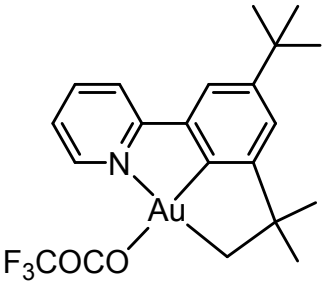


Figure S 7. ^{13}C NMR (151 MHz, $CDCl_3$) of 2-(*tert*-butyl)-6-(*p*-tolyl)pyridine (**L_2**).

NMR spectra of Au(III) complex 1



1

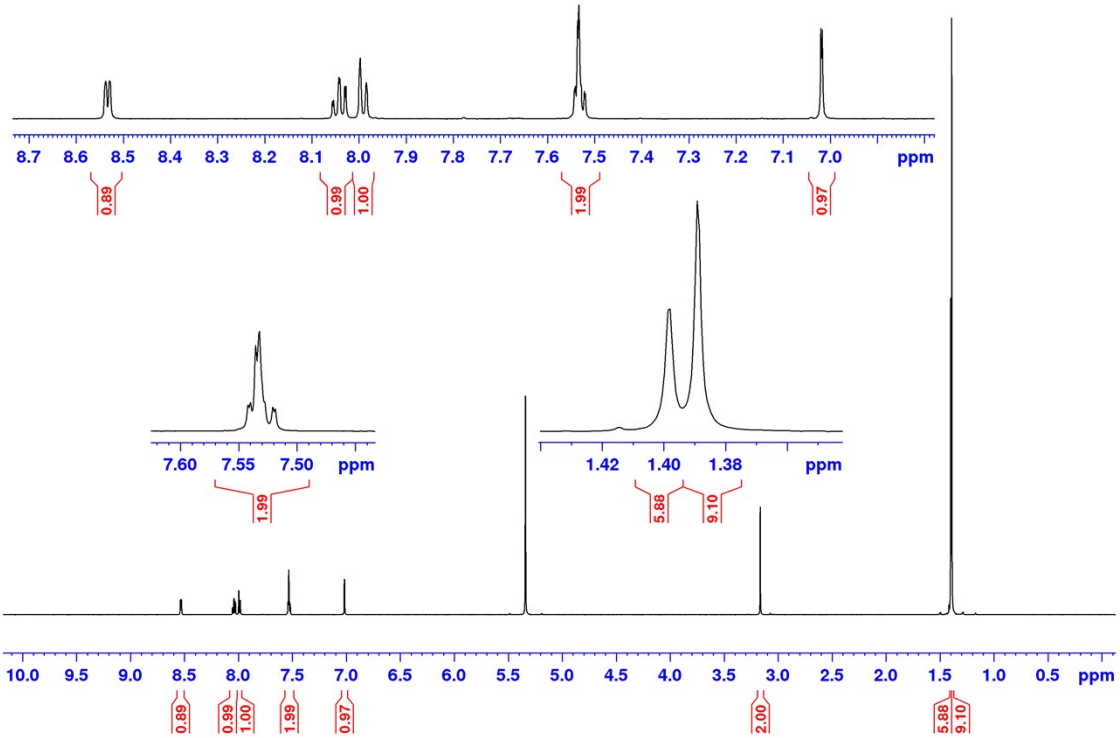


Figure S 8. ^{1}H NMR (600 MHz, CD_2Cl_2) of Au(III) complex **1**.

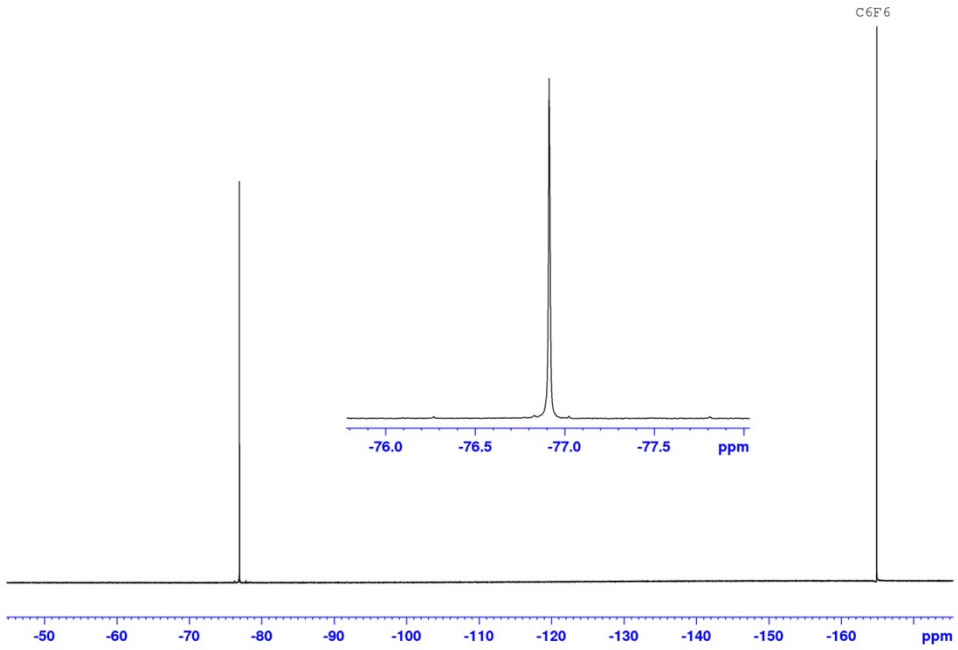


Figure S 9. ^{19}F NMR (188 MHz, CD_2Cl_2) of Au(III) complex **1**.

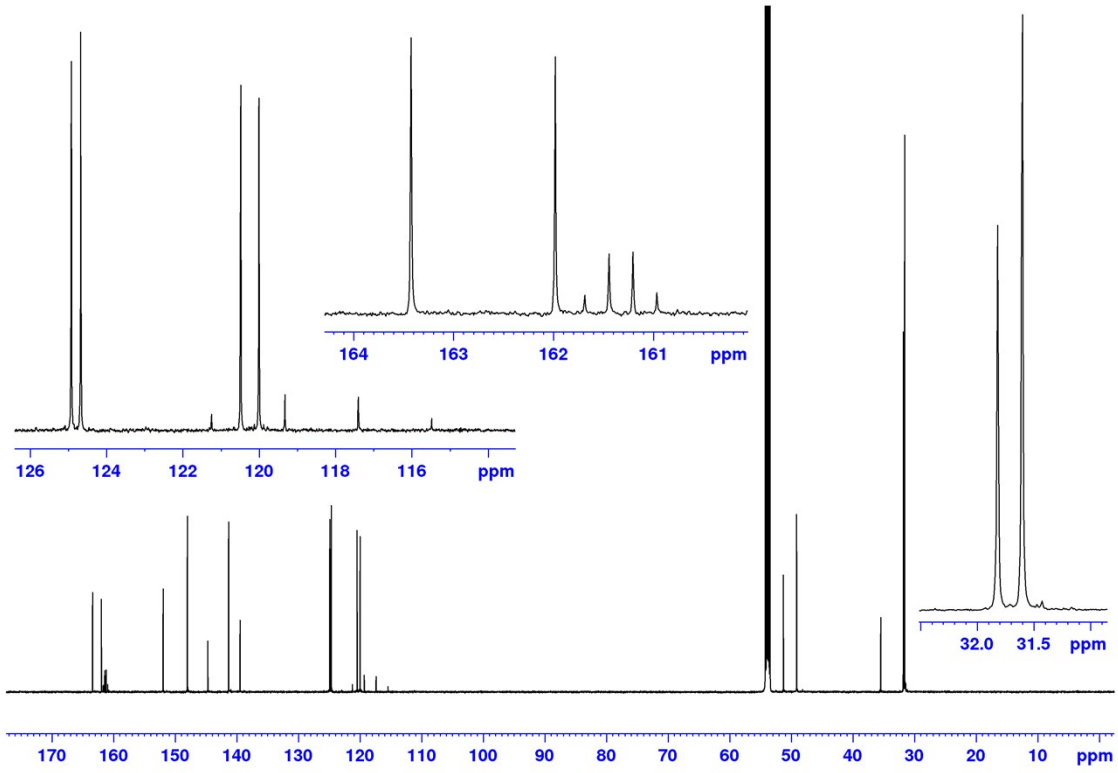


Figure S 10. ^{13}C NMR (151 MHz, CD_2Cl_2, d1 = 6 s, ns = 10240) of Au(III) complex **1**. The two left insets shows the quartets arising from the coupling to ^{19}F.

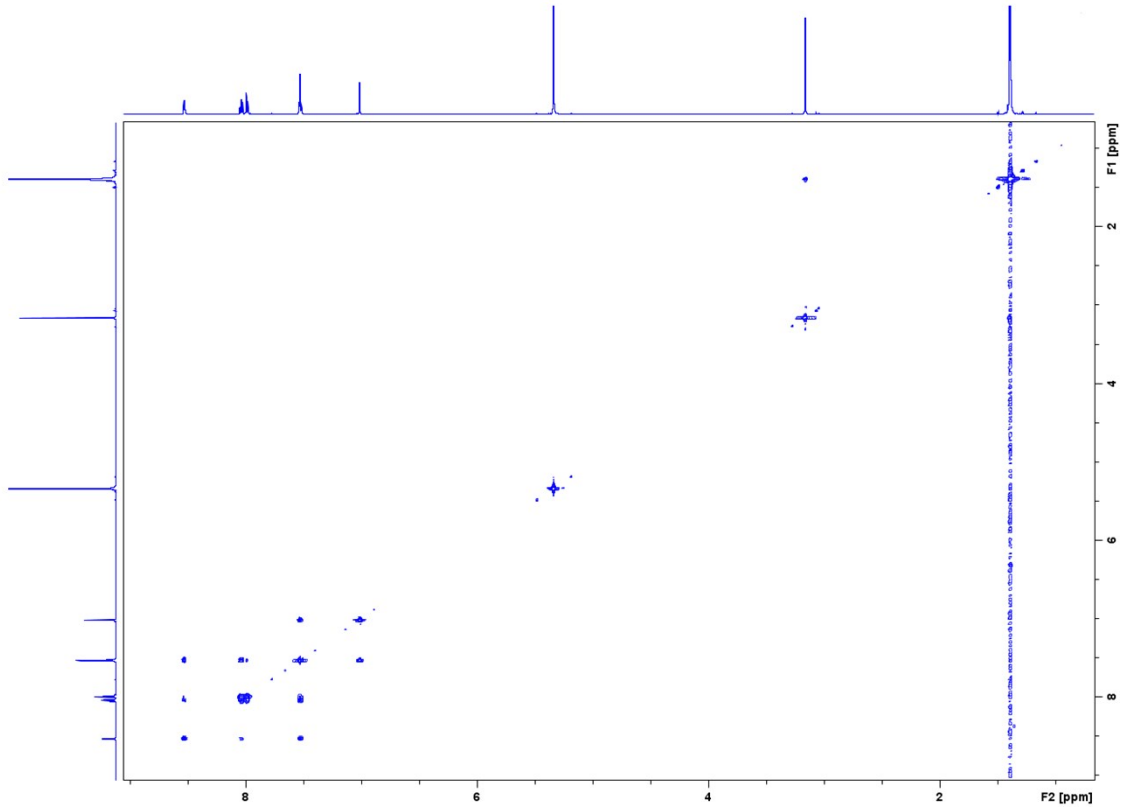


Figure S 11. COSY (600 MHz, CD_2Cl_2) of Au(III) complex **1**.

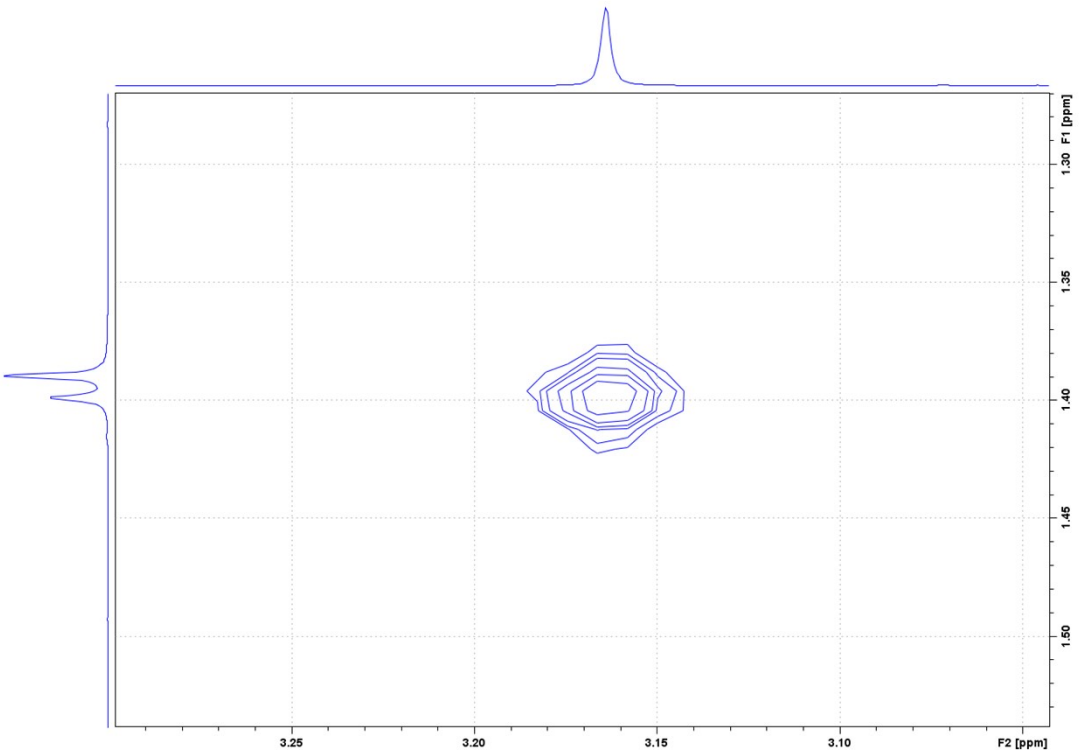


Figure S 12. COSY (600 MHz, CD_2Cl_2) of Au(III) complex **1**. Close up of the COSY correlation between Au$C\mathbf{H_2}$ and $C(C\mathbf{H_3})_2$.

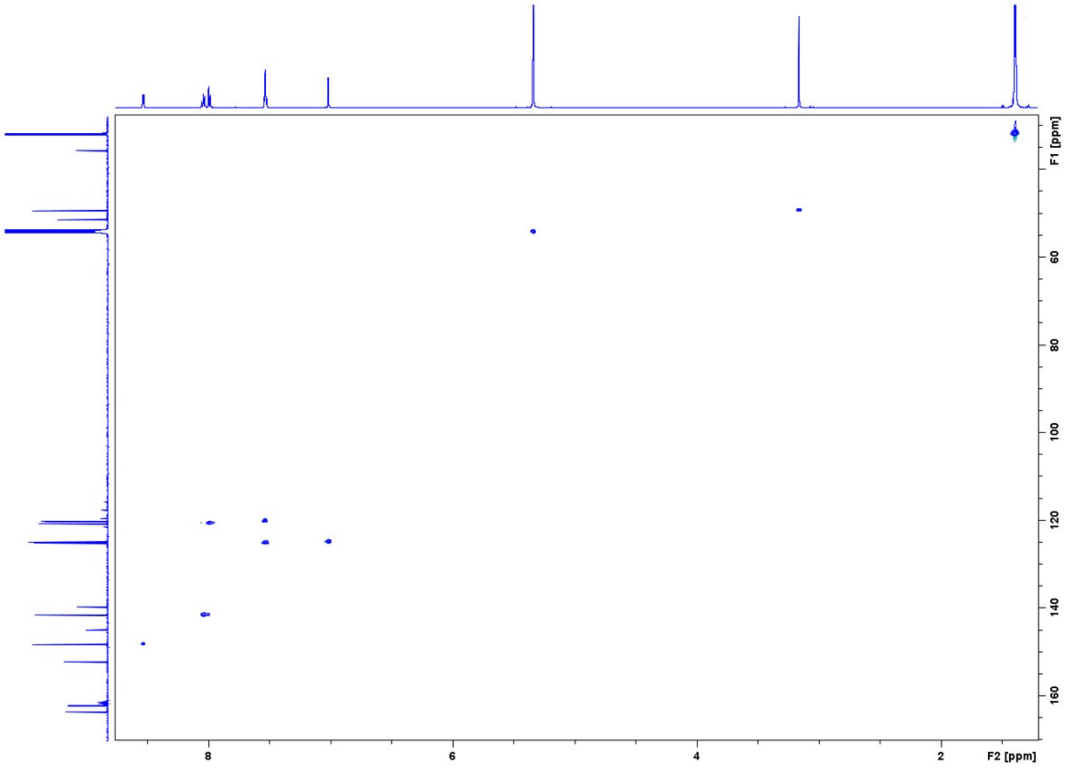


Figure S 13. HSQC (600 MHz, CD_2Cl_2) of Au(III) complex **1**.

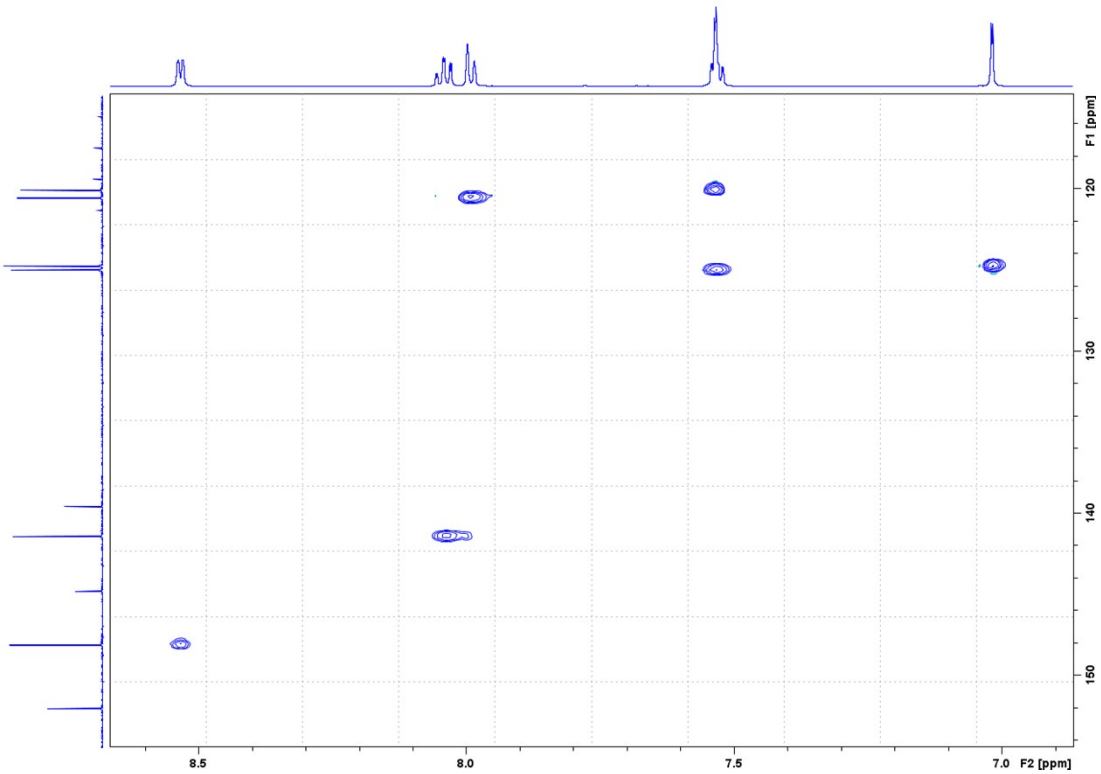


Figure S 14. HSQC (600 MHz, CD_2Cl_2) of Au(III) complex **1**. Close up of the aromatic region.

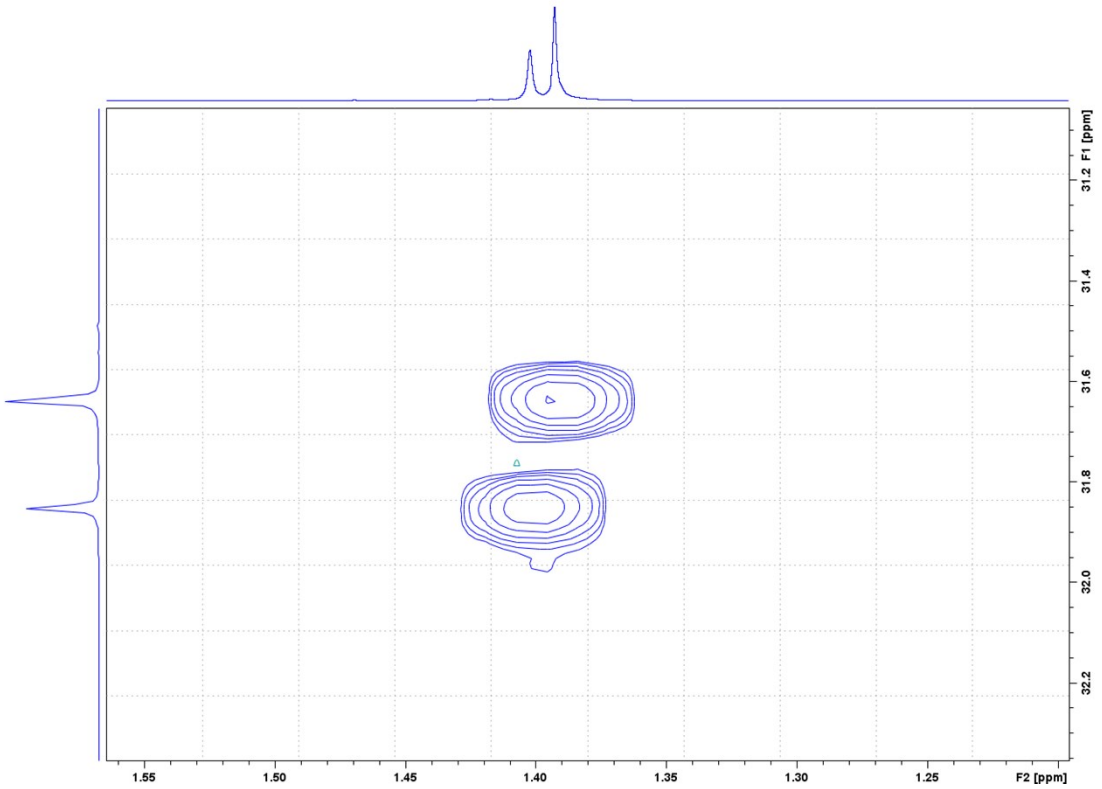


Figure S 15. Selective HSQC (800 MHz, CD_2Cl_2) of the aliphatic region in Au(III) complex **1**.

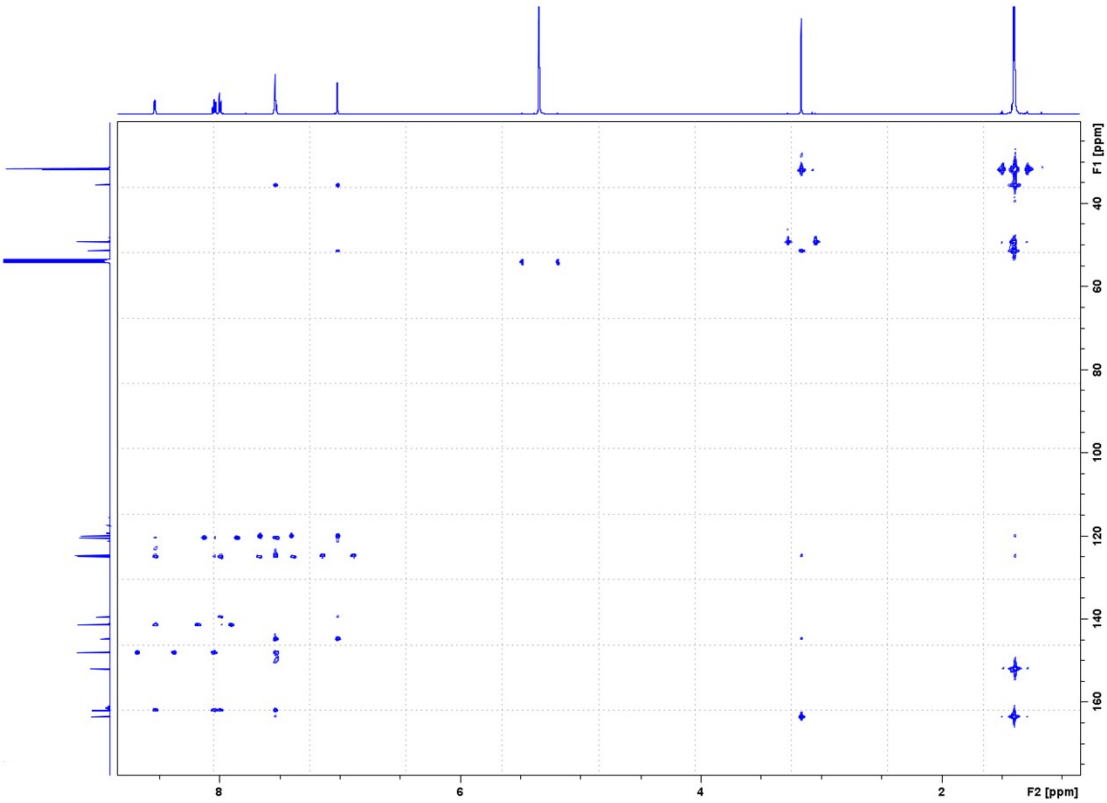


Figure S 16. HMBC (600 MHz, CD_2Cl_2, no decoupling) of Au(III) complex **1**.

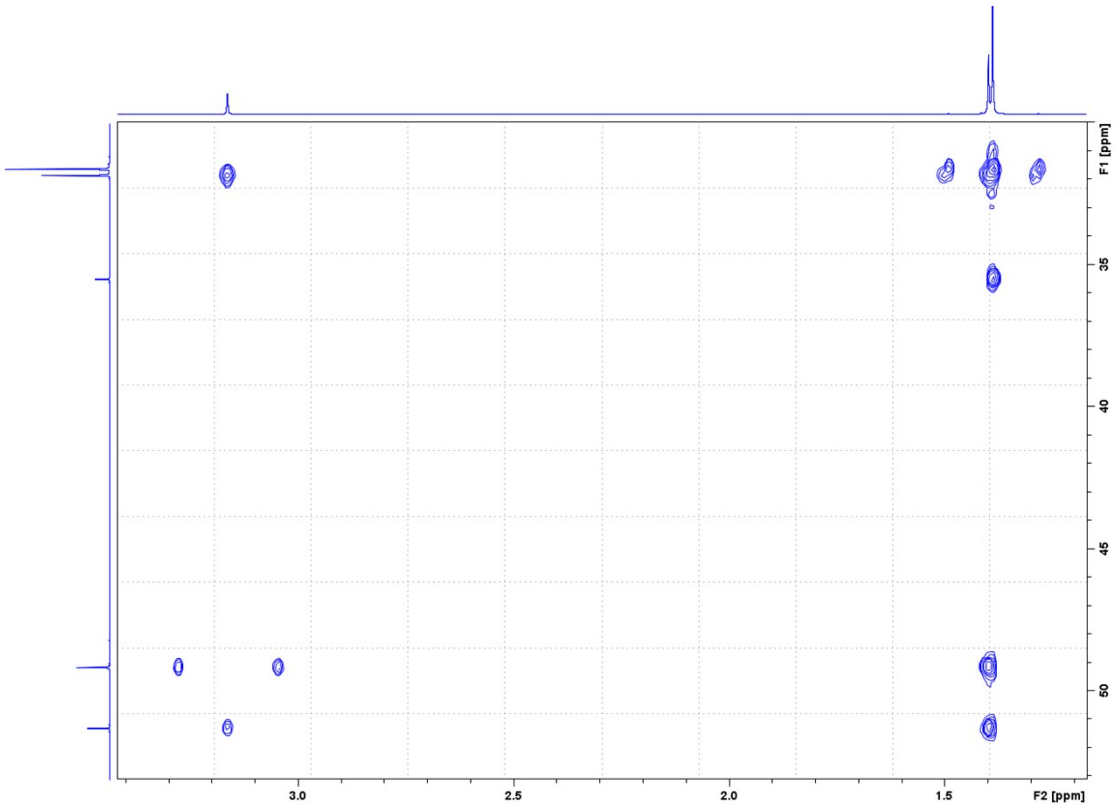


Figure S 17. HMBC (600 MHz, CD_2Cl_2, no decoupling) of Au(III) complex **1**. Close up of the aliphatic region.

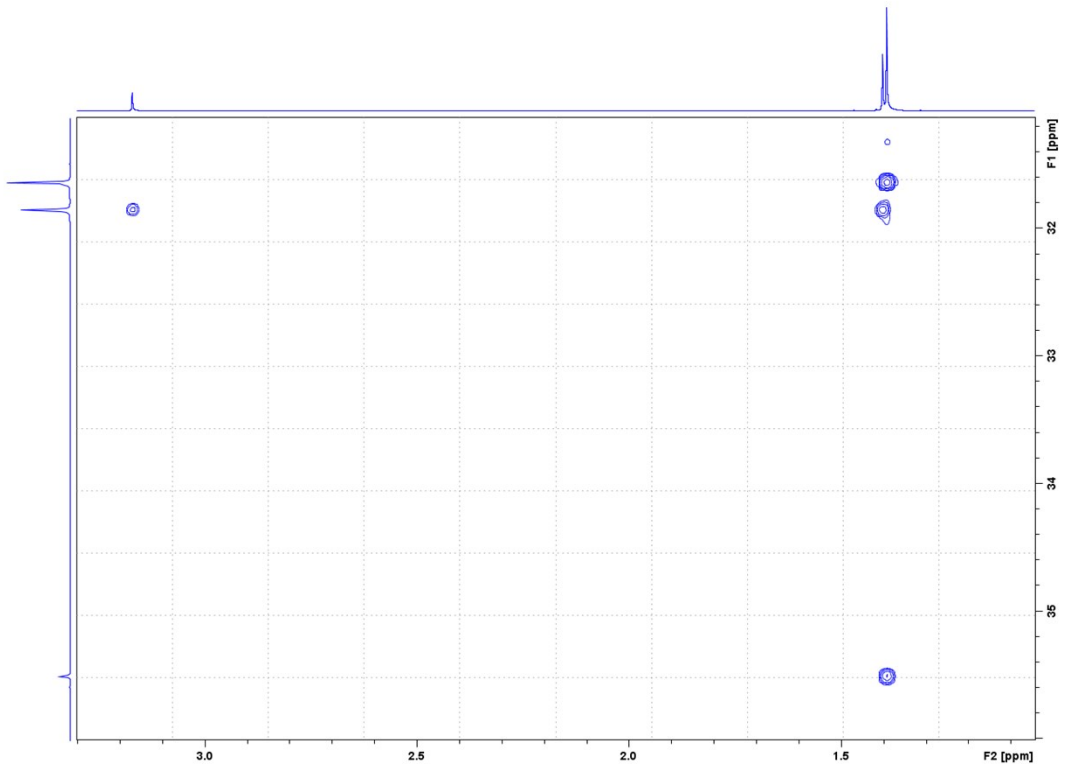


Figure S 18. Selective HMBC (800 MHz, CD_2Cl_2) of the aliphatic region in **1** showing the correlation between Au**C**$\mathbf{H_2}$ and $C(\mathbf{C}H_3)_2$.

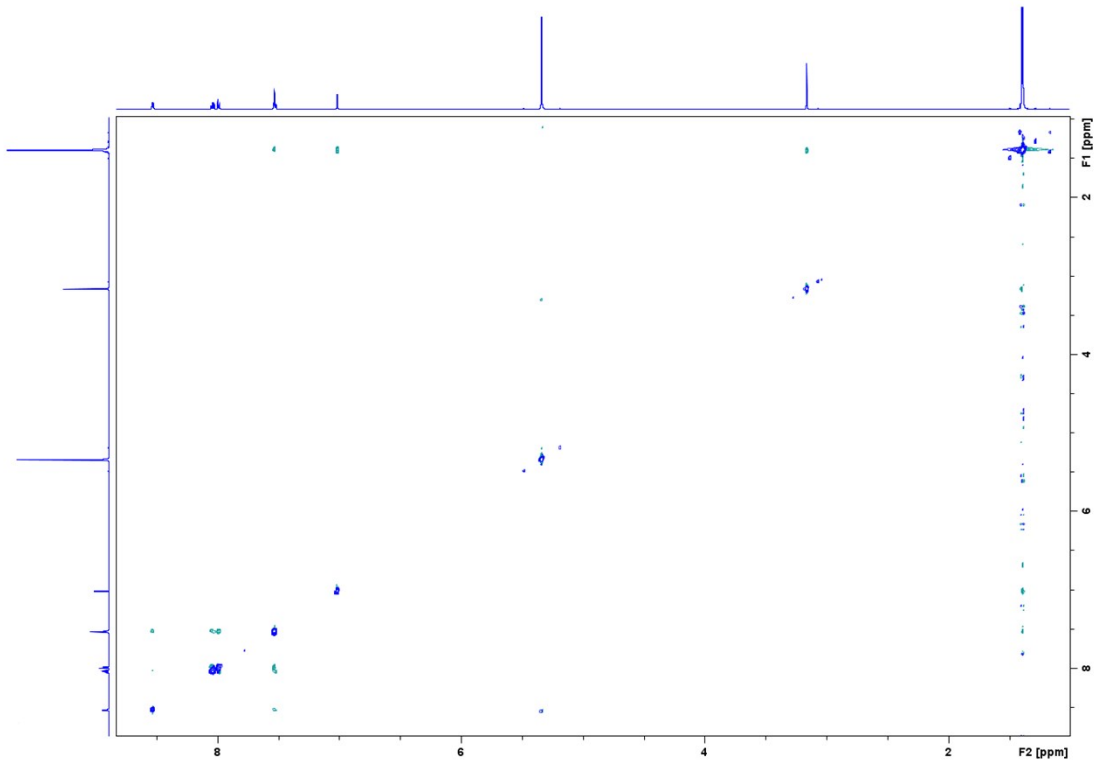


Figure S 19. NOESY (600 MHz, CD_2Cl_2, mixing time = 1 s) of Au(III) complex **1**.

Miscellaneous NMR spectra

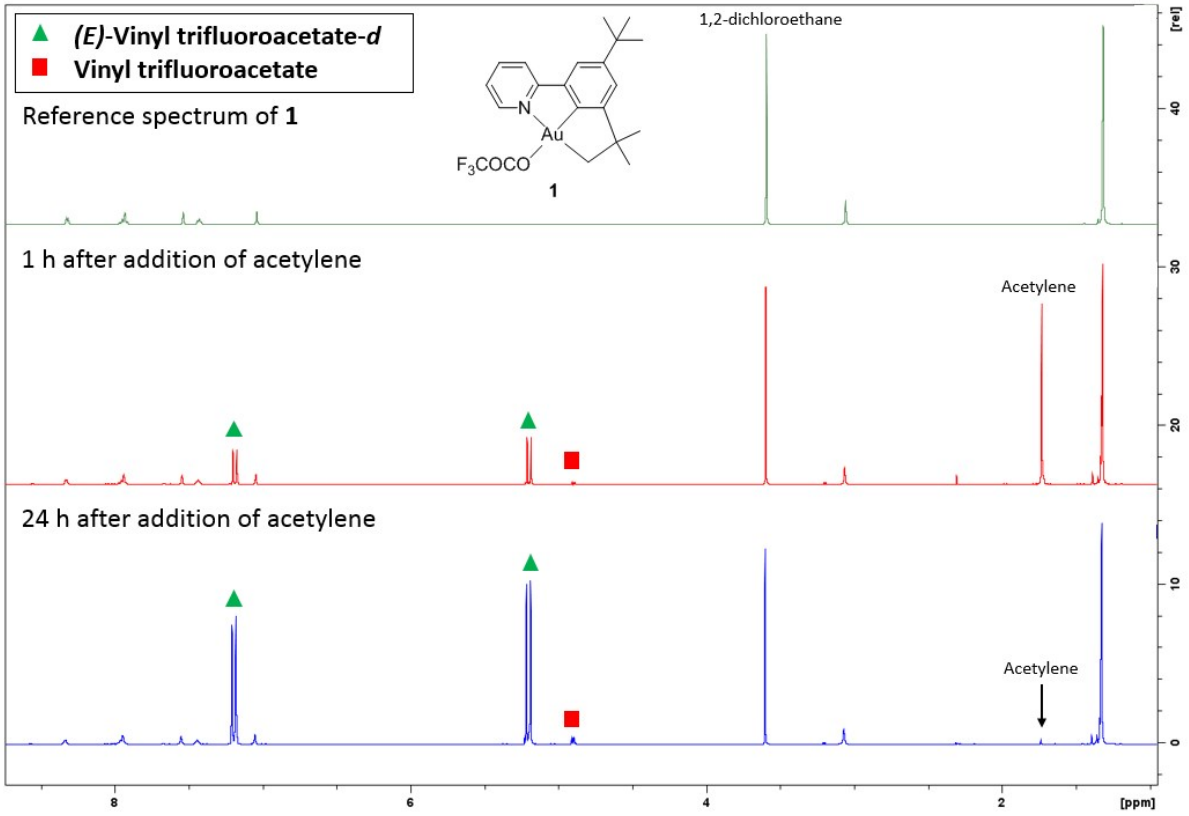


Figure S 20. Stacked ^{1}H NMR (500 MHz, CF_3COOD) spectra showing the catalytic transformation of acetylene into *(E)*-vinyl trifluoroacetate-*d* at **1**. Top: Reference spectrum of **1**. Middle: Reaction mixture 1 h after addition of acetylene. Bottom: Reaction mixture 24 h after addition of acetylene.

Crystallographic methods

Crystals suitable for X-ray diffraction analysis of **1** were grown by the vapor diffusion technique.[4] A small vial containing **1** dissolved in CH_2Cl_2 was placed in a capped larger vial containing pentane and placed in a refrigerator (*ca*. 10 ^{o}C) slowly producing crystals of **1**.

Single crystal diffraction data was acquired on a Bruker D8 Venture equipped with a Photon 100 detector and using Mo Kα radiation (λ = 0.71073 Å) from an Incoatec iμS microsource. Data reduction was performed with the Bruker Apex3 Suite,[5] the structure was solved with ShelXT[6] and refined with ShelXL.[7] Olex2 was used as user interface.[8] The cif files were edited with enCIFer v1.4,[9] and molecular graphics were produced with Diamond v4.4.0.[10]

Full details of the data collection, structure solution and refinement are contained in the cif file, available as ESI and from https://www.ccdc.cam.ac.uk/ (CCDC number: 1853366); and are summarized in Table S 2.

Crystallographic structure determination of 1

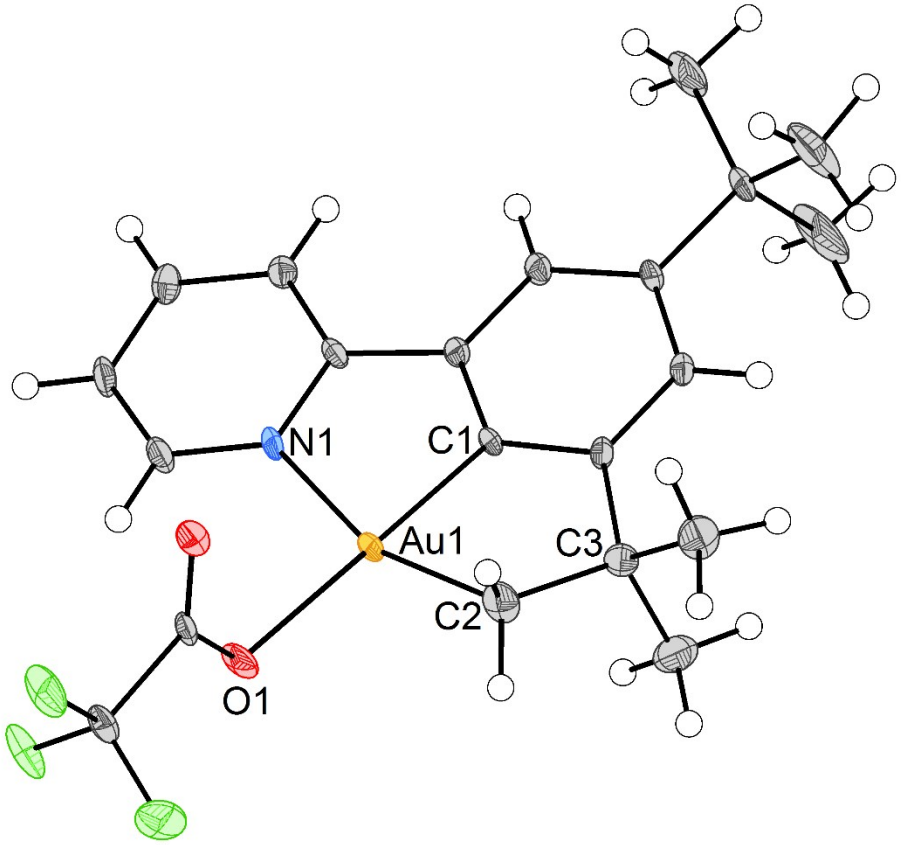
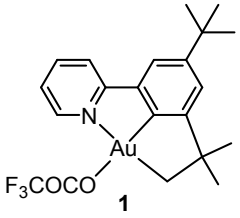


Figure S 21. ORTEP plot of **1** with 50% ellipsoids. Selected bond distances [Å] and angles [º]: Au1-N1, 2.135(3); Au1-C1, 1.944(3); Au1-O1, 2.119(3); Au1-C2, 2.049(4); C2-C3, 1.557(6); O1-Au1-N1, 99.62(11); N1-Au1-C1, 80.36(13); C1-Au1-C2, 81.66(15); C2-Au1-O1, 98.30(14); C1-Au1-O1, 179.34(13); N1-Au1-C2, 161.36(14).

Crystal and structure refinement data for 1

Table S 2. Crystal and structure refinement data for **1**.

	 **1**
Crystal data	
Identification code	MSH-699-SOE_pl
Chemical formula	$C_{21}H_{23}AuF_3NO_2$
M_r	575.37
Crystal system, space group	Triclinic, *P*-1
Temperature (K)	105
a, *b*, *c* (Å)	8.7448 (5), 9.6069 (6), 12.4327 (7)
α, β, γ (°)	94.949(2), 95.354(2), 104.902(2)
V (Å^3)	998.32(10)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	7.41
Crystal size (mm)	1 x 0.33 x 0.21
Data Collection	
Diffractometer	Bruker D8 Venture, CMOS detector diffractometer
Absorption correction	Multi-scan SADABS2016/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1755 before and 0.0840 after correction. The Ratio of minimum to maximum transmission is 0.2143. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.160, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26763, 6990, 6325
R_{int}	0.046
(sin θ/λ)max (Å^{-1})	0.749
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.033, 0.081, 1.08
No. of reflections	6990
No. of parameters	258
No. of restraints	0
H-atom treatment	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 3.1444P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.66, −2.86

Free energy profile for the formation of 1 and 1'

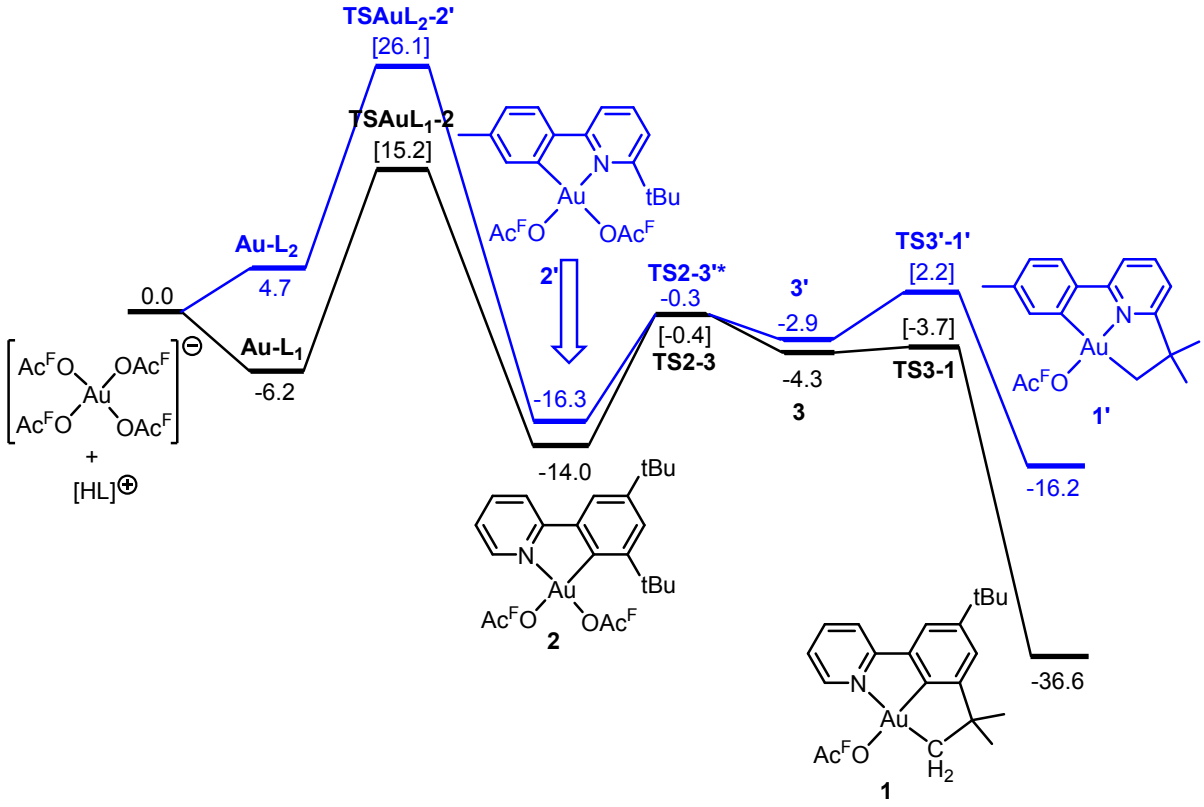


Figure S 22. Reaction pathway for the formation of complexes **1** (in black) and **1'** (in blue) from **[Au(OAc^F)$_4$]$^-$** and **[L$_1$H]$^+$** and [**L$_2$H**]$^+$, respectively. Gibbs energies in HOAc^F solvent (SMD) are given in kcal/mol. * Estimated energy for the dissociative ligand substitution transition state. Transition state energies are showed in brackets.

Computational details

Calculations were carried out at the DFT level as implemented in the Gaussian09 software package.[11] The hybrid PBE0+GD3 functional[12, 13] including Grimme's model for dispersion forces was used to optimize all geometries. This methodology was selected because previous studies have proven its solid performance in the modeling of Au(III) complexes.[3, 14-17] C, H, N and O were described with the all-electron triple-ζ 6-311+G** basis set,[18, 19] whereas Au was described with the Stuttgart–Köln basis set including a small-core quasi-relativistic pseudopotential.[20, 21] Geometries were fully optimized without any constraint. Vibrational frequencies were computed at the same level of theory to classify all stationary points as either saddle points (transition states, with a single imaginary frequency) or energy minima (reactants, intermediates and products, with only real frequencies). These calculations were also used to obtain the thermochemistry corrections (zero-point, thermal and entropy energies) at the experimental p = 1 atm and T = 298.15 K. All optimizations needed for the mechanism proposal

were carried out in solvent (trifluoroacetic acid), which was defined using eps=8.55, epsinf=2.26 and rsolv=13.7 with the SMD solvation model.[22] In the bimolecular steps, these energies were corrected for the 1M standard state.

Optimized coordinates and energies

1
G = -1453.214496

Au	-0.769000	-0.283000	-0.188000
F	-5.906000	-0.259000	1.341000
F	-5.444000	0.672000	-0.550000
F	-5.439000	-1.484000	-0.372000
O	-2.888000	-0.381000	-0.411000
O	-3.289000	-0.210000	1.802000
N	-0.514000	1.883000	-0.242000
C	1.732000	1.110000	-0.005000
C	1.170000	-0.161000	-0.069000
C	5.855000	-0.629000	1.604000
C	1.606000	-3.760000	0.606000
C	6.098000	-0.521000	-0.889000
C	5.947000	1.568000	0.449000
C	1.219000	-2.972000	-1.739000
C	3.300000	-1.200000	0.094000
C	-3.611000	-0.307000	0.634000
C	5.438000	0.130000	0.335000
C	3.917000	0.060000	0.184000
C	1.120000	-2.594000	-0.254000
C	-1.462000	2.813000	-0.351000
C	0.159000	4.551000	-0.197000
C	-5.119000	-0.347000	0.267000
C	1.145000	3.582000	-0.077000
C	-1.169000	4.167000	-0.337000
C	3.123000	1.208000	0.124000
C	-0.360000	-2.271000	0.090000
C	1.921000	-1.327000	-0.041000
C	0.791000	2.236000	-0.104000
H	-2.479000	2.450000	-0.457000
H	-1.966000	4.894000	-0.431000
H	0.428000	5.602000	-0.181000
H	2.185000	3.865000	0.034000
H	3.583000	2.187000	0.174000
H	5.392000	-0.189000	2.493000
H	5.566000	-1.683000	1.560000
H	6.942000	-0.586000	1.729000
H	7.189000	-0.485000	-0.794000
H	5.807000	-1.570000	-0.998000
H	5.820000	0.004000	-1.809000
H	5.719000	2.156000	-0.446000
H	5.525000	2.082000	1.319000
H	7.035000	1.560000	0.567000

H	2.258000	-3.161000	-2.029000
H	0.637000	-3.877000	-1.940000
H	0.830000	-2.166000	-2.371000
H	1.591000	-3.499000	1.669000
H	0.960000	-4.632000	0.460000
H	2.626000	-4.055000	0.340000
H	-1.057000	-2.892000	-0.481000
H	-0.553000	-2.422000	1.158000
H	3.913000	-2.096000	0.126000

2

G = -1979.61823

Au	-0.457000	0.366000	-0.235000
F	-5.071000	1.893000	1.908000
F	-4.744000	2.558000	-0.119000
F	-5.149000	0.470000	0.285000
O	-2.471000	1.038000	-0.255000
O	-2.476000	1.296000	1.986000
N	0.228000	2.218000	-0.538000
C	2.275000	1.155000	-0.061000
C	1.557000	-0.061000	-0.141000
C	6.090000	-0.806000	1.936000
C	2.770000	-3.747000	-0.516000
C	6.574000	-0.765000	-0.522000
C	6.454000	1.360000	0.765000
C	0.808000	-2.719000	-1.537000
C	3.645000	-1.181000	0.171000
C	-2.992000	1.276000	0.890000
C	5.855000	-0.040000	0.625000
C	4.357000	0.006000	0.333000
C	1.686000	-2.682000	-0.278000
C	-0.578000	3.232000	-0.883000
C	1.269000	4.732000	-0.768000
C	-4.511000	1.557000	0.746000
C	2.088000	3.669000	-0.429000
C	-0.083000	4.514000	-1.011000
C	3.648000	1.184000	0.185000
C	0.957000	-3.095000	1.011000
C	2.270000	-1.274000	-0.086000
C	1.550000	2.389000	-0.324000
H	-1.620000	2.990000	-1.047000
H	-0.753000	5.317000	-1.292000
H	1.687000	5.729000	-0.852000
H	3.145000	3.827000	-0.257000
H	4.150000	2.140000	0.258000
H	5.583000	-0.317000	2.774000
H	5.726000	-1.836000	1.874000
H	7.161000	-0.841000	2.160000
H	7.651000	-0.799000	-0.327000
H	6.223000	-1.795000	-0.635000
H	6.417000	-0.248000	-1.474000

H	6.348000	1.942000	-0.156000
H	5.991000	1.921000	1.584000
H	7.523000	1.279000	0.984000
H	1.445000	-2.696000	-2.428000
H	0.225000	-3.645000	-1.569000
H	0.121000	-1.882000	-1.624000
H	3.395000	-3.925000	0.364000
H	2.271000	-4.692000	-0.749000
H	3.416000	-3.497000	-1.364000
H	0.464000	-4.063000	0.872000
H	1.685000	-3.202000	1.822000
H	4.200000	-2.106000	0.245000
H	0.205000	-2.375000	1.324000
O	-1.337000	-1.397000	0.235000
C	-2.170000	-1.897000	-0.610000
O	-2.375000	-1.605000	-1.763000
C	-2.978000	-3.072000	0.001000
F	-2.781000	-3.245000	1.308000
F	-2.646000	-4.219000	-0.613000
F	-4.287000	-2.875000	-0.192000

3

G = -1979.602676

Au	0.373000	0.446000	-0.493000
F	5.408000	0.557000	-2.326000
F	4.806000	2.207000	-1.072000
F	5.107000	0.245000	-0.211000
O	2.427000	0.954000	-0.561000
O	2.821000	-0.030000	-2.549000
N	-0.096000	2.073000	0.629000
C	-2.252000	1.129000	0.391000
C	-1.571000	0.164000	-0.348000
C	-6.447000	-0.208000	-1.335000
C	-1.166000	-3.171000	-0.834000
C	-6.120000	-1.603000	0.723000
C	-6.469000	0.850000	0.914000
C	0.023000	-1.294000	-2.010000
C	-3.571000	-1.006000	-0.792000
C	3.147000	0.548000	-1.535000
C	-5.823000	-0.247000	0.068000
C	-4.309000	-0.069000	-0.056000
C	-1.344000	-1.924000	-1.708000
C	0.816000	2.944000	1.069000
C	-0.893000	4.161000	2.203000
C	4.639000	0.891000	-1.290000
C	-1.828000	3.245000	1.745000
C	0.446000	4.012000	1.864000
C	-3.634000	1.001000	0.533000
C	-1.973000	-2.309000	-3.049000
C	-2.188000	-0.913000	-0.958000
C	-1.416000	2.185000	0.948000

H 1.841000 2.760000 0.769000
H 1.204000 4.705000 2.208000
H -1.211000 4.989000 2.828000
H -2.875000 3.340000 2.006000
H -4.176000 1.742000 1.108000
H -7.532000 -0.343000 -1.266000
H -6.255000 0.753000 -1.824000
H -6.052000 -1.000000 -1.979000
H -7.202000 -1.744000 0.819000
H -5.728000 -2.437000 0.133000
H -5.679000 -1.660000 1.723000
H -6.082000 0.858000 1.939000
H -6.321000 1.844000 0.479000
H -7.548000 0.675000 0.971000
H 0.707000 -1.270000 -1.045000
H 0.731000 -1.979000 -2.494000
H -0.042000 -0.436000 -2.687000
H -2.134000 -3.641000 -0.642000
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H -1.315000 -2.999000 -3.587000
H -2.931000 -2.815000 -2.902000
H -4.089000 -1.841000 -1.253000
H -2.140000 -1.430000 -3.679000
O 1.950000 -2.145000 0.300000
C 1.729000 -1.751000 1.454000
O 1.045000 -0.798000 1.862000
C 2.396000 -2.569000 2.601000
F 1.465000 -3.102000 3.420000
F 3.156000 -3.586000 2.171000
F 3.186000 -1.790000 3.366000

5

G = -1530.435928
Au -0.002000 -1.306000 0.269000
N 0.749000 0.658000 0.902000
C -1.266000 -2.709000 -0.572000
C -2.751000 -2.329000 -0.358000
C -0.191000 1.628000 0.757000
C -1.508000 1.157000 0.304000
C 1.975000 0.963000 1.331000
H 2.687000 0.150000 1.420000
C -1.627000 -0.215000 0.080000
C -2.813000 -0.821000 -0.292000
C -3.929000 -0.005000 -0.486000
C 0.123000 2.951000 1.045000
H -0.627000 3.724000 0.925000
C -3.855000 1.381000 -0.302000
C 2.344000 2.265000 1.633000
H 3.352000 2.471000 1.971000
C -2.639000 1.946000 0.106000

H -2.579000 3.017000 0.270000
C 1.400000 3.271000 1.484000
H 1.655000 4.302000 1.707000
C 1.519000 -3.044000 0.787000
H 1.067000 -3.853000 1.325000
C 2.169000 -2.220000 0.166000
H 2.864000 -1.530000 -0.356000
H -0.995000 -2.659000 -1.632000
H -1.044000 -3.713000 -0.201000
H -4.865000 -0.462000 -0.786000
C -3.227000 -2.885000 0.992000
H -4.259000 -2.585000 1.198000
H -3.181000 -3.980000 0.987000
H -2.594000 -2.517000 1.807000
C -3.597000 -2.924000 -1.483000
H -3.464000 -4.011000 -1.520000
H -4.662000 -2.727000 -1.326000
H -3.312000 -2.512000 -2.456000
C -5.059000 2.297000 -0.535000
C -5.373000 3.071000 0.754000
C -4.721000 3.291000 -1.657000
C -6.310000 1.520000 -0.945000
H -5.613000 2.387000 1.574000
H -4.533000 3.697000 1.070000
H -6.235000 3.728000 0.596000
H -4.487000 2.765000 -2.588000
H -5.574000 3.952000 -1.845000
H -3.862000 3.919000 -1.400000
H -7.136000 2.220000 -1.102000
H -6.162000 0.969000 -1.879000
H -6.621000 0.810000 -0.171000
O 3.929000 -0.377000 -1.123000
C 4.788000 0.070000 -0.337000
C 5.809000 1.060000 -0.981000
O 4.979000 -0.161000 0.860000
F 5.376000 1.619000 -2.121000
F 6.962000 0.420000 -1.278000
F 6.132000 2.072000 -0.155000

6

G = -1530.458565
Au 0.180000 -0.451000 0.237000
N -0.021000 1.737000 0.346000
C -0.353000 -2.402000 -0.122000
C -1.866000 -2.644000 0.157000
C -1.304000 2.156000 0.172000
C -2.299000 1.084000 0.004000
C 0.959000 2.624000 0.527000
H 1.953000 2.212000 0.663000
C -1.783000 -0.211000 0.049000
C -2.595000 -1.329000 -0.043000

C	-3.968000	-1.142000	-0.218000
C	-1.594000	3.518000	0.179000
H	-2.617000	3.850000	0.042000
C	-4.521000	0.145000	-0.289000
C	0.728000	3.990000	0.543000
H	1.553000	4.676000	0.694000
C	-3.673000	1.255000	-0.168000
H	-4.096000	2.254000	-0.205000
C	-0.575000	4.439000	0.364000
H	-0.797000	5.501000	0.370000
C	2.225000	-0.776000	0.429000
H	2.604000	-1.532000	1.122000
C	3.148000	-0.128000	-0.267000
H	2.997000	0.644000	-1.013000
O	4.520000	-0.455000	-0.092000
C	5.432000	0.371000	-0.550000
C	6.831000	-0.229000	-0.286000
O	5.280000	1.427000	-1.096000
F	6.982000	-1.390000	-0.933000
F	7.017000	-0.461000	1.019000
F	7.782000	0.602000	-0.698000
H	-0.135000	-2.533000	-1.188000
H	0.271000	-3.102000	0.440000
H	-4.617000	-2.008000	-0.294000
C	-2.044000	-3.067000	1.622000
H	-3.102000	-3.200000	1.868000
H	-1.525000	-4.013000	1.814000
H	-1.631000	-2.307000	2.295000
C	-2.376000	-3.756000	-0.760000
H	-1.781000	-4.666000	-0.622000
H	-3.420000	-4.008000	-0.542000
H	-2.310000	-3.462000	-1.813000
C	-6.023000	0.377000	-0.481000
C	-6.575000	1.146000	0.728000
C	-6.254000	1.201000	-1.757000
C	-6.804000	-0.932000	-0.610000
H	-6.428000	0.578000	1.652000
H	-6.086000	2.118000	0.849000
H	-7.649000	1.325000	0.605000
H	-5.860000	0.679000	-2.636000
H	-7.325000	1.368000	-1.912000
H	-5.770000	2.180000	-1.702000
H	-7.866000	-0.708000	-0.751000
H	-6.473000	-1.522000	-1.471000
H	-6.714000	-1.551000	0.288000

7

G = -2056.878703

Au	0.140000	-0.679000	0.082000
N	0.259000	1.062000	-1.283000
C	0.602000	-2.097000	1.504000

C	1.872000	-1.627000	2.258000
C	1.525000	1.532000	-1.390000
C	2.509000	0.736000	-0.628000
C	-0.736000	1.672000	-1.925000
H	-1.725000	1.245000	-1.793000
C	2.059000	0.236000	0.618000
C	2.691000	-0.880000	1.207000
C	3.889000	-1.318000	0.655000
C	1.816000	2.640000	-2.172000
H	2.836000	3.001000	-2.234000
C	4.445000	-0.703000	-0.475000
C	-0.516000	2.790000	-2.716000
H	-1.351000	3.264000	-3.218000
C	3.709000	0.292000	-1.146000
H	4.049000	0.669000	-2.105000
C	0.779000	3.277000	-2.841000
H	0.979000	4.154000	-3.447000
H	-0.249000	-2.235000	2.174000
C	-1.600000	-1.607000	-0.320000
H	-1.574000	-2.618000	-0.723000
C	-2.757000	-1.001000	-0.107000
H	-2.903000	-0.014000	0.316000
O	-3.937000	-1.700000	-0.418000
C	-5.075000	-1.033000	-0.461000
C	-6.218000	-2.026000	-0.770000
O	-5.258000	0.138000	-0.301000
F	-6.295000	-2.974000	0.170000
F	-6.018000	-2.630000	-1.947000
F	-7.383000	-1.392000	-0.821000
H	1.387000	0.885000	1.215000
H	4.395000	-2.168000	1.095000
H	0.790000	-3.017000	0.943000
C	2.591000	-2.854000	2.813000
H	3.493000	-2.566000	3.363000
H	1.930000	-3.382000	3.507000
H	2.874000	-3.556000	2.024000
C	1.498000	-0.692000	3.413000
H	2.396000	-0.319000	3.914000
H	0.911000	0.168000	3.080000
H	0.900000	-1.242000	4.146000
C	5.777000	-1.154000	-1.064000
C	5.526000	-1.768000	-2.451000
H	5.079000	-1.048000	-3.143000
H	6.475000	-2.102000	-2.882000
H	4.859000	-2.633000	-2.382000
C	6.699000	0.068000	-1.203000
H	7.659000	-0.244000	-1.625000
H	6.274000	0.828000	-1.865000
H	6.890000	0.531000	-0.230000
C	6.481000	-2.194000	-0.191000
H	6.671000	-1.818000	0.819000

H	5.905000	-3.122000	-0.112000
H	7.446000	-2.445000	-0.640000
O	0.356000	2.404000	1.926000
C	-0.827000	2.443000	1.550000
O	-1.656000	1.542000	1.380000
C	-1.338000	3.894000	1.273000
F	-1.553000	4.554000	2.434000
F	-0.449000	4.627000	0.574000
F	-2.491000	3.941000	0.588000

8

G = -2056.878703

Au	-0.682000	0.231000	-0.190000
O	-3.810000	-0.082000	-0.054000
O	-3.597000	-0.775000	2.092000
C	-2.458000	1.625000	-0.944000
H	-2.686000	1.281000	-1.948000
F	-4.507000	-2.718000	-0.409000
F	-5.312000	-2.769000	1.596000
C	-2.973000	0.999000	0.135000
H	-2.912000	1.367000	1.155000
C	1.846000	-0.447000	1.018000
C	1.444000	0.710000	1.832000
C	1.240000	-1.822000	-0.914000
F	-6.177000	-1.450000	0.118000
C	-4.053000	-0.872000	0.998000
C	-0.174000	2.378000	2.091000
H	-1.087000	2.814000	1.702000
C	0.495000	2.927000	3.173000
C	3.012000	-1.202000	1.174000
H	3.703000	-0.949000	1.969000
C	-5.039000	-1.980000	0.568000
C	1.680000	2.333000	3.584000
H	2.234000	2.737000	4.425000
C	2.403000	-2.561000	-0.727000
C	2.162000	1.219000	2.909000
H	3.087000	0.746000	3.215000
C	3.296000	-2.269000	0.318000
H	-1.949000	2.581000	-0.815000
C	-1.077000	-1.286000	-1.531000
H	-1.701000	-0.929000	-2.355000
C	0.233000	-1.937000	-2.036000
C	0.987000	-0.795000	-0.019000
N	0.284000	1.304000	1.449000
H	0.093000	3.804000	3.666000
H	2.626000	-3.379000	-1.406000
C	4.550000	-3.131000	0.484000
C	5.423000	-2.674000	1.652000
H	5.781000	-1.648000	1.519000
H	4.892000	-2.735000	2.608000
H	6.301000	-3.323000	1.723000

C	5.389000	-3.065000	-0.801000
H	6.293000	-3.672000	-0.690000
H	4.838000	-3.442000	-1.668000
H	5.696000	-2.036000	-1.018000
C	4.127000	-4.586000	0.738000
H	3.521000	-4.666000	1.647000
H	3.543000	-4.992000	-0.094000
H	5.013000	-5.218000	0.863000
C	0.763000	-1.141000	-3.237000
H	1.715000	-1.550000	-3.589000
H	0.044000	-1.179000	-4.062000
H	0.922000	-0.092000	-2.968000
C	-0.045000	-3.381000	-2.453000
H	-0.825000	-3.407000	-3.221000
H	0.851000	-3.851000	-2.874000
H	-0.380000	-3.983000	-1.603000
H	-1.655000	-2.000000	-0.933000
O	-0.519000	4.124000	-0.461000
C	0.205000	3.726000	-1.388000
O	-0.074000	3.292000	-2.512000
C	1.744000	3.750000	-1.104000
F	2.077000	4.213000	0.112000
F	2.280000	2.513000	-1.199000
F	2.402000	4.521000	-1.998000

L_1

G = -792.799262

N	3.051000	1.055000	-0.518000
C	0.960000	-0.019000	-0.005000
C	0.236000	-1.208000	-0.032000
C	-2.807000	2.658000	-1.147000
C	-3.435000	-2.345000	-0.086000
C	-2.766000	2.572000	1.356000
C	-0.982000	3.777000	0.114000
C	-1.539000	-3.385000	1.136000
C	-1.812000	0.025000	0.002000
C	-1.900000	2.554000	0.087000
C	-1.115000	1.242000	0.033000
C	-1.918000	-2.536000	-0.087000
C	4.381000	1.093000	-0.531000
C	4.559000	-1.040000	0.510000
C	3.174000	-1.089000	0.535000
C	5.186000	0.073000	-0.038000
C	0.273000	1.202000	0.019000
C	-1.527000	-3.289000	-1.367000
C	-1.163000	-1.206000	-0.034000
C	2.443000	-0.022000	-0.001000
H	4.830000	1.985000	-0.963000
H	6.266000	0.155000	-0.079000
H	5.143000	-1.857000	0.923000
H	2.665000	-1.935000	0.982000

H	0.857000	2.113000	0.037000
H	-2.217000	2.639000	-2.070000
H	-3.530000	1.838000	-1.192000
H	-3.370000	3.598000	-1.123000
H	-3.336000	3.506000	1.411000
H	-3.481000	1.744000	1.370000
H	-2.146000	2.498000	2.256000
H	-0.327000	3.778000	0.991000
H	-0.355000	3.835000	-0.782000
H	-1.588000	4.687000	0.153000
H	-1.814000	-2.877000	2.066000
H	-2.065000	-4.346000	1.105000
H	-0.465000	-3.593000	1.169000
H	-3.775000	-1.773000	-0.956000
H	-3.925000	-3.323000	-0.122000
H	-3.782000	-1.834000	0.818000
H	-2.066000	-4.241000	-1.424000
H	-1.775000	-2.704000	-2.258000
H	-2.896000	0.050000	0.007000
H	-0.456000	-3.510000	-1.398000
H	0.767000	-2.153000	-0.076000

Au-L_1

G = -2506.045423

Au	-0.712000	-0.885000	-0.147000
F	2.687000	-4.582000	1.340000
F	3.490000	-2.884000	0.271000
F	2.784000	-2.654000	2.304000
O	0.918000	-1.674000	0.703000
O	0.474000	-3.793000	0.050000
N	0.111000	-1.195000	-1.966000
C	1.529000	0.749000	-1.576000
C	2.824000	0.862000	-1.089000
C	-0.135000	4.246000	1.217000
C	4.852000	3.338000	1.030000
C	0.422000	5.278000	-1.001000
C	-1.470000	3.669000	-0.794000
C	5.641000	1.937000	-0.866000
C	2.237000	2.955000	-0.096000
C	1.147000	-2.941000	0.568000
C	-0.063000	4.001000	-0.298000
C	0.927000	2.872000	-0.585000
C	4.606000	2.038000	0.264000
C	-0.317000	-2.249000	-2.686000
C	1.399000	-1.862000	-4.293000
C	2.548000	-3.274000	1.148000
C	1.817000	-0.774000	-3.545000
C	0.303000	-2.603000	-3.865000
C	0.582000	1.751000	-1.331000
C	4.789000	0.859000	1.231000
C	3.196000	1.970000	-0.322000

C	1.150000	-0.431000	-2.375000
H	-1.151000	-2.810000	-2.282000
H	-0.065000	-3.456000	-4.421000
H	1.917000	-2.123000	-5.209000
H	2.649000	-0.155000	-3.862000
H	-0.411000	1.652000	-1.751000
H	-0.433000	3.336000	1.746000
H	0.824000	4.574000	1.626000
H	-0.871000	5.027000	1.432000
H	-0.263000	6.107000	-0.791000
H	1.419000	5.572000	-0.659000
H	0.463000	5.138000	-2.086000
H	-1.503000	3.527000	-1.879000
H	-1.862000	2.765000	-0.319000
H	-2.147000	4.494000	-0.551000
H	5.534000	2.765000	-1.575000
H	6.653000	1.974000	-0.451000
H	5.545000	1.000000	-1.423000
H	4.176000	3.442000	1.885000
H	5.876000	3.344000	1.416000
H	4.734000	4.219000	0.389000
H	5.788000	0.891000	1.680000
H	4.049000	0.897000	2.037000
H	2.510000	3.824000	0.490000
H	4.680000	-0.103000	0.722000
O	-1.605000	-0.711000	1.637000
C	-1.091000	0.100000	2.508000
O	-0.120000	0.803000	2.423000
C	-1.961000	0.084000	3.793000
F	-2.072000	-1.153000	4.290000
F	-3.196000	0.532000	3.529000
F	-1.436000	0.861000	4.735000
H	3.532000	0.061000	-1.279000
O	-2.226000	0.136000	-0.969000
C	-3.420000	-0.369000	-0.915000
O	-3.778000	-1.451000	-0.536000
C	-4.439000	0.686000	-1.422000
F	-4.061000	1.214000	-2.592000
F	-5.643000	0.148000	-1.582000
F	-4.544000	1.685000	-0.536000

TS2-3

G = -1979.596598

Au	0.396000	0.463000	-0.255000
F	5.361000	0.896000	-2.111000
F	4.779000	2.440000	-0.717000
F	5.128000	0.423000	-0.019000
O	2.448000	0.992000	-0.192000
O	2.741000	0.492000	-2.368000
N	-0.220000	2.235000	0.535000
C	-2.301000	1.129000	0.395000

C	-1.559000	0.128000	-0.239000
C	-6.425000	-0.434000	-1.334000
C	-1.040000	-3.201000	-0.721000
C	-6.098000	-1.671000	0.821000
C	-6.523000	0.778000	0.834000
C	-0.026000	-1.346000	-2.086000
C	-3.535000	-1.084000	-0.697000
C	3.121000	0.822000	-1.265000
C	-5.828000	-0.355000	0.079000
C	-4.318000	-0.139000	-0.024000
C	-1.332000	-1.993000	-1.620000
C	0.626000	3.222000	0.844000
C	-1.176000	4.454000	1.807000
C	4.620000	1.139000	-1.030000
C	-2.037000	3.416000	1.487000
C	0.172000	4.362000	1.480000
C	-3.685000	0.982000	0.505000
C	-2.070000	-2.457000	-2.880000
C	-2.149000	-0.974000	-0.843000
C	-1.544000	2.291000	0.837000
H	1.664000	3.072000	0.575000
H	0.874000	5.153000	1.716000
H	-1.557000	5.334000	2.315000
H	-3.089000	3.469000	1.741000
H	-4.259000	1.757000	0.999000
H	-7.506000	-0.597000	-1.274000
H	-6.252000	0.495000	-1.887000
H	-5.996000	-1.257000	-1.913000
H	-7.177000	-1.843000	0.896000
H	-5.658000	-2.529000	0.303000
H	-5.686000	-1.641000	1.835000
H	-6.159000	0.867000	1.863000
H	-6.391000	1.743000	0.334000
H	-7.597000	0.576000	0.881000
H	0.713000	-1.195000	-1.231000
H	0.598000	-2.028000	-2.674000
H	-0.190000	-0.451000	-2.690000
H	-1.971000	-3.702000	-0.443000
H	-0.405000	-3.920000	-1.248000
H	-0.532000	-2.893000	0.196000
H	-1.428000	-3.133000	-3.454000
H	-2.983000	-3.006000	-2.635000
H	-4.025000	-1.943000	-1.144000
H	-2.337000	-1.611000	-3.522000
O	2.561000	-2.160000	-0.151000
C	1.994000	-2.037000	0.926000
O	1.024000	-1.305000	1.260000
C	2.500000	-2.904000	2.117000
F	1.509000	-3.654000	2.635000
F	3.485000	-3.740000	1.773000
F	2.969000	-2.131000	3.115000

TS3-1

G = -1979.601818

Au	0.263000	0.447000	-0.460000
F	5.325000	0.515000	-2.226000
F	4.667000	2.299000	-1.204000
F	4.965000	0.463000	-0.099000
O	2.300000	1.016000	-0.562000
O	2.738000	-0.049000	-2.500000
N	-0.295000	2.175000	0.488000
C	-2.399000	1.095000	0.341000
C	-1.659000	0.089000	-0.276000
C	-6.482000	-0.670000	-1.274000
C	-1.018000	-3.213000	-0.296000
C	-6.136000	-1.782000	0.945000
C	-6.606000	0.655000	0.826000
C	0.064000	-1.405000	-1.685000
C	-3.582000	-1.242000	-0.598000
C	3.040000	0.578000	-1.508000
C	-5.887000	-0.503000	0.133000
C	-4.380000	-0.262000	0.012000
C	-1.260000	-2.114000	-1.340000
C	0.560000	3.142000	0.832000
C	-1.228000	4.385000	1.804000
C	4.522000	0.963000	-1.261000
C	-2.105000	3.371000	1.446000
C	0.122000	4.273000	1.497000
C	-3.774000	0.904000	0.484000
C	-1.809000	-2.734000	-2.626000
C	-2.205000	-1.087000	-0.753000
C	-1.624000	2.252000	0.780000
H	1.598000	2.984000	0.564000
H	0.835000	5.043000	1.765000
H	-1.600000	5.260000	2.326000
H	-3.160000	3.440000	1.685000
H	-4.369000	1.672000	0.963000
H	-7.560000	-0.850000	-1.206000
H	-6.324000	0.230000	-1.877000
H	-6.035000	-1.516000	-1.805000
H	-7.212000	-1.965000	1.033000
H	-5.687000	-2.660000	0.470000
H	-5.721000	-1.695000	1.955000
H	-6.248000	0.804000	1.850000
H	-6.489000	1.596000	0.278000
H	-7.676000	0.436000	0.880000
H	0.858000	-1.331000	-0.686000
H	0.841000	-2.098000	-2.035000
H	-0.038000	-0.705000	-2.522000
H	-1.956000	-3.725000	-0.063000
H	-0.307000	-3.951000	-0.680000
H	-0.614000	-2.797000	0.631000

H	-1.078000	-3.430000	-3.048000
H	-2.727000	-3.296000	-2.429000
H	-4.046000	-2.153000	-0.963000
H	-2.029000	-1.968000	-3.377000
O	1.983000	-1.979000	0.244000
C	1.953000	-1.609000	1.443000
O	1.211000	-0.806000	2.005000
C	3.023000	-2.324000	2.318000
F	3.147000	-1.786000	3.537000
F	2.702000	-3.623000	2.493000
F	4.239000	-2.294000	1.749000

TS1-5

G = -1530.42586

Au	0.636000	-0.695000	-0.821000
N	0.702000	1.476000	-0.994000
C	1.747000	2.228000	-1.336000
H	2.671000	1.696000	-1.542000
C	1.663000	3.608000	-1.418000
H	2.536000	4.188000	-1.693000
C	0.444000	4.211000	-1.135000
H	0.339000	5.289000	-1.188000
C	-0.643000	3.426000	-0.776000
H	-1.597000	3.883000	-0.544000
C	-0.496000	2.044000	-0.706000
C	-1.547000	1.098000	-0.303000
C	-2.850000	1.422000	0.079000
H	-3.169000	2.459000	0.059000
C	-3.752000	0.434000	0.496000
C	-3.321000	-0.897000	0.550000
C	-2.024000	-1.256000	0.178000
C	-1.184000	-0.248000	-0.257000
C	2.824000	-1.357000	-2.262000
C	1.892000	-1.364000	-3.032000
H	3.647000	-1.346000	-1.579000
H	1.117000	-1.391000	-3.770000
O	2.864000	-0.599000	0.392000
C	2.856000	0.121000	1.421000
O	1.934000	0.646000	2.032000
C	4.299000	0.393000	1.949000
F	5.028000	-0.733000	2.056000
F	4.966000	1.207000	1.098000
F	4.326000	0.987000	3.149000
C	-1.373000	-2.616000	0.289000
C	-0.122000	-2.597000	-0.629000
H	0.664000	-3.267000	-0.265000
H	-0.388000	-2.890000	-1.650000
C	-0.931000	-2.809000	1.746000
H	-1.789000	-2.774000	2.424000
H	-0.436000	-3.779000	1.866000
H	-0.227000	-2.025000	2.043000

C	-2.298000	-3.760000	-0.124000
H	-1.758000	-4.712000	-0.090000
H	-3.157000	-3.842000	0.551000
H	-2.675000	-3.618000	-1.142000
H	-3.998000	-1.672000	0.891000
C	-5.175000	0.844000	0.884000
C	-5.120000	1.866000	2.029000
C	-5.865000	1.478000	-0.334000
C	-6.017000	-0.346000	1.346000
H	-4.618000	1.444000	2.906000
H	-4.585000	2.776000	1.740000
H	-6.134000	2.156000	2.325000
H	-5.916000	0.768000	-1.166000
H	-6.888000	1.773000	-0.076000
H	-5.336000	2.370000	-0.681000
H	-7.020000	0.003000	1.614000
H	-6.130000	-1.099000	0.560000
H	-5.590000	-0.831000	2.230000

TS5-6

G = -1530.42273

Au	0.094000	-0.761000	-0.013000
N	0.295000	1.423000	0.087000
C	-0.774000	-2.602000	-0.324000
C	-2.261000	-2.606000	0.116000
C	-0.913000	2.045000	0.042000
C	-2.078000	1.149000	-0.011000
C	1.423000	2.135000	0.150000
H	2.359000	1.581000	0.179000
C	-1.797000	-0.218000	-0.024000
C	-2.779000	-1.191000	-0.021000
C	-4.112000	-0.774000	-0.050000
C	-0.981000	3.434000	0.060000
H	-1.945000	3.927000	0.022000
C	-4.446000	0.586000	-0.060000
C	1.413000	3.521000	0.173000
H	2.350000	4.062000	0.225000
C	-3.416000	1.538000	-0.026000
H	-3.667000	2.594000	-0.010000
C	0.190000	4.177000	0.126000
H	0.145000	5.261000	0.141000
C	2.142000	-1.518000	0.362000
H	2.297000	-2.079000	1.266000
C	2.634000	-0.959000	-0.624000
H	2.741000	-0.435000	-1.549000
H	-0.687000	-2.727000	-1.409000
H	-0.203000	-3.397000	0.163000
H	-4.896000	-1.523000	-0.057000
C	-2.346000	-3.001000	1.597000
H	-3.380000	-2.959000	1.955000
H	-1.974000	-4.021000	1.741000

H	-1.744000	-2.324000	2.212000
C	-3.040000	-3.615000	-0.728000
H	-2.587000	-4.608000	-0.644000
H	-4.080000	-3.695000	-0.392000
H	-3.042000	-3.329000	-1.785000
C	-5.900000	1.066000	-0.093000
C	-6.189000	1.899000	1.164000
C	-6.119000	1.936000	-1.340000
C	-6.894000	-0.095000	-0.139000
H	-6.037000	1.307000	2.072000
H	-5.546000	2.782000	1.224000
H	-7.229000	2.245000	1.154000
H	-5.926000	1.367000	-2.255000
H	-7.155000	2.290000	-1.372000
H	-5.468000	2.815000	-1.345000
H	-7.913000	0.301000	-0.179000
H	-6.747000	-0.721000	-1.025000
H	-6.822000	-0.732000	0.748000
O	4.885000	-0.949000	-0.641000
C	5.252000	0.169000	-0.218000
C	6.791000	0.230000	0.044000
O	4.612000	1.195000	0.016000
F	7.490000	0.016000	-1.090000
F	7.180000	-0.714000	0.923000
F	7.204000	1.407000	0.534000

TS6-7

G = -2056.875846

Au	-0.140000	-0.769000	-0.082000
N	0.177000	0.921000	-1.485000
C	0.300000	-2.301000	1.217000
C	1.663000	-2.042000	1.914000
C	1.490000	1.224000	-1.652000
C	2.422000	0.387000	-0.872000
C	-0.759000	1.625000	-2.120000
H	-1.786000	1.327000	-1.940000
C	1.842000	-0.246000	0.246000
C	2.525000	-1.260000	0.935000
C	3.853000	-1.505000	0.604000
C	1.874000	2.265000	-2.490000
H	2.925000	2.505000	-2.602000
C	4.486000	-0.793000	-0.427000
C	-0.440000	2.678000	-2.965000
H	-1.230000	3.230000	-3.459000
C	3.745000	0.132000	-1.187000
H	4.204000	0.617000	-2.042000
C	0.899000	2.998000	-3.151000
H	1.183000	3.821000	-3.799000
H	-0.506000	-2.439000	1.940000
C	-2.027000	-1.448000	-0.432000
H	-2.184000	-2.420000	-0.901000

C	-3.090000	-0.734000	-0.094000
H	-3.099000	0.233000	0.395000
O	-4.375000	-1.267000	-0.339000
C	-5.415000	-0.460000	-0.285000
C	-6.700000	-1.288000	-0.511000
O	-5.434000	0.721000	-0.094000
F	-6.848000	-2.209000	0.448000
F	-6.659000	-1.925000	-1.687000
F	-7.769000	-0.502000	-0.502000
H	1.273000	0.670000	0.965000
H	4.400000	-2.277000	1.132000
H	0.358000	-3.182000	0.571000
C	2.277000	-3.391000	2.292000
H	3.204000	-3.258000	2.858000
H	1.580000	-3.952000	2.922000
H	2.495000	-3.995000	1.406000
C	1.456000	-1.208000	3.185000
H	2.414000	-0.973000	3.658000
H	0.942000	-0.267000	2.970000
H	0.847000	-1.770000	3.900000
C	5.949000	-1.039000	-0.791000
C	6.024000	-1.606000	-2.218000
H	5.606000	-0.915000	-2.956000
H	7.069000	-1.790000	-2.487000
H	5.481000	-2.553000	-2.293000
C	6.713000	0.294000	-0.730000
H	7.765000	0.127000	-0.981000
H	6.315000	1.028000	-1.436000
H	6.667000	0.728000	0.274000
C	6.631000	-2.027000	0.156000
H	6.609000	-1.678000	1.194000
H	6.172000	-3.019000	0.115000
H	7.680000	-2.138000	-0.134000
O	1.044000	1.880000	1.553000
C	-0.160000	2.274000	1.598000
O	-1.201000	1.646000	1.506000
C	-0.248000	3.819000	1.756000
F	0.518000	4.271000	2.761000
F	0.179000	4.425000	0.629000
F	-1.494000	4.242000	1.984000

TS6-8

G = -2056.883373

Au	-0.121000	-0.120000	-0.354000
O	-4.113000	-1.218000	-0.115000
O	-4.594000	-1.692000	2.052000
C	-2.276000	0.099000	-0.791000
H	-2.588000	-0.120000	-1.812000
F	-5.510000	-3.557000	-0.514000
F	-6.686000	-3.143000	1.250000
C	-3.021000	-0.424000	0.188000

H	-2.862000	-0.281000	1.252000
C	2.348000	-0.278000	1.144000
C	1.483000	0.434000	2.097000
C	2.480000	-1.171000	-1.125000
F	-6.772000	-1.802000	-0.442000
C	-4.804000	-1.774000	0.881000
C	-0.626000	1.388000	2.413000
H	-1.595000	1.600000	1.977000
C	-0.298000	1.817000	3.688000
C	3.677000	-0.660000	1.362000
H	4.142000	-0.448000	2.317000
C	-5.971000	-2.588000	0.282000
C	0.973000	1.532000	4.172000
H	1.269000	1.851000	5.166000
C	3.796000	-1.547000	-0.880000
C	1.869000	0.839000	3.372000
H	2.866000	0.615000	3.730000
C	4.408000	-1.307000	0.363000
H	-1.939000	1.379000	-0.576000
O	-1.790000	2.626000	-0.328000
C	-1.196000	3.274000	-1.253000
O	-0.995000	2.974000	-2.412000
C	-0.638000	4.624000	-0.720000
F	-1.553000	5.311000	-0.019000
F	0.406000	4.398000	0.102000
F	-0.206000	5.419000	-1.701000
C	0.202000	-1.191000	-2.079000
H	-0.384000	-0.776000	-2.903000
C	1.713000	-1.258000	-2.427000
C	1.781000	-0.560000	-0.094000
N	0.231000	0.714000	1.645000
H	-1.024000	2.364000	4.277000
H	4.364000	-2.035000	-1.668000
C	5.854000	-1.760000	0.580000
C	6.372000	-1.410000	1.976000
H	6.371000	-0.329000	2.155000
H	5.783000	-1.891000	2.764000
H	7.404000	-1.759000	2.078000
C	6.764000	-1.082000	-0.455000
H	7.802000	-1.397000	-0.307000
H	6.480000	-1.342000	-1.479000
H	6.723000	0.008000	-0.360000
C	5.935000	-3.284000	0.406000
H	5.294000	-3.796000	1.132000
H	5.626000	-3.596000	-0.596000
H	6.964000	-3.626000	0.560000
C	2.090000	-0.036000	-3.277000
H	3.163000	-0.027000	-3.495000
H	1.546000	-0.050000	-4.228000
H	1.840000	0.892000	-2.754000
C	2.003000	-2.537000	-3.211000

H 1.368000 -2.586000 -4.103000
H 3.045000 -2.570000 -3.545000
H 1.809000 -3.428000 -2.605000
H -0.186000 -2.187000 -1.839000

1'

G = -1335.437612
Au 0.119000 -0.382000 -0.129000
F -4.887000 -1.402000 1.138000
F -4.516000 -0.433000 -0.753000
F -4.059000 -2.532000 -0.502000
O -1.826000 -0.891000 -0.440000
O -2.368000 -0.817000 1.751000
C 2.308000 1.410000 0.224000
C 3.113000 -3.385000 0.554000
C 2.570000 -2.454000 -1.711000
C 4.239000 -0.582000 0.404000
C -2.603000 -0.974000 0.575000
C 4.586000 0.754000 0.575000
C 2.370000 -2.278000 -0.194000
C -1.214000 2.487000 -0.308000
C 0.110000 4.473000 -0.000000
C -4.038000 -1.339000 0.113000
C 1.251000 3.697000 0.153000
C -1.138000 3.885000 -0.228000
C 3.631000 1.756000 0.474000
C 0.858000 -2.317000 0.129000
C 2.915000 -0.906000 0.143000
C 1.158000 2.306000 0.077000
H -2.184000 2.027000 -0.490000
H 0.186000 5.555000 0.058000
H 2.206000 4.185000 0.328000
H 3.903000 2.797000 0.592000
H 3.627000 -2.391000 -1.985000
H 2.192000 -3.435000 -2.016000
H 2.021000 -1.689000 -2.270000
H 3.056000 -3.239000 1.637000
H 2.651000 -4.349000 0.318000
H 4.168000 -3.444000 0.267000
H 0.357000 -3.083000 -0.469000
H 0.698000 -2.551000 1.189000
H 4.985000 -1.364000 0.464000
C -0.092000 1.687000 -0.160000
N 2.013000 0.092000 0.087000
C -2.375000 4.723000 -0.347000
H -3.059000 4.320000 -1.099000
H -2.917000 4.740000 0.606000
H -2.137000 5.757000 -0.610000
H 5.618000 1.019000 0.781000

2'

G = -1861.869856

Au	-0.167000	0.223000	0.196000
F	4.873000	0.575000	-1.173000
F	4.352000	1.297000	0.794000
F	4.369000	-0.828000	0.388000
O	1.832000	0.254000	0.489000
O	2.268000	0.638000	-1.696000
C	-2.414000	1.647000	-0.753000
C	-4.542000	-1.811000	1.465000
C	-2.165000	-1.511000	1.995000
C	-4.278000	-0.331000	-0.951000
C	2.576000	0.437000	-0.548000
C	-4.456000	0.837000	-1.669000
C	-3.139000	-1.703000	0.830000
C	0.700000	3.056000	0.708000
C	-0.554000	4.895000	-0.212000
C	4.069000	0.368000	-0.132000
C	-1.535000	4.025000	-0.669000
C	0.562000	4.436000	0.491000
C	-3.545000	1.869000	-1.517000
C	-2.851000	-2.999000	0.062000
C	-3.160000	-0.515000	-0.136000
C	-1.410000	2.656000	-0.438000
H	1.573000	2.677000	1.230000
H	-0.662000	5.959000	-0.398000
H	-2.399000	4.418000	-1.194000
H	-3.693000	2.829000	-1.995000
H	-2.299000	-0.535000	2.472000
H	-2.370000	-2.279000	2.746000
H	-1.118000	-1.631000	1.723000
H	-5.320000	-2.075000	0.746000
H	-4.518000	-2.603000	2.219000
H	-4.829000	-0.879000	1.962000
H	-2.841000	-3.841000	0.761000
H	-3.629000	-3.188000	-0.685000
H	-5.028000	-1.108000	-0.993000
H	-1.888000	-2.958000	-0.447000
O	0.116000	-1.816000	-0.367000
C	0.793000	-2.628000	0.351000
O	1.086000	-2.574000	1.526000
C	1.281000	-3.831000	-0.499000
F	2.194000	-3.426000	-1.399000
F	0.276000	-4.404000	-1.180000
F	1.849000	-4.780000	0.248000
C	-0.275000	2.201000	0.243000
N	-2.192000	0.428000	-0.165000
H	-5.326000	0.960000	-2.306000
C	1.606000	5.380000	1.002000
H	2.603000	5.079000	0.665000
H	1.421000	6.401000	0.662000

H	1.623000	5.384000	2.097000

3'

G = -1861.855972

Au	-0.445000	0.137000	-0.490000
F	4.387000	0.535000	-2.436000
F	3.549000	2.414000	-1.778000
F	4.072000	0.894000	-0.332000
O	1.400000	0.937000	-0.703000
O	1.822000	-0.176000	-2.619000
C	-3.144000	0.459000	0.387000
C	-1.236000	-3.624000	0.218000
C	-0.547000	-2.097000	-1.643000
C	-4.029000	-2.104000	-0.063000
C	2.127000	0.517000	-1.680000
C	-4.887000	-1.165000	0.485000
C	-1.738000	-2.765000	-0.955000
C	-0.417000	3.004000	0.369000
C	-2.384000	4.060000	1.275000
C	3.562000	1.088000	-1.550000
C	-3.112000	2.889000	1.116000
C	-1.038000	4.140000	0.913000
C	-4.449000	0.130000	0.712000
C	-2.429000	-3.652000	-1.999000
C	-2.723000	-1.752000	-0.393000
C	-2.506000	1.752000	0.581000
H	0.629000	3.034000	0.084000
H	-2.872000	4.934000	1.695000
H	-4.156000	2.861000	1.412000
H	-5.104000	0.875000	1.146000
H	0.233000	-1.701000	-0.922000
H	0.094000	-2.851000	-2.109000
H	-0.838000	-1.417000	-2.449000
H	-2.064000	-4.157000	0.692000
H	-0.519000	-4.361000	-0.156000
H	-0.736000	-3.008000	0.970000
H	-1.697000	-4.355000	-2.409000
H	-3.241000	-4.241000	-1.567000
H	-4.364000	-3.119000	-0.231000
H	-2.831000	-3.056000	-2.824000
N	-2.326000	-0.489000	-0.153000
C	-1.156000	1.857000	0.216000
C	-0.245000	5.394000	1.111000
H	0.480000	5.263000	1.922000
H	0.322000	5.647000	0.210000
H	-0.890000	6.237000	1.366000
H	-5.904000	-1.446000	0.741000
O	2.113000	-1.878000	0.189000
C	1.748000	-1.545000	1.320000
O	0.670000	-1.053000	1.706000
C	2.778000	-1.749000	2.473000

F 2.266000 -2.505000 3.467000
F 3.913000 -2.345000 2.083000
F 3.128000 -0.569000 3.025000

4'

G = -1861.895918
Au 0.754000 -0.392000 0.005000
F 4.058000 3.412000 -1.428000
F 3.065000 3.641000 0.474000
F 4.668000 2.204000 0.254000
O 2.125000 1.077000 0.285000
O 2.344000 1.445000 -1.932000
C -1.719000 -2.063000 -0.504000
C 2.551000 -4.217000 -0.290000
C 2.040000 -2.910000 1.787000
C -0.409000 -4.406000 0.151000
C 2.587000 1.653000 -0.767000
C -1.782000 -4.422000 -0.051000
C 1.757000 -3.041000 0.283000
C -2.370000 1.014000 -2.565000
C -4.181000 0.736000 -1.019000
C 3.608000 2.749000 -0.364000
C -3.586000 -0.409000 -0.514000
C -3.583000 1.472000 -2.048000
C -2.436000 -3.251000 -0.397000
C 2.161000 -1.768000 -0.462000
C 0.272000 -3.204000 0.069000
C -2.356000 -0.840000 -1.017000
H -1.892000 1.559000 -3.374000
H -5.124000 1.077000 -0.599000
H -4.059000 -0.954000 0.297000
H -3.493000 -3.245000 -0.633000
H 1.743000 -3.819000 2.317000
H 3.112000 -2.751000 1.944000
H 1.502000 -2.064000 2.226000
H 2.306000 -4.394000 -1.341000
H 3.621000 -3.999000 -0.218000
H 2.364000 -5.137000 0.273000
H 3.137000 -1.388000 -0.156000
H 2.122000 -1.888000 -1.549000
H 0.135000 -5.315000 0.374000
C -1.760000 -0.124000 -2.057000
N -0.400000 -2.059000 -0.206000
C -4.223000 2.729000 -2.555000
H -3.699000 3.120000 -3.430000
H -5.270000 2.560000 -2.825000
H -4.210000 3.504000 -1.780000
H -2.335000 -5.353000 0.025000
H -0.820000 -0.465000 -2.482000
O -0.670000 1.110000 0.611000
C -1.362000 0.890000 1.650000

C	-2.267000	2.089000	2.045000
O	-1.397000	-0.087000	2.378000
F	-1.772000	2.688000	3.146000
F	-2.373000	3.026000	1.100000
F	-3.510000	1.682000	2.346000

L_2

G = -675.05209

N	-0.855000	-0.101000	-0.036000
C	1.498000	0.382000	0.030000
C	2.534000	1.218000	-0.402000
C	4.178000	-0.526000	-0.025000
C	3.142000	-1.359000	0.402000
C	-2.142000	0.237000	-0.006000
C	-1.573000	2.552000	0.263000
C	-0.232000	2.192000	0.235000
C	-2.543000	1.572000	0.137000
C	1.826000	-0.918000	0.427000
C	3.847000	0.770000	-0.431000
C	0.091000	0.844000	0.072000
H	-3.595000	1.833000	0.161000
H	-1.857000	3.592000	0.391000
H	0.542000	2.941000	0.355000
H	1.036000	-1.581000	0.761000
H	2.314000	2.225000	-0.744000
H	4.630000	1.436000	-0.783000
H	3.371000	-2.373000	0.721000
C	5.603000	-0.996000	-0.045000
H	6.070000	-0.803000	-1.016000
H	6.200000	-0.471000	0.709000
H	5.672000	-2.067000	0.159000
C	-3.183000	-0.876000	-0.109000
C	-4.146000	-0.578000	-1.267000
C	-2.526000	-2.233000	-0.350000
C	-3.971000	-0.930000	1.209000
H	-4.688000	0.360000	-1.120000
H	-3.608000	-0.515000	-2.219000
H	-4.888000	-1.380000	-1.350000
H	-1.848000	-2.503000	0.464000
H	-3.301000	-3.003000	-0.420000
H	-1.949000	-2.241000	-1.279000
H	-4.719000	-1.729000	1.166000
H	-3.307000	-1.130000	2.056000
H	-4.497000	0.010000	1.404000

Au-L_2

G = -2388.283566

Au	0.162000	-0.016000	-0.195000
F	-3.717000	-3.004000	-2.158000
F	-2.177000	-3.974000	-0.994000
F	-3.610000	-2.673000	-0.028000

O	-1.168000	-1.504000	-0.342000
O	-1.965000	-1.010000	-2.402000
N	1.417000	-1.389000	0.651000
C	0.107000	-0.723000	2.624000
C	-1.100000	-1.367000	2.906000
C	-1.975000	0.667000	3.898000
C	-1.933000	-1.636000	-1.378000
C	-0.760000	1.295000	3.622000
C	2.393000	-2.086000	0.021000
C	3.078000	-2.960000	2.179000
C	-2.883000	-2.841000	-1.136000
C	2.031000	-2.278000	2.778000
C	3.247000	-2.858000	0.814000
C	0.276000	0.612000	2.996000
C	-2.124000	-0.675000	3.535000
C	1.218000	-1.483000	1.996000
H	4.060000	-3.387000	0.338000
H	3.755000	-3.568000	2.770000
H	1.840000	-2.332000	3.842000
H	1.215000	1.116000	2.792000
O	-0.942000	1.455000	-0.995000
C	-2.200000	1.585000	-0.729000
O	-2.916000	0.933000	-0.017000
C	-2.750000	2.812000	-1.507000
F	-2.614000	2.644000	-2.827000
F	-2.095000	3.930000	-1.166000
F	-4.042000	3.000000	-1.247000
H	-1.238000	-2.405000	2.623000
O	1.513000	1.400000	0.243000
C	2.085000	2.057000	-0.716000
O	1.980000	1.933000	-1.906000
C	3.043000	3.111000	-0.097000
F	4.024000	2.501000	0.586000
F	3.603000	3.861000	-1.038000
F	2.397000	3.918000	0.751000
H	-3.061000	-1.184000	3.742000
H	-0.617000	2.334000	3.902000
C	-3.105000	1.413000	4.542000
H	-3.856000	1.687000	3.792000
H	-3.608000	0.800000	5.295000
H	-2.758000	2.333000	5.017000
C	2.664000	-2.085000	-1.491000
C	2.831000	-3.546000	-1.954000
C	1.578000	-1.484000	-2.379000
C	3.975000	-1.317000	-1.723000
H	3.680000	-4.054000	-1.494000
H	1.926000	-4.127000	-1.751000
H	2.999000	-3.549000	-3.035000
H	1.470000	-0.401000	-2.270000
H	1.876000	-1.637000	-3.420000
H	0.616000	-1.984000	-2.252000

H 4.208000 -1.322000 -2.792000
H 3.890000 -0.275000 -1.400000
H 4.813000 -1.774000 -1.189000

TS2-3'

G = -1335.850577

Au -0.047000 -0.249000 0.084000
F 4.719000 -2.359000 -0.595000
F 4.576000 -0.208000 -0.491000
F 4.348000 -1.396000 1.302000
O 1.962000 -0.421000 0.282000
O 2.069000 -2.359000 -0.868000
C -2.329000 1.451000 -0.079000
C -2.784000 -2.763000 1.491000
C -1.057000 -2.544000 -0.302000
C -4.283000 -0.481000 -0.106000
C 2.550000 -1.439000 -0.256000
C -4.636000 0.857000 -0.139000
C -2.527000 -2.313000 0.044000
C 1.269000 2.441000 0.047000
C -0.037000 4.463000 -0.084000
C 4.078000 -1.354000 -0.009000
C -1.216000 3.729000 -0.107000
C 1.212000 3.845000 -0.011000
C -3.655000 1.838000 -0.128000
C -3.354000 -3.168000 -0.927000
C -2.941000 -0.852000 -0.060000
C -1.175000 2.336000 -0.057000
H 2.225000 1.934000 0.112000
H -0.088000 5.547000 -0.124000
H -2.170000 4.242000 -0.165000
H -3.911000 2.890000 -0.155000
H -0.356000 -2.187000 0.510000
H -0.810000 -3.609000 -0.254000
H -0.784000 -2.218000 -1.311000
H -3.838000 -2.644000 1.755000
H -2.520000 -3.819000 1.596000
H -2.181000 -2.184000 2.197000
H -3.004000 -4.202000 -0.879000
H -4.414000 -3.171000 -0.666000
H -5.047000 -1.247000 -0.106000
H -3.248000 -2.816000 -1.957000
N -2.014000 0.124000 -0.045000
C 0.090000 1.741000 0.018000
H -5.683000 1.139000 -0.173000
C 2.482000 4.636000 0.002000
H 3.083000 4.394000 0.885000
H 3.092000 4.401000 -0.877000
H 2.281000 5.709000 0.003000

TS3-1'

G = -1861.84794

Au	-0.494000	0.073000	-0.417000
F	3.972000	1.876000	-2.557000
F	2.939000	3.208000	-1.207000
F	3.943000	1.452000	-0.441000
O	1.217000	1.153000	-0.557000
O	1.671000	0.545000	-2.686000
C	-3.245000	-0.077000	0.334000
C	-0.579000	-3.631000	0.274000
C	-0.070000	-1.880000	-1.467000
C	-3.616000	-2.736000	-0.330000
C	1.909000	1.101000	-1.641000
C	-4.671000	-1.988000	0.171000
C	-1.125000	-2.874000	-0.950000
C	-1.015000	2.889000	0.614000
C	-3.192000	3.549000	1.406000
C	3.215000	1.919000	-1.463000
C	-3.689000	2.278000	1.151000
C	-1.858000	3.875000	1.150000
C	-4.493000	-0.654000	0.512000
C	-1.456000	-3.868000	-2.067000
C	-2.370000	-2.140000	-0.494000
C	-2.850000	1.295000	0.627000
H	0.025000	3.122000	0.405000
H	-3.854000	4.305000	1.817000
H	-4.730000	2.057000	1.364000
H	-5.309000	-0.067000	0.913000
H	0.801000	-2.439000	-1.830000
H	-0.410000	-1.358000	-2.370000
H	-1.305000	-4.368000	0.630000
H	0.339000	-4.158000	-0.002000
H	-0.351000	-2.946000	1.096000
H	-0.535000	-4.361000	-2.390000
H	-2.147000	-4.647000	-1.732000
H	-3.750000	-3.778000	-0.588000
H	-1.894000	-3.362000	-2.933000
N	-2.238000	-0.845000	-0.164000
C	-1.508000	1.629000	0.356000
C	-1.319000	5.241000	1.446000
H	-0.848000	5.677000	0.559000
H	-2.107000	5.917000	1.785000
H	-0.552000	5.193000	2.226000
H	-5.644000	-2.451000	0.302000
H	0.869000	-1.517000	-0.547000
O	2.026000	-1.661000	0.143000
C	1.977000	-1.347000	1.370000
O	1.054000	-0.884000	2.020000
C	3.306000	-1.666000	2.109000
F	3.373000	-1.084000	3.309000
F	3.415000	-2.996000	2.304000

F 4.383000 -1.279000 1.414000

TS(Au-L_2-2')

G = -2388.249523

Au	-0.088000	0.020000	0.118000
F	-3.984000	3.432000	-0.524000
F	-3.302000	2.429000	-2.306000
F	-4.636000	1.414000	-0.940000
O	-1.649000	0.948000	-0.926000
O	-2.359000	1.907000	0.993000
N	-1.346000	-1.461000	0.728000
C	-0.331000	-0.562000	2.662000
C	-0.526000	0.407000	3.637000
C	1.808000	1.128000	3.401000
C	-2.414000	1.675000	-0.191000
C	2.012000	0.138000	2.457000
C	-2.230000	-2.184000	0.013000
C	-3.406000	-2.650000	2.091000
C	-3.593000	2.259000	-1.018000
C	-2.440000	-1.950000	2.802000
C	-3.284000	-2.776000	0.721000
C	0.961000	-0.718000	2.071000
C	0.533000	1.227000	3.997000
C	-1.417000	-1.368000	2.089000
H	-4.014000	-3.354000	0.172000
H	-4.240000	-3.113000	2.606000
H	-2.474000	-1.842000	3.879000
H	1.192000	-1.661000	1.573000
O	1.065000	1.628000	-0.141000
C	1.372000	1.982000	-1.349000
O	1.008000	1.539000	-2.404000
C	2.360000	3.178000	-1.276000
F	3.473000	2.842000	-0.610000
F	1.806000	4.221000	-0.640000
F	2.715000	3.582000	-2.491000
H	-1.508000	0.555000	4.072000
O	1.975000	-0.950000	-0.806000
C	2.337000	-2.126000	-0.570000
O	1.753000	-3.034000	0.017000
C	3.784000	-2.424000	-1.065000
F	4.676000	-1.992000	-0.147000
F	4.008000	-3.731000	-1.244000
F	4.079000	-1.809000	-2.218000
C	-2.129000	-2.445000	-1.489000
C	-0.852000	-1.937000	-2.151000
C	-2.151000	-3.976000	-1.682000
C	-3.344000	-1.821000	-2.190000
H	-0.802000	-0.848000	-2.215000
H	0.038000	-2.325000	-1.657000
H	-0.839000	-2.299000	-3.183000
H	-3.079000	-4.436000	-1.336000

H	-2.054000	-4.193000	-2.750000
H	-1.313000	-4.449000	-1.161000
H	-3.306000	-2.073000	-3.254000
H	-4.291000	-2.194000	-1.790000
H	-3.333000	-0.733000	-2.100000
C	2.895000	2.075000	3.796000
H	2.616000	3.101000	3.532000
H	3.063000	2.052000	4.877000
H	3.833000	1.836000	3.291000
H	0.367000	1.998000	4.744000
H	2.988000	0.005000	2.002000

$[Au(OAc^F)_4]^-$

G = -2239.241531

Au	0.000164	-0.550872	-0.560469
F	4.939791	-1.172344	0.991733
F	4.522213	-1.412949	-1.112072
F	4.515177	0.559805	-0.224669
O	1.991210	-0.450891	-0.705481
O	2.308938	-1.314025	1.359202
C	2.683193	-0.869547	0.306273
C	4.194591	-0.722866	-0.013317
O	-0.040890	1.271119	0.260481
C	-0.130222	2.283577	-0.542453
O	-0.183560	2.306441	-1.743670
C	-0.164067	3.593176	0.289280
F	0.960786	3.735105	1.001504
F	-1.192866	3.592051	1.145069
F	-0.287303	4.655773	-0.500136
O	-1.996494	-0.561693	-0.652826
C	-2.639391	-0.923192	0.411958
O	-2.214990	-1.275746	1.480544
C	-4.164825	-0.846807	0.137726
F	-4.513771	-1.678185	-0.852090
F	-4.860704	-1.181561	1.219931
F	-4.526900	0.390686	-0.220511
O	0.046820	-2.462025	-1.144083
C	0.087231	-2.694344	-2.417726
C	0.135092	-4.227008	-2.655674
F	-0.961322	-4.820059	-2.166940
F	1.198400	-4.773327	-2.054241
F	0.208873	-4.505494	-3.953547
O	0.090596	-1.920185	-3.338026

$[L_2H]^+$

G = -675.492155

N	0.864439	-0.022332	0.049198
C	-1.516068	0.393036	-0.052162
C	-2.522944	1.182394	0.516309
C	-4.176463	-0.525829	0.035084
C	-3.167616	-1.303714	-0.536261

C	2.181540	0.249934	0.002304
C	1.568811	2.547107	-0.318296
C	0.222829	2.206773	-0.278407
C	2.548907	1.574249	-0.185669
C	-1.854703	-0.856375	-0.581388
C	-3.828822	0.724442	0.558968
C	-0.135338	0.881810	-0.092233
H	3.598519	1.833434	-0.231303
H	1.855883	3.582282	-0.470476
H	-0.548945	2.953271	-0.415163
H	-1.102795	-1.472189	-1.066881
H	-2.275144	2.146267	0.948848
H	-4.595547	1.343770	1.015650
H	-3.415280	-2.271167	-0.962206
C	-5.597053	-0.998732	0.073740
H	-6.015625	-0.903609	1.080299
H	-6.222757	-0.394071	-0.592227
H	-5.681246	-2.041850	-0.238456
C	3.180840	-0.883384	0.135045
C	4.138223	-0.564789	1.292592
C	2.500752	-2.226477	0.401870
C	3.965779	-0.967258	-1.183683
H	4.691718	0.362111	1.120544
H	3.597727	-0.475100	2.239676
H	4.865913	-1.375741	1.388999
H	1.846390	-2.533678	-0.422079
H	3.268847	-2.996996	0.500000
H	1.928650	-2.221411	1.336350
H	4.701548	-1.773982	-1.113630
H	3.301720	-1.180860	-2.026786
H	4.501559	-0.037447	-1.393112
H	0.595735	-0.985831	0.230687

$[L_1H]^+$

G = -793.236624

N	3.074773	0.930813	-0.628065
C	0.948110	-0.021075	0.022096
C	0.233391	-1.215029	-0.015361
C	-2.790839	2.671989	-1.130176
C	-3.437308	-2.336511	-0.120279
C	-2.781990	2.554677	1.374365
C	-0.983208	3.777327	0.168349
C	-1.555268	-3.393886	1.111976
C	-1.807654	0.026354	0.000502
C	-1.900836	2.555464	0.116219
C	-1.115895	1.245607	0.053795
C	-1.921541	-2.534592	-0.107077
C	4.412520	1.033857	-0.688538
C	4.564711	-0.955619	0.604672
C	3.182175	-1.025611	0.652774
C	5.195520	0.089772	-0.069416

C	0.271667	1.206136	0.060637
C	-1.516865	-3.273456	-1.391783
C	-1.163844	-1.208128	-0.034985
C	2.413492	-0.053043	0.019664
H	4.802820	1.875401	-1.246380
H	6.273740	0.170442	-0.116712
H	5.157856	-1.712847	1.106128
H	2.683926	-1.815544	1.199689
H	0.838865	2.126921	0.136677
H	-2.189697	2.670196	-2.045578
H	-3.510285	1.851002	-1.197278
H	-3.356864	3.608861	-1.097424
H	-3.353579	3.487096	1.431668
H	-3.495080	1.725292	1.369827
H	-2.172740	2.473018	2.280557
H	-0.343560	3.772284	1.057108
H	-0.344633	3.846376	-0.718928
H	-1.591195	4.686178	0.206865
H	-1.837326	-2.892882	2.043853
H	-2.085088	-4.351315	1.066925
H	-0.483164	-3.608446	1.152118
H	-3.767412	-1.757857	-0.989087
H	-3.928944	-3.312795	-0.168565
H	-3.791771	-1.833118	0.784953
H	-2.058242	-4.222707	-1.463409
H	-1.755787	-2.678056	-2.279176
H	-2.890592	0.052743	-0.007489
H	-0.446144	-3.498010	-1.412208
H	0.770266	-2.156599	-0.060987
H	2.526994	1.626676	-1.128016

TS1’-4’

G = -1861.858491

Au	-0.192937	-0.671644	-0.038280
F	-5.412254	-0.990717	-0.484897
F	-4.504900	0.938839	-0.819371
F	-4.312885	-0.623167	-2.304973
O	-2.019431	-0.290540	-0.836241
O	-3.084401	-1.652419	0.616250
C	2.123079	-0.270982	1.611749
C	2.279536	-3.469600	-2.065751
C	0.264340	-2.154559	-1.385641
C	3.665620	-2.178494	0.324823
C	-3.035899	-0.861832	-0.297288
C	4.227422	-1.363098	1.299884
C	1.493984	-2.923608	-0.873552
C	-1.074664	1.597307	2.166630
C	0.182052	1.639311	4.202447
C	-4.338992	-0.382015	-0.986625
C	1.232290	0.967462	3.587716
C	-0.996627	1.947509	3.515094

C	3.454400	-0.423537	1.969933
C	1.031510	-4.083630	0.026271
C	2.325136	-2.019863	0.004278
C	1.131226	0.603185	2.248499
H	-1.959757	1.876768	1.599770
H	0.272363	1.913732	5.250006
H	2.108534	0.697829	4.169519
H	3.874817	0.194231	2.753994
H	0.170137	1.523246	0.344885
H	0.487468	-1.568933	-2.284045
H	-0.588565	-2.810259	-1.569332
H	3.097592	-4.118539	-1.738832
H	1.614671	-4.067473	-2.696033
H	2.693691	-2.659268	-2.672342
H	0.416315	-4.772631	-0.560151
H	1.886882	-4.635316	0.426559
H	4.253928	-2.936944	-0.176655
H	0.431747	-3.714345	0.864114
O	0.350235	2.386845	-0.665996
C	1.466289	2.236816	-1.252821
O	2.368595	1.450509	-1.024943
C	1.623951	3.224622	-2.442984
F	2.835685	3.161395	-3.001907
F	0.725922	2.952699	-3.407768
F	1.425812	4.497142	-2.062878
N	1.630344	-1.047191	0.620620
C	-0.026114	0.949747	1.505371
C	-2.135524	2.626269	4.213475
H	-1.785034	3.472279	4.812116
H	-2.878647	2.990499	3.500639
H	-2.637555	1.931619	4.896406
H	5.276548	-1.473224	1.553730

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