Electronic Supplementary Information (ESI)

Gold complexes with remote-substituted amino N-heterocyclic carbenes

Sofie M. P. Vanden Broeck,[†a] Nikolaos V. Tzouras,[†ab] Marina Saab,[a] Kristof Van Hecke,[a] Busra Dereli,[c] Ida Ritacco,[d] Luigi Cavallo,[c,d] Georgios C. Vougioukalakis,[b] Pierre Braunstein,[e] Steven P. Nolan,*[a] Andreas A. Danopoulos*[b] and Catherine S. J. Cazin*[a]

---

[a] S. M. P. Vanden Broek, N. V. Tzouras, M. Saab, Prof. Dr. K. Van Hecke, Prof. Dr. C. S. J. Cazin, Prof. Dr. S. P. Nolan
Department of Chemistry and Centre for Sustainable Chemistry
Ghent University
Krijgslaan 281, S-3, 9000 Ghent, Belgium
E-mail: steven.nolan@ugent.be

[b] N. V. Tzouras, Prof. Dr. G. C. Vougioukalakis, Prof. Dr. A. A. Danopoulos
Department of Chemistry
National and Kapodistrian University of Athens
Panepistimiopolis
15771 Athens
Greece
E-mail: A.Danopoulos@chem.uoa.gr

[c] Dr. Busra Dereli, Prof. Dr. L. Cavallo
KAUST Catalysis Center, Physical Sciences and Engineering Division
King Abdullah University of Science and Technology
Thuwal 23955-6900, Saudi Arabia

[d] Dr. Ida Ritacco, Prof. Dr. L. Cavallo
Dipartimento di Chimica e Biologia, Università di Salerno, Fisciano 84084, Italy

[e] Prof. Dr. P. Braunstein
Université de Strasbourg, CNRS, Institut de Chimie UMR 7177, Strasbourg 67081, Cedex, France.

† Equal contribution

Table of contents

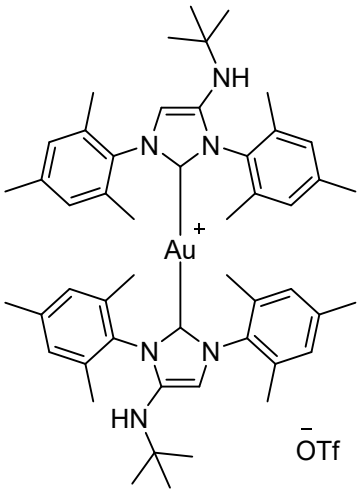
General considerations

All chemicals used were either used as received or prepared from commercially available starting products. When these chemicals were used for experiments under inert atmosphere (glovebox), they were either dried under vacuum (solids) or degassed using argon (liquids). All solvents were used as received when reactions were performed in air, and dry solvents were used when experiments were performed under inert atmosphere. Solid Lithium diisopropylamide (LDA) was purchased commercially and stored in the glovebox. ^{1}H, ^{19}F and $^{13}C\{^{1}H\}$ Nuclear Magnetic Resonance (NMR) spectra were recorded using Bruker-300, 400 or 500 MHz spectrometers at room temperature using $CDCl_3$ as solvent. Chemical shifts (ppm) are referenced to the residual solvent peaks ($CHCl_3$: 7.26 ppm in ^{1}H-NMR and 77.16 ppm in $^{13}C\{^{1}H\}$-NMR). Coupling constants (J) are given in Hertz. Abbreviations used in the designation of the signals: s = singlet, d = doublet, dd = doublet of doublets, m = multiplet, q = quadruplet. In ^{1}H-NMR spectra in $CDCl_3$, peaks appearing at 1.56 ppm, at 0.85 and 1.25 ppm, at 0.07 ppm, at 5.32 ppm, and at 3.76 and 1.85 ppm are attributed to water, H-grease, silicon grease, dichloromethane and tetrahydrofuran, respectively. HRMS was recorded with direct injection by an Agilent 1100 Series HPLC on an Agilent 6220A time of flight HRMS using ESI/APCI-multimode ionization source. Elemental analysis was performed by Université de Namur (Belgium).

Following products were prepared according to literature procedures: [AuCl(DMS)],[1] IPrAuN(iPr)$_2$,[2] AC$^{i\text{-Pr}}$•HOTf,[3a] AC$^{t\text{-Bu}}$ •HOTf,[3a] [AuCl(IMe)][3b] and [AuCl(MeImDipp)].[3b]

Procedures

Synthesis of [Au(AC$^{t\text{-Bu}}$)$_2$][OTf] (1)



In a 4 mL scintillation vial, the [Au(DMS)Cl] (22.4 mg, 0.076 mmol) and AC$^{t\text{-Bu}}$ •HOTf (1 equiv., 40mg, 0.076 mmol) were dissolved in acetone (0.4 mL) and put to stir at 30°C to evaporate the DMS. Afterwards, K_2CO_3 (3 equiv., 31.6mg, 0.228 mmol) was added and the closed scintillation vial was put to stir at 60 °C for 3h. The reaction mixture was then filtered over silica and dichloromethane (2 mL)

was used to wash the silica plug. The solution was subsequently concentrated on the rotary evaporator and pentane (5 mL) was added to crash out the product, which was collected by filtration. The final product was dried *in vacuo* and collected in 23% yield (19.2mg, 0.017 mmol).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92 (s, 2H, CH_{arom}), 6.87 (s, 2H, CH_{arom}) 6.12 (s, 2H, $CH_{backbone}$), 2.77 (s, 2H, NH), 2.45 (s, 6H, CH_3), 2.43 (s, 6H, CH_3) 1.75 (s, 12H, CH_3), 1.69 (s, 12H, CH_3), 1.14 (s, 18H, $CH_{3,\ t\text{-Bu}}$).

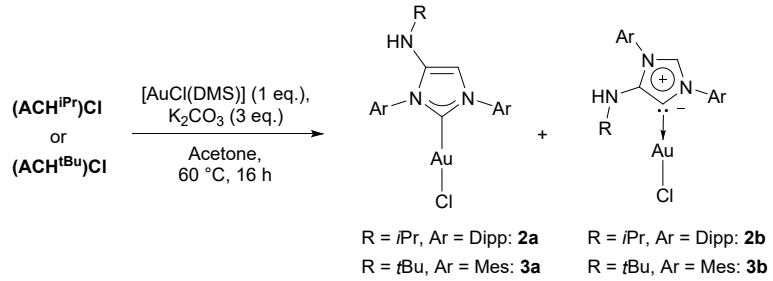
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 178.9 ($C_{q,\ carbene}$), 140.2 (C_qCH_3), 139.1 (C_qCH_3), 137.7 ($C_{q,\ backbone}$), 135.9 (C_qCH_3), 135.0 ($NC_{q,\ arom}$), 134.9 (C_qCH_3), 129.7 (CH_{arom}), 129.0 (CH_{arom}), 100.7 ($CH_{backbone}$), 51.8 ($C_{q,\ tBu}$), 28.9 ($CH_{3,\ tBu}$), 21.5 (CH_3), 21.4 (CH_3), 17.4 (CH_3), 17.1 (CH_3).

^{19}F NMR (376 MHz, $CDCl_3$) δ -78.03.

HRMS m/z calcd for $C_{50}H_{66}AuN_6^+$ $[M\text{-}OTf]^+$ 947.50; found 947.4988.

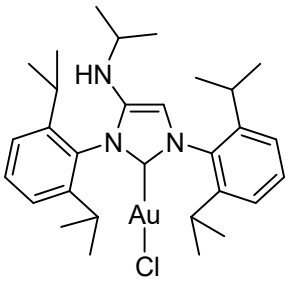
Synthesis of 2a and 3a from the NHC•HCl salts *via* the weak base route

After conversion of the precursors to $(ACH)^+Cl^-$ *via* anion exchange using the Amberlite® IRA402 chloride form of the resin, the same approach afforded the desired [AuCl(AC$^{i\text{-Pr}}$)] (**2a**) and [AuCl(AC$^{t\text{-Bu}}$)] (**3a**) (Scheme S1). However, in the reaction mixture the NMR clearly showed the presence of additional gold species (*ca*. 7% of total, assuming that the impurity is not a bis-NHC complex). This second species was assigned the structure of **3b**, where the ligand is coordinated to gold *via* the C5 instead of C2 position. Interestingly, an analogous regio-isomer (**2b**) was detected in the course of the synthesis of **2a**, but here both isomers appear in almost equal amounts. The assignments of the abnormal NHC coordinated structures are tentative, as they are only based on NMR data, and formation of bis-NHC species cannot be excluded.



Scheme S1. The weak base route from the AC•HCl salts using K_2CO_3 and [Au(DMS)Cl] lead to the desired [Au(AC)Cl] complexes, possibly as a mixture of isomers.

Synthesis of [Au(AC$^{i\text{-Pr}}$)Cl] (2a)



Inside a glovebox, a vial was charged with the ligand precursor AC$^{i\text{-Pr}}$•HOTf (50mg, 0.084 mmol) and the gold source [Au(DMS)Cl] (1 equiv., 28 mg, 0.084 mmol). THF (0.6 mL) was added to solubilize the

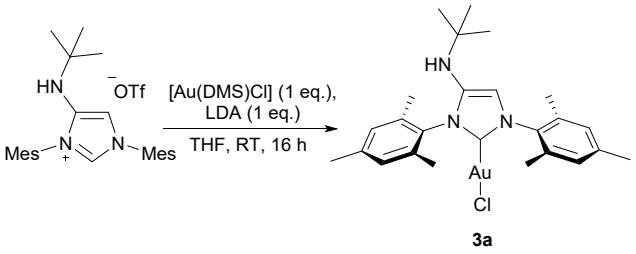
solids and the solution was put to stir. After 5 min, when everything was dissolved, solid LDA (1 equiv., 10.2 mg, 0.084 mmol) was added and the reaction was stirred for 16 h at room temperature. Afterwards, the solvent was removed in vacuo, the resulting product was dissolved in DCM (4 mL) and passed through a syringe filter. After removing the solvent in vacuo, an off-white product was obtained in 98% yield (55.7mg, 0.082 mmol).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (t, *J* = 7.8 Hz, 1H, $C_{Ar}H$), 7.45 (t, *J* = 7.8 Hz, 1H, $C_{Ar}H$), 7.31 (d, *J* = 7.8 Hz, 2H, $C_{Ar}H$), 7.25 (d, *J* = 7.8 Hz, 2H, $C_{Ar}H$), 6.19 (s, 1H, $CH_{backbone}$), 3.41 – 3.23 (m, 1H, NH), 2.76 – 2.66 (m, 3H, C*H*$(CH_3)_2$), 2.66 – 2.58 (m, 2H, C*H*$(CH_3)_2$), 1.38 (d, *J* = 6.5 Hz, 2H, CH_3), 1.34 (dd, *J* = 6.9, 1.3 Hz, 10H, CH_3), 1.23 (dd, *J* = 6.9, 6.1 Hz, 12H, CH_3), 1.14 (d, *J* = 6.3, 6H, CH_3).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 168.5 ($C_{q,\ carbene}$), 146.9 (CH_{arom}), 145.9 (CH_{arom}), 140.1 ($NC_{q,\ backbone}$), 135.0 (CH_{arom}), 131.3 ($NC_{q,\ arom}$), 130.4 ($NC_{q,\ arom}$), 129.7 (CH_{arom}), 124.9 ($C_{q,\ arom}$), 124.2 ($C_{q,\ arom}$), 99.89 ($CH_{backbone}$), 46.8 (N*C*H$(CH_3)_2$), 28.9 (*C*H$(CH_3)_2$), 28.8 (*C*H$(CH_3)_2$), 24.9 (CH_3), 24.6 (CH_3), 24.3 (CH_3), 23.8 (CH_3), 22.3 (CH_3).

HRMS m/z calcd for $C_{30}H_{47}AuClN_4^+$ $[M+NH_4]^+$ 695.3149; found 695.3148.

Synthesis of [Au(AC$^{t\text{-}Bu}$)Cl] (3a)



3a

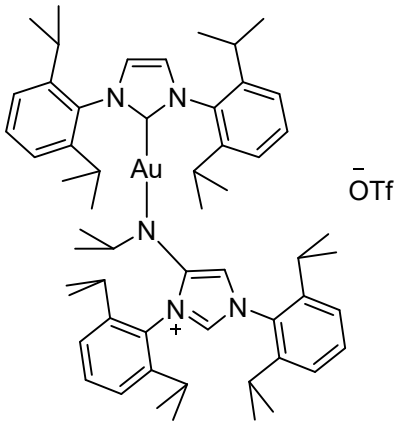
Inside a glovebox, a vial was charged with the ligand AC$^{t\text{-}Bu}$ •HOTf (50mg, 0.095 mmol) and the gold precursor [Au(DMS)Cl] (1 equiv., 28mg, 0.095 mmol). THF (0.6 mL) was added to solubilize the solids and the solution was put to stir. After 5 min, when everything was dissolved, solid LDA (1 equiv., 11.5 mg, 0.095 mmol) was added and the reaction was stirred for 16h at room temperature. Afterwards, the solvent was removed in vacuo, the resulting product was dissolved in DCM (4 mL) and passed through a syringe filter. After removing the solvent in vacuo, an off-white solid was obtained in 96% yield (55.4mg, 0.091 mmol). A mixture of complexes was obtained with **3a** as a primary component and the following assignments are provided, based on NMR data.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00-6.96 (overlapping singlets, 4H, CH_{arom}), 6.24 (s, 1H, $CH_{backbone}$), 2.84 (broad, 1H, NH), 2.34 (s, 3H, CH_3), 2.32 (s, 3H, CH_3), 2.16 (s, 6H, CH_3), 2.09 (s, 6H, CH_3), 1.21 (s, 9H, $CH_{3,tBu}$).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 165.8 ($C_{q,\ carbene}$), 140.4 (C_qCH_3), 139.4 (C_qCH_3), 137.2 ($C_{q,\ backbone}$), 136.1 (C_qCH_3), 135.1 (C_qCH_3), 130.2 ($NC_{q,\ arom}$), 130.1 (CH_{arom}), 129.4 (CH_{arom}), 129.1 ($NC_{q,\ arom}$), 100.5 ($CH_{backbone}$), 51.8 ($C_{q,\ tBu}$), 29.0 ($CH_{3,\ tBu}$), 21.4 (CH_3), 21.2 (CH_3), 18.0 (CH_3), 17.8 (CH_3).

HRMS m/z calcd for $C_{25}H_{37}AuClN_4^+$ $[M+NH_4]^+$ 625.2367; found 625.2355.

Synthesis of [Au(IPr)(AC$^{i\text{-Pr}}$)][OTf] (4)



Method 1: Inside a glovebox, IPrAuN(iPr)$_2$ (65.1mg, 0.09 mmol) and AC$^{i\text{-Pr}}$•HOTf (1 equiv., 50mg, 0.09 mmol) were stirred in 0.4 mL THF for 3h at room temperature. The solvent was subsequently removed and recrystallisation was performed in DCM/pentane. The crystalline product was filtered of and dried under vacuum, which afforded the off-white product in excellent yield (99%, 105.1mg, 0.089mmol).

Method 2: Inside a glovebox, a 20 mL scintillation vial was charged with AC$^{i\text{-Pr}}$•HOTf (25mg, 0.042 mmol), a stirring bar and THF (2mL). The mixture was put to stir at room temperature and the solid LDA (1.1 equiv., 4.9mg, 0.046 mmol) was added. After mixing for 10 minutes at room temperature, the [Au(IPr)Cl] (1 equiv., 26mg, 0.042 mmol) was added and the reaction was stirred for an additional 3h. Afterwards, the THF was removed *in vacuo* and the resulting solid was redissolved in dichloromethane (4 mL) and subsequently passed through a syringe filter. Removal of the solvent *in vacuo* afforded the final product in 93% yield (46.1mg, 0.039 mmol).

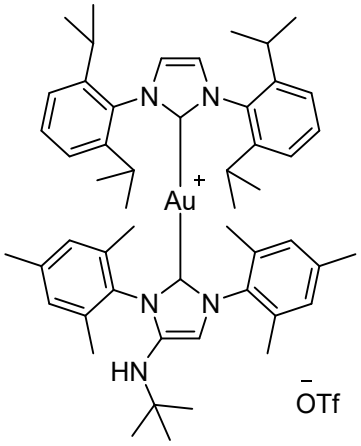
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (t, *J* = 7.8 Hz, 1H, CH_{arom}), 7.56 – 7.41 (m, 3H, CH_{arom}), 7.39 (d, *J* = 7.8 Hz, 1H, CH_{arom}), 7.32 (s, 1H, $CH_{backbone}$(IPr)), 7.30 – 7.27 (m, 1H, CH_{arom}), 7.23 (s, 1H, $CH_{backbone}$(IPr)), 7.21 (d, *J* = 3.7 Hz, 2H, $CH_{backbone+carbene}$(AC$^{i\text{-Pr}}$)), 7.19 – 6.97 (m, 6H, CH_{arom}), 2.50 (m, 7H, C*H*$(CH_3)_2$), 2.38 – 2.22 (m, 2H, C*H*$(CH_3)_2$), 1.41 – 0.95 (m, 45H, CH_3), 0.89 (d, J = 6.8 Hz, 2H, CH_3), 0.82 (m, 2H, CH_3), 0.58 (d, J = 6.3 Hz, 2H, CH_3), 0.39 (d, J = 6.2 Hz, 3H, CH_3).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 189.5 ($C_{q,\ carbene}$(IPr)), 177.3 ($C_{q,\ backbone}$(AC$^{i\text{-Pr}}$)), 146.1 ($C_{q,\ arom}$), 145.9 ($C_{q,\ arom}$), 145.7 ($C_{q,\ arom}$), 145.6 ($C_{q,\ arom}$), 145.3 ($C_{q,\ arom}$), 145.0 ($C_{q,\ arom}$), 144.6 ($C_{q,\ arom}$), 134.4 ($C_{q,\ arom}$), 134.3 ($C_{q,\ arom}$), 130.8 (CH_{arom}), 130.8 (CH_{arom}), 130.7 (CH_{arom}), 130.6 (CH_{arom}), 130.3 (CH_{arom}), 127.6 ($C_{q,\ arom}$), 125.0 ($CH_{backbone}$(IPr)), 125.0 ($CH_{backbone+carbene}$(AC$^{i\text{-Pr}}$)), 124.6 (CH_{arom}), 124.5 (CH_{arom}), 124.4 (CH_{arom}), 124.4 (CH_{arom}), 124.4 (CH_{arom}), 124.3 (CH_{arom}), 124.1 (CH_{arom}), 123.6 ($CH_{backbone}$(IPr)), 29.4 (***C***H$(CH_3)_2$), 29.2 (***C***H$(CH_3)_2$), 29.1 (***C***H$(CH_3)_2$), 28.9 (***C***H$(CH_3)_2$), 28.9 (***C***H$(CH_3)_2$), 28.8 (***C***H$(CH_3)_2$), 28.8 (***C***H$(CH_3)_2$), 28.7 (***C***H$(CH_3)_2$), 28.6 (***C***H$(CH_3)_2$), 26.1 (CH_3), 25.7 (CH_3), 25.4 (CH_3), 25.4 (CH_3), 25.0 (CH_3), 24.8 (CH_3), 24.6 (CH_3), 24.6 (CH_3), 24.5 (CH_3), 24.4 (CH_3), 24.3 (CH_3), 24.2 (CH_3), 24.2 (CH_3), 24.2 (CH_3), 23.9 (CH_3), 23.0 (CH_3), 22.7 (CH_3), 22.5 (CH_3).

^{19}F NMR (376 MHz, $CDCl_3$) δ -78.35.

Anal. Calcd for $C_{58}H_{79}AuF_3N_5O_3S$: C, 59.02; H, 6.75; N, 5.93. Found: C, 59.06; H, 6.86; N, 5.78.

Synthesis of [Au(IPr)(AC$^{t\text{-}Bu}$)][OTf] (5)



Inside a glovebox, IPrAuN(iPr)$_2$ (40mg, 0.06 mmol) and AC$^{t\text{-}Bu}$ •HOTf (1 equiv., 30.7mg, 0.06 mmol) were stirred in 0.35 mL THF for 3h at room temperature. The solvent was subsequently removed, which afforded the off-white product in excellent yield (99%, 65.9mg, 0.059mmol).

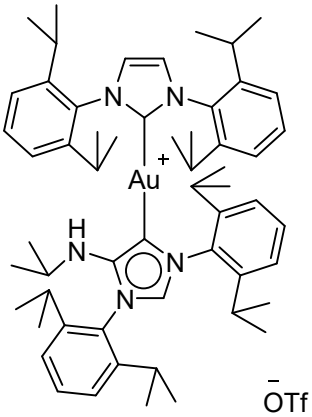
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (t, *J* = 7.8 Hz, 2H, CH_{arom}(IPr)), 7.21 (s, 2H, $CH_{backbone}$(IPr)), 7.14 (d, *J* = 7.8 Hz, 4H, CH_{arom}(IPr)), 6.82 (s, 2H, CH_{arom}(AC$^{t\text{-}Bu}$)), 6.76 (s, 2H, CH_{arom}(AC$^{t\text{-}Bu}$)), 6.03 (s, 1H, $CH_{backbone}$(AC$^{t\text{-}Bu}$)), 2.39 (d, *J* = 9.9 Hz, 6H, $CH_{3,\ arom}$(AC$^{t\text{-}Bu}$)), 2.32 – 2.20 (m, 4H, C*H*$(CH_3)_2$), 1.73 (s, 6H, $CH_{3,\ arom}$(AC$^{t\text{-}Bu}$)), 1.67 (s, 6H, $CH_{3,\ arom}$(AC$^{t\text{-}Bu}$)), 1.11 (d, *J* = 6.9 Hz, 12H, CH(C*H*$_3)_2$), 1.09 (s, 9H, CH_3(*t*-Bu)), 0.86 (d, *J* = 6.9 Hz, 12H, CH(C*H*$_3)_2$).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 186.8 ($C_{q,\ carbene}$(IPr)), 176.5 ($C_{q,\ carbene}$(AC$^{t\text{-}Bu}$)), 145.3 ($C_{q,\ arom}$(IPr)), 140.1 ($C_{q,\ arom}$(AC$^{t\text{-}Bu}$)), 139.0 ($C_{q,\ arom}$(AC$^{t\text{-}Bu}$)), 137.8 ($C_{q,\ backbone}$(AC$^{t\text{-}Bu}$)), 135.5 ($C_{q,\ arom}$(AC$^{t\text{-}Bu}$)), 134.5 ($NC_{q,\ arom}$(AC$^{t\text{-}Bu}$)), 133.7 (NC_q(IPr)), 130.7 (CH_{arom}(IPr)), 130.4 (CH_{arom}(AC$^{t\text{-}Bu}$)), 129.6 (CH_{arom}(AC$^{t\text{-}Bu}$)), 124.2 ($CH_{backbone}$(IPr)), 124.0 (CH_{arom}(IPr)), 101.2 ($CH_{backbone}$(AC$^{t\text{-}Bu}$)), 51.7 ($C_{q,\ t\text{-}Bu}$(AC$^{t\text{-}Bu}$)), 28.7 (CH_3(*t*-Bu)), 28.6 (C*H*$(CH_3)_2$), 24.1 (CH(C*H*$_3)_2$), 23.9 (CH(C*H*$_3)_2$), 21.5 ($CH_{3,\ arom}$(AC$^{t\text{-}Bu}$)), 21.3 ($CH_{3,\ arom}$(AC$^{t\text{-}Bu}$)), 17.4 ($CH_{3,\ arom}$(AC$^{t\text{-}Bu}$)), 17.1 ($CH_{3,\ arom}$(AC$^{t\text{-}Bu}$)).

^{19}F NMR (376 MHz, $CDCl_3$) δ -78.10.

Anal. Calcd for $C_{53}H_{69}AuF_3N_5O_3S$: C, 57.34; H, 6.26; N, 6.31. Found: C, 57.38; H, 6.26; N, 6.29.

Synthesis of [Au(IPr)(AC$^{i\text{-}Pr}$)][OTf] (6)



The [Au(IPr)(AC$^{i\text{-}Pr}$)][OTf] (20mg, 0.017 mmol) was dissolved in 0.2 mL benzene and heated for 4h at 80 °C. Subsequently, the solvent was removed *in vacuo* and recrystallisation was performed in

DCM/pentane. The crystalline product was filtered of and dried under vacuum, which afforded the off-white product in excellent yield (99%, 19.8mg, 0.0168 mmol).

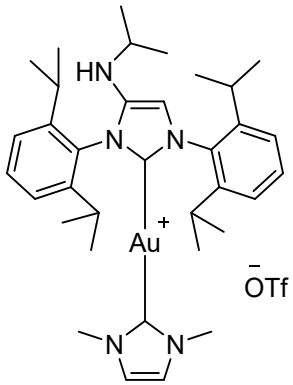
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.26 (m, 3H), 7.25 – 6.91 (m, 12H), 2.51 – 2.31 (m, 6H), 2.30 – 2.13 (m, 3H), 1.24 (d, *J* = 6.9 Hz, 6H), 1.24 – 1.14 (m, 9H), 1.16 – 1.08 (m, 12H), 1.07 (d, *J* = 6.9 Hz, 6H), 1.02 (d, *J* = 6.8 Hz, 6H), 0.98 – 0.91 (d, *J* = 6.9 Hz, 6H), 0.90 (d, *J* = 6.9 Hz, 3H), 0.80 (d, *J* = 6.8 Hz, 3H), 0.48 (d, *J* = 6.3 Hz, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 189.5 ($C_{q,\ carbene}$(IPr)), 150.8 ($C_{q,\ arom}$), 146.2 ($C_{q,\ arom}$), 146.2 ($C_{q,\ arom}$), 146.1 ($C_{q,\ arom}$), 145.9 ($C_{q,\ arom}$), 145.7 ($C_{q,\ arom}$), 145.6 ($C_{q,\ arom}$), 145.2 ($C_{q,\ arom}$), 145.0($C_{q,\ arom}$), 144.6 ($C_{q,\ arom}$), 134.4 ($C_{q,\ arom}$), 132.0 (C_q(AC$^{i\text{-Pr}}$), 130.8 (CH_{arom}), 130.8 (CH_{arom}), 130.7 (CH_{arom}), 130.3 (CH_{arom}), 128.5 (CH_{arom}), 127.6 (N**C**$_q$(AC$^{i\text{-Pr}}$), 125.5 (CH_{arom}), 125.0 (CH_{arom}), 125.0 (CH_{arom}), 124.7 (CH_{arom}), 124.5 (CH_{arom}), 124.4 (CH_{arom}), 124.4 (CH_{arom}), 124.3 (CH_{arom}), 124.1 (CH_{arom}), 123.2 (CH_{arom}), 28.9 (***C***H(CH_3)$_2$), 28.8 (***C***H(CH_3)$_2$), 28.6 (*C*H(CH_3)$_2$), 25.4 (CH_3), 25.0 (CH_3), 24.7 (CH_3), 24.6 (CH_3), 24.5 (CH_3), 24.2 (CH_3), 24.2 (CH_3), 24.1 (CH_3), 23.5 (CH_3), 23.0 (CH_3), 22.5 (CH_3), 22.1 (CH_3).

^{19}F NMR (471 MHz, $CDCl_3$) δ -78.01.

Anal. Calcd for $C_{58}H_{79}AuF_3N_5O_3S$: C, 59.02; H, 6.75; N, 5.93. Found: C, 59.21; H, 6.69; N, 5.50.

Synthesis of [Au(IMe)(AC$^{i\text{-Pr}}$)][OTf] (7)



Inside a glovebox, a 20 mL scintillation vial was charged with AC$^{i\text{-Pr}}$•HOTf (54.4mg, 0.091 mmol), a stirring bar and THF (4mL). The mixture was put to stir at room temperature and the solid LDA (1.1 equiv., 10.8mg, 0.100 mmol) was added. After mixing for 10 minutes at room temperature, the [Au(IMe)Cl] (1 equiv., 30mg, 0.091 mmol) was added and the reaction was stirred for an additional 3h. Afterwards, the THF was removed *in vacuo* and the resulting solid was redissolved in dichloromethane (6 mL) and subsequently passed through a syringe filter. Removal of the solvent *in vacuo* afforded the final product in 97% yield (79mg, 0.0889 mmol).

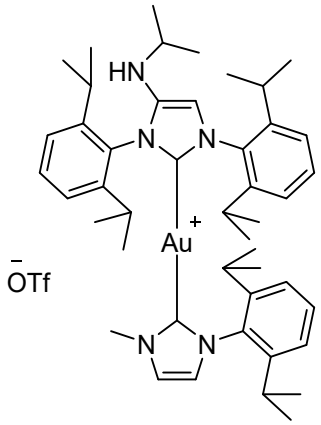
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (t, J = 7.8 Hz, 1H, CH_{arom}), 7.50 (t, J = 7.8 Hz, 1H, CH_{arom}), 7.37 (d, J = 7.9 Hz, 2H, CH_{arom}), 7.30 (d, J = 7.8 Hz, 2H, CH_{arom}), 7.05 (s, 2H, $CH_{backbone}$), 6.34 (s, 1H, $CH_{backbone}$), 3.38 (m, 1H, NC*H*(CH_3)$_2$), 3.16 (s, 6H, CH_3), 2.91 (d, J = 7.7 Hz, 1H, NH), 2.68 (m, 2H, C*H*(CH_3)$_2$), 2.60 (m, 2H, C*H*(CH_3)$_2$), 1.35 – 1.23 (m, 24H, CH_3), 1.19 (d, J = 6.3 Hz, 6H, CH_3).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 182.6 ($C_{q,\ carbene}$), 181.9 ($C_{q,\ carbene}$), 147.2 ($C_{q,\ arom}$), 146.1 ($C_{q,\ arom}$), 141.0 ($C_{q,\ backbone}$), 134.5 ($C_{q,\ arom}$), 131.7 (CH_{arom}), 130.7 (CH_{arom}), 129.3 ($C_{q,\ arom}$), 124.9 (CH_{arom}), 124.2 (CH_{arom}), 123.2 (CH_{arom}), 100.5 (CH_{arom}), 47.0 (N*C*H(CH_3)$_2$), 37.0 (CH_3), 29.0 (*C*H(CH_3)$_2$), 28.9 (*C*H(CH_3)$_2$), 25.0 (CH_3), 24.7 (CH_3), 24.3 (CH_3), 23.8 (CH_3), 22.4 (CH_3).

^{19}F NMR (376 MHz, $CDCl_3$) δ -78.21.

HRMS m/z calcd for $C_{35}H_{51}AuN_5^+$ [M-OTf]$^+$ 738.38; found 738.3801.

Synthesis of [Au(MeImDipp)(AC$^{i\text{-}Pr}$)][OTf] (8)



Inside a glovebox, a 20 mL scintillation vial was charged with AC$^{i\text{-}Pr}$•HOTf (50.2mg, 0.084 mmol), a stirring bar and THF (4 mL). The mixture was put to stir at room temperature and the solid LDA (1.1 equiv., 9.9mg, 0.093 mmol) was added. After mixing for 10 minutes at room temperature, the [Au(MeImDipp)Cl] (1 equiv., 40mg, 0.084 mmol) was added and the reaction was stirred for an additional 3h. Afterwards, the THF was removed *in vacuo* and the resulting solid was redissolved in dichloromethane (6 mL) and subsequently passed through a syringe filter. Removal of the solvent *in vacuo* afforded the final product in 98% yield (85.1mg, 0.0823 mmol).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 1.8 Hz, 1H, $CH_{backbone\ MeImDipp}$), 7.55 (t, J = 7.8 Hz, 1H, CH_{arom}), 7.45 (t, J = 7.8 Hz, 1H, CH_{arom}), 7.33 (t, J = 7.8 Hz, 1H, CH_{arom}), 7.28 (d, J = 7.8 Hz, 2H, CH_{arom}), 7.18 (d, J = 7.8 Hz, 2H, CH_{arom}), 6.99 (d, J = 7.8 Hz, 2H, CH_{arom}), 6.71 (d, J = 1.8 Hz, 1H, $CH_{backbone\ MeImDipp}$), 6.20 (s, 1H, $CH_{backbone\ AC}$), 3.33 (s, 3H, $CH_{3,\ MeImDipp}$), 3.32 – 3.24 (m, 1H, NCH), 2.77 (d, J = 7.6 Hz, 1H, NH), 2.51 (m, 4H, CH), 2.02 (h, J = 6.9 Hz, 2H, CH), 1.18 (dd, J = 6.9, 2.5 Hz, 12H, CH_3), 1.13 (d, J = 6.3 Hz, 6H, CH_3), 1.06 (dd, J = 7.8, 6.9 Hz, 12H, CH_3), 0.91 (d, J = 6.9 Hz, 6H, CH_3), 0.70 (d, J = 6.9 Hz, 6H, CH_3).

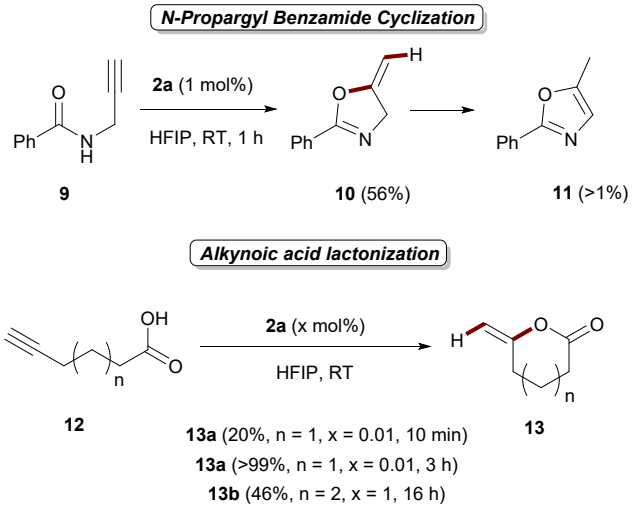
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 183.5 ($C_{q,\ carbene\ MeImDipp}$), 180.8 ($C_{q,\ carbene\ AC}$), 146.7 ($C_{q,\ arom\ MeImDipp}$), 145.7 ($C_{q,\ arom\ AC}$), 145.6 ($C_{q,\ arom\ AC}$), 140.8 ($C_{q,\ backbone\ AC}$), 134.5 ($C_{q,\ arom\ AC}$), 134.1 ($C_{q,\ arom\ MelùmDipp}$), 131.6 ($CH_{arom}$), 130.6 ($CH_{arom}$), 130.1 ($CH_{arom}$), 129.4 ($C_{q,\ arom\ AC}$), 125.0 ($CH_{arom}$), 124.3 ($CH_{backbone\ MeImDipp}$), 124.2 ($CH_{arom}$), 123.9 ($CH_{arom}$), 122.8 ($CH_{backbone\ MeImDipp}$), 100.8 (, $CH_{backbone\ AC}$), 46.9 (N*C*H$_{AC}$), 37.8 ($CH_{3,\ MeImDipp}$), 28.9 (CH_{AC}), 28.7 (CH_{AC}), 28.0 ($CH_{MeImDipp}$), 24.8 (CH_3), 24.7 (CH_3), 24.6 (CH_3), 24.5 (CH_3), 24.0 (CH_3), 23.8 (CH_3), 22.3 (CH_3).

^{19}F NMR (376 MHz, $CDCl_3$) δ -78.16.

HRMS m/z calcd for $C_{46}H_{65}AuN_5^+$ [M-OTf]$^+$ 884.4900; found 884.4901.

Catalysis with complex 2a

With complex **2a** in hand, we thought it would be informative to test its catalytic activity in two benchmark reactions and compare to that of [AuCl(IPr)] (Scheme S2). The catalytic system chosen for this purpose was recently reported,[3b] and does not require activation or further functionalization of the gold-chloride bond. This novel complex exhibited slightly higher catalytic activity than [AuCl(IPr)] in propargylamide cyclization (50% yield is reached when [AuCl(IPr)] is used under identical conditions). Backbone substitution on the NHC is not expected to be beneficial in this case, according to the reported data, however the isopropylamine moiety is expected to affect both the steric and electronic properties of the complex. In the case of lactonization, the catalyst led to complete conversion of 5-hexynoic acid after 3 hours (99% yield is reached when [AuCl(IPr)] is used at 0.01 mol% loading for 10 minutes of reaction time under identical conditions), while it only led to 46% yield after 16 hours when a 7-membered ring-closure was attempted (88% yield is reached when [AuCl(IPr)] is used under identical conditions). [AuCl(IPr)] is the best-performing catalyst in this case, and this may be because of a negative effect of the amine moiety on the backbone**,** which can react with the carboxylic acid group, leading to species which do not form when simpler NHCs are examined.



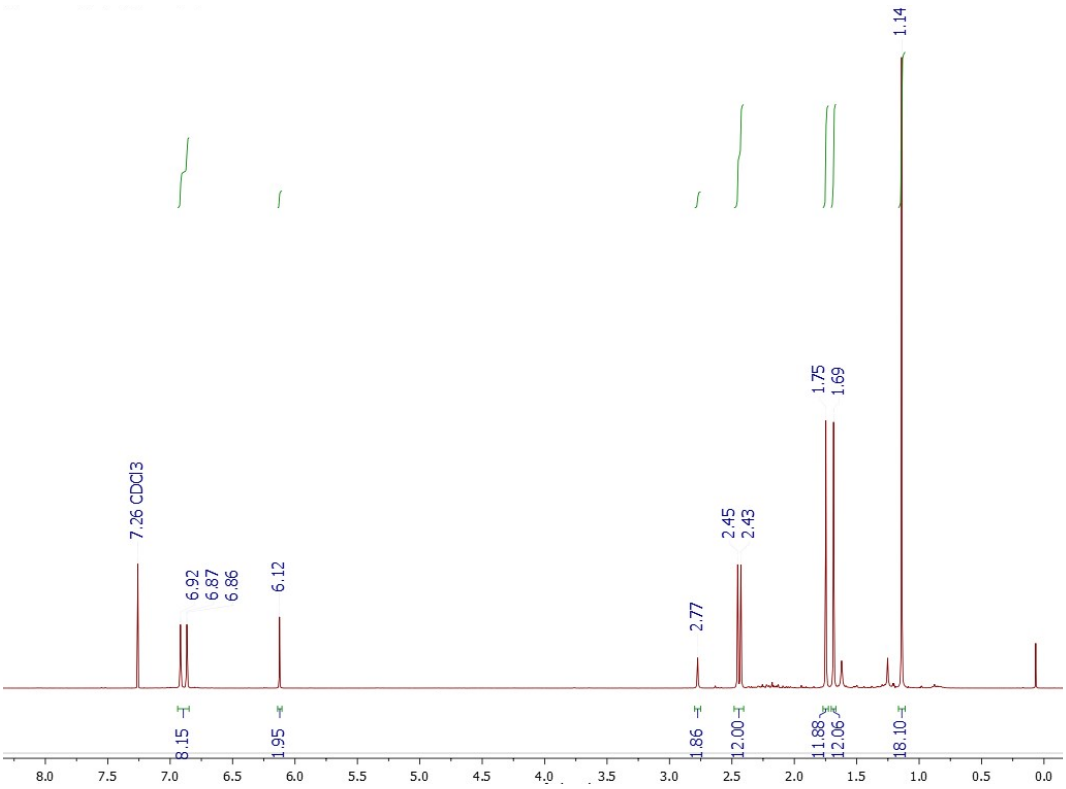
Scheme S2. 2a as a catalyst in propargylamide cyclization and alkynoic acid lactonization. Conditions: 0.5 mmol of substrate, 0.250 mL hexafluoroisopropanol (HFIP), yield determined by ^{1}H-NMR using 1, 3, 5-trimethoxybenzene as internal standard according to the reported procedures.[3b]

Computational details

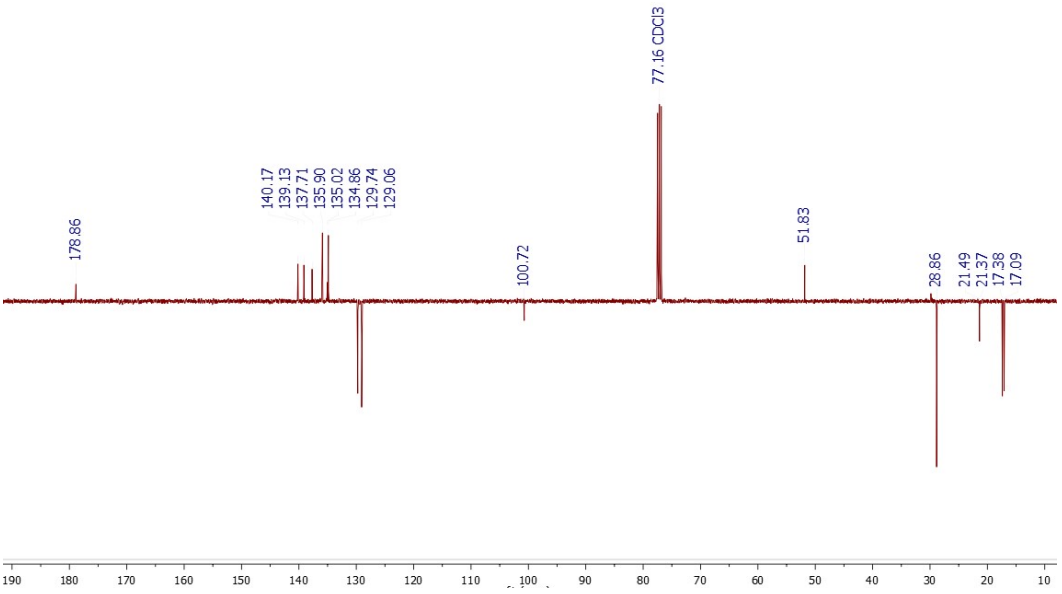
Full geometry optimizations were performed at the generalized-gradient approximation (GGA) hybrid PBE functional[4] in Gaussian 16[5] Numerical integrations were performed with an ultrafine grid. For geometry optimizations, the SVP[6] basis set was used for non-metal atoms and the SDD[i] pseudopotential and its associated double-ζ basis set was employed for Au. Optimizations were performed in gas phase. The natures of all stationary points were determined by calculation of the analytical vibrational frequencies. These were also used to compute the molecular partition functions (298 K, 1 atm) with the conventional particle-in-a-box, rigid-rotator, quantum-mechanical harmonic oscillator approximation, except that all vibrational frequencies below 50 cm^{-1} were replaced with values of 50 cm^{-1} (the quasi-harmonic-oscillator approximation). Single point energy calculations were carried out at M06[7] level of theory using TZVP[6] and SMD[8] solvation model with solvent parameters of THF (ε = 7.6). The ΔG value was obtained by augmenting the electronic energies at M06(SMD-THF)/TZVP with the respective free energy corrections at the PBE/SVP level.

NMR spectra

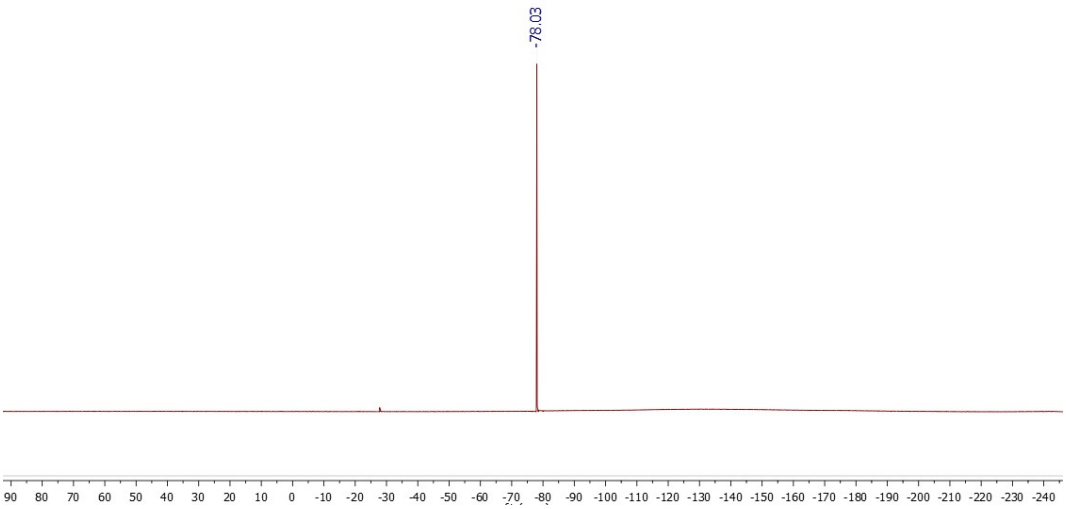
^{1}H NMR (400 MHz, Chloroform-d) of [Au(AC$^{t\text{-}Bu}$)$_2$][OTf] (1)



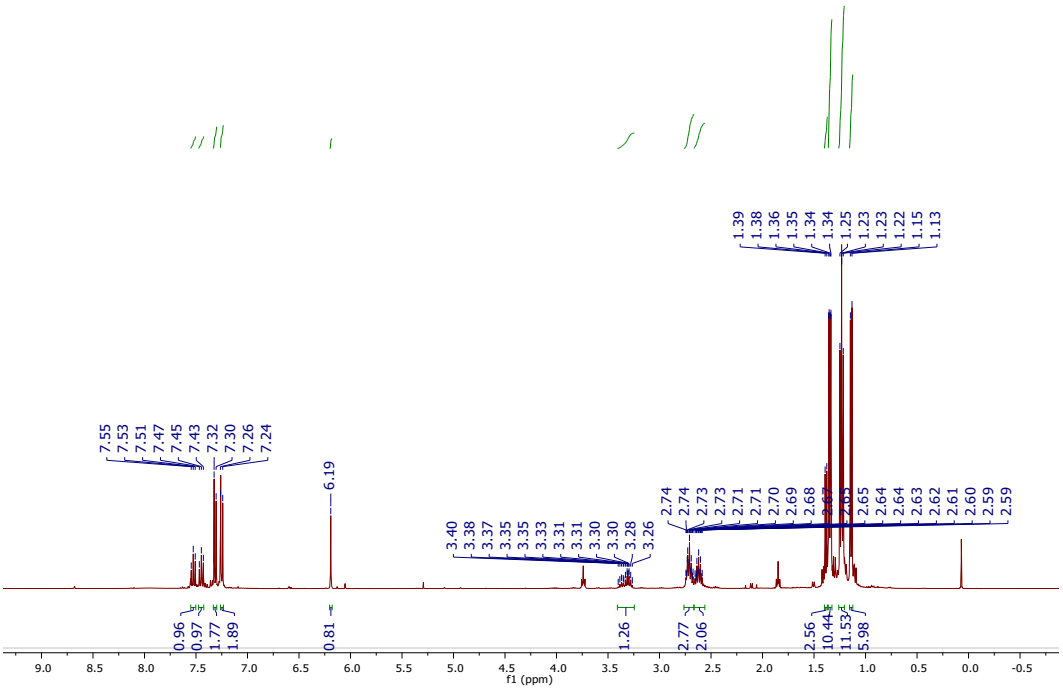
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) of [Au(AC$^{t\text{-}Bu}$)$_2$][OTf] (1)



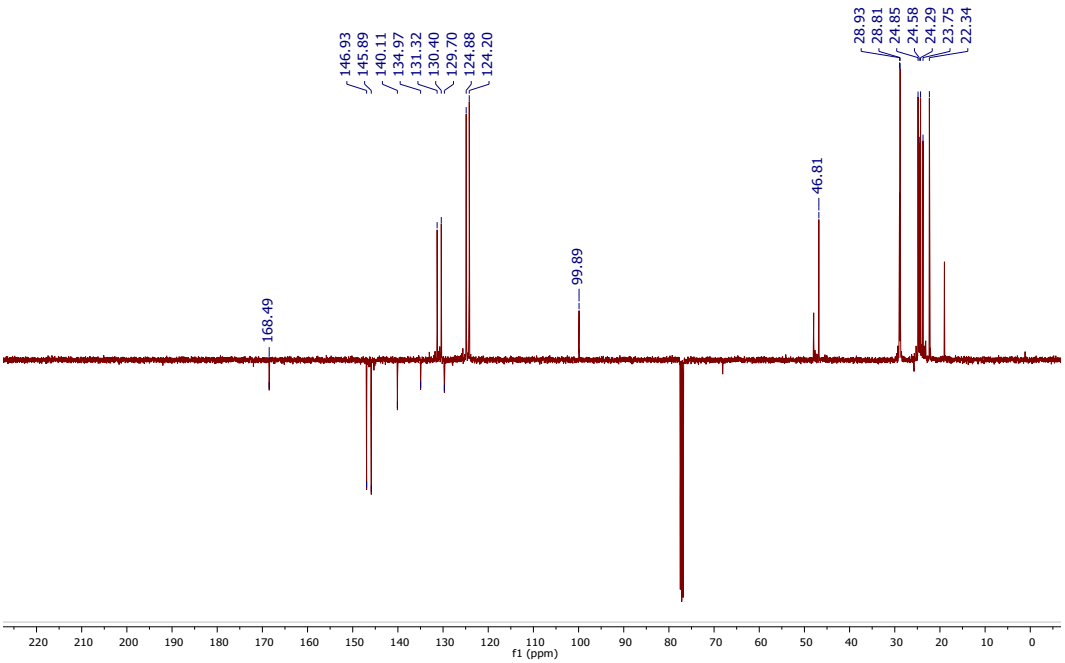
^{19}F NMR (376 MHz, Chloroform-*d*) of [Au(AC$^{t\text{-}Bu}$)$_2$][OTf] (1)



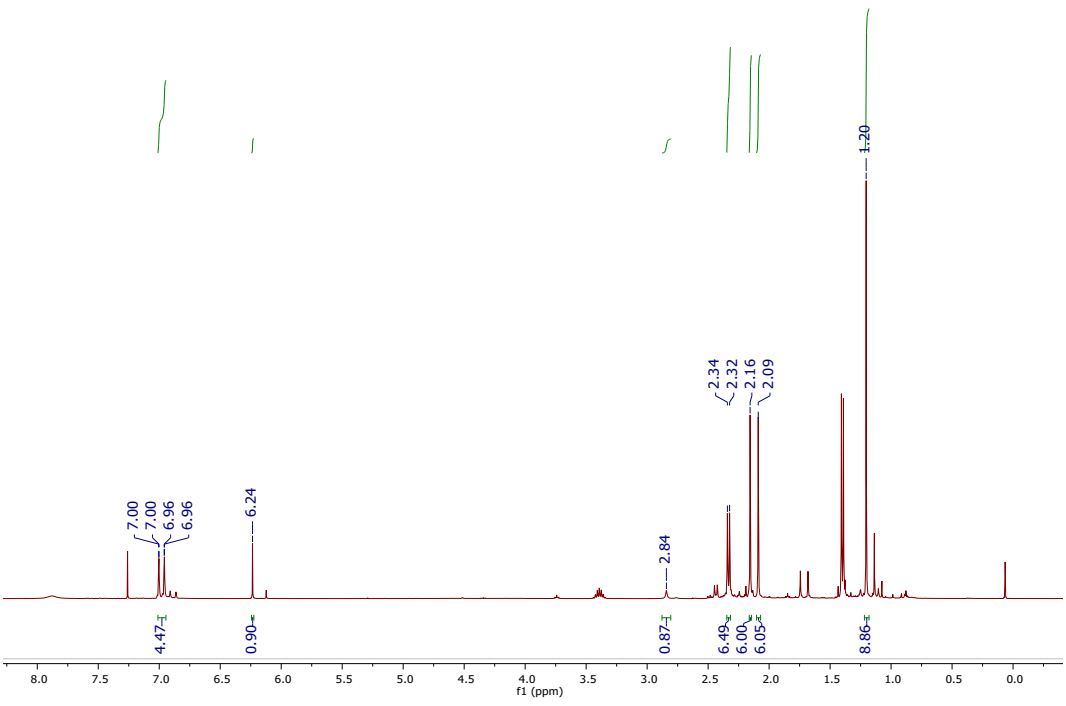
^{1}H NMR (400 MHz, Chloroform-d) of [Au(AC$^{i\text{-Pr}}$)Cl] (2a)



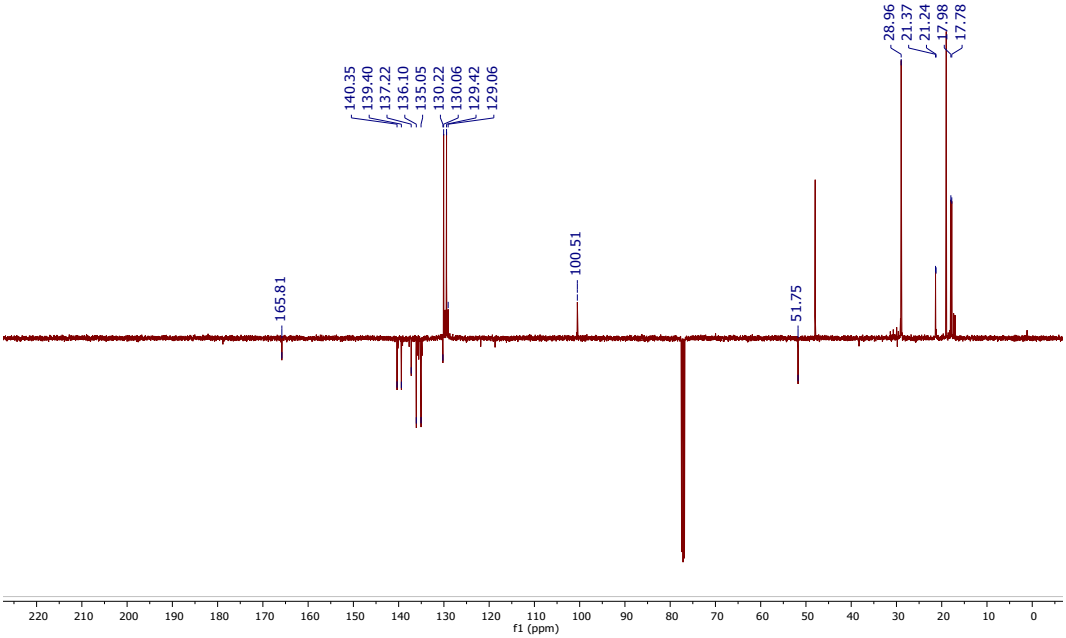
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) of [Au(AC$^{i\text{-Pr}}$)Cl] (2a)



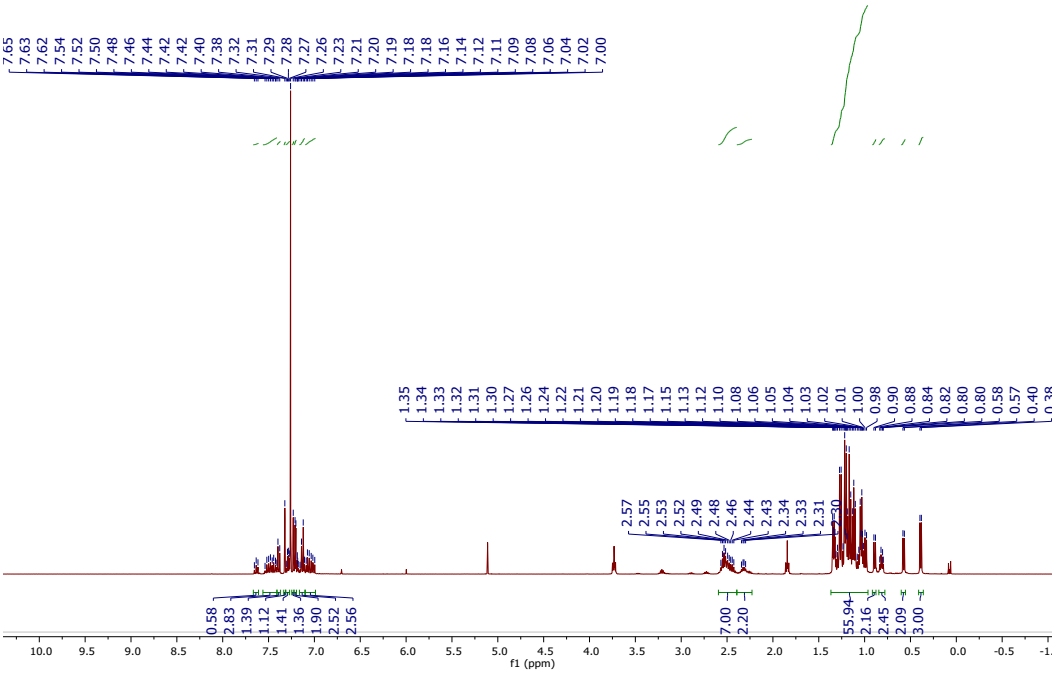
^{1}H NMR (400 MHz, Chloroform-d) of [Au(AC$^{t\text{-}Bu}$)Cl] (3a)



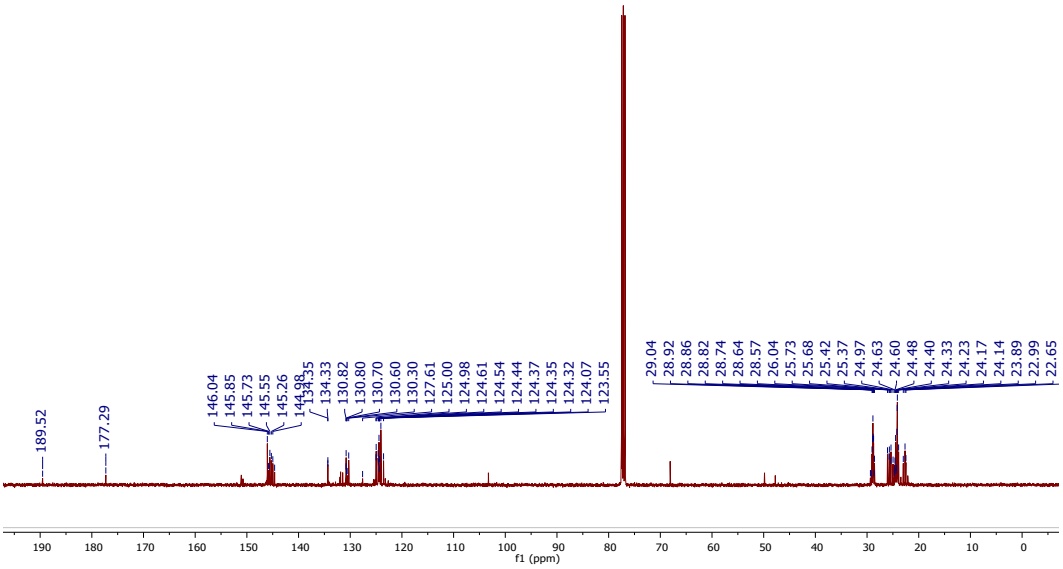
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) of [Au(AC$^{t\text{-}Bu}$)Cl] (3a)



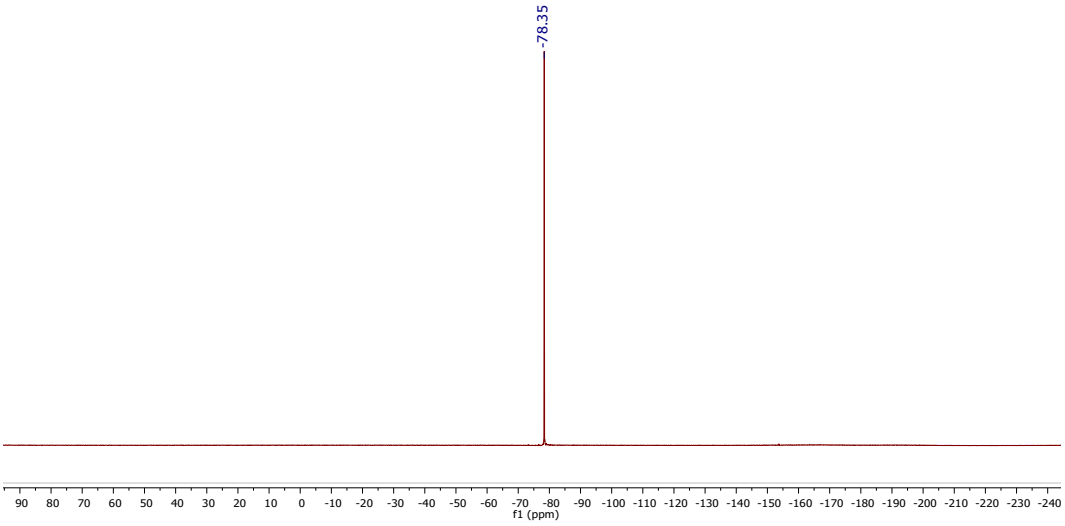
^{1}H NMR (400 MHz, Chloroform-d) of [Au(IPr)(AC$^{i\text{-Pr}}$)][OTf] (4)



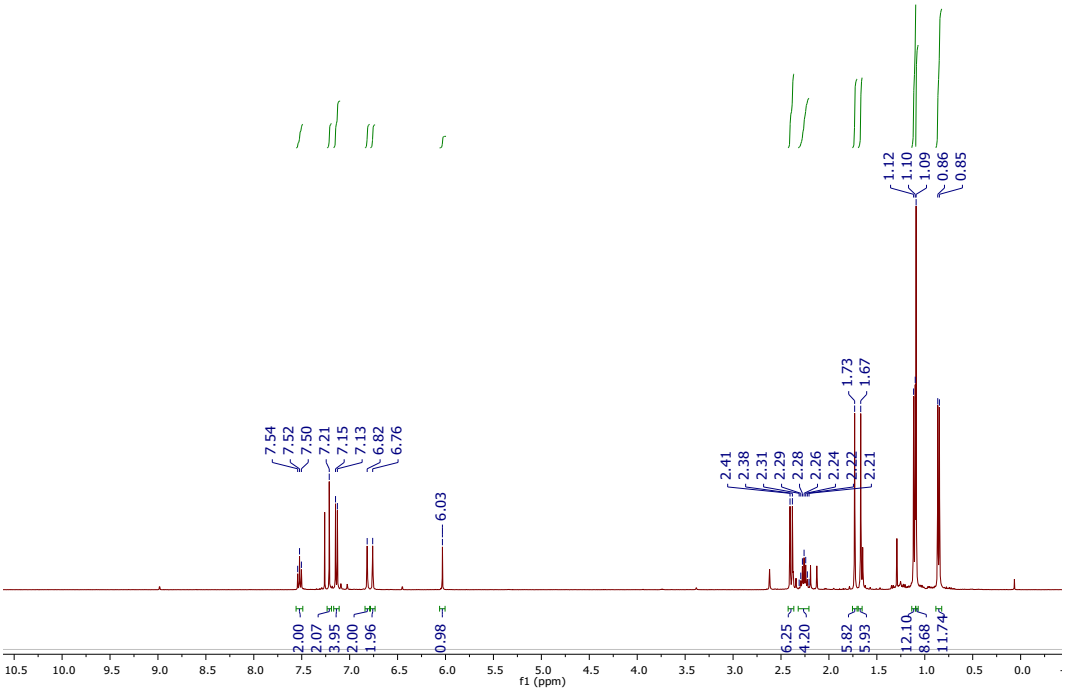
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) of [Au(IPr)(AC$^{i\text{-Pr}}$)][OTf] (4)



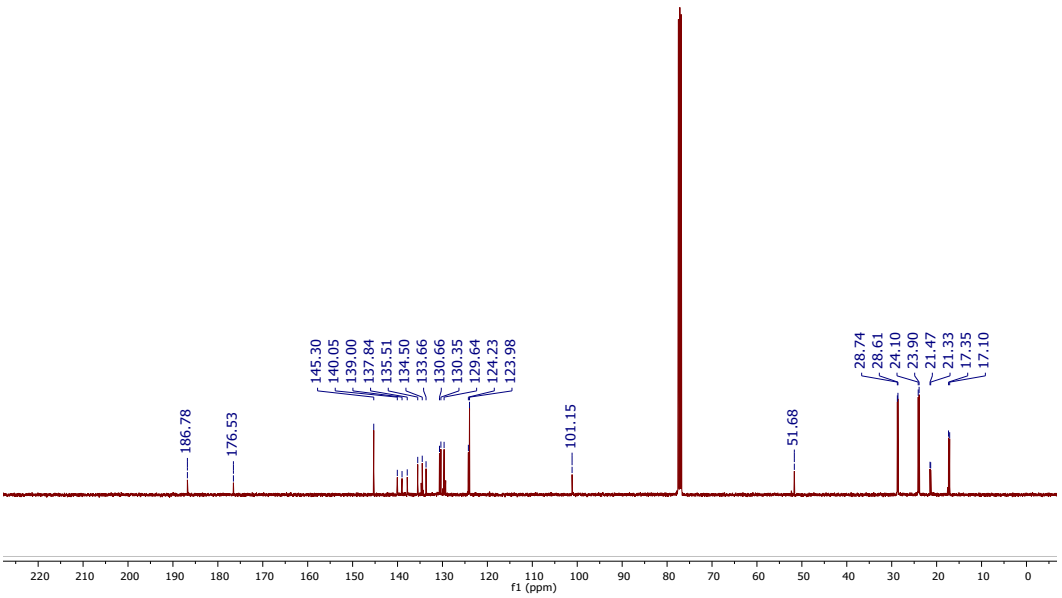
^{19}F NMR (376 MHz, Chloroform-*d*) of [Au(IPr)(AC$^{i\text{-Pr}}$)][OTf] (4)



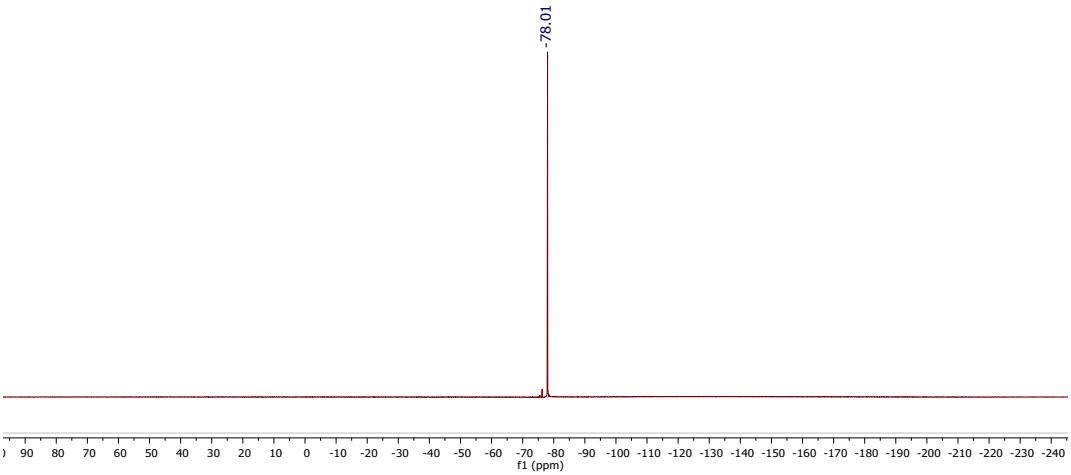
^{1}H NMR (400 MHz, Chloroform-d) of [Au(IPr)(AC$^{t\text{-Bu}}$)][OTf] (5)



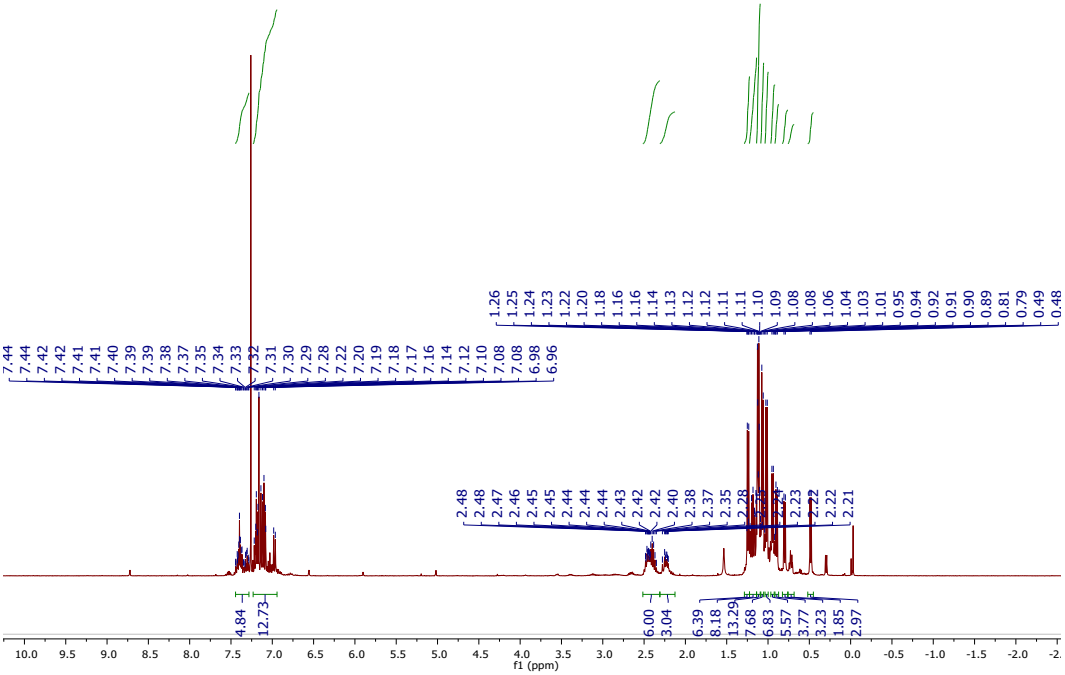
$^{13}C\{^{1}H\}$ NMR (101 MHz, Chloroform-*d*) of [Au(IPr)(AC$^{t\text{-}Bu}$)][OTf] (5)



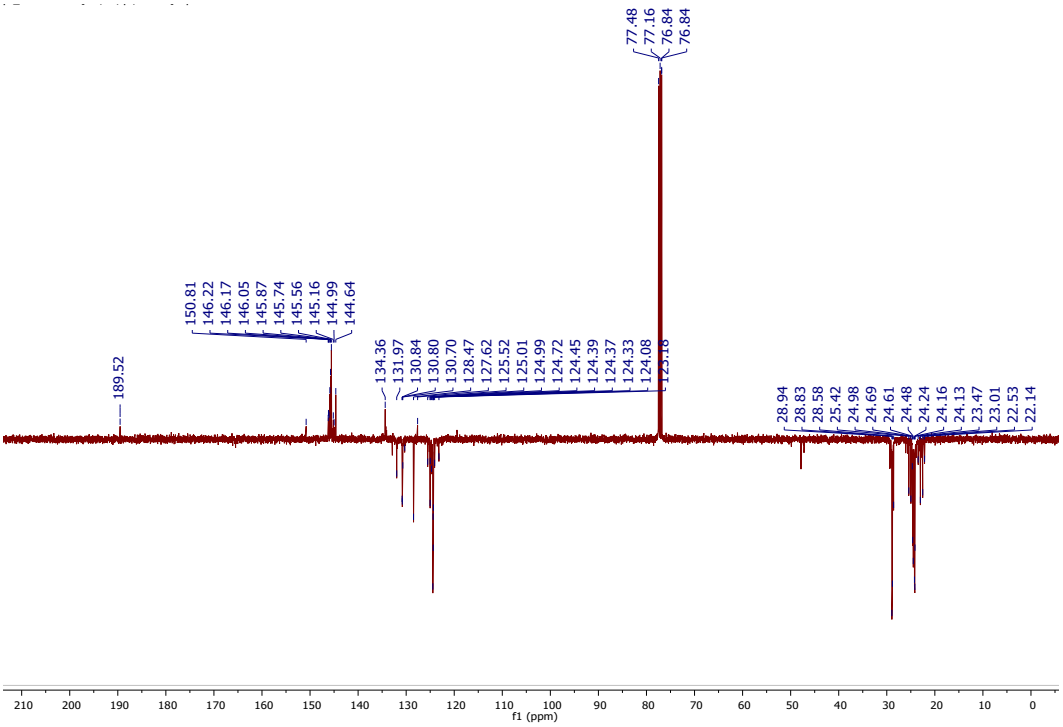
^{19}F NMR (376 MHz, Chloroform-*d*) of [Au(IPr)(AC$^{t\text{-}Bu}$)][OTf] (5)



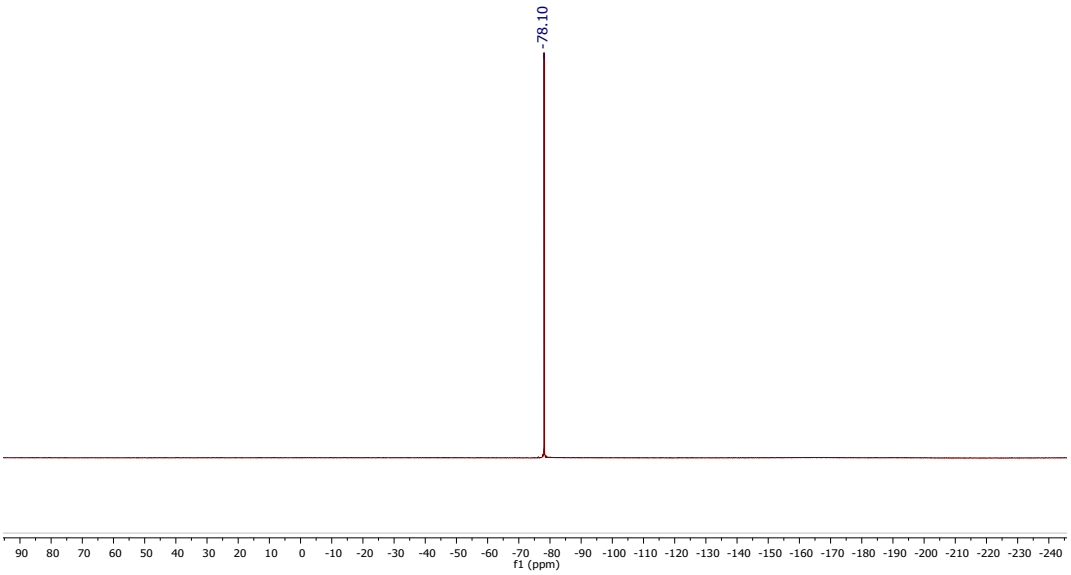
^{1}H NMR (400 MHz, Chloroform-d) of [Au(IPr)(AC$^{i\text{-Pr}}$)][OTf] (6)



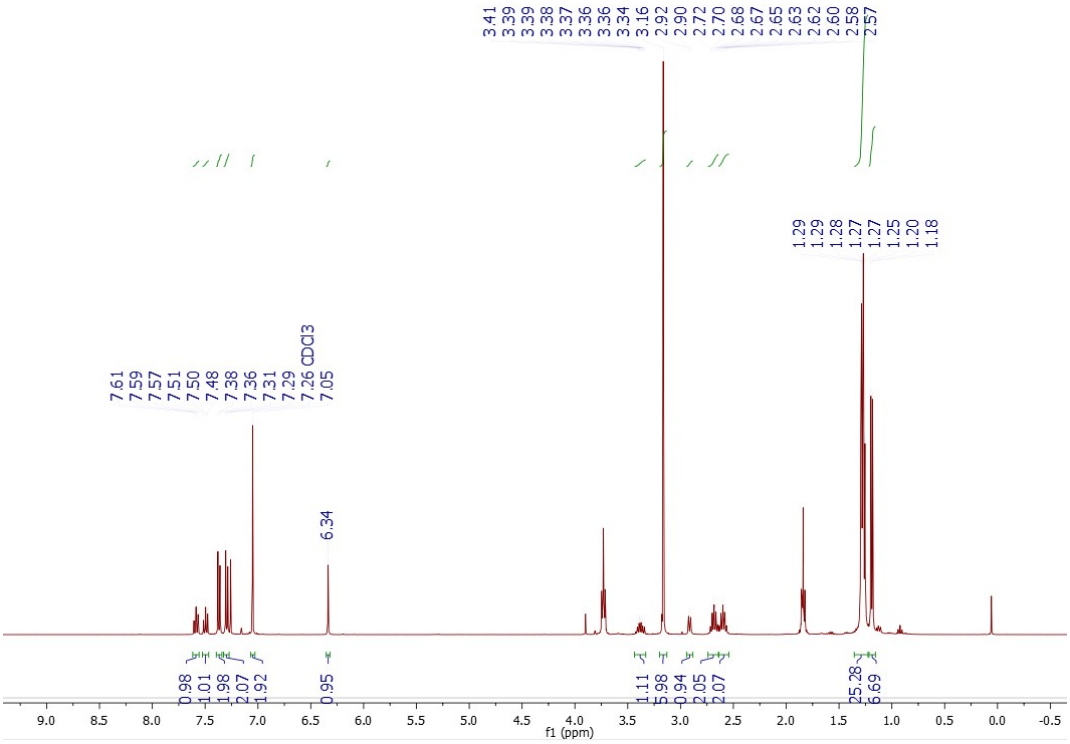
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) of [Au(IPr)(AC$^{i\text{-Pr}}$)][OTf] (6)



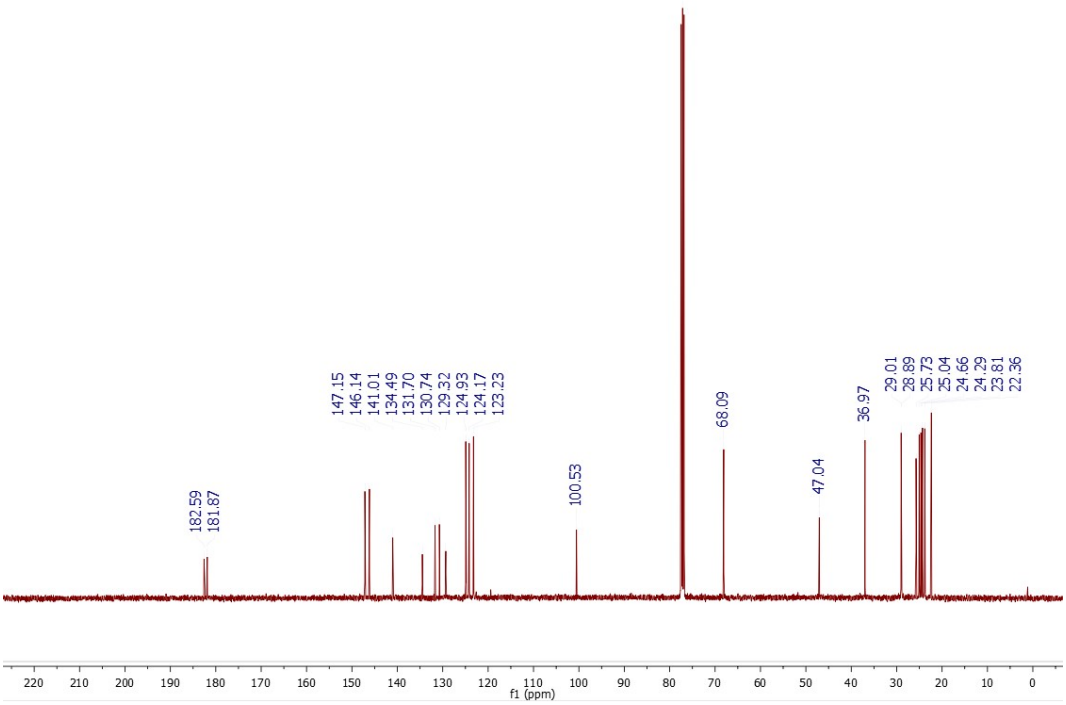
^{19}F NMR (471 MHz, Chloroform-*d*) of [Au(IPr)(AC$^{i\text{-Pr}}$)][OTf] (6)



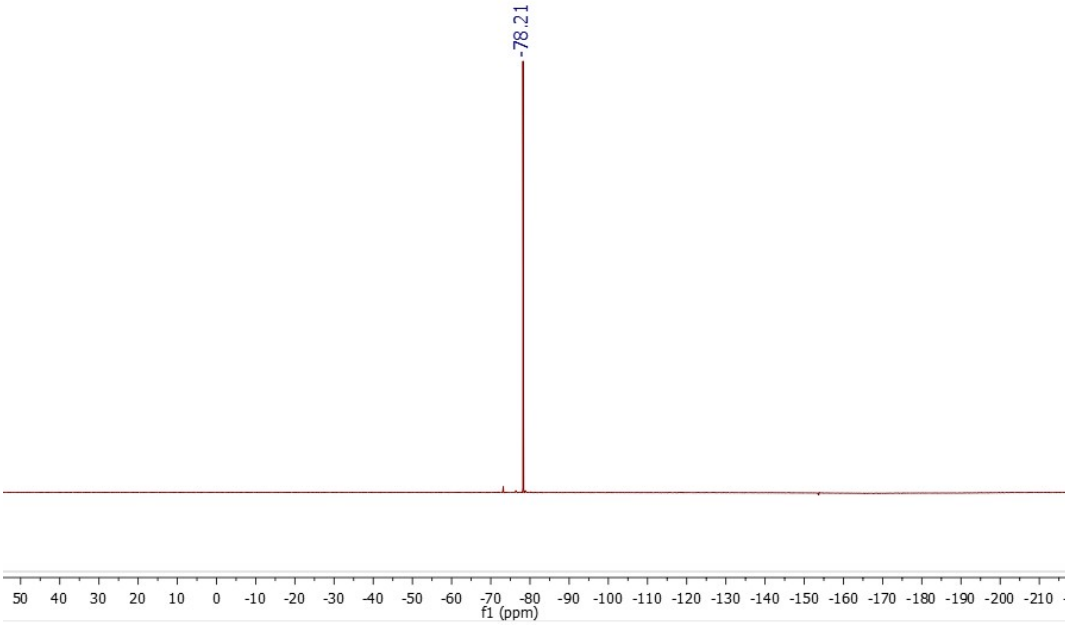
^{1}H NMR (400 MHz, Chloroform-d) of [Au(IMe)(AC$^{i\text{-Pr}}$)][OTf] (7)



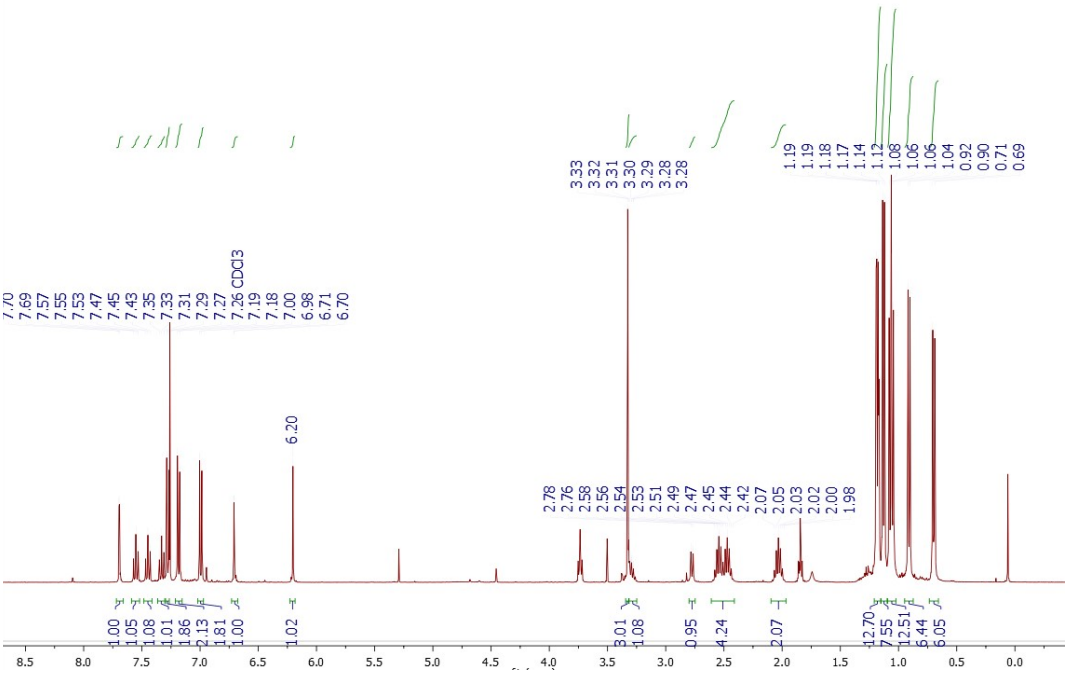
$^{13}C\{^{1}H\}$ NMR (101 MHz, Chloroform-*d*) of [Au(IMe)(AC$^{i\text{-}Pr}$)][OTf] (7)



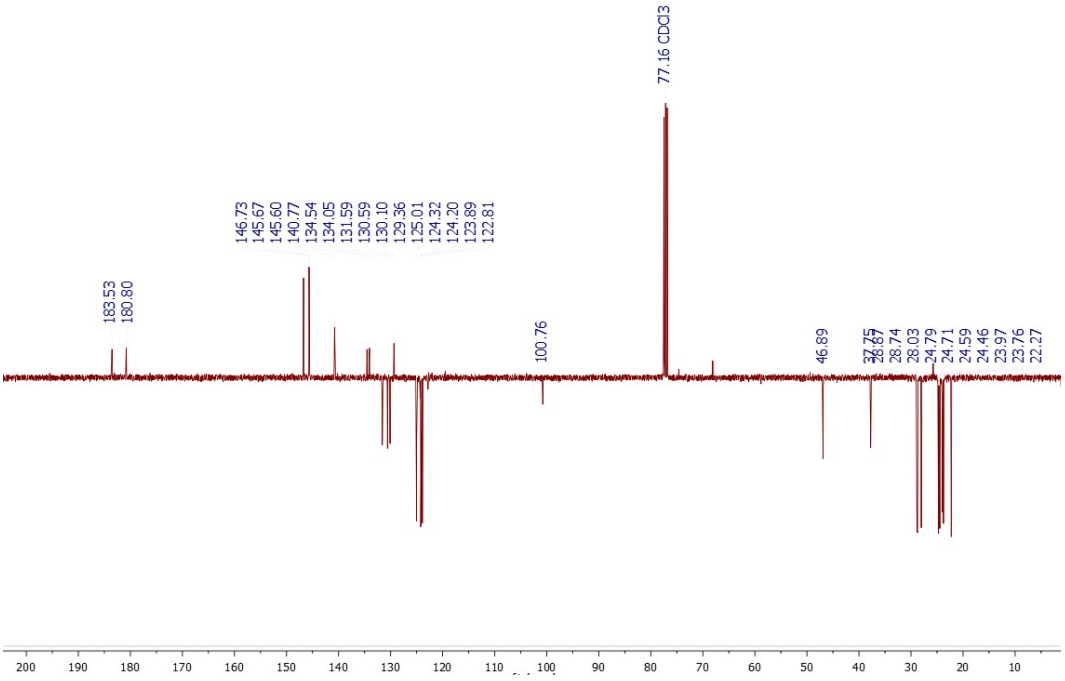
^{19}F NMR (376 MHz, Chloroform-*d*) of [Au(IMe)(AC$^{i\text{-}Pr}$)][OTf] (7)



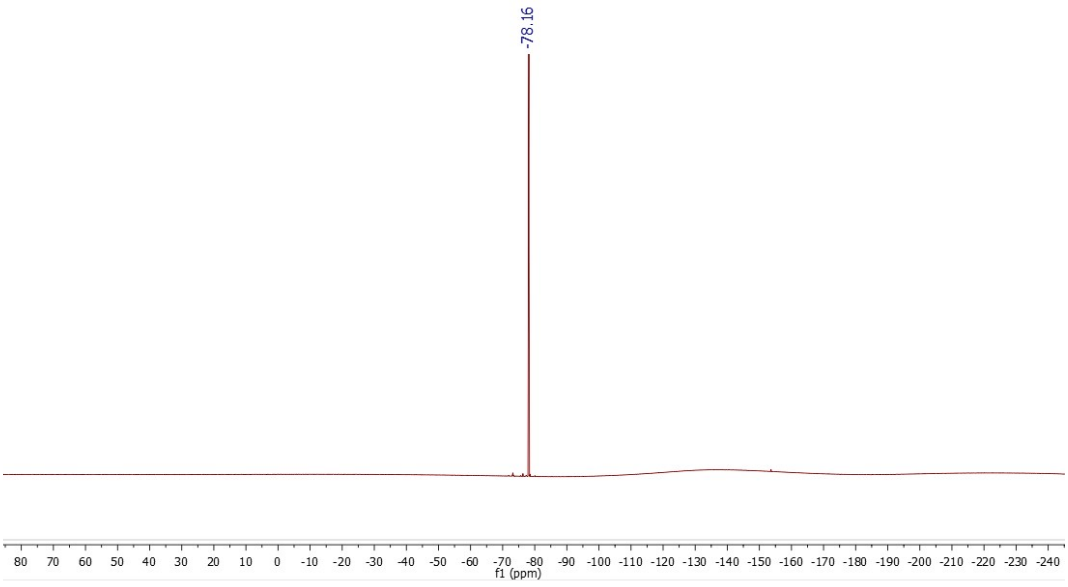
^{1}H NMR (400 MHz, Chloroform-d) of [Au(MeImDipp)(AC$^{i\text{-}Pr}$)][OTf] (8)



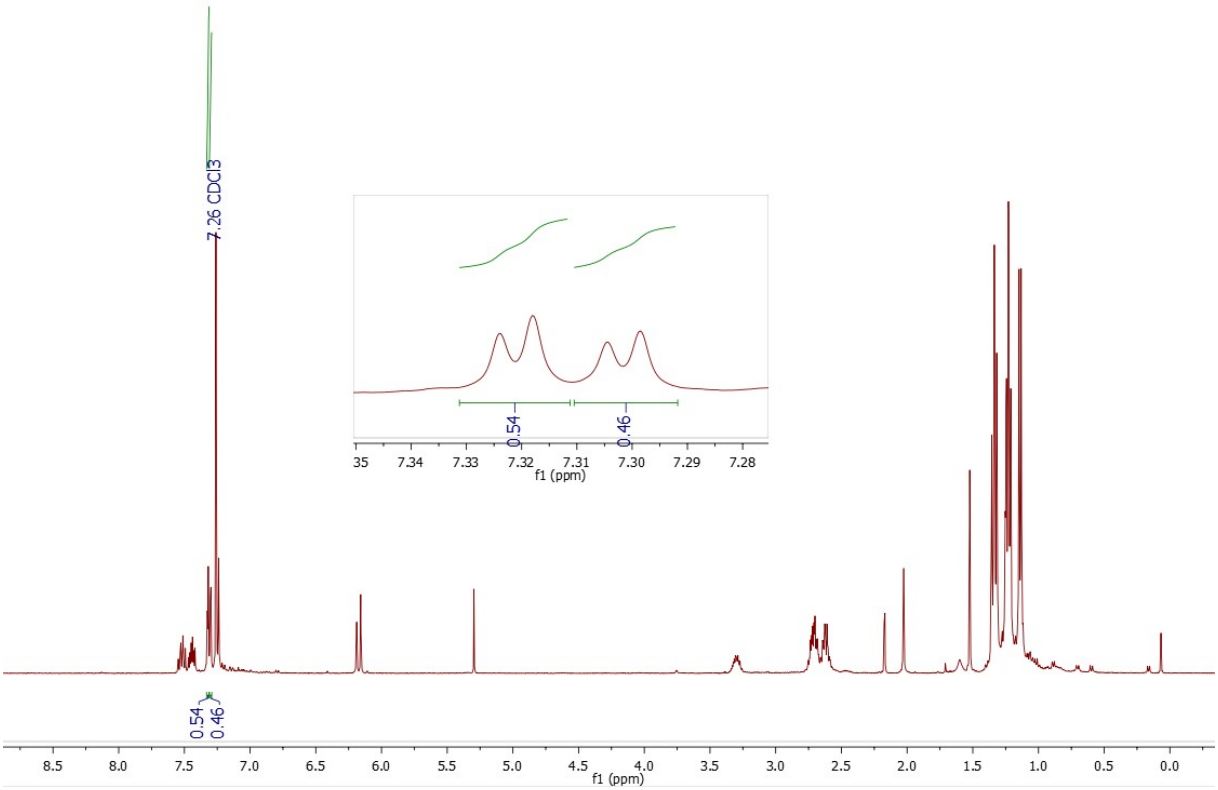
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) of [Au(MeImDipp)(AC$^{i\text{-}Pr}$)][OTf] (8)



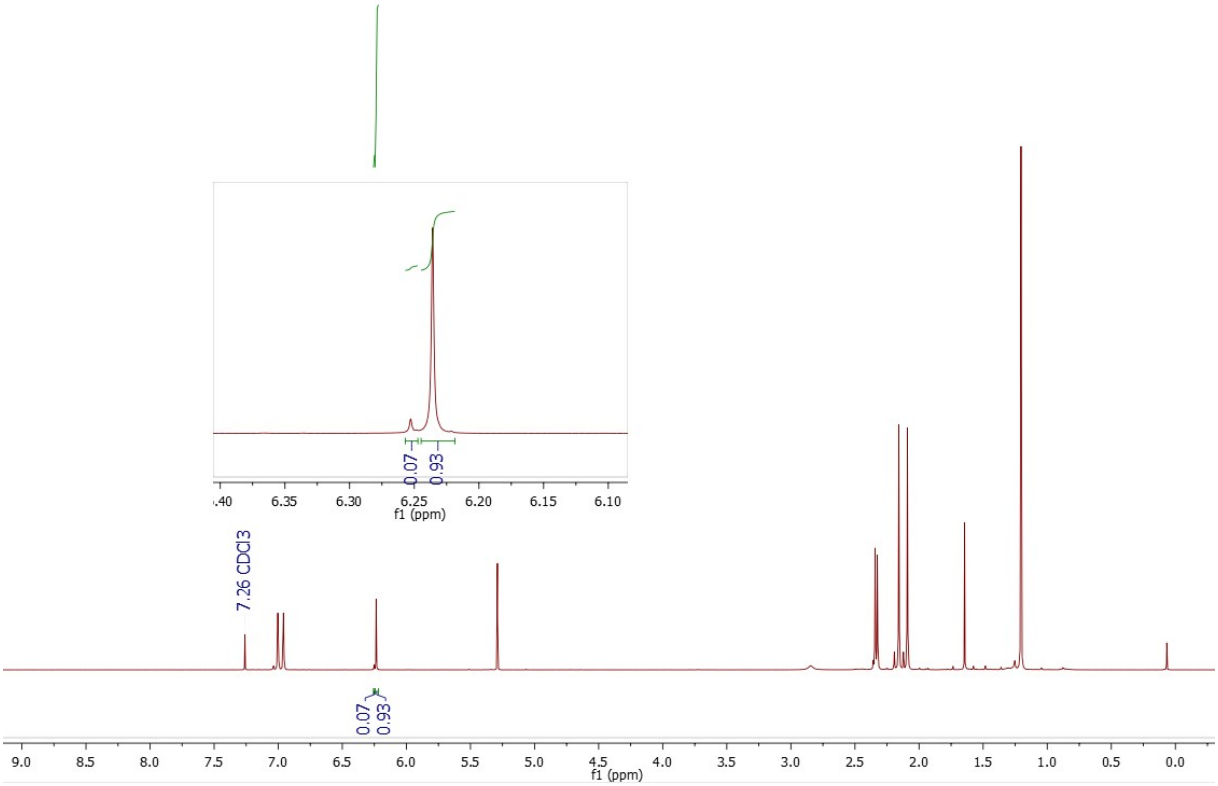
^{19}F NMR (376 MHz, Chloroform-*d*) of [Au(MeImDipp)(AC$^{i\text{-}Pr}$)][OTf] (8)



^{1}H NMR (400 MHz, Chloroform-d) of the mixture of isomers 2a and 2b

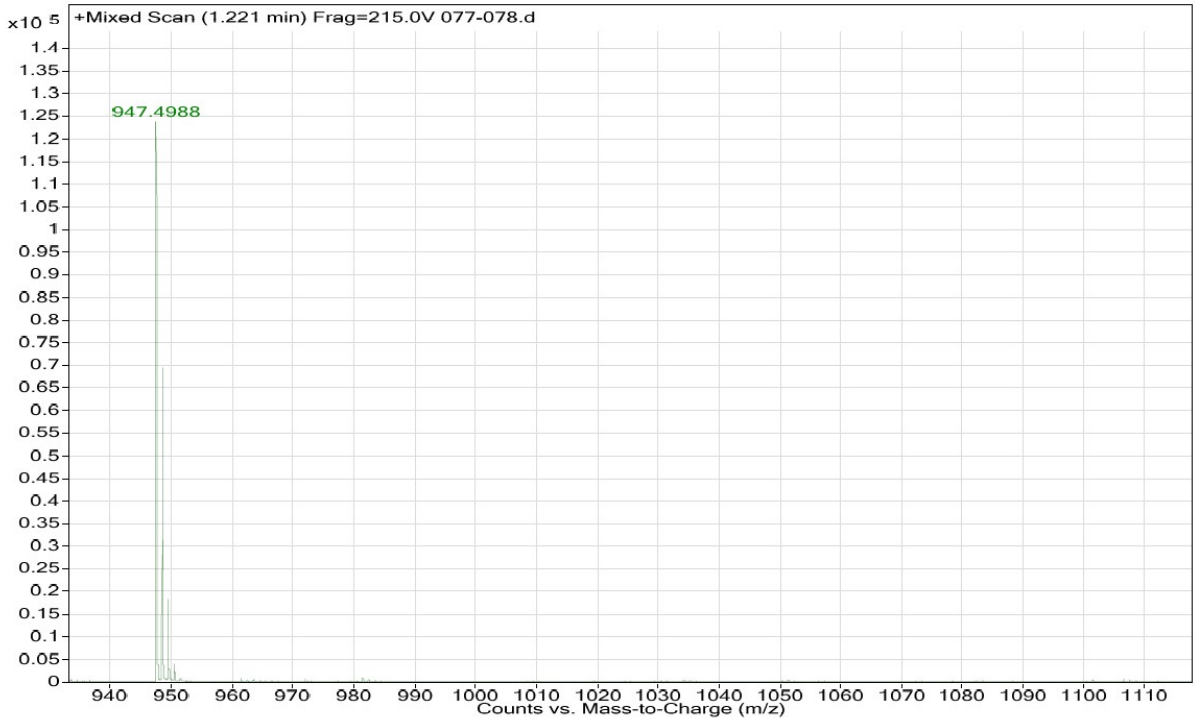


^{1}H NMR (400 MHz, Chloroform-d) of the mixture of isomers 3a and 3b

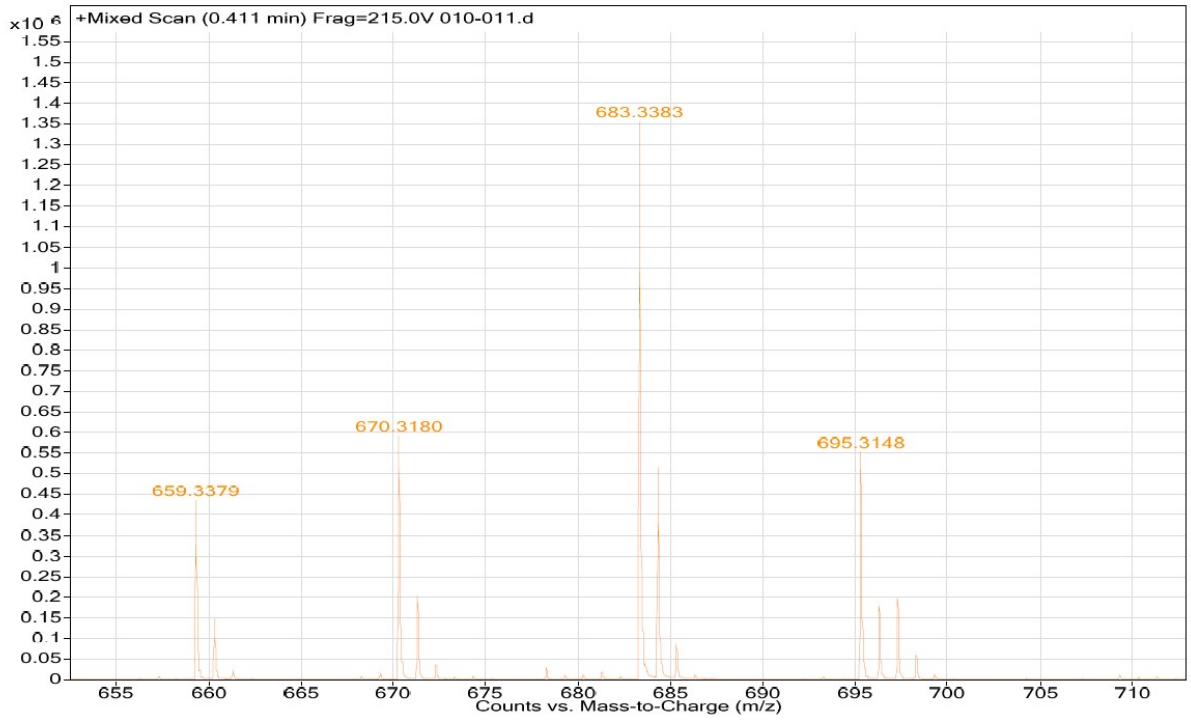


HRMS spectra

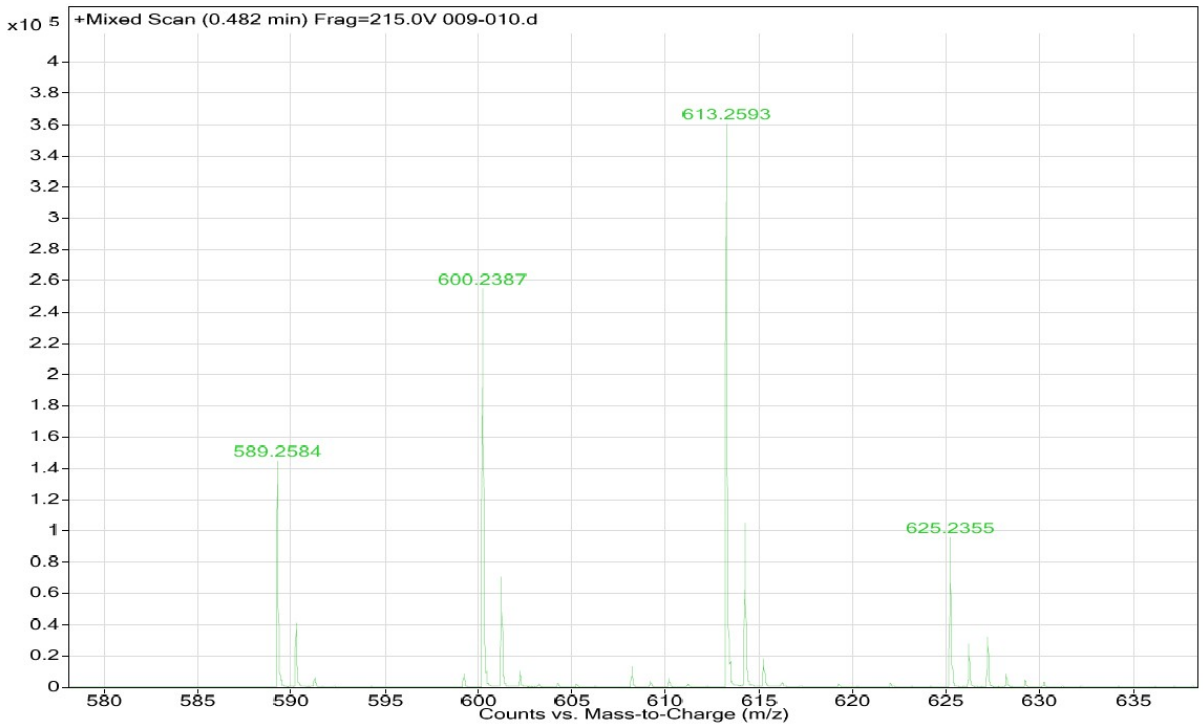
HRMS data for [Au(AC$^{t\text{-}Bu}$)$_2$][OTf] (1)



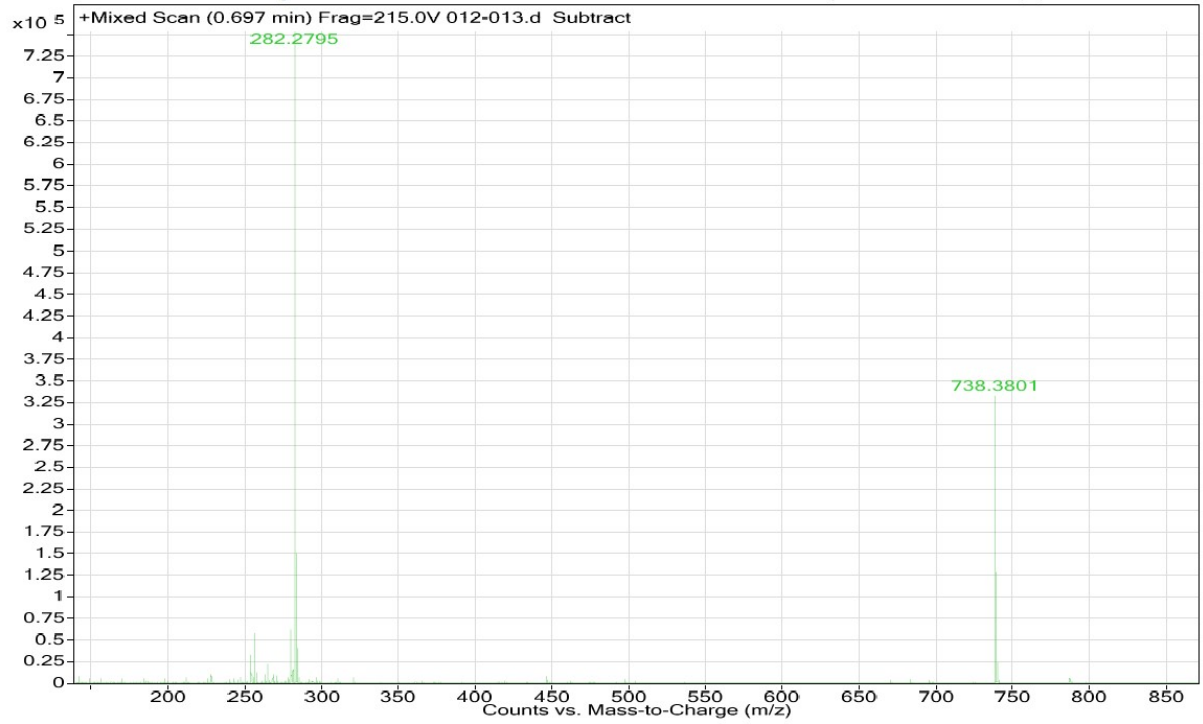
HRMS data for [Au(AC$^{i\text{-}Pr}$)Cl] (2a)



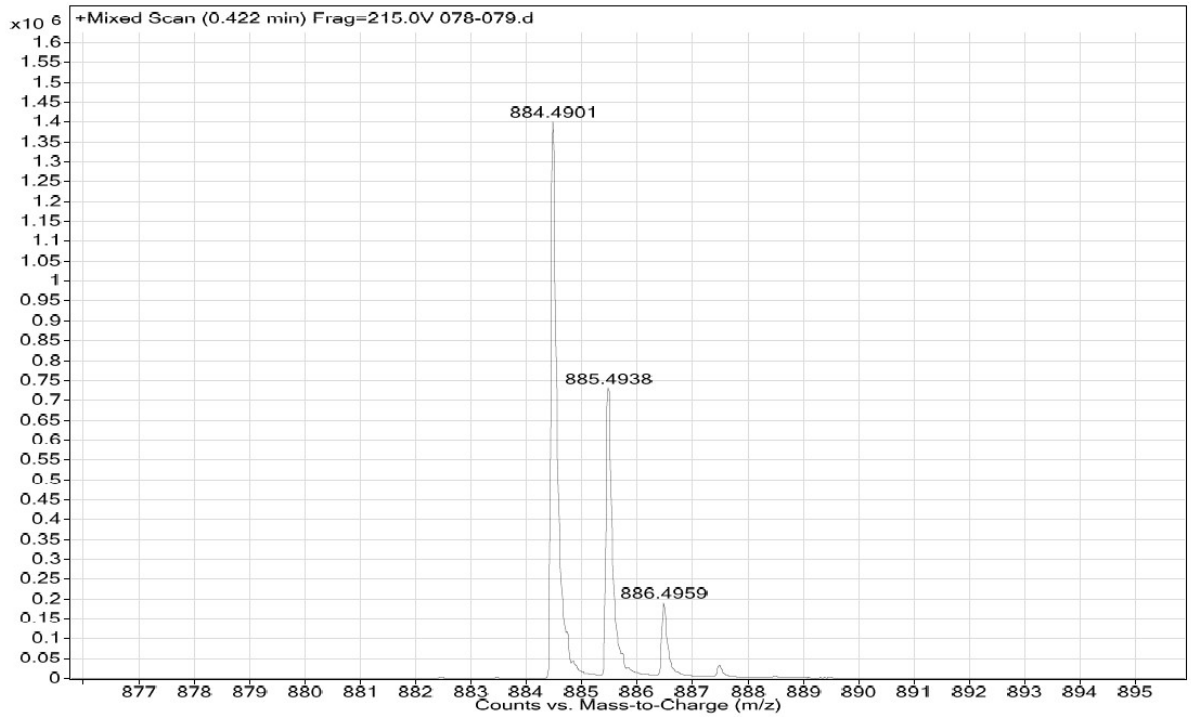
HRMS data for [Au(AC$^{t\text{-}Bu}$)Cl] (3a)



HRMS data for [Au(IMe)(AC$^{i\text{-}Pr}$)][OTf] (7)



HRMS data for [Au(MeImDipp)(AC$^{i\text{-}Pr}$)][OTf] (8)



References

[1] F. Nahra, N. V. Tzouras, A. Collado, S. P. Nolan, *Nat. Protoc.* **2021**, *16*, 1476-1493.

[2] M. W. Johnson, S. L. Shevick, F. D. Toste, R. G. Bergman, *Chem. Sci.* **2013**, *4*, 1023-1027.

[3] a) A. A. Danopoulos, P. Braunstein, *Chem. Commun.* **2014**, *50*, 3055-3057; b) N. V. Tzouras, A. Gobbo, N. B. Pozsoni, S. G. Chalkidis, S. Bhandary, K. V. Hecke, G. C. Vougioukalakis and S. P. Nolan, *Chem. Commun.*, 2022, **58**, 8516-8519.

[4] J. P. Perdew, K. Burke, M. Ernzerhof, *Physical Review Letters* **1996**, *77*, 3865-3868.

[5] G. W. T. M. J. Frisch, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji,, X. L. M. Caricato, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida,, Y. H. T. Nakajima, O. Kitao, H. Nakai, T. Vreven, J. E. Jr. Peralta, F. Ogliaro, m. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R., J. N. Kobayashi, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M.; Millam, M. Klene, J. E. Knox, J. B., V. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K., V. G. Z. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, J. B. Farkas; J. B. Foresman, J. V. Ortiz, J. Cioslowski,, G. D. J. Fox, revision D.01 2013, Gaussian Inc., Wallingford, CT, *Gaussian 09, revision D.01 2013, Gaussian Inc., Wallingford, CT.*

[6] P. J. Hay, *The Journal of Chemical Physics* **1977**, *66*, 4377-4384.

[7] Y. Zhao, D. G. Truhlar, *Theoretical Chemistry Accounts* **2008**, *120*, 215-241.

[8] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *The Journal of Physical Chemistry B* **2009**, *113*, 6378-6396.

Cartesian coordinates

---

4 gas phase : -2624.25731513 A.U.

N	3.232751	1.960561	0.105147
N	3.905144	0.056749	0.895684
C	2.875621	0.646360	0.218283
C	4.475658	2.185545	0.690112
C	4.899135	0.981487	1.193976
C	2.444642	2.949371	-0.591655
C	3.901928	-1.343744	1.243866
C	1.467530	3.678982	0.132476
C	4.523405	-2.257398	0.359823
C	2.673655	3.124715	-1.975608
C	3.223330	-1.739407	2.420447
C	1.249132	3.460832	1.625937
C	5.204430	-1.801179	-0.925362
C	3.668330	2.272116	-2.752789
C	2.555483	-0.737076	3.354005
C	0.722681	4.633992	-0.583450
C	4.436484	-3.623859	0.685449
C	1.898832	4.095486	-2.640366
C	3.167572	-3.118638	2.696002
C	0.939338	4.844931	-1.952599
C	3.763145	-4.050754	1.837407
H	4.948547	3.171389	0.681632
H	5.809346	0.700974	1.731462
H	-0.044683	5.222936	-0.061977
H	4.901755	-4.367350	0.021807
H	2.049259	4.259890	-3.717750
H	2.647621	-3.467748	3.600906
H	5.372975	-0.706826	-0.848150
H	1.468202	2.390974	1.835220
H	2.781154	0.281406	2.976344
Au	1.221606	-0.262689	-0.407297
H	3.706046	-5.124603	2.070723
H	0.344269	5.598983	-2.489418
H	4.228580	1.649748	-2.025364
C	6.577487	-2.458388	-1.132213
H	7.240844	-2.303286	-0.258149
H	7.077223	-2.030361	-2.024139
H	6.490968	-3.550951	-1.301425
C	4.279016	-2.032815	-2.134321
H	3.310034	-1.509387	-2.001769
H	4.064693	-3.112929	-2.269548
H	4.749556	-1.658677	-3.066316
C	1.025083	-0.894778	3.337180
H	0.547733	-0.122994	3.973997
H	0.717554	-1.888036	3.724614
H	0.625405	-0.792675	2.306164
C	3.118778	-0.828177	4.782098
H	2.665587	-0.049284	5.428133
H	4.218132	-0.689074	4.794990
H	2.899704	-1.811778	5.245532
C	2.918913	1.308057	-3.690178
H	2.356020	1.861381	-4.469609
H	2.193839	0.691060	-3.121448
H	3.628987	0.627830	-4.202527
C	4.697244	3.125133	-3.511616
H	5.246252	3.804385	-2.829206
H	4.217162	3.748910	-4.292920

H	5.438105	2.475207	-4.019121
C	-0.193587	3.731363	2.074441
H	-0.322984	3.430899	3.132320
H	-0.937610	3.173072	1.472608
H	-0.451756	4.807995	2.012386
C	2.228708	4.314738	2.455732
H	2.086425	4.129079	3.539724
H	2.057705	5.394526	2.268443
H	3.285566	4.094151	2.212310
N	-2.920952	-1.335856	-0.305997
N	-3.176125	0.729693	0.389465
C	-3.807212	-0.440029	0.214796
C	-1.659472	-0.693936	-0.507111
C	-1.864595	0.618107	-0.045659
C	-3.250017	-2.722591	-0.525869
C	-3.770089	1.971291	0.824977
C	-4.129540	-3.050518	-1.590961
C	-4.028267	2.165737	2.205602
C	-2.684641	-3.687852	0.347005
C	-4.019402	2.951877	-0.163636
C	-4.740512	-1.977324	-2.495330
C	-3.758083	1.071108	3.234472
C	-1.833887	-3.274517	1.546713
C	-3.795655	2.694474	-1.649939
C	-4.397224	-4.417285	-1.794721
C	-4.525798	3.425784	2.584396
C	-2.984337	-5.037504	0.085135
C	-4.512269	4.195303	0.278144
C	-3.821889	-5.398088	-0.977049
C	-4.753252	4.432532	1.635335
H	-1.179660	1.468213	-0.047078
H	-5.067092	-4.722778	-2.609488
H	-4.741702	3.624512	3.643061
H	-2.559604	-5.820793	0.727527
H	-4.718450	4.985919	-0.458817
H	-4.000562	0.101201	2.751848
H	-5.064948	-1.138412	-1.842296
H	-3.461018	1.644050	-1.771113
H	-5.138091	5.410701	1.960547
H	-4.040888	-6.460024	-1.163896
H	-1.177832	-2.441936	1.214655
C	-2.266844	1.017592	3.616696
H	-1.615397	0.871575	2.733207
H	-2.079508	0.180085	4.318551
H	-1.960248	1.958392	4.117424
C	-4.638061	1.177913	4.486000
H	-5.713768	1.253362	4.231211
H	-4.370539	2.057859	5.106003
H	-4.498941	0.281764	5.122502
C	-5.103295	2.846534	-2.446340
H	-4.937384	2.586005	-3.511367
H	-5.486309	3.886890	-2.415065
H	-5.898565	2.183792	-2.049866
C	-2.678061	3.589802	-2.211737
H	-2.499278	3.362901	-3.282240
H	-1.722944	3.442091	-1.669749
H	-2.944597	4.664413	-2.136972
C	-2.729118	-2.755317	2.689264
H	-3.394462	-3.560316	3.062331
H	-3.371385	-1.911787	2.369139

H	-2.108519	-2.401578	3.537462
C	-0.914569	-4.384927	2.071342
H	-0.277077	-4.813691	1.273166
H	-1.486162	-5.212911	2.538055
H	-0.240691	-3.974826	2.849319
C	-5.989173	-2.453180	-3.248208
H	-6.461245	-1.598752	-3.772021
H	-6.743374	-2.894236	-2.566763
H	-5.741621	-3.208833	-4.021445
C	-3.706439	-1.396257	-3.479235
H	-3.296391	-2.189406	-4.137116
H	-2.857028	-0.913509	-2.959912
H	-4.181460	-0.630121	-4.124988
N	-0.516115	-1.251108	-0.941654
C	-0.458975	-2.320461	-1.955361
H	-1.479614	-2.730159	-2.097224
C	0.012231	-1.752658	-3.301880
H	-0.629199	-0.911553	-3.630792
H	-0.003867	-2.533180	-4.089349
H	1.051135	-1.371503	-3.215879
C	0.445484	-3.464383	-1.490433
H	0.049648	-3.939257	-0.574431
H	1.463645	-3.084945	-1.262412
H	0.532283	-4.242230	-2.274829
H	-4.856219	-0.642785	0.444201

4-6a gas phase : -2624.21034485 A.U.

N	-2.033922	1.437216	1.555919
N	-3.006883	3.332519	1.140023
C	-1.844032	2.642790	0.934933
C	-3.296367	1.371917	2.135976
C	-3.910488	2.569074	1.875469
C	-1.061767	0.371409	1.560451
C	-3.292431	4.630236	0.580654
C	-0.172293	0.272424	2.656706
C	-3.808478	4.687857	-0.734850
C	-1.036918	-0.519360	0.460533
C	-3.051843	5.777239	1.373089
C	-0.172346	1.280483	3.798072
C	-4.119393	3.434305	-1.543339
C	-1.975207	-0.378638	-0.731198
C	-2.488251	5.666370	2.783905
C	0.766093	-0.776169	2.631946
C	-4.041283	5.966788	-1.276168
C	-0.077919	-1.549913	0.489337
C	-3.315622	7.028741	0.786898
C	0.810592	-1.680682	1.563410
C	-3.794406	7.123190	-0.526805
H	-3.637174	0.483714	2.675260
H	-4.902866	2.947361	2.136485
H	1.477365	-0.882167	3.464551
H	-4.434623	6.055414	-2.299954
H	-0.029722	-2.263487	-0.346803
H	-3.141889	7.945817	1.368436
H	-3.941553	2.556199	-0.889490
H	-1.074909	1.916791	3.690106
H	-2.684181	4.633612	3.140803
Au	-0.195039	3.131729	-0.052973
H	-3.988414	8.112498	-0.967766
H	1.550211	-2.495498	1.566074

H	-2.670263	0.459821	-0.521068
C	-5.596327	3.390320	-1.970029
H	-6.275329	3.468366	-1.097483
H	-5.818213	2.439309	-2.494931
H	-5.845945	4.217685	-2.665156
C	-3.172710	3.296850	-2.745800
H	-2.115004	3.286516	-2.416130
H	-3.303257	4.135287	-3.460504
H	-3.374933	2.355053	-3.295368
C	-0.960777	5.854624	2.775800
H	-0.549130	5.705856	3.793379
H	-0.690291	6.880390	2.448876
H	-0.465119	5.135695	2.090425
C	-3.162764	6.625736	3.775153
H	-2.799276	6.431435	4.804043
H	-4.264746	6.509867	3.771971
H	-2.933154	7.686270	3.545647
C	-1.188724	-0.005702	-2.000041
H	-0.473046	-0.805186	-2.282162
H	-0.614954	0.932758	-1.853904
H	-1.877852	0.145008	-2.855480
C	-2.829868	-1.640254	-0.937034
H	-3.411698	-1.891007	-0.027576
H	-2.204800	-2.520999	-1.189547
H	-3.543820	-1.491212	-1.772007
C	1.051774	2.206495	3.686780
H	1.048455	2.954938	4.504947
H	1.054927	2.746165	2.718061
H	2.001429	1.637354	3.758747
C	-0.250340	0.603350	5.175409
H	-0.323515	1.366228	5.976416
H	0.651786	-0.006712	5.385319
H	-1.132562	-0.062874	5.253641
N	3.042043	4.819364	-1.598580
N	3.350483	3.763226	0.327741
C	3.796270	4.733022	-0.469972
C	1.991288	3.830161	-1.517440
C	2.215207	3.148221	-0.265151
C	3.031899	5.988459	-2.441080
C	3.978084	3.331679	1.553601
C	3.774753	5.972300	-3.645685
C	3.905175	4.166305	2.697900
C	2.248216	7.093866	-2.024765
C	4.622314	2.069709	1.559532
C	4.646291	4.778181	-4.014710
C	3.286051	5.558715	2.664171
C	1.451771	7.100830	-0.723079
C	4.770828	1.209612	0.308614
C	3.707361	7.117166	-4.459284
C	4.483402	3.678416	3.884677
C	2.216066	8.212048	-2.880727
C	5.164545	1.627925	2.781083
C	2.932379	8.223041	-4.083160
C	5.092601	2.419109	3.932970
H	2.152560	2.054583	-0.177870
H	4.268507	7.144502	-5.404180
H	4.448794	4.297334	4.792599
H	1.614605	9.089064	-2.598683
H	5.667666	0.650441	2.823211
H	2.611174	5.608724	1.783551

H	4.228825	3.893356	-3.487679
H	4.391494	1.791359	-0.556180
H	5.527308	2.056525	4.876410
H	2.889294	9.106906	-4.737020
H	1.733499	6.199954	-0.139621
C	2.436848	5.868624	3.905487
H	1.682810	5.080431	4.087126
H	1.904621	6.831061	3.771136
H	3.059727	5.967082	4.817355
C	4.381507	6.630638	2.495237
H	4.996380	6.474296	1.586374
H	5.075711	6.616004	3.360021
H	3.933874	7.642715	2.434896
C	6.247756	0.892680	0.015399
H	6.338327	0.331635	-0.936434
H	6.701006	0.267541	0.811150
H	6.851600	1.817882	-0.071255
C	3.928470	-0.074299	0.410807
H	3.997134	-0.663797	-0.525730
H	2.858244	0.140156	0.605146
H	4.284327	-0.719283	1.240441
C	1.798129	8.322063	0.145540
H	1.453546	9.267635	-0.319925
H	2.889957	8.409258	0.313960
H	1.300906	8.242373	1.133866
C	-0.063180	7.002427	-0.973785
H	-0.330747	6.055007	-1.478899
H	-0.424527	7.842311	-1.601872
H	-0.616355	7.036504	-0.015597
C	6.082218	4.984587	-3.494823
H	6.714330	4.102816	-3.723889
H	6.104573	5.144182	-2.397643
H	6.548745	5.872473	-3.968473
C	4.638413	4.463613	-5.516717
H	5.131630	5.259991	-6.110033
H	3.606493	4.341669	-5.902958
H	5.191561	3.523966	-5.713881
N	0.947109	3.635268	-2.272686
C	0.898965	3.875553	-3.715643
H	1.928485	4.094161	-4.081585
C	0.432410	2.587668	-4.410516
H	1.087266	1.734730	-4.143589
H	0.444096	2.708559	-5.512381
H	-0.600683	2.333312	-4.100299
C	0.011010	5.066503	-4.094372
H	0.430889	6.018721	-3.721158
H	-1.005613	4.945225	-3.672298
H	-0.079813	5.142610	-5.196393
H	4.623820	5.409434	-0.232007

6a gas phase : -2624.24258680 A.U.

N	0.183790	-0.185930	3.259741
N	-1.412239	1.273881	3.374507
C	-0.231369	1.009470	2.741634
C	-0.721482	-0.660442	4.203354
C	-1.732342	0.264148	4.275939
C	1.341985	-0.901009	2.777515
C	-2.279107	2.373634	3.025256
C	2.562635	-0.769438	3.480985
C	-3.222917	2.167262	1.990228

C	1.200082	-1.687212	1.609491	H	-2.290087	1.553606	-0.545538
C	-2.145156	3.597046	3.719878	H	-4.078651	1.572420	-0.689182
C	2.668762	0.102347	4.725240	H	-3.205933	0.020073	-0.765149
C	-3.345429	0.839924	1.252518	C	0.062563	4.681441	4.203845
C	-0.135384	-1.870598	0.898067	H	0.877061	4.803921	4.945419
C	-1.070215	3.810840	4.776276	H	-0.310884	5.692725	3.939749
C	3.684630	-1.432436	2.951546	H	0.490389	4.225820	3.286078
C	-4.069324	3.245109	1.670323	C	-1.630971	4.396400	6.081175
C	2.355800	-2.329930	1.125370	H	-0.832499	4.467900	6.846761
C	-3.014449	4.642352	3.355112	H	-2.445979	3.768053	6.492113
C	3.584465	-2.198279	1.782385	H	-2.035582	5.418549	5.933755
C	-3.968497	4.468266	2.344504	C	-0.105919	-1.300388	-0.529470
H	-0.566697	-1.607852	4.727494	H	0.653965	-1.808942	-1.157218
H	-2.645180	0.295040	4.877425	H	0.124080	-0.215198	-0.517150
H	4.653129	-1.349239	3.464881	H	-1.090826	-1.432781	-1.020496
H	-4.819820	3.122561	0.875552	C	-0.572847	-3.345626	0.912891
H	2.287344	-2.948325	0.217774	H	-0.618528	-3.745305	1.945672
H	-2.945181	5.608589	3.876871	H	0.127466	-3.984394	0.336891
H	-2.501452	0.196455	1.572967	H	-1.577016	-3.456285	0.455980
H	1.656805	0.160585	5.178761	C	3.076335	1.532525	4.330687
H	-0.631458	2.820593	5.017536	H	3.093066	2.195342	5.219905
Au	0.621804	2.049972	1.223414	H	2.377392	1.960811	3.583003
H	-4.641432	5.297304	2.078334	H	4.086440	1.541865	3.873209
H	4.474833	-2.709217	1.385681	C	3.612024	-0.472246	5.790893
H	-0.901338	-1.297184	1.458764	H	3.558776	0.136217	6.715615
C	-4.646142	0.114138	1.639437	H	4.669654	-0.459031	5.457102
H	-4.708808	-0.056892	2.733033	H	3.350714	-1.517097	6.051554
H	-4.708572	-0.870832	1.133822	N	1.225663	5.152917	-1.276310
H	-5.537930	0.702863	1.341321	N	2.656457	3.684490	-0.402826
C	-3.217888	1.011938	-0.269705	C	2.467811	4.925250	-0.813400

C	0.460956	3.897664	-1.206947
C	1.391506	2.930916	-0.522533
C	0.825818	6.438203	-1.794282
C	3.855926	3.179779	0.212892
C	1.109406	6.733684	-3.151591
C	4.350506	3.791725	1.398216
C	0.176137	7.345793	-0.922328
C	4.489105	2.056903	-0.379963
C	1.786232	5.715684	-4.062961
C	3.772660	5.073748	1.987702
C	-0.086994	7.006479	0.539653
C	4.052771	1.464068	-1.715446
C	0.733775	8.003602	-3.624598
C	5.480235	3.208320	2.001942
C	-0.183048	8.598939	-1.452072
C	5.596630	1.502912	0.287224
C	0.095037	8.926015	-2.785081
C	6.085675	2.064590	1.470669
H	1.549597	2.045822	-1.169215
H	0.934696	8.272525	-4.671508
H	5.889582	3.660848	2.916581
H	-0.689535	9.332442	-0.808029
H	6.097630	0.624269	-0.145138
H	2.745490	5.207960	1.587441
H	1.610732	4.710944	-3.622007
H	3.270520	2.123206	-2.143889
H	6.957847	1.620218	1.973013
H	-0.194300	9.912249	-3.177689
H	-0.019709	5.903122	0.648823
C	3.637095	5.043080	3.516789
H	3.048760	4.171071	3.852488
H	3.124364	5.961089	3.867108
H	4.623968	5.010253	4.020590
C	4.629889	6.283189	1.561405
H	4.739816	6.369233	0.460712
H	5.655630	6.191708	1.972560
H	4.197632	7.230801	1.940999
C	5.208091	1.451017	-2.731951
H	4.848527	1.086117	-3.715140
H	6.031200	0.780439	-2.412593
H	5.634309	2.464137	-2.874743
C	3.447420	0.061742	-1.528613
H	3.059536	-0.331741	-2.490053
H	2.620646	0.063832	-0.791431
H	4.209772	-0.651503	-1.154139
C	1.002581	7.635295	1.428860
H	0.943497	8.742536	1.397097
H	2.019953	7.353381	1.095227
H	0.885874	7.315399	2.484236
C	-1.486208	7.425169	1.014048
H	-2.279197	7.018585	0.356858
H	-1.599782	8.527706	1.045707
H	-1.668143	7.044953	2.038778
C	3.309275	5.944365	-4.112977
H	3.799971	5.183918	-4.753753
H	3.776071	5.891444	-3.108665
H	3.542392	6.944917	-4.531116
C	1.190423	5.695925	-5.478761
H	1.423255	6.624247	-6.038605
H	0.089155	5.578619	-5.456210

H	1.614371	4.852885	-6.059821
N	-0.700199	3.616560	-1.634461
C	-1.612854	4.484695	-2.364800
H	-1.176965	5.489065	-2.554006
C	-1.913958	3.834613	-3.721541
H	-0.988387	3.707596	-4.317490
H	-2.618818	4.460242	-4.304955
H	-2.366839	2.832711	-3.577646
C	-2.891588	4.674860	-1.540393
H	-2.663486	5.087330	-0.538542
H	-3.404899	3.705417	-1.392148
H	-3.584998	5.367438	-2.057931
H	3.237457	5.706328	-0.778801

---

6 gas phase : -2624.27759181 A.U.

N	-1.777296	0.958949	1.573916
N	-2.929347	2.767373	1.275605
C	-1.706924	2.206091	1.026376
C	-3.021459	0.739499	2.158132
C	-3.750370	1.887220	1.971945
C	-0.701906	-0.001218	1.515201
C	-3.293574	4.082637	0.806422
C	0.192543	-0.077165	2.609276
C	-4.035476	4.177318	-0.396726
C	-0.588861	-0.809695	0.360393
C	-2.852040	5.213980	1.533611
C	0.062933	0.847826	3.812807
C	-4.415161	2.943735	-1.207533
C	-1.540314	-0.681280	-0.822903
C	-2.075312	5.100361	2.839071
C	1.244513	-1.006736	2.514565
C	-4.341601	5.468725	-0.865448
C	0.475147	-1.731506	0.325566
C	-3.178234	6.481156	1.011610
C	1.382298	-1.827730	1.387849
C	-3.915056	6.609128	-0.171597
H	-3.271439	-0.206495	2.646820
H	-4.769561	2.153609	2.266314
H	1.966055	-1.091043	3.339883
H	-4.920401	5.582369	-1.793795
H	0.594961	-2.382853	-0.553013
H	-2.850316	7.384716	1.546607
H	-4.344288	2.061372	-0.538970
H	-0.980164	1.227079	3.834645
H	-1.811189	4.033415	2.986450
Au	-0.161304	3.194440	0.156479
H	-4.160329	7.609397	-0.559001
H	2.207914	-2.553567	1.337706
H	-2.349483	0.020537	-0.534177
C	-5.853856	2.993269	-1.741428
H	-6.586573	3.163865	-0.927836
H	-6.110232	2.037299	-2.240009
H	-5.989555	3.796863	-2.493683
C	-3.397016	2.733325	-2.344328
H	-2.361033	2.673238	-1.952271
H	-3.440960	3.572461	-3.069317
H	-3.612628	1.796925	-2.897883
C	-0.755494	5.887327	2.790686
H	-0.187174	5.743430	3.730908
H	-0.928174	6.976710	2.672623

H	-0.121351	5.544818	1.946970
C	-2.950941	5.529353	4.030323
H	-2.400559	5.401655	4.984426
H	-3.881471	4.929737	4.087313
H	-3.244702	6.596110	3.950274
C	-0.816096	-0.064549	-2.033258
H	-0.001912	-0.726041	-2.392655
H	-0.367378	0.916388	-1.771027
H	-1.522421	0.089725	-2.873768
C	-2.203759	-2.021217	-1.179828
H	-2.738149	-2.454899	-0.311177
H	-1.460140	-2.768308	-1.524658
H	-2.936208	-1.883302	-2.000594
C	0.989275	2.066453	3.648113
H	0.859026	2.770846	4.495019
H	0.781644	2.612091	2.703240
H	2.053358	1.756574	3.618071
C	0.312980	0.132957	5.148706
H	0.101188	0.817521	5.994228
H	1.368396	-0.191500	5.252350
H	-0.329925	-0.762532	5.261834
N	2.253886	6.166417	-1.668085
N	2.634859	4.413554	-0.419897
C	3.220022	5.453172	-1.043509
C	1.021021	5.535737	-1.441801
C	1.249810	4.406919	-0.648791
C	2.457458	7.448102	-2.294914
C	3.342494	3.467879	0.409181
C	2.960981	7.491232	-3.617473
C	3.757420	3.887900	1.694901
C	2.123504	8.603290	-1.548228
C	3.564335	2.161921	-0.095630
C	3.320642	6.222118	-4.380885
C	3.513469	5.301576	2.212691
C	1.607720	8.533331	-0.115332
C	3.150053	1.782133	-1.513818
C	3.137748	8.762498	-4.194039
C	4.442184	2.945052	2.486772
C	2.308104	9.846852	-2.181644
C	4.231098	1.257305	0.749770
C	2.809834	9.926681	-3.486593
C	4.670910	1.645368	2.023119
H	-0.953002	5.616531	-1.378597
H	3.532779	8.842086	-5.217370
H	4.790550	3.234443	3.489092
H	2.060182	10.770495	-1.637313
H	4.416985	0.231500	0.403899
H	2.751319	5.774669	1.558667
H	2.845472	5.369132	-3.851853
H	2.176075	2.279004	-1.710301
H	5.199703	0.921813	2.661782
H	2.949685	10.910353	-3.959300
H	1.568679	7.465879	0.182803
C	2.947796	5.319058	3.641108
H	2.036241	4.697608	3.720757
H	2.686549	6.355703	3.934767
H	3.682841	4.945310	4.382419
C	4.799559	6.144903	2.126175
H	5.196680	6.195459	1.092614
H	5.597966	5.713190	2.763746

H	4.612506	7.181712	2.471421
C	4.168205	2.319964	-2.540530
H	3.840333	2.082225	-3.573067
H	5.163912	1.856580	-2.384326
H	4.295515	3.418391	-2.473114
C	2.938457	0.276658	-1.704879
H	2.515990	0.079955	-2.710213
H	2.239705	-0.136930	-0.952166
H	3.891557	-0.287509	-1.639936
C	2.569729	9.240133	0.855602
H	2.625282	10.329794	0.656540
H	3.597273	8.831857	0.778006
H	2.226161	9.110345	1.902229
C	0.174510	9.080318	-0.002403
H	-0.510344	8.511003	-0.660705
H	0.124685	10.153147	-0.280013
H	-0.190290	8.987744	1.041200
C	4.842670	5.986516	-4.361725
H	5.099206	5.034700	-4.869189
H	5.241038	5.939690	-3.328235
H	5.376714	6.806894	-4.883464
C	2.779487	6.223102	-5.818895
H	3.271970	6.994135	-6.445248
H	1.688070	6.412379	-5.844805
H	2.968468	5.242783	-6.300252
N	-0.175066	6.083564	-1.862739
C	-0.451331	6.253311	-3.308991
H	0.346720	6.915015	-3.706775
C	-0.414834	4.922037	-4.069245
H	0.555347	4.403864	-3.927283
H	-0.560508	5.080775	-5.156415
H	-1.214669	4.242202	-3.710748
C	-1.786592	6.977031	-3.462508
H	-1.773134	7.950311	-2.934099
H	-2.613259	6.367776	-3.039973
H	-2.012072	7.160311	-4.530769
H	4.286122	5.692756	-1.047716

6a-OTS gas phase : -3584.64196488 A.U.

N	0.082404	-0.239729	3.251912
N	-1.427536	1.291036	3.492198
C	-0.281295	0.999854	2.802466
C	-0.815583	-0.714665	4.202222
C	-1.774338	0.253698	4.352160
C	1.186685	-1.002628	2.721535
C	-2.245728	2.448824	3.227980
C	2.446261	-0.898392	3.356037
C	-3.138933	2.389770	2.132655
C	0.951889	-1.821378	1.591173
C	-2.116699	3.580986	4.065864
C	2.675494	0.057341	4.518842
C	-3.301756	1.133731	1.287079
C	-0.399246	-1.886551	0.890145
C	-1.102150	3.606027	5.201516
C	3.501837	-1.659745	2.822086
C	-3.913653	3.537343	1.876912
C	2.043475	-2.563295	1.101419
C	-2.913577	4.699933	3.763554
C	3.301081	-2.487538	1.710332
C	-3.799182	4.679655	2.677474

H	-0.690642	-1.693083	4.674085
H	-2.667903	0.299815	4.980739
H	4.499372	-1.596531	3.280991
H	-4.617174	3.531418	1.031684
H	1.905276	-3.198686	0.214223
H	-2.836004	5.604074	4.384510
H	-2.443221	0.467680	1.504512
H	1.682296	0.318436	4.940524
H	-0.918617	2.554011	5.505793
Au	0.569104	2.042807	1.278314
H	-4.408757	5.567896	2.452376
H	4.140602	-3.071767	1.304247
H	-1.130226	-1.328519	1.511088
C	-4.581693	0.379517	1.692805
H	-4.581462	0.117737	2.770805
H	-4.678403	-0.559821	1.110875
H	-5.484610	0.994229	1.496353
C	-3.258498	1.429414	-0.217004
H	-2.342090	1.988758	-0.498151
H	-4.138211	2.021698	-0.544191
H	-3.272620	0.482527	-0.793353
C	0.237004	4.169242	4.695338
H	1.018309	4.099706	5.479422
H	0.130638	5.237348	4.413533
H	0.590044	3.622278	3.797358
C	-1.594477	4.360517	6.443526
H	-0.864621	4.253271	7.271056
H	-2.573617	3.978210	6.795371
H	-1.704572	5.447228	6.249418
C	-0.341194	-1.193153	-0.482415
H	0.394317	-1.672938	-1.158188
H	-0.052093	-0.126779	-0.395590
H	-1.330622	-1.229731	-0.980784
C	-0.915918	-3.330526	0.778257
H	-0.967539	-3.826696	1.768837
H	-0.266337	-3.947595	0.124303
H	-1.931421	-3.339981	0.333118
C	3.311973	1.358515	4.000010
H	3.436295	2.093331	4.821934
H	2.689945	1.819987	3.205053
H	4.309860	1.165474	3.557921
C	3.504036	-0.563561	5.652788
H	3.566839	0.136750	6.510190
H	4.544257	-0.778013	5.332768
H	3.058959	-1.512424	6.014123
N	1.214905	5.054518	-1.471341
N	2.594291	3.641124	-0.425140
C	2.458642	4.813284	-1.020250
C	0.378226	3.881718	-1.171977
C	1.305066	2.919380	-0.468057
C	0.779520	6.356447	-1.920042
C	3.784512	3.221959	0.279771
C	0.729031	6.613735	-3.313494
C	4.217120	3.967207	1.414306
C	0.398162	7.317038	-0.944704
C	4.487395	2.072973	-0.165641
C	1.178065	5.563762	-4.312961
C	3.485803	5.196194	1.938865
C	0.532517	7.048264	0.553145
C	4.081663	1.278391	-1.391715

C	0.246795	7.869832	-3.723712
C	5.386437	3.546401	2.073799
C	-0.087708	8.552383	-1.416012
C	5.627512	1.677659	0.561662
C	-0.169990	8.823675	-2.787324
C	6.085058	2.407158	1.661426
H	1.406055	2.038698	-1.148300
H	0.186325	8.092786	-4.798662
H	5.743792	4.116704	2.943547
H	-0.402118	9.319233	-0.694207
H	6.177669	0.784585	0.230560
H	2.458421	5.169102	1.522227
H	1.062152	4.571288	-3.838474
H	3.299912	1.838722	-1.936353
H	6.990187	2.089158	2.201316
H	-0.556274	9.796298	-3.128854
H	1.414608	6.389260	0.671423
C	3.333635	5.191633	3.467810
H	2.906188	4.237922	3.825390
H	2.660944	6.013325	3.786518
H	4.304646	5.347581	3.980542
C	4.172401	6.499212	1.487432
H	4.264736	6.577257	0.386222
H	5.200199	6.555421	1.900999
H	3.612006	7.386487	1.844296
C	5.249334	1.135843	-2.382223
H	4.891553	0.647353	-3.307411
H	6.079854	0.522364	-1.973194
H	5.659375	2.127311	-2.660977
C	3.497309	-0.087026	-0.996002
H	3.074975	-0.584208	-1.890153
H	2.678978	0.022897	-0.256807
H	4.268864	-0.745823	-0.544021
C	0.827044	8.317706	1.365217
H	-0.056528	8.986321	1.421930
H	1.666981	8.900027	0.936497
H	1.090389	8.045788	2.407708
C	-0.661523	6.290421	1.162892
H	-0.846362	5.316659	0.672616
H	-1.591470	6.890673	1.088736
H	-0.475448	6.089461	2.237377
C	2.679596	5.698990	-4.622915
H	3.006639	4.832719	-5.230017
H	3.291536	5.691679	-3.698314
H	2.898063	6.640650	-5.169787
C	0.346370	5.533559	-5.600143
H	0.553869	6.399799	-6.263691
H	-0.740008	5.515402	-5.379374
H	0.578294	4.601877	-6.150983
N	-0.839991	3.658530	-1.451696
C	-1.712473	4.407931	-2.351642
H	-1.128878	5.090331	-3.002767
C	-2.434347	3.411314	-3.269040
H	-1.697683	2.799247	-3.823042
H	-3.058859	3.963388	-4.001562
H	-3.094504	2.742947	-2.681775
C	-2.712489	5.262728	-1.561307
H	-2.217206	6.113180	-1.057242
H	-3.221690	4.650440	-0.789872
H	-3.480444	5.673759	-2.246751

H	3.269381	5.547068	-1.107394
S	1.290908	1.759744	-3.963020
C	2.190640	0.669945	-5.211841
O	2.346872	2.750610	-3.547366
O	0.187803	2.335748	-4.784480
O	0.895779	0.804735	-2.878093
F	1.323430	-0.121299	-5.863728
F	2.843066	1.425938	-6.114107
F	3.100975	-0.130273	-4.601593

6a-6-OTS gas phase : -3584.61345400 A.U.

N	-1.863239	0.734046	1.831504
N	-3.104295	2.483565	1.568067
C	-1.805648	2.050708	1.451809
C	-3.160403	0.358196	2.175132
C	-3.945550	1.465904	2.000546
C	-0.768212	-0.198664	1.805022
C	-3.543990	3.805487	1.202154
C	0.052345	-0.311628	2.950356
C	-3.677699	4.099938	-0.174183
C	-0.607667	-1.003670	0.650630
C	-3.820704	4.736970	2.231518
C	-0.129754	0.604041	4.153102
C	-3.470188	3.034615	-1.243557
C	-1.479825	-0.809333	-0.585419
C	-3.607786	4.375269	3.699026
C	1.073799	-1.280023	2.917150
C	-4.069629	5.408461	-0.513487
C	0.421467	-1.962519	0.675982
C	-4.239652	6.017790	1.834001
C	1.249301	-2.102584	1.797751
C	-4.344383	6.355731	0.477960
H	-3.395867	-0.657800	2.503191
H	-5.019153	1.623596	2.135679
H	1.738356	-1.392723	3.786381
H	-4.154420	5.688274	-1.572856
H	0.580512	-2.607285	-0.200568
H	-4.460420	6.775295	2.596980
H	-2.865704	2.222912	-0.793135
H	-1.132691	1.071092	4.068006
H	-3.921554	3.316844	3.828810
Au	-0.246854	3.188554	0.779887
H	-4.634634	7.377679	0.191818
H	2.048825	-2.859120	1.794847
H	-2.401720	-0.281944	-0.263853
C	-4.824054	2.425413	-1.653815
H	-5.362831	1.995643	-0.784398
H	-4.677859	1.617509	-2.400567
H	-5.481600	3.194713	-2.109522
C	-2.677634	3.547079	-2.450651
H	-1.746932	4.061051	-2.126773
H	-3.269708	4.261817	-3.059341
H	-2.409455	2.701149	-3.116526
C	-2.114293	4.457585	4.070793
H	-1.947898	4.098209	5.107441
H	-1.757748	5.502382	4.003007
H	-1.483222	3.856411	3.387149
C	-4.449019	5.219368	4.664417
H	-4.347085	4.831447	5.697742
H	-5.524851	5.210288	4.397045

H	-4.108724	6.275279	4.681324
C	-0.776909	0.099639	-1.611927
H	0.153228	-0.374433	-1.987241
H	-0.503819	1.080138	-1.169321
H	-1.440649	0.288420	-2.480257
C	-1.919085	-2.136041	-1.221591
H	-2.411546	-2.801855	-0.484466
H	-1.062511	-2.689126	-1.658930
H	-2.635037	-1.945041	-2.046198
C	0.908975	1.737403	4.113700
H	0.748546	2.450480	4.947626
H	0.850200	2.304476	3.161038
H	1.939155	1.338064	4.196113
C	-0.089768	-0.153150	5.488828
H	-0.318160	0.537398	6.325666
H	0.912819	-0.584092	5.688955
H	-0.826242	-0.981625	5.514530
N	2.484990	5.647467	-1.431312
N	2.560943	4.385119	0.371400
C	3.301839	5.116450	-0.473471
C	1.099350	5.264685	-1.137979
C	1.203577	4.395409	0.021793
C	3.046070	6.355862	-2.549908
C	3.158996	3.696208	1.484502
C	3.638567	5.616539	-3.605986
C	3.193371	4.345614	2.740622
C	3.026341	7.774642	-2.545513
C	3.738424	2.422851	1.267780
C	3.720833	4.093862	-3.585625
C	2.577264	5.718735	2.944631
C	2.434155	8.534621	-1.370211
C	3.662964	1.721822	-0.081205
C	4.202125	6.338292	-4.676884
C	3.844984	3.685219	3.799722
C	3.600349	8.446755	-3.638281
C	4.365735	1.799288	2.363871
C	4.181244	7.736937	-4.697679
C	4.427569	2.425881	3.614886
H	-0.400080	5.732399	0.758746
H	4.662658	5.789855	-5.512323
H	3.896471	4.172791	4.785125
H	3.588131	9.546290	-3.659628
H	4.820579	0.806497	2.229766
H	2.065285	6.004056	2.007354
H	3.005447	3.732642	-2.816861
H	3.359305	2.477302	-0.833748
H	4.933700	1.925386	4.454865
H	4.622593	8.280235	-5.547316
H	1.706600	7.863539	-0.876942
C	1.505250	5.695865	4.043751
H	0.726000	4.943450	3.815484
H	1.013193	6.684907	4.114702
H	1.935569	5.457097	5.039050
C	3.650034	6.785157	3.217829
H	4.410006	6.805951	2.410855
H	4.178316	6.601129	4.177070
H	3.181101	7.788233	3.266187
C	5.014969	1.139383	-0.519466
H	4.934590	0.705694	-1.536898
H	5.348627	0.323544	0.154461

H	5.809862	1.911135	-0.537194
C	2.575587	0.638015	-0.048892
H	2.458889	0.164277	-1.045036
H	1.597607	1.069716	0.245009
H	2.827477	-0.156997	0.680668
C	3.527959	8.851115	-0.334265
H	4.299074	9.523748	-0.765040
H	4.035725	7.928579	0.011990
H	3.082201	9.339704	0.554256
C	1.668524	9.799949	-1.776377
H	0.916717	9.582292	-2.561134
H	2.343014	10.597955	-2.151504
H	1.124467	10.201762	-0.899497
C	5.134094	3.642249	-3.172008
H	5.202260	2.536347	-3.141407
H	5.411842	4.027017	-2.171311
H	5.890287	4.011090	-3.895715
C	3.328344	3.446168	-4.923457
H	4.057739	3.682188	-5.725499
H	2.329306	3.780778	-5.264126
H	3.303804	2.342268	-4.819635
N	-0.016490	5.641819	-1.705613
C	-0.096320	6.399692	-2.939474
H	0.697065	7.180495	-2.999130
C	0.083763	5.492428	-4.170765
H	1.046423	4.950433	-4.121187
H	0.073794	6.082463	-5.111114
H	-0.727647	4.738302	-4.221034
C	-1.440679	7.136667	-3.008150
H	-1.562809	7.797198	-2.130480
H	-2.277313	6.409471	-3.009612
H	-1.509671	7.746109	-3.932859
H	4.379212	5.281576	-0.394924
S	-0.465270	7.902567	1.139220
C	-1.410887	8.604861	2.622041
O	-1.043827	8.569763	-0.034055
O	0.966998	8.049000	1.460477
O	-0.953879	6.377452	1.316459
F	-1.212131	7.879404	3.732537
F	-0.944378	9.842227	2.818961
F	-2.720851	8.664137	2.362406

6-OTS gas phase : -3584.68025800 A.U.

N	-1.871777	0.857355	1.667310
N	-3.145899	2.598016	1.766457
C	-1.862150	2.215136	1.470036
C	-3.123250	0.406429	2.075827
C	-3.928209	1.510646	2.137460
C	-0.774289	-0.050142	1.456560
C	-3.686105	3.932490	1.657210
C	0.022857	-0.405810	2.570497
C	-4.219474	4.331394	0.412277
C	-0.610248	-0.620413	0.172475
C	-3.711708	4.746108	2.812286
C	-0.123873	0.309205	3.907074
C	-4.213046	3.407818	-0.798426
C	-1.438762	-0.168300	-1.023883
C	-3.191053	4.233265	4.150513
C	0.998497	-1.400264	2.372245
C	-4.734259	5.636126	0.323814

C	0.381476	-1.609445	0.030160
C	-4.227563	6.044989	2.663725
C	1.165523	-2.006460	1.120019
C	-4.723848	6.487998	1.432505
H	-3.314352	-0.650376	2.280146
H	-4.981849	1.631170	2.403440
H	1.636936	-1.705047	3.214158
H	-5.135708	5.995588	-0.635275
H	0.539148	-2.077097	-0.953213
H	-4.224977	6.728421	3.522745
H	-3.998062	2.379137	-0.440256
H	-1.140000	0.754279	3.940837
H	-3.375071	3.136472	4.174813
Au	-0.263351	3.323163	0.823660
H	-5.100046	7.516529	1.335976
H	1.928770	-2.788578	0.988431
H	-2.264069	0.466243	-0.641526
C	-5.574187	3.358612	-1.509332
H	-6.389605	3.082300	-0.810841
H	-5.554601	2.613261	-2.330737
H	-5.836136	4.336792	-1.961945
C	-3.084606	3.794429	-1.765305
H	-2.102574	3.787502	-1.250930
H	-3.241471	4.818017	-2.161870
H	-3.044045	3.092052	-2.623726
C	-1.674749	4.454329	4.281940
H	-1.307618	4.054040	5.250080
H	-1.436432	5.531919	4.210205
H	-1.116163	3.956403	3.463981
C	-3.931746	4.838210	5.351363
H	-3.616259	4.333168	6.286692
H	-5.031662	4.734728	5.255972
H	-3.698303	5.915571	5.471564
C	-0.594363	0.714767	-1.960554
H	0.271748	0.153318	-2.368515
H	-0.206986	1.604696	-1.422197
H	-1.205268	1.070394	-2.814905
C	-2.077779	-1.346716	-1.774409
H	-2.688257	-1.978376	-1.097989
H	-1.313929	-1.998265	-2.246710
H	-2.736327	-0.973995	-2.584982
C	0.886899	1.467758	3.983295
H	0.757404	2.044553	4.921315
H	0.766154	2.169057	3.131350
H	1.927209	1.087759	3.952175
C	0.004504	-0.628815	5.115119
H	-0.211983	-0.075321	6.050822
H	1.031125	-1.037997	5.213383
H	-0.697958	-1.484274	5.050167
N	2.670664	5.636040	-1.265518
N	2.645572	4.409778	0.547295
C	3.429813	5.160038	-0.252434
C	1.348657	5.164529	-1.088257
C	1.330665	4.351686	0.058838
C	3.213344	6.355319	-2.392639
C	3.184920	3.729350	1.700858
C	3.945626	5.619071	-3.358479
C	3.046292	4.334290	2.973262
C	2.977408	7.748815	-2.506088
C	3.879038	2.512038	1.495093

C	4.146824	4.111007	-3.258694
C	2.337627	5.667361	3.140445
C	2.186939	8.506232	-1.453124
C	3.942637	1.855657	0.122049
C	4.488046	6.329598	-4.446204
C	3.642447	3.675223	4.065644
C	3.533032	8.403013	-3.621836
C	4.456204	1.897966	2.622842
C	4.286136	7.707755	-4.576448
C	4.344680	2.476361	3.893521
H	-0.567675	5.715022	-1.261873
H	5.067134	5.788283	-5.209387
H	3.554748	4.117906	5.068145
H	3.368891	9.482988	-3.741978
H	5.001568	0.950863	2.502075
H	1.583166	5.763550	2.334722
H	3.468399	3.731426	-2.466292
H	3.834861	2.657458	-0.636411
H	4.806943	1.982284	4.762034
H	4.712934	8.245953	-5.436637
H	1.435397	7.813520	-1.025172
C	1.597683	5.804646	4.475760
H	0.979496	4.912191	4.689668
H	0.918514	6.678135	4.426756
H	2.292736	5.957261	5.328562
C	3.327974	6.831586	2.953016
H	3.864061	6.763815	1.986279
H	4.087216	6.843098	3.763503
H	2.779450	7.793750	2.958779
C	5.274006	1.145661	-0.155507
H	5.295896	0.772115	-1.199356
H	5.417546	0.263849	0.502261
H	6.141192	1.821518	-0.013634
C	2.753239	0.897541	-0.051221
H	2.729407	0.474568	-1.076737
H	1.788518	1.411710	0.133862
H	2.824082	0.056044	0.665149
C	3.100413	8.930559	-0.289366
H	3.853511	9.676706	-0.620320
H	3.639721	8.064643	0.140851
H	2.485376	9.367208	0.521502
C	1.427691	9.714827	-2.013430
H	0.791029	9.434157	-2.876812
H	2.109818	10.528627	-2.338909
H	0.767335	10.132720	-1.230425
C	5.590050	3.771466	-2.845824
H	5.726813	2.675442	-2.751867
H	5.858237	4.230349	-1.873384
H	6.314733	4.142513	-3.599690
C	3.762505	3.385026	-4.558611
H	4.447458	3.641158	-5.392680
H	2.732024	3.638806	-4.874610
H	3.816328	2.286653	-4.413906
N	0.297414	5.626360	-1.827804
C	0.199947	5.557197	-3.284840
H	1.152356	5.942190	-3.708490
C	0.014644	4.119511	-3.796908
H	0.800697	3.454204	-3.385386
H	0.072141	4.078856	-4.904583
H	-0.965714	3.710283	-3.484702

C	-0.918687	6.492813	-3.743398
H	-0.739265	7.523439	-3.380757
H	-1.896815	6.161890	-3.337308
H	-0.994721	6.506702	-4.848304
H	4.506926	5.305885	-0.141762
S	-0.869046	7.166950	1.178495
C	-1.553566	8.770221	0.446143
O	0.605755	7.318967	0.967642
O	-1.313056	7.201282	2.598777
O	-1.532097	6.127053	0.310220
F	-2.834776	8.971985	0.807072
F	-0.830496	9.833836	0.853541
F	-1.503713	8.728487	-0.906357
