Electronic Supplementary Information

for

Simple synthesis of [Au(NHC)X] complexes utilizing aqueous ammonia: revisiting the *weak base route* mechanism

Riku Saito,[a] Alberto Prato,[b] Alessandro Rubbi,[b] Laura Orian,[b] Thomas Scattolin*[b] and Steven P. Nolan*[a]

[a.] *Department of Chemistry and Center for Sustainable Chemistry, Ghent University, Krijgslaan 281 (S-3), 9000 Ghent, Belgium. E-mail: steven.nolan@ugent.be*

[b.] *Dipartimento di Scienze Chimiche, Università degli Studi di Padova, via Marzolo 1, 35131 Padova (Italy). E-mail: thomas.scattolin@unipd.it*

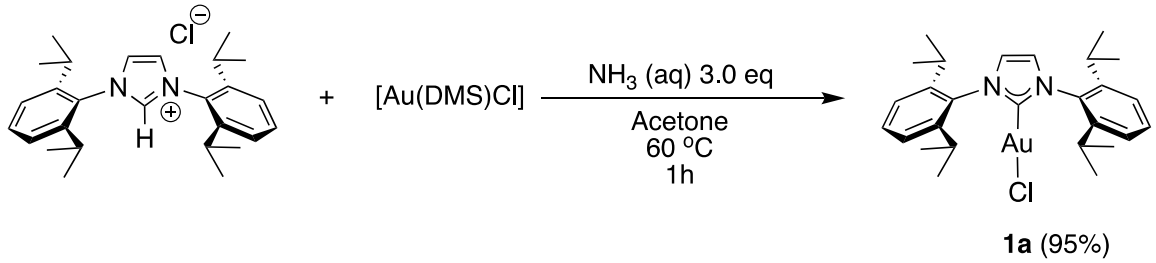
Table of Contents

General information

All syntheses were carried out in atmospheric conditions. Solvents and other reagents were obtained and utilized as supplied without additional purification unless specified otherwise. ^{1}H Nuclear Magnetic Resonance (NMR) spectra were measured using a Bruker Advance 300 or 400 Ultrashield spectrometer at 298 K. Chemical shifts (in parts per million) are referenced to the residual solvent peaks ($CDCl_3$, δ = 7.26 ppm).

Experimental procedure

Synthesis of [Au(IPr)Cl] (1a)



1a (95%)

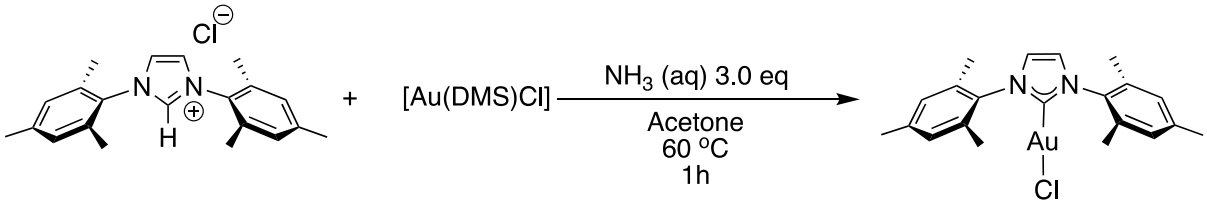
A 4 mL vial was charged with 99.9 mg of IPr·HCl (0.235 mmol, 1.0 equiv.), 69.2 mg of [Au(DMS)Cl] (0.235 mmol, 1.0 equiv.), and 1.0 mL of acetone. The reaction mixture was stirred at 60 °C for 10 minutes. Then, 47.3 µL of NH_4OH aqueous solution (12.1 mg of NH_3, 0.708 mmol, 3.0 equiv. 28-30 wt% of NH_3 dissolved in water) was added. The resulting reaction mixture was stirred at 60 °C for 50 minutes. The full conversion of [Au(IPr)Cl] was confirmed by NMR analysis of an aliquot after 1 hour of the total reaction time. After the solvent was removed under vacuum, the resulting crude product was transferred to a separation funnel using dichloromethane (10 mL), and the organic layer was extracted with water (10 mL). The collected organic layer was washed with brine (10 mL), dried over anhydrous magnesium sulfate, filtered, and concentrated to dryness. Minor impurities in the obtained solid were removed by trituration of a saturated dichloromethane solution with pentane, affording a white solid product after being dried under vacuum.

Yield: 139 mg (95%)

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.50 (t, J = 7.8 Hz, 2H), 7.29 (d, J = 7.8 Hz, 4H), 7.17 (s, 2H), 2.56 (sept, J = 6.9 Hz , 4H), 1.34 (d, J = 6.9 Hz, 12H), 1.22 (d, J = 6.9 Hz, 12H).

The data agree with the reported values.[1]

Synthesis of [Au(IMes)Cl] (1b)



1b (86%)

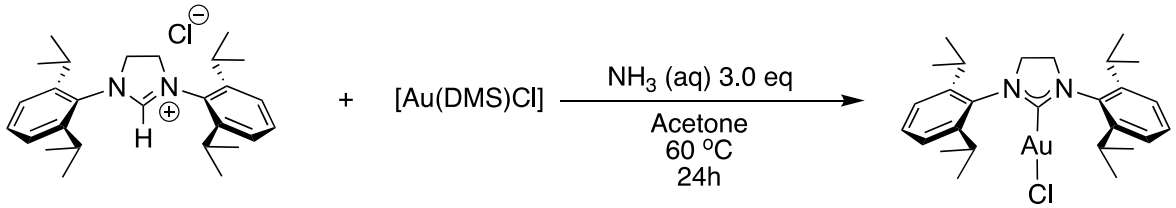
Complex [Au(IMes)Cl] **1b** was prepared in the same manner as **1a**, using 100 mg of IMes·HCl (0.293 mmol, 1.0 equiv.), 86.4 mg of [Au(DMS)Cl] (0.293 mmol, 1.0 equiv.), 58.8 µL of NH_4OH aqueous solution (15.0 mg of NH_3, 0.880 mmol, 3.0 equiv.), and 1.0 mL of acetone.

Yield: 136 mg (86%) as a white solid.

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 7.09 (s, 2H), 6.99 (s, 4H), 2.34 (s, 6H), 2.10 (s, 12H).

The data agree with the reported values.[1]

Synthesis of [Au(SIPr)Cl] (1c)



1c (84%)

Complex [Au(SIPr)Cl] **1c** was prepared analogously as **1a**, using 100 mg of SIPr·HCl (0.234 mmol, 1.0 equiv.), 68.9 mg of [Au(DMS)Cl] (0.234 mmol, 1.0 equiv.), 47.0 µL of NH_4OH aqueous solution (12.0 mg of NH_3, 0.703 mmol, 3.0 equiv.), and 1.0 mL of acetone.

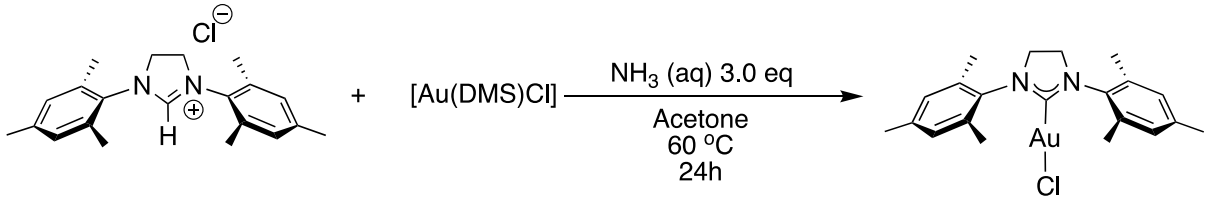
Reaction time: 24h

Yield: 122 mg (84 %) as a white solid.

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 7.42 (t, J = 7.7 Hz, 2H), 7.24 (d, J = 7.7 Hz ,4H), 4.04 (s, 4H), 3.06 (sept, J = 6.8 Hz, 4H), 1.42 (d, J = 6.8 Hz, 12H), 1.34 (d, J = 6.9 Hz, 12H).

The data agree with the reported values.[1]

Synthesis of [Au(SIMes)Cl] (1d)



1d (65%)

Complex [Au(SIMes)Cl] **1d** was prepared analogously as **1a**, using 99.9 mg of SIMes·HCl (0.291 mmol, 1.0 equiv.), 85.8 mg of [Au(DMS)Cl] (0.291 mmol, 1.0 equiv.), 58.5 µL of NH_4OH aqueous solution (14.9 mg of NH_3, 0.875 mmol, 3.0 equiv.), and 1.0 mL of acetone.

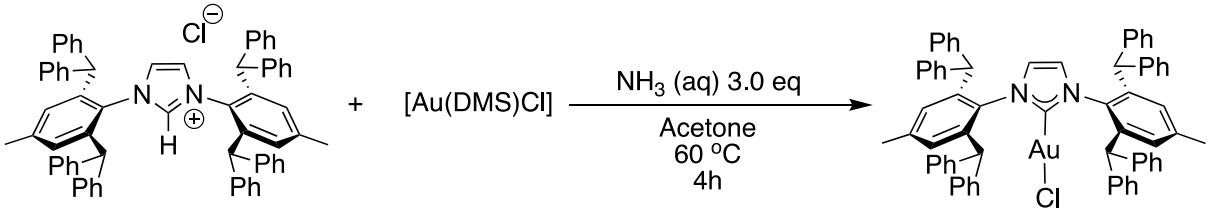
Reaction time: 24h

Yield: 102 mg (65 %) as a white solid.

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 6.94 (s, 4H), 3.98 (s, 4H), 2.32 (s, 12H), 2.30 (s, 6H).

The data agree with the reported values.[1]

Synthesis of [Au(IPr*)Cl] (1e)



1e (84%)

Complex [Au(IPr*)Cl] **1e** was prepared analogously as **1a**, using 100 mg of IPr*·HCl (0.105 mmol, 1.0 equiv.), 31.0 mg of [Au(DMS)Cl] (0.105 mmol, 1.0 equiv.), 21.1 µL of NH_4OH aqueous solution (5.4 mg of NH_3, 0.316 mmol, 3.0 equiv.), and 1.0 mL of acetone.

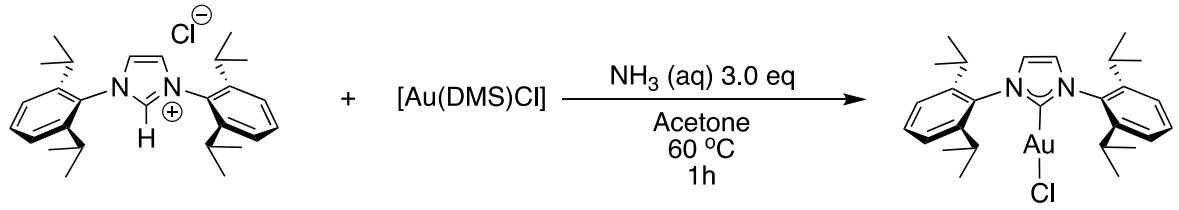
Reaction time: 4h

Yield: 101 mg (84%) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.16 (m, 24H), 7.08 (dd, J = 7.3, 1.7 Hz, 8H), 6.88 (dd, J = 6.7, 2.8 Hz, 8H), 6.84 (s, 4H), 5.80 (s, 2H), 5.26 (s, 4H), 2.22 (s, 6H).

The data agree with the reported values.[9]

Large scale synthesis of [Au(IPr)Cl] (1a)



1a (92%)

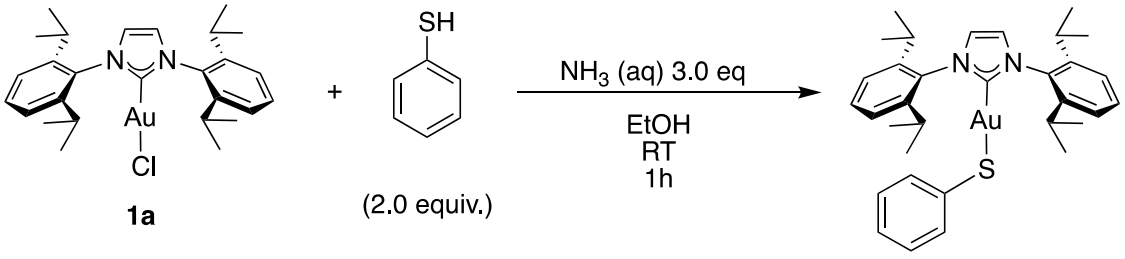
A 40 mL vial was charged with 1000 mg of IPr·HCl (2.353 mmol, 1.0 equiv.), 693.1 mg of [Au(DMS)Cl] (2.353 mmol, 1.0 equiv.), and 10 mL of acetone. The reaction mixture was stirred at 60 °C for 1 hour. Then, 472.0 µL of NH_4OH aqueous solution (120.3 mg of NH_3, 7.062 mmol, 3.0 equiv. 28-30 wt% of NH_3 dissolved in water) was added. The resulting reaction mixture was stirred at 60 °C for 1h After 1h, the full conversion of [Au(IPr)Cl] was confirmed by NMR analysis of an aliquot. After the solvent was removed under vacuum, the resulting crude product was transferred to a separation funnel using dichloromethane (50 mL), and the organic layer was extracted with water (50 mL). The collected organic layer was washed with brine (50 mL), dried over anhydrous magnesium sulfate, filtered, and concentrated to dryness. Minor impurities present in the obtained solid were removed by trituration of a saturated dichloromethane solution with pentane, affording a white solid product after being dried under vacuum.

Yield: 1.3 g (92%)

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 7.50 (t, J = 7.8 Hz, 2H), 7.29 (d, J = 7.8 Hz, 4H), 7.16 (s, 2H), 2.56 (sept, J = 6.9 Hz, 4H), 1.35 (d, J = 6.8 Hz, 12H), 1.22 (d, J = 6.9 Hz , 12H).

The data agree with the reported values.[1]

Synthesis of [Au(IPr)(SPh)] (2a)



2a (88%)

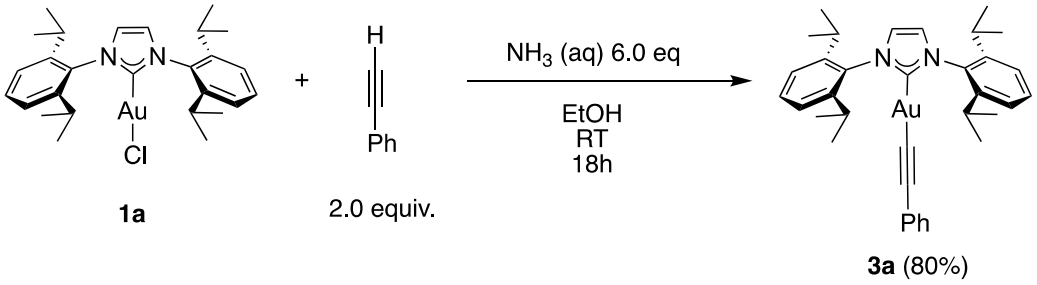
A 4 mL vial was charged with 100 mg of [Au(IPr)Cl] (0.161 mmol, 1.0 equiv.), 33.1 µL of thiophenol (35.5 mg, 0.322 mmol, 2.0 equiv.), 32.3 µL of NH_4OH aqueous solution (8.20 mg of NH_3, 0.483 mmol, 3.0 equiv.), and 1.0 mL of ethanol. The reaction mixture was stirred at room temperature for 1h. After 1 h, the full conversion of [Au(IPr)(SPh)] was confirmed by NMR analysis of an aliquot. After the solvent was removed under vacuum, the resulting crude product was transferred to a separation funnel using dichloromethane (10 mL), and the organic layer was extracted with water (10 mL). The collected organic layer was washed with brine (10 mL), dried over anhydrous magnesium sulfate, filtered, and concentrated to dryness. Minor impurities in the obtained solid were removed by trituration of a saturated dichloromethane solution with pentane, affording a white solid product after being dried under vacuum.

Yield: 97.5 mg (88%)

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.54 (t, J = 7.8 Hz, 2H), 7.32 (d, J = 7.8 Hz, 4H), 7.20 (s, 2H), 6.86-6.82 (m, 2H), 6.77-6.74 (m, 3H), 2.62 (sept, J = 6.9 Hz, 4H), 1.33 (d, J = 6.8 Hz, 12H), 1.23 (d, J = 6.9 Hz, 12H).

The data agree with the reported values.[1]

Synthesis of [Au(IPr)(C≡CPh)] (3a)



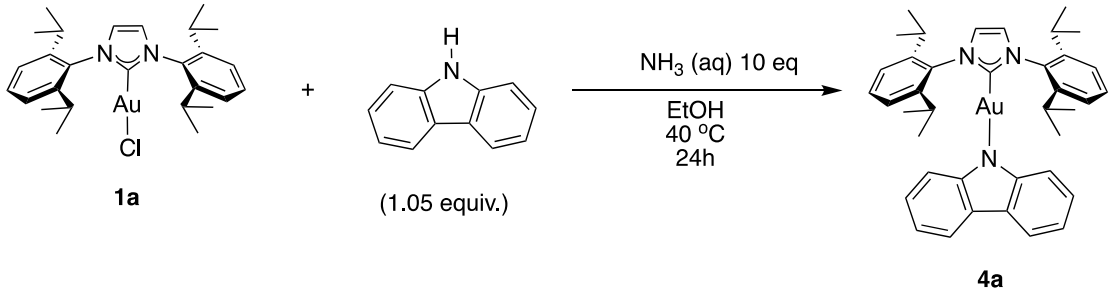
A 4 mL vial was charged with 100 mg of [Au(IPr)Cl] (0.161 mmol, 1.0 equiv.), 35.4 µL of thiophenol (32.9 mg, 0.322 mmol, 2.0 equiv.), 64.6 µL of NH_4OH aqueous solution (16.5 mg of NH_3, 0.967 mmol, 6.0 equiv.), and 1.0 mL of ethanol. The reaction mixture was stirred at room temperature for 18h. After 118h, the full conversion of [Au(IPr)(C≡CPh)] was confirmed by NMR analysis of an aliquot. After the solvent was removed under vacuum, the resulting crude product was transferred to a separation funnel using dichloromethane (10 mL), and the organic layer was extracted with water (10 mL). The collected organic layer was washed with brine (10 mL), dried over anhydrous magnesium sulfate, filtered, and concentrated to dryness. Minor impurities in the obtained solid were removed by trituration of a saturated dichloromethane solution with pentane, affording a white solid product after being dried under vacuum.

Yield: 88 mg (88%)

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.49 (t, J = 7.8 Hz, 2H), 7.31-7.28 (m, 6H), 7.12 (s, 2H), 7.11-7.01 (m, 3H), 2.60 (sept, J = 6.8 Hz, 4H), 1.38 (d, J = 6.9 Hz, 12H), 1.21 (d, J = 6.9 Hz, 12H).

The data agree with the reported values.[1]

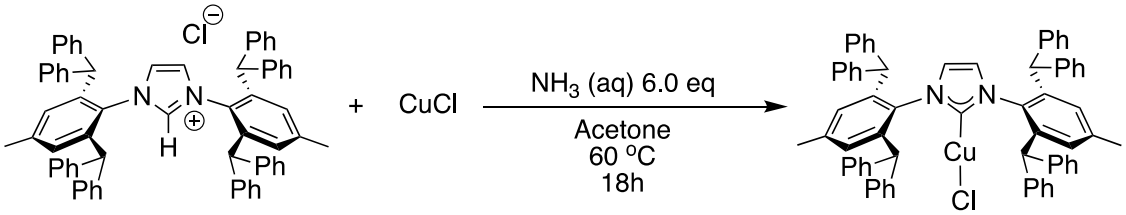
Synthesis of [Au(IPr)(cbz)] (4a)



A 4 mL vial was charged with 20.0 mg of [Au(IPr)Cl] (0.0322 mmol, 1.0 equiv.), 5.7 mg of carbazole (0.034 mmol, 1.05 equiv.), 21.5 µL of NH_4OH aqueous solution (5.48 mg of NH_3, 0.322 mmol, 10 equiv.), and 0.2 mL of ethanol. The reaction mixture was stirred at 40 °C for 24h. After 24h, the reaction progress was monitored by the ^{1}H NMR analysis of the aliquot of the reaction mixture.

Conversion: 74%.

Synthesis of [Cu(IPr*)Cl] (5a)



5a (87%)

Complex [Cu(IPr*)Cl] was prepared in the same manner as **1a**, using 100 mg of IPr*·HCl (0.11 mmol, 1.0 equiv.), 10.4 mg of CuCl (0.11 mmol, 1.0 equiv.), 42.2 µL of NH_4OH aqueous solution (10.8 mg of NH_3, 0.63 mmol, 6.0 equiv.), and 1.0 mL of acetone.

Yield: 97 mg (87%) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.20-7.14 (m, 24H), 7.01-7.00 (m, 8H), 6.90-6.87 (m, 8H), 6.84 (s, 4H), 5.80 (s, 2H), 5.19 (s, 4H), 2.22 (6H).

The data agree with the reported values.[10]

Table S1. Optimization for 4a.

Entry	Carbazole [equiv.]	Temp. [°C]	Time [h]	NMR conversion [%]
1	1.05	RT	24	37
2	**1.05**	**40**	**24**	**74**
3	1.05	60	24	34
4	1.05	40	48	67
5	2.0	RT	24	22
6	2.0	40	24	43
7	2.0	60	24	34

NMR spectra

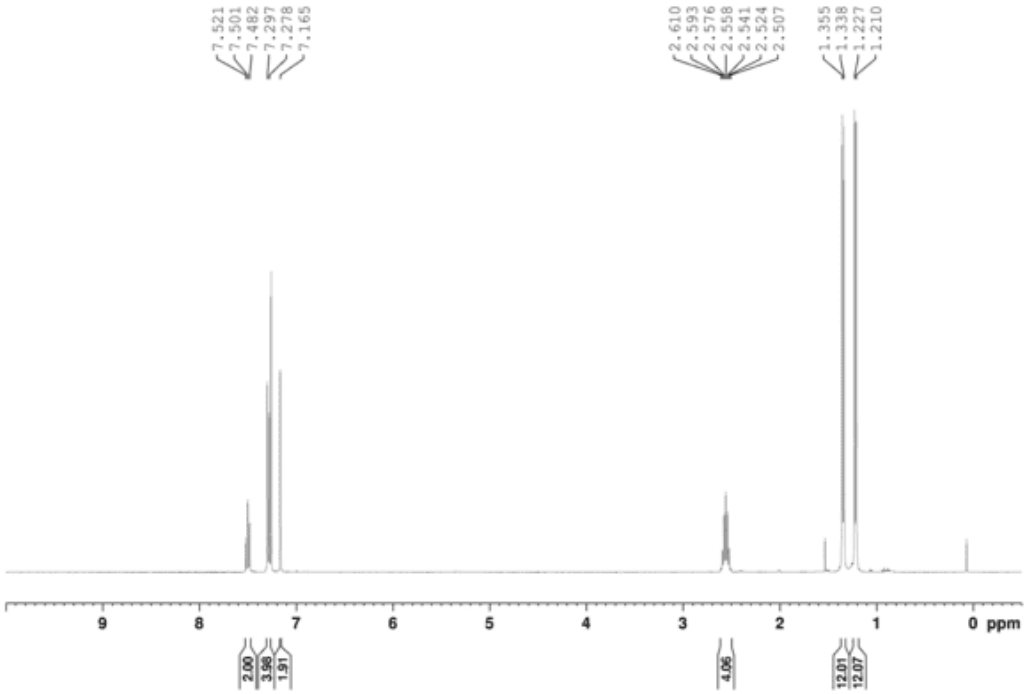


Figure S1: ^{1}H NMR spectrum of [Au(IPr)Cl] (**1a**) in $CDCl_3$ at 298 K.

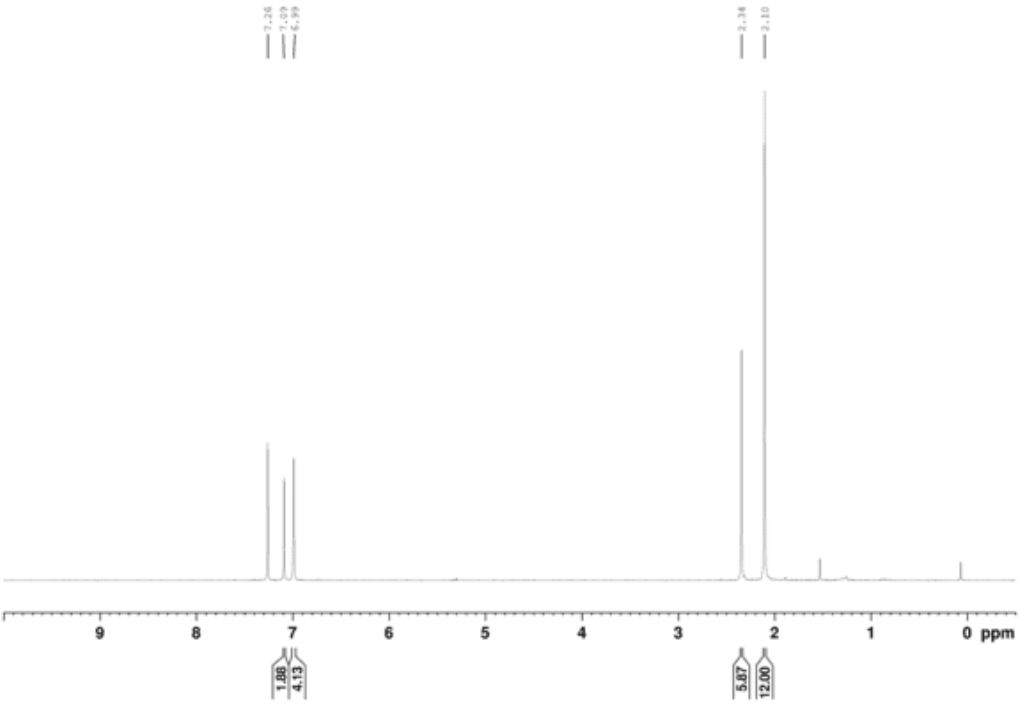


Figure S2: ^{1}H NMR spectrum of [Au(IMes)Cl] (**1b**) in $CDCl_3$ at 298 K.

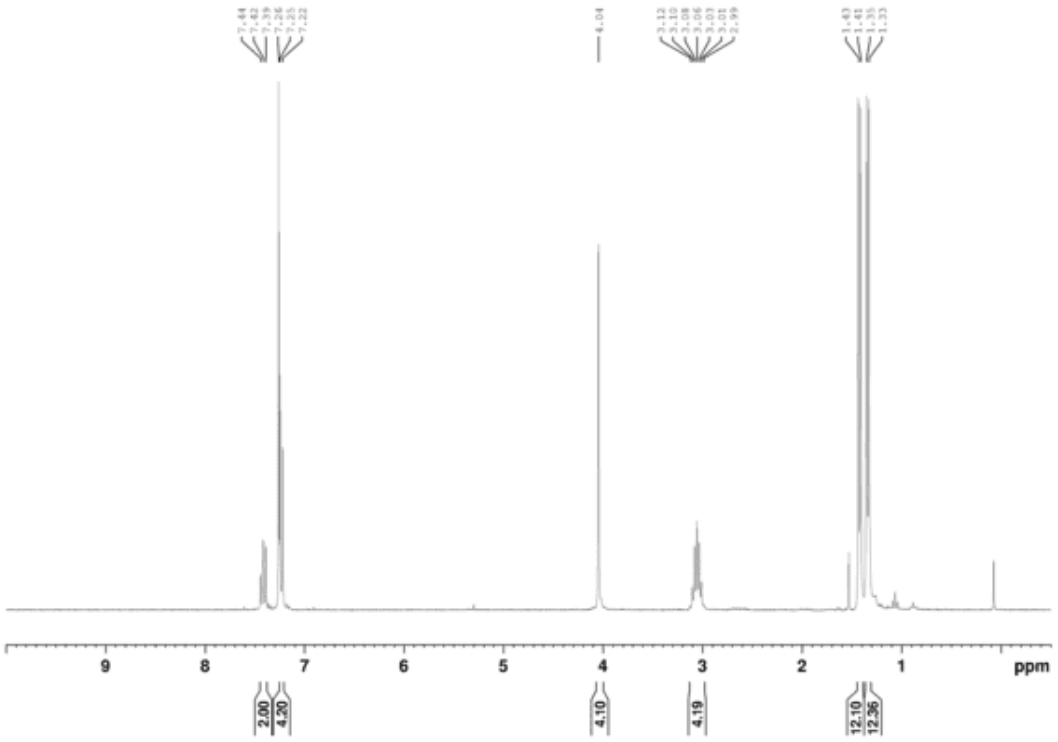


Figure S3: ^{1}H NMR spectrum of [Au(SIPr)Cl] (**1c**) in $CDCl_3$ at 298 K.

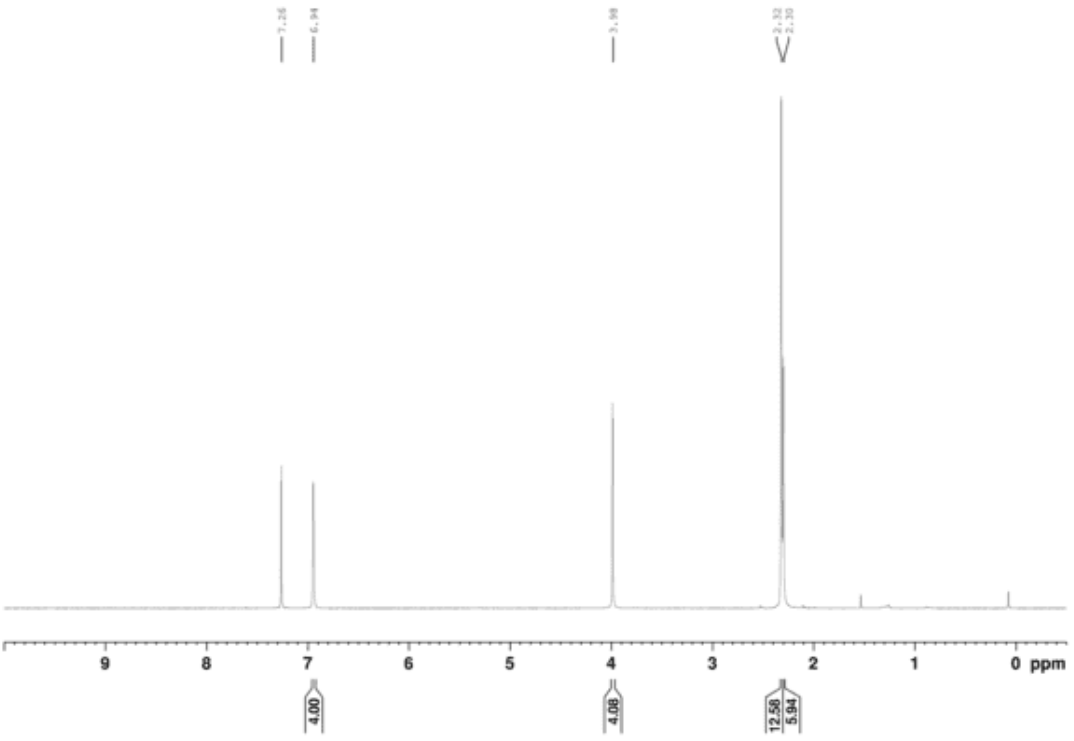


Figure S4: ^{1}H NMR spectrum of [Au(SIMes)Cl] (**1d**) in $CDCl_3$ at 298 K.

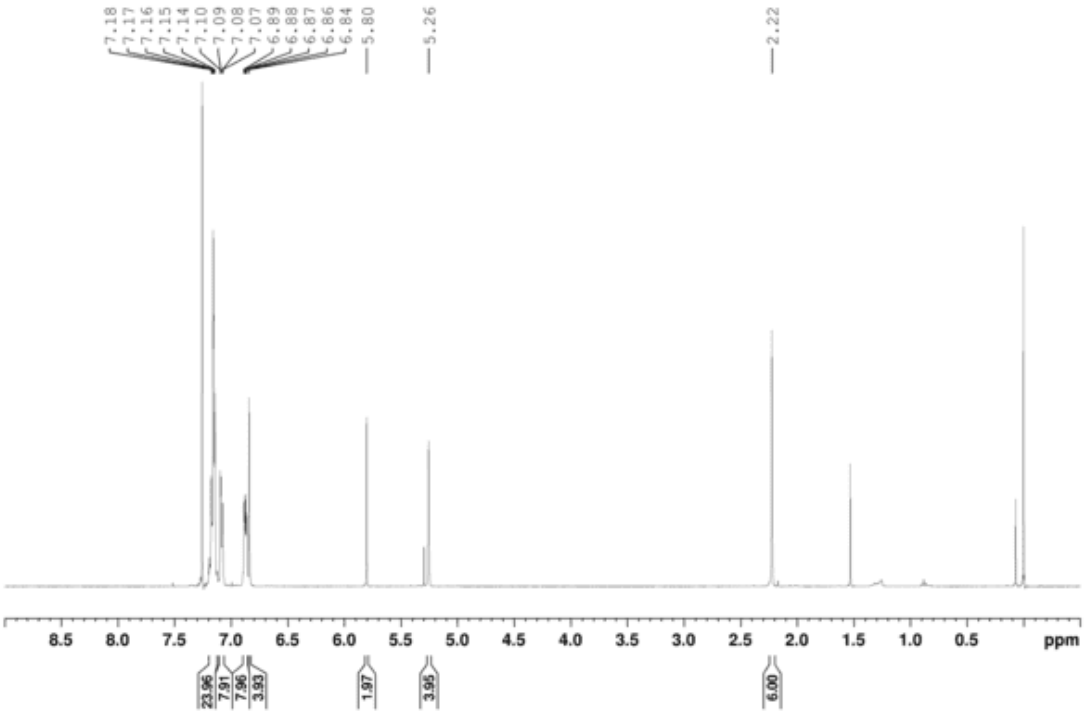


Figure S5: ^{1}H NMR spectrum of [Au(IPr*)Cl] (**1e**) in $CDCl_3$ at 298 K.

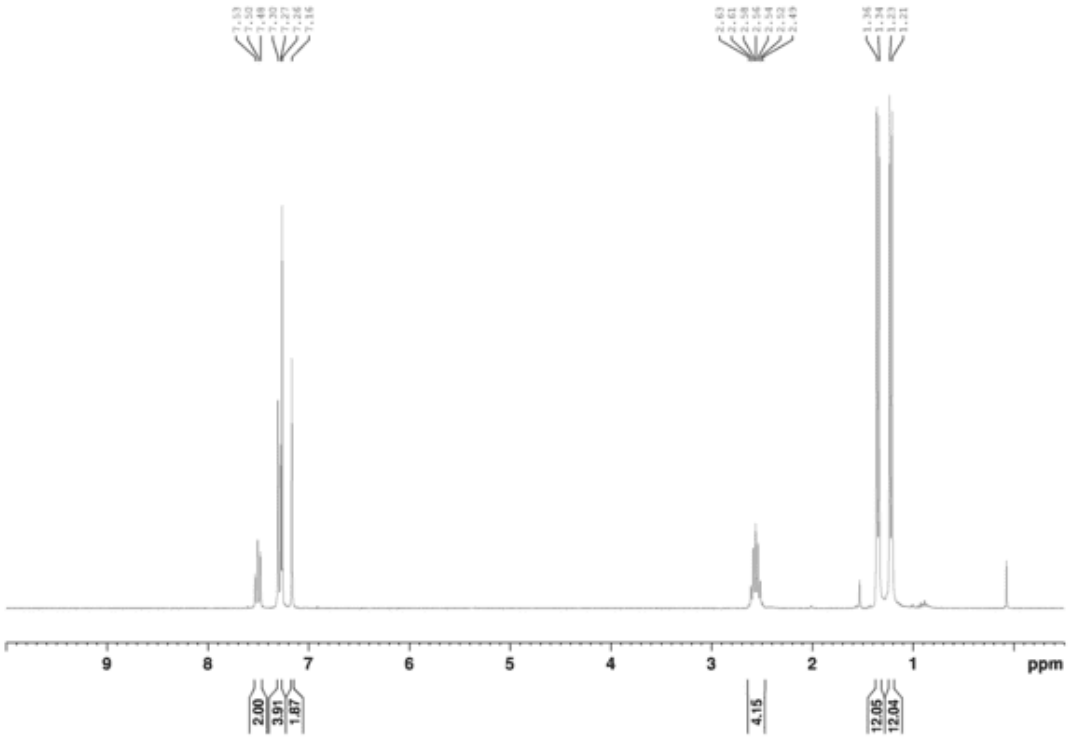


Figure S6: ^{1}H NMR spectrum of [Au(IPr)Cl] (**1a**, large scale) in $CDCl_3$ at 298 K.

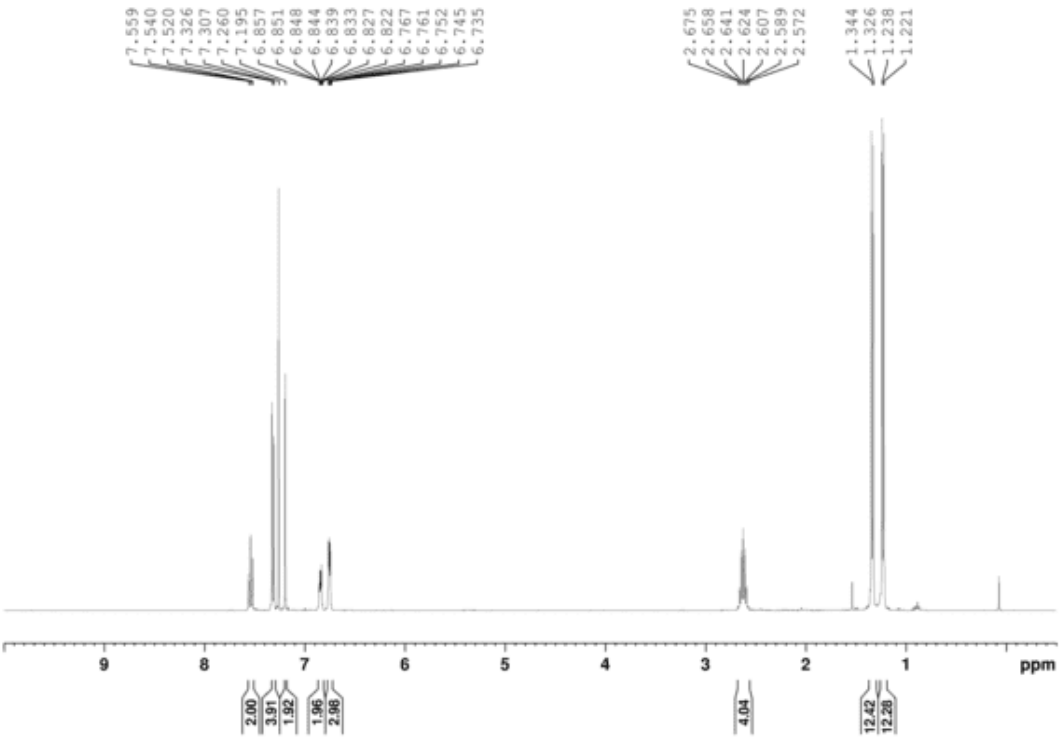


Figure S7: ^{1}H NMR spectrum of [Au(IPr)(SPh)] (**2a**) in $CDCl_3$ at 298 K.

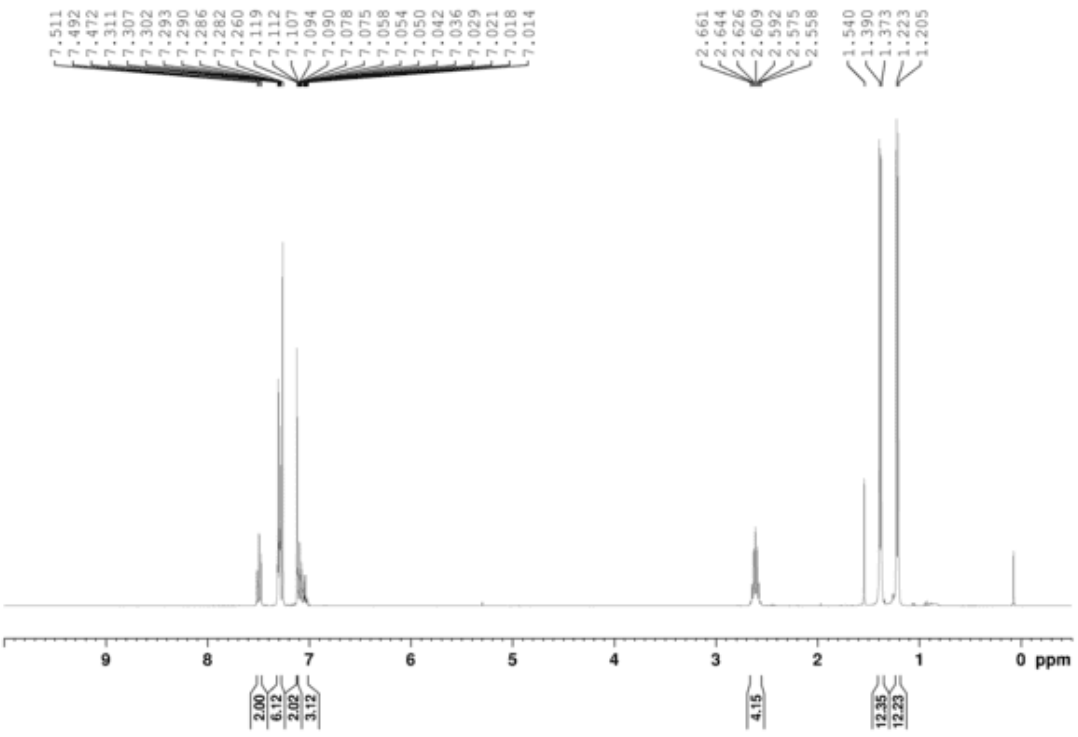


Figure S8: ^{1}H NMR spectrum of [Au(IPr)(C≡CPh)] (**3a**) in $CDCl_3$ at 298 K.

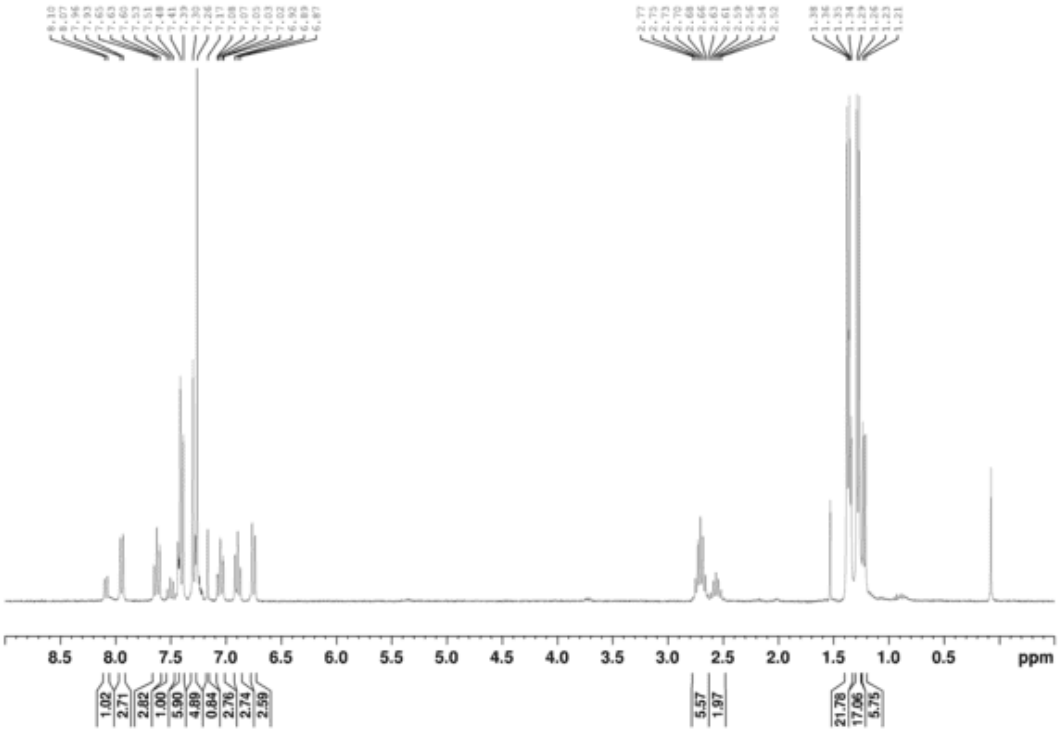


Figure S9: ^{1}H NMR spectrum of [Au(IPr)(cbz)] (**4a)** in $CDCl_3$ at 298 K.

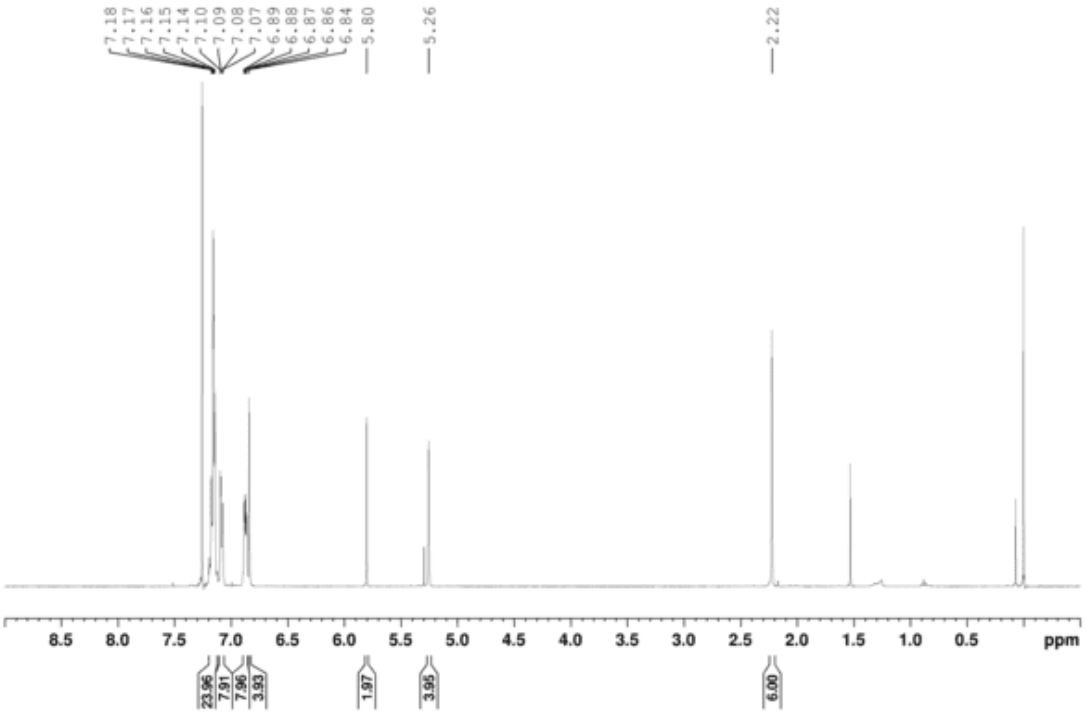


Figure S10: ^{1}H NMR spectrum of [Cu(IPr*)Cl] (**5a**) in $CDCl_3$ at 298 K.

Computational details

All DFT calculations have been performed using the Gaussian16 (revA.03) package.[2] Geometry optimizations of reactants and transition states have all been conducted with the hybrid functional PBE0[3], with the inclusion of dispersion interactions according to Grimme's DFT-D3 approach, corrected with the Becke-Johnson damping function.[4] The 6-31G split-valence basis set has been adopted for all elements, along with two sets of polarization functions (p-type for hydrogen atoms and d-type for the other elements), with the only exception of gold, for which the quasi-relativistic Stuttgart-Dresden effective core potential was used (SDD keyword in Gaussian16).[5] We denote this level of theory as PBE0-D3(BJ)/SDD,6-31G(d,p). Gas-phase vibrational frequencies calculations have been performed at the same level of theory of the optimization procedure. All minima display positive frequencies, while all transition states display a single imaginary frequency associated with the motion along the reaction coordinate. Solvation effects to the electronic energy have been included by means of the SMD model for acetone or ethanol,[6] depending on the reaction conditions. On account of this, all electronic energies discussed in the paper have been computed as single-point calculations at the SMD-PBE0-D3(BJ)/SDD,6-31G(d,p) level of theory on the gas-phase optimized geometries. Zero point and thermodynamic corrections obtained from gas-phase vibrational frequencies calculations have been then applied to compute the corresponding Gibbs free energies, along with standard state corrections.[7] The gas-phase free energy of the chloride ion has been estimated based on commonly available experimental data.[8]

References

1. T. Scattolin, N. V. Tzouras, L. Falivene, L. Cavallo and S. P. Nolan, *Dalton Trans.*, 2020, **49**, 9694–9700.
2. Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
3. C. Adamo, V. Barone, *J. Chem. Phys.* 1999, *110*, 6158-6170.
4. S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* 2011, *32*, 1456-1465.
5. D. Andrae, U. Häußermann, M. Dolg, H. Stoll, H. Preuß, *Theor. Chim. Acta* 1990, *77*, 123-141.
6. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* 2009, *113*, 6378-6396.
7. J. H. Jensen, *Phys. Chem. Chem. Phys.* 2015, *17*, 12441-12451.

8. Haynes, W.M. (Ed.). (2016). CRC Handbook of Chemistry and Physics (97th ed.). CRC Press. https://doi.org/10.1201/9781315380476

9. G. Pisanò and C. S. J. Cazin, *ACS Sustain. Chem. Eng.*, 2021, **9**, 9625–9631.

10. O. Santoro, A. Collado, A. M. Z. Slawin, S. P. Nolan and C. S. J. Cazin, *Chem. Commun.*, 2013, **49**, 10483.

Figure S11

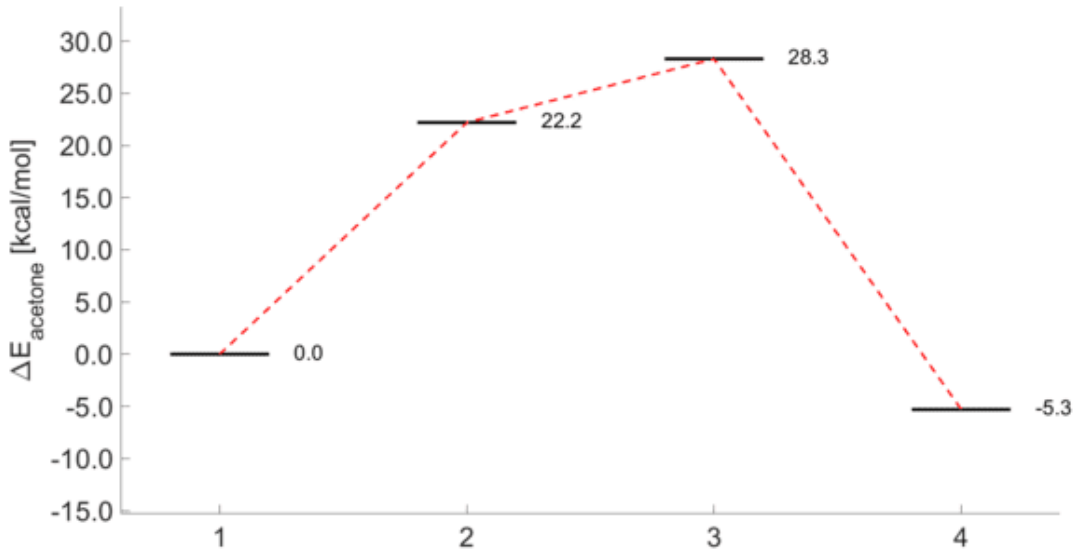


Figure S11: Computed reaction pathway for the reaction of IPr·HCl with $AuCl_2^-$: on the y-axis are plotted the electronic energies in acetone relative to the reactants of (1) NH_3, $IPrH^+$, $AuCl_2^-$; (2) NH_4^+, IPr, $AuCl_2^-$; (3) NH_4^+, $[IPr{\cdot}AuCl_2]^-_‡$; (4) NH_4^+, **1a**, Cl^- [level of theory: SMD-PBE0-D3(BJ)/SDD,6-31G(d,p)//PBE0-D3(BJ)/SDD,6-31G(d,p)].

Table S2

Entry	E(acetone) [H] [(a)]	G°(acetone) [H] [(b)]
1a	-1754.7221	-1754.2102
$AuCl_2^-$	-1056.0528	-1056.0718
Cl^-	-460.1906	-460.2191
IPr	-1158.8162	-1158.2970
IPr H^+	-1159.3233	-1158.7961
$[IPr{\cdot}AuCl_2]^-_‡$	-2214.8593	-2214.3510
NH_3	-56.4943	-56.4748
NH_4^+	-56.9661	-56.9303

Table S2: Electronic energies (a) and Gibbs standard free energies (b) in acetone [level of theory: SMD-PBE0-D3(BJ)/SDD,6-31G(d,p)//PBE0-D3(BJ)/SDD,6-31G(d,p)].

Figure S12

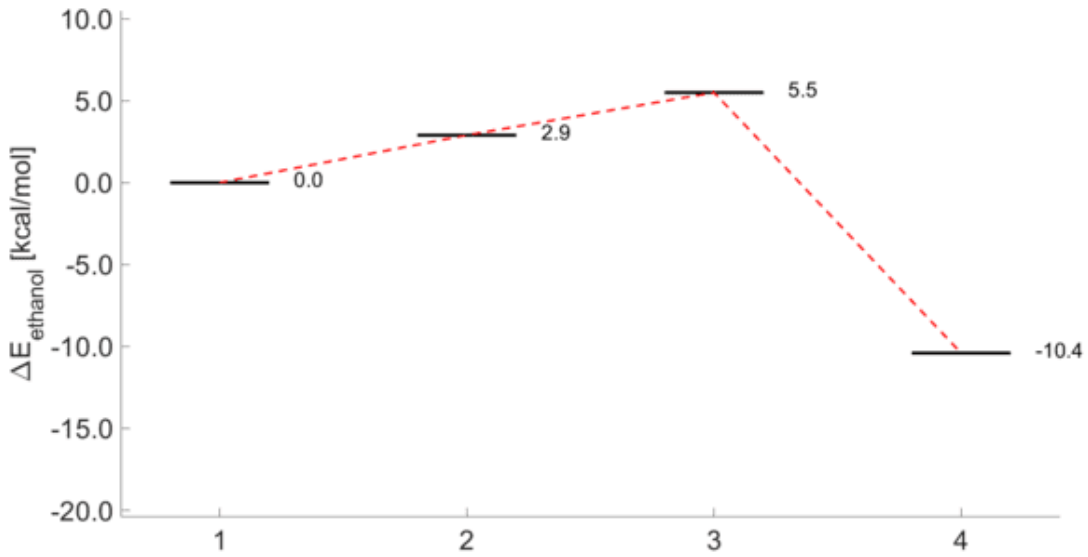


Figure S12: Computed reaction pathway for the reaction of **1a** with PhSH: on the y-axis are plotted the electronic energies in ethanol relative to the reactants of (1) NH_3, PhSH, **1a** ; (2) NH_4^+, PhS^-, **1a**; (3) NH_4^+, [**1a**·PhS]$^-_‡$; (4) NH_4^+, **2a**, Cl^- [level of theory: SMD-PBE0-D3(BJ)/SDD,6-31G(d,p)//PBE0-D3(BJ)/SDD,6-31G(d,p)].

Table S3

Entry	E(ethanol) [H] [(a)]	G°(ethanol) [H] [(b)]
1a	-1754.7184	-1754.2065
[**1a**·PhS]$^-_‡$	-2384.2704	-2383.6745
2a	-1924.1042	-1923.5081
Cl^-	-460.1916	-460.2201
NH_3	-56.4945	-56.4747
NH_4^+	-56.9673	-56.9315
PhS^-	-629.5562	-629.4913
PhSH	-630.0337	-629.9610

Table S3: Electronic energies (a) and Gibbs standard free energies (b) in ethanol [level of theory: SMD-PBE0-D3(BJ)/SDD,6-31G(d,p)//PBE0-D3(BJ)/SDD,6-31G(d,p)].

Figure S13

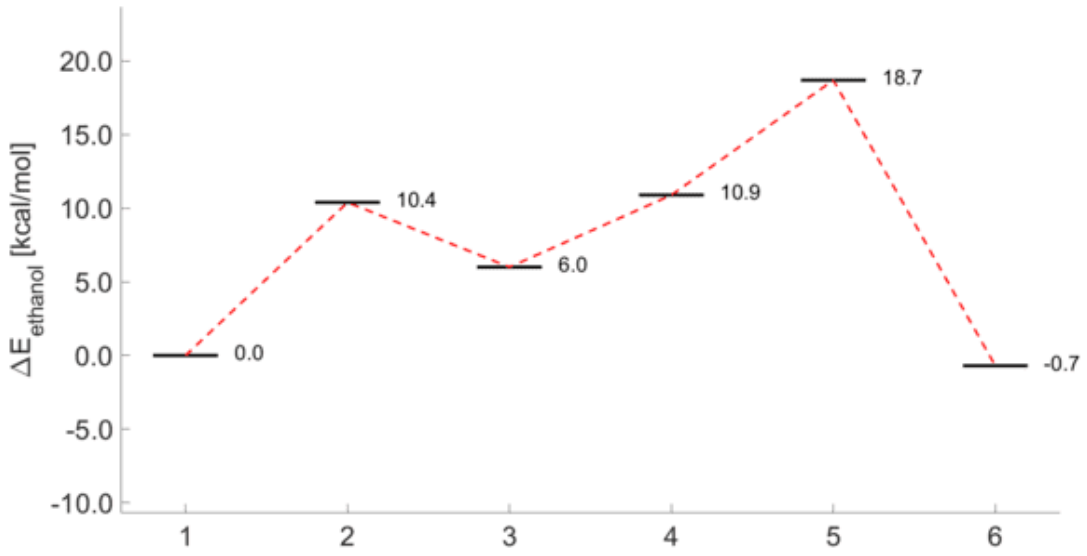


Figure S13: Computed reaction pathway for the reaction of **1a** with phenylacetylene: on the y-axis are plotted the electronic energies in ethanol relative to the reactants of (1) NH_3, phenylacetylene, **1a** ; (2) NH_3, [**1a**·phenylacetylene]$_‡$; (3) NH_3, [AuCl(I^{i}Pr)(η^2-phenylacetylene)] ; (4) NH_3, [Au(I^{i}Pr)(η^2-phenylacetylene)]$^+$, Cl^- ; (5) NH_4^+, [AuCl(I^{i}Pr)(η^2-phenylethynyl)], Cl^- ; (6) NH_4^+, **3a**, Cl^- [level of theory: SMD-PBE0-D3(BJ)/SDD,6-31G(d,p)//PBE0-D3(BJ)/SDD,6-31G(d,p)].

Table S4

Entry	E(ethanol) [H] [(a)]	G°(ethanol) [H] [(b)]
1a	-1754.7184	-1754.2065
[**1a**·phenylacetylene]$_‡$	-2062.7492	-2062.1374
3a	-1602.1024	-1601.5011
Cl^-	-460.1916	-460.2201
NH_3	-56.4945	-56.4747
NH_4^+	-56.9673	-56.9315
phenylacetylene	-308.0474	-307.9637
[AuCl(IPr)(η^2-phenylacetylene)]	-2062.7562	-2062.1411
[Au(IPr)(η^2-phenylacetylene)]$^+$	-1602.5568	-1601.9419
[AuCl(IPr)(η^2-phenylethynyl)] [(c)]	-1602.0715	-1601.4673

Table S4: Electronic energies (a) and Gibbs standard free energies (b) in ethanol [level of theory: SMD-PBE0-D3(BJ)/SDD,6-31G(d,p)//PBE0-D3(BJ)/SDD,6-31G(d,p)]. (c) The energy of the deprotonated gold-alkynyl complex has been computed as a single point on the optimized geometry of [Au(IPr)(η^2-phenylacetylene)]$^+$ after the removal of the acidic proton. Optimization of the deprotonated complex [Au(IPr)(η^2-phenylethynyl)] leads directly to the formation of the **3a** product.

Figure S14

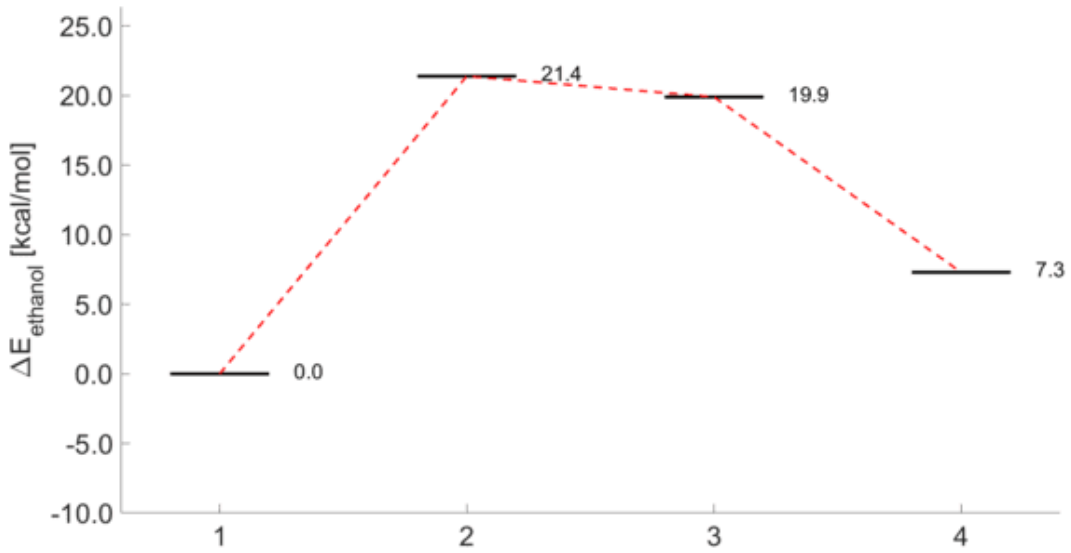


Figure S14: Computed reaction pathway for the reaction of **1a** with carbazole (CbzH): on the y-axis are plotted the electronic energies in ethanol relative to the reactants of (1) NH_3, CbzH, **1a** ; (2) NH_4^+, Cbz^-, **1a**; (3) NH_4^+, $[\mathbf{1a}\cdot Cbz]^-_{\ddagger}$; (4) NH_4^+, **4a**, Cl^- [level of theory: SMD-PBE0-D3(BJ)/SDD,6-31G(d,p)//PBE0-D3(BJ)/SDD,6-31G(d,p)].

Table S5

Entry	E(ethanol) [H] [(a)]	G°(ethanol) [H] [(b)]
1a	-1754.7184	-1754.2065
$[\mathbf{1a}\cdot Cbz]^-_{\ddagger}$	-2271.1411	-2270.4746
4a	-1810.9695	-1810.3040
Cbz^-	-516.4202	-516.2862
CbzH	-516.9271	-516.7788
Cl^-	-460.1916	-460.2201
NH_3	-56.4945	-56.4747
NH_4^+	-56.9673	-56.9315

Table S5: Electronic energies (a) and Gibbs standard free energies (b) in ethanol [level of theory: SMD-PBE0-D3(BJ)/SDD,6-31G(d,p)//PBE0-D3(BJ)/SDD,6-31G(d,p)].

Coordinates

Cartesian coordinates [in Å], gas-phase electronic energies [in Hartree], number and value of the imaginary frequencies [in cm^{-1}] of species reported in tables **S2**, **S3**, **S4** and **S5**.
Level of theory: PBE0-D3(BJ)/SDD,6-31G(d,p)

1a/ $AuC_{27}N_2H_{36}Cl$

-2215.31921055 Nimag=0

C	2.907500000	-0.792226000	2.352197000
N	1.968404000	-1.649937000	1.811112000
C	0.832726000	-1.664064000	2.549130000
N	1.077667000	-0.799525000	3.562644000
C	2.343565000	-0.253865000	3.461416000
Au	-0.815751000	-2.713657000	2.218791000
Cl	-2.726113000	-3.930160000	1.835824000
H	3.875419000	-0.651154000	1.899008000
H	2.714632000	0.457072000	4.181851000
C	2.154917000	-2.432026000	0.625933000
C	2.686918000	-3.721223000	0.757965000
C	1.768704000	-1.880259000	-0.602291000
C	2.843470000	-4.468910000	-0.409676000
C	1.945870000	-2.669318000	-1.739467000
C	2.479242000	-3.948493000	-1.645155000
H	3.243915000	-5.476405000	-0.347230000
H	1.649787000	-2.279946000	-2.709026000
H	2.603476000	-4.548920000	-2.541552000
C	0.134059000	-0.501367000	4.597942000
C	0.134644000	-1.301033000	5.748067000
C	-0.761249000	0.557000000	4.396180000
C	-0.805414000	-0.999877000	6.734333000
C	-1.681300000	0.816296000	5.412634000
C	-1.702258000	0.048118000	6.569955000
H	-0.842298000	-1.603139000	7.636577000
H	-2.398253000	1.622485000	5.289041000
H	-2.430241000	0.262436000	7.346859000
C	1.136907000	-0.507634000	-0.708243000
H	1.186357000	-0.034184000	0.278246000
C	3.033726000	-4.317035000	2.106810000
H	2.941614000	-3.527592000	2.860507000
C	1.073295000	-2.478401000	5.913118000
H	1.780957000	-2.468342000	5.077194000
C	-0.781738000	1.363070000	3.113771000
H	0.088768000	1.071883000	2.516055000
C	-0.342397000	-0.628304000	-1.083983000
H	-0.460074000	-1.082392000	-2.073615000
H	-0.881850000	-1.250318000	-0.362920000
H	-0.812360000	0.360538000	-1.107785000
C	1.893070000	0.392556000	-1.686188000
H	2.947347000	0.488989000	-1.408605000
H	1.850924000	0.000823000	-2.707706000
H	1.449617000	1.393213000	-1.700122000
C	-2.031687000	1.029044000	2.294927000
H	-2.087742000	-0.043119000	2.082247000
H	-2.941221000	1.312018000	2.835395000
H	-2.021251000	1.570733000	1.343205000
C	-0.670472000	2.864489000	3.381168000
H	-1.534764000	3.239027000	3.939168000
H	0.228637000	3.103238000	3.957722000
H	-0.627505000	3.414857000	2.435991000
C	1.888189000	-2.379443000	7.203365000
H	1.245874000	-2.425326000	8.088821000
H	2.596660000	-3.211287000	7.268572000
H	2.453752000	-1.443539000	7.249076000
C	0.296236000	-3.795384000	5.838254000
H	-0.260516000	-3.870308000	4.898991000
H	0.981247000	-4.647308000	5.903403000
H	-0.421479000	-3.875047000	6.661625000
C	2.036464000	-5.419095000	2.474711000
H	2.090161000	-6.249763000	1.762991000
H	2.254304000	-5.814065000	3.472633000
H	1.010234000	-5.038670000	2.469620000
C	4.474924000	-4.826101000	2.152110000
H	5.187502000	-4.034738000	1.899519000
H	4.714400000	-5.195614000	3.154221000
H	4.631633000	-5.653043000	1.451916000

$AuCl_2^-$

-1055.97536144 Nimag=0

Cl	-1.133673000	-3.426987000	-1.335156000
Au	-1.134697000	-3.424242000	0.985309000
Cl	-1.134583000	-3.424548000	3.305770000

IPr / $C_{27}N_2H_{36}$

-1158.78671282 Nimag=0

C	0.771908000	2.893153000	-1.162273000
C	0.595144000	3.172530000	0.148441000
N	0.869970000	1.994089000	0.830204000
C	1.212524000	0.958322000	0.006615000
N	1.138857000	1.554886000	-1.221032000
H	0.302438000	4.080150000	0.653123000
H	0.676297000	3.507899000	-2.043809000
C	1.401998000	0.881171000	-2.453901000
C	2.731449000	0.659743000	-2.835529000
C	0.312314000	0.483635000	-3.245742000
C	2.956767000	0.020943000	-4.057050000
C	0.588165000	-0.140646000	-4.461717000
C	1.898544000	-0.368135000	-4.865551000
H	3.975921000	-0.171264000	-4.377981000
H	-0.230377000	-0.458723000	-5.098880000
H	2.094085000	-0.857594000	-5.815373000
C	-1.108800000	0.647686000	-2.743387000
H	-1.146944000	1.561051000	-2.138839000
C	3.887152000	1.031019000	-1.930643000
H	3.521874000	1.773089000	-1.212565000
C	-2.141880000	0.793956000	-3.856427000
H	-1.874520000	1.591959000	-4.556072000
H	-2.259271000	-0.133056000	-4.427725000
H	-3.120095000	1.030623000	-3.426913000
C	-1.454909000	-0.525104000	-1.819442000
H	-2.450176000	-0.391935000	-1.380764000
H	-1.452082000	-1.466021000	-2.380559000
H	-0.724778000	-0.609411000	-1.010042000
C	5.060997000	1.654785000	-2.682673000

H	5.818182000	1.999551000	-1.971284000
H	5.549880000	0.936215000	-3.348900000
H	4.743540000	2.511219000	-3.285313000
C	4.322558000	-0.202559000	-1.134274000
H	5.142431000	0.046045000	-0.452050000
H	3.482353000	-0.585475000	-0.548194000
H	4.667764000	-0.994047000	-1.808904000
C	0.803595000	1.894521000	2.254597000
C	-0.316183000	1.290687000	2.840787000
C	1.859218000	2.426258000	3.013125000
C	-0.363945000	1.230861000	4.235455000
C	1.760716000	2.352619000	4.402116000
C	0.658100000	1.762404000	5.008608000
H	-1.215420000	0.763131000	4.720037000
H	2.557531000	2.755906000	5.018248000
H	0.599589000	1.712489000	6.092146000
C	-1.405745000	0.659342000	2.000190000
H	-1.338172000	1.086094000	0.993686000
C	3.099259000	2.974048000	2.334125000
H	2.787480000	3.436980000	1.390852000
C	-1.143955000	-0.844785000	1.879469000
H	-1.905824000	-1.321805000	1.253825000
H	-0.161974000	-1.018974000	1.430652000
H	-1.166449000	-1.319706000	2.866728000
C	-2.810516000	0.942220000	2.528554000
H	-3.557011000	0.555672000	1.827429000
H	-2.992222000	0.454702000	3.492136000
H	-2.984478000	2.015101000	2.655451000
C	4.036580000	1.812928000	1.984445000
H	3.517372000	1.063622000	1.380909000
H	4.906495000	2.172790000	1.423649000
H	4.396419000	1.325725000	2.897317000
C	3.826084000	4.040660000	3.147425000
H	4.633007000	4.477122000	2.550974000
H	3.152673000	4.847619000	3.452592000
H	4.285376000	3.622385000	4.049425000

IPr H^+ / $C_{27}N_2H_{37}^+$

-1159.23671401 Nimag=0

C	1.481057000	0.922663000	-1.050287000
C	1.244533000	1.630301000	0.088841000
N	1.181262000	0.719725000	1.121057000
C	1.372844000	-0.502887000	0.627014000
N	1.557310000	-0.405564000	-0.689364000
H	1.116254000	2.686557000	0.263746000
H	1.601869000	1.233104000	-2.075897000
C	1.798336000	-1.519446000	-1.573408000
C	3.127647000	-1.905397000	-1.789784000
C	0.687638000	-2.146499000	-2.152592000
C	3.328587000	-3.001330000	-2.629280000
C	0.951028000	-3.236406000	-2.982794000
C	2.253992000	-3.658466000	-3.215630000
H	4.338709000	-3.344048000	-2.826809000
H	0.125798000	-3.760690000	-3.452938000
H	2.434674000	-4.509264000	-3.865068000
C	-0.733669000	-1.707120000	-1.861032000
H	-0.700640000	-0.690712000	-1.449603000
C	4.292355000	-1.209853000	-1.112873000
H	3.950577000	-0.225561000	-0.769430000
C	-1.599491000	-1.651294000	-3.119291000
H	-1.141510000	-1.032094000	-3.895389000
H	-1.770964000	-2.646942000	-3.538707000
H	-2.579577000	-1.229705000	-2.879250000
C	-1.362182000	-2.617546000	-0.800870000
H	-2.375836000	-2.283997000	-0.559369000
H	-1.422291000	-3.648752000	-1.162404000
H	-0.779121000	-2.628019000	0.125874000
C	5.464539000	-0.968272000	-2.063347000
H	6.232004000	-0.370102000	-1.564262000
H	5.936990000	-1.905375000	-2.372048000
H	5.148438000	-0.436078000	-2.964629000
C	4.739397000	-2.003190000	0.119591000
H	5.556725000	-1.488000000	0.633054000
H	3.922728000	-2.140414000	0.835975000
H	5.093834000	-2.997801000	-0.168187000
C	0.951398000	1.021974000	2.511765000
C	-0.372476000	1.033119000	2.969698000
C	2.067082000	1.283965000	3.317437000
C	-0.562606000	1.323988000	4.320981000
C	1.814064000	1.569467000	4.659542000
C	0.516371000	1.589448000	5.154624000
H	-1.570124000	1.341190000	4.724481000
H	2.646195000	1.777292000	5.324840000
H	0.343925000	1.813674000	6.202572000
C	-1.556515000	0.728046000	2.074165000
H	-1.192472000	0.595834000	1.048229000
C	3.488618000	1.252583000	2.792843000
H	3.458497000	1.047998000	1.715919000
C	-2.230148000	-0.580931000	2.494464000
H	-3.056257000	-0.819350000	1.818014000
H	-1.526485000	-1.419106000	2.482962000
H	-2.638944000	-0.506694000	3.506750000
C	-2.555414000	1.886649000	2.052631000
H	-3.371721000	1.669336000	1.357790000
H	-2.998123000	2.051301000	3.039468000
H	-2.079595000	2.820730000	1.740587000
C	4.287746000	0.124721000	3.450581000
H	3.811706000	-0.848873000	3.298657000
H	5.297851000	0.080045000	3.032751000
H	4.381057000	0.282757000	4.529276000
C	4.178951000	2.605687000	2.976863000
H	5.183973000	2.580142000	2.545916000
H	3.619016000	3.410903000	2.492534000
H	4.280104000	2.860793000	4.035984000
H	1.377657000	-1.417688000	1.197916000

$[IPr{\cdot}AuCl_2]^{-}_{‡}$ / $AuC_{27}N_2H_{36}Cl_2^-$

-2214.75225769 Nimag=1, ν=-55.3072

C	0.774634000	2.811139000	-1.145290000
C	0.603323000	3.087354000	0.168107000
N	0.887954000	1.911296000	0.846212000
C	1.227601000	0.887213000	0.015376000
N	1.145560000	1.476158000	-1.209801000
H	0.310907000	3.991434000	0.679329000
H	0.671306000	3.424308000	-2.027105000
C	1.421071000	0.812211000	-2.444855000

C	2.751323000	0.658654000	-2.844939000
C	0.338254000	0.352654000	-3.208543000
C	2.987708000	0.034932000	-4.071166000
C	0.624157000	-0.258735000	-4.427079000
C	1.937196000	-0.414526000	-4.856109000
H	4.011842000	-0.114642000	-4.401911000
H	-0.187114000	-0.637433000	-5.040528000
H	2.140592000	-0.907316000	-5.803125000
C	-1.078626000	0.451386000	-2.678511000
H	-1.139409000	1.354012000	-2.058237000
C	3.909422000	1.112460000	-1.982117000
H	3.496858000	1.601975000	-1.095106000
C	-2.127958000	0.589531000	-3.779195000
H	-1.893722000	1.410229000	-4.465961000
H	-2.218052000	-0.329895000	-4.367912000
H	-3.110212000	0.782756000	-3.335281000
C	-1.385228000	-0.748542000	-1.775858000
H	-2.388946000	-0.652228000	-1.343596000
H	-1.332206000	-1.680918000	-2.346114000
H	-0.653241000	-0.839543000	-0.969191000
C	4.787311000	2.132712000	-2.708790000
H	5.591606000	2.479578000	-2.050527000
H	5.253870000	1.697381000	-3.599839000
H	4.206378000	3.004687000	-3.028295000
C	4.720245000	-0.089799000	-1.495919000
H	5.509455000	0.236707000	-0.809348000
H	4.073376000	-0.804145000	-0.977259000
H	5.191567000	-0.613073000	-2.335810000
C	0.812140000	1.806835000	2.269458000
C	-0.340577000	1.264739000	2.844232000
C	1.897284000	2.267543000	3.028857000
C	-0.401058000	1.208702000	4.237636000
C	1.788877000	2.194617000	4.415745000
C	0.648699000	1.672296000	5.015424000
H	-1.277311000	0.777548000	4.714028000
H	2.613031000	2.531112000	5.036640000
H	0.588690000	1.610934000	6.098795000
C	-1.479275000	0.723161000	2.006666000
H	-1.230025000	0.886696000	0.954258000
C	3.165243000	2.749063000	2.351933000
H	2.879377000	3.201531000	1.394437000
C	-1.623410000	-0.786525000	2.204746000
H	-2.392895000	-1.185434000	1.534224000
H	-0.675819000	-1.292705000	1.996637000
H	-1.911576000	-1.023823000	3.235350000
C	-2.787983000	1.461092000	2.293842000
H	-3.588318000	1.082191000	1.648511000
H	-3.106314000	1.321248000	3.333232000
H	-2.686891000	2.537497000	2.117603000
C	4.078769000	1.557824000	2.043746000
H	3.561155000	0.800626000	1.449238000
H	4.971862000	1.893757000	1.502357000
H	4.390060000	1.064021000	2.969342000
C	3.909315000	3.816646000	3.150896000
H	4.740962000	4.213019000	2.558872000
H	3.254755000	4.650925000	3.425752000
H	4.338789000	3.405424000	4.070940000
Cl	2.179210000	-1.430822000	2.986697000
Au	1.845043000	-1.606410000	0.621291000
Cl	1.725147000	-2.648295000	-1.531960000

NH_3

-56.4879050732 Nimag=0

N	-0.034787000	-0.000003000	-1.470383000
H	-0.034816000	0.935899000	-1.077674000
H	0.775713000	-0.467971000	-1.077676000
H	-0.845263000	-0.467925000	-1.077679000

NH_4^+

-56.8375585659 Nimag=0

N	-0.753513000	-1.928560000	-0.869522000
H	-0.527289000	-2.608737000	-0.137038000
H	-1.651040000	-2.174488000	-1.298810000
H	-0.018810000	-1.939057000	-1.584005000
H	-0.816667000	-0.991985000	-0.458204000

$[1a\cdot PhS]^-_‡$ / $AuC_{33}N_2H_{41}SCl^-$

-2384.16103575 Nimag=1, v=-24.4807

C	1.761497000	-7.068092000	-2.357957000
N	0.704841000	-6.248257000	-1.992213000
C	1.009798000	-5.493931000	-0.899770000
N	2.302120000	-5.826098000	-0.629052000
C	2.767174000	-6.806182000	-1.491500000
Au	-0.155315000	-4.227622000	0.093232000
Cl	-1.726315000	-3.815589000	1.874208000
H	1.693879000	-7.746906000	-3.192915000
H	3.764279000	-7.207991000	-1.410867000
C	-0.582496000	-6.254762000	-2.610438000
C	-1.488765000	-7.256250000	-2.240817000
C	-0.891764000	-5.241534000	-3.532173000
C	-2.733045000	-7.265342000	-2.874577000
C	-2.147509000	-5.296448000	-4.137064000
C	-3.053941000	-6.302519000	-3.820960000
H	-3.464568000	-8.021271000	-2.603734000
H	-2.427921000	-4.527097000	-4.848422000
H	-4.029222000	-6.319364000	-4.300310000
C	3.031103000	-5.321475000	0.493698000
C	2.931803000	-6.026720000	1.699786000
C	3.779076000	-4.138900000	0.352943000
C	3.667968000	-5.554668000	2.788093000
C	4.495165000	-3.712579000	1.472469000
C	4.450986000	-4.416083000	2.670690000
H	3.605046000	-6.075324000	3.739827000
H	5.063836000	-2.791890000	1.417880000
H	5.010895000	-4.052207000	3.528212000
C	0.094325000	-4.129091000	-3.830177000
H	0.583906000	-3.867594000	-2.883888000
C	-1.182013000	-8.236111000	-1.126711000
H	-0.107901000	-8.187526000	-0.919976000
C	2.020672000	-7.226493000	1.861882000
H	1.559733000	-7.436673000	0.892062000
C	3.753344000	-3.322666000	-0.928198000
H	2.692883000	-3.202851000	-1.198251000
C	-0.574736000	-2.849582000	-4.320358000
H	-0.993386000	-2.960826000	-5.328960000
H	-1.365560000	-2.532850000	-3.635545000

H	0.164638000	-2.045071000	-4.345339000
C	1.167429000	-4.590009000	-4.821358000
H	1.719134000	-5.459499000	-4.452555000
H	0.717770000	-4.855268000	-5.786022000
H	1.890319000	-3.785178000	-4.991888000
C	4.323736000	-1.918261000	-0.752865000
H	3.867962000	-1.390966000	0.086799000
H	5.413117000	-1.942294000	-0.614539000
H	4.115701000	-1.333465000	-1.653175000
C	4.487319000	-4.010715000	-2.085270000
H	5.540521000	-4.178381000	-1.827807000
H	4.045351000	-4.969099000	-2.363282000
H	4.457619000	-3.367108000	-2.971144000
C	2.801298000	-8.472830000	2.282264000
H	3.271929000	-8.338191000	3.262581000
H	2.131261000	-9.336633000	2.353127000
H	3.592351000	-8.710965000	1.562986000
C	0.884083000	-6.910696000	2.837238000
H	0.301760000	-6.048766000	2.494863000
H	0.208192000	-7.769385000	2.920349000
H	1.272380000	-6.690230000	3.838154000
C	-1.912195000	-7.812904000	0.152154000
H	-2.997889000	-7.846131000	0.006608000
H	-1.658360000	-8.488781000	0.976905000
H	-1.640579000	-6.792584000	0.443845000
C	-1.506249000	-9.679692000	-1.509997000
H	-0.987171000	-9.979436000	-2.426643000
H	-1.203468000	-10.359469000	-0.706515000
H	-2.580121000	-9.824940000	-1.670247000
S	0.190075000	-1.749457000	-0.969727000
C	1.178719000	-0.925750000	0.211985000
C	1.717784000	0.348158000	-0.069640000
C	2.561066000	0.997441000	0.823505000
C	2.902416000	0.407001000	2.041301000
C	2.358541000	-0.840409000	2.349450000
C	1.510853000	-1.491584000	1.461088000
H	1.469794000	0.812021000	-1.020701000
H	2.963978000	1.974572000	0.561971000
H	3.567903000	0.911948000	2.736884000
H	2.598695000	-1.322127000	3.295165000
H	1.086614000	-2.456282000	1.725376000

2a/ $AuC_{33}N_2H_{41}S$

-1924.06315049 Nimag=0

C	2.615791000	-0.993841000	2.082389000
N	1.661655000	-1.941651000	1.762294000
C	0.631969000	-1.919935000	2.642337000
N	0.958303000	-0.942055000	3.519691000
C	2.170865000	-0.360818000	3.195898000
Au	-1.033677000	-3.029495000	2.535281000
H	3.509575000	-0.865070000	1.493467000
H	2.593304000	0.438275000	3.783500000
C	1.735260000	-2.844917000	0.652429000
C	2.378049000	-4.075825000	0.843638000
C	1.135956000	-2.470937000	-0.557495000
C	2.438886000	-4.942038000	-0.248534000
C	1.226318000	-3.372817000	-1.618539000
C	1.877120000	-4.590207000	-1.469627000
H	2.923526000	-5.907388000	-0.137151000
H	0.760705000	-3.123987000	-2.567136000
H	1.933974000	-5.278429000	-2.308215000
C	0.120922000	-0.551432000	4.613408000
C	0.294275000	-1.192623000	5.846892000
C	-0.853320000	0.429178000	4.385774000
C	-0.549928000	-0.809448000	6.889640000
C	-1.671367000	0.776973000	5.461665000
C	-1.520823000	0.166324000	6.700108000
H	-0.452939000	-1.290018000	7.858487000
H	-2.443610000	1.527649000	5.321858000
H	-2.171395000	0.447236000	7.523169000
C	0.379490000	-1.169566000	-0.725281000
H	0.487968000	-0.592162000	0.199353000
C	2.927930000	-4.495337000	2.191393000
H	2.916503000	-3.620474000	2.850329000
C	1.307315000	-2.302560000	6.037863000
H	1.968466000	-2.310600000	5.164371000
C	-1.057226000	1.067435000	3.027116000
H	-0.261646000	0.713539000	2.362931000
C	-1.114731000	-1.435903000	-0.927801000
H	-1.298679000	-2.033009000	-1.826721000
H	-1.536653000	-1.985800000	-0.081545000
H	-1.656376000	-0.489446000	-1.029318000
C	0.959451000	-0.326803000	-1.862547000
H	2.024475000	-0.124770000	-1.710255000
H	0.849087000	-0.829184000	-2.829112000
H	0.434810000	0.631637000	-1.928655000
C	-2.390222000	0.623708000	2.418706000
H	-2.444213000	-0.466987000	2.342644000
H	-3.233578000	0.962333000	3.030095000
H	-2.509672000	1.045651000	1.415242000
C	-0.950662000	2.591514000	3.096868000
H	-1.744039000	3.021478000	3.716996000
H	0.009552000	2.907254000	3.516730000
H	-1.045493000	3.023850000	2.095745000
C	2.183020000	-2.082061000	7.271253000
H	1.597630000	-2.123304000	8.195473000
H	2.947413000	-2.862836000	7.335265000
H	2.687080000	-1.111313000	7.236916000
C	0.597928000	-3.658951000	6.089225000
H	0.001537000	-3.824832000	5.186298000
H	1.327632000	-4.470970000	6.175851000
H	-0.074979000	-3.713352000	6.951737000
C	2.017491000	-5.554349000	2.820280000
H	1.997321000	-6.463247000	2.209204000
H	2.375894000	-5.825573000	3.818999000
H	0.990614000	-5.185347000	2.909269000
C	4.374680000	-4.980761000	2.101911000
H	5.024431000	-4.223235000	1.652843000
H	4.757824000	-5.212053000	3.100792000
H	4.458574000	-5.892354000	1.501456000
S	-2.976624000	-4.250717000	2.241824000
C	-2.891781000	-4.483066000	0.477785000
C	-1.771700000	-5.043831000	-0.152489000
C	-3.986380000	-4.113454000	-0.313945000
C	-1.748428000	-5.216973000	-1.532189000
C	-3.959301000	-4.291236000	-1.693900000
C	-2.839469000	-4.841330000	-2.312876000

H	-0.914623000	-5.334268000	0.448422000
H	-4.855913000	-3.674079000	0.165600000
H	-0.867216000	-5.649618000	-1.997366000
H	-4.818976000	-3.993275000	-2.288559000
H	-2.819427000	-4.980420000	-3.390040000

PhS^- / $C_6H_5S^-$

-629.464882471 Nimag=0

C	-0.002388000	0.000000000	-1.434621000
C	-1.146122000	-0.350893000	-0.714190000
C	1.141346000	0.350893000	-0.714190000
H	-2.055186000	-0.629790000	-1.247436000
H	2.050410000	0.629790000	-1.247436000
C	-1.147210000	-0.351244000	0.674247000
C	1.142434000	0.351244000	0.674247000
H	-2.046356000	-0.627132000	1.219352000
H	2.041580000	0.627132000	1.219352000
C	-0.002388000	0.000000000	1.435057000
H	-0.002388000	0.000000000	-2.522204000
S	-0.002388000	0.000000000	3.170045000

PhSH / C_6H_6S

-630.022447562 Nimag=0

C	-0.025665000	0.023423000	-1.370897000
C	-1.126549000	-0.406137000	-0.636679000
C	1.138183000	0.392990000	-0.702414000
H	-2.041234000	-0.697601000	-1.144638000
H	2.005124000	0.730102000	-1.262955000
C	-1.070695000	-0.467608000	0.751593000
C	1.204865000	0.335091000	0.684352000
H	-1.937969000	-0.804603000	1.312303000
H	2.117119000	0.624950000	1.197709000
C	0.097859000	-0.096564000	1.420213000
H	-0.073963000	0.069822000	-2.454152000
S	0.249009000	-0.145976000	3.185502000
H	-0.988506000	-0.604080000	3.435021000

$[1a\cdot phenylacetylene]_‡$ / $AuC_{35}N_2H_{42}Cl$

-2062.70269231 Nimag=1, v=-101.3263

C	5.252452000	-0.757089000	1.444276000
N	3.964451000	-0.626216000	1.936114000
C	3.237162000	-1.748797000	1.718036000
N	4.088034000	-2.578897000	1.067249000
C	5.330500000	-1.992801000	0.894481000
Au	1.329365000	-2.125031000	2.259673000
Cl	0.364098000	-3.024067000	4.300819000
H	5.982532000	0.029882000	1.543674000
H	6.142827000	-2.511845000	0.411851000
C	3.472083000	0.496384000	2.674581000
C	2.794480000	1.510497000	1.982431000
C	3.667171000	0.510950000	4.061061000
C	2.333608000	2.595180000	2.727460000
C	3.183623000	1.618055000	4.761523000
C	2.530247000	2.650274000	4.103016000
H	1.805906000	3.402294000	2.229569000
H	3.313140000	1.661905000	5.838873000
H	2.159558000	3.501648000	4.666473000
C	3.748280000	-3.921231000	0.705401000
C	3.149587000	-4.148829000	-0.541999000
C	4.002824000	-4.939120000	1.632676000
C	2.836775000	-5.467528000	-0.869480000
C	3.666825000	-6.241671000	1.258019000
C	3.096693000	-6.504132000	0.020187000
H	2.375113000	-5.686789000	-1.826909000
H	3.845305000	-7.056401000	1.953544000
H	2.840634000	-7.524142000	-0.251338000
C	4.361565000	-0.616850000	4.795757000
H	4.616076000	-1.391318000	4.065351000
C	2.591593000	1.439076000	0.482659000
H	2.642225000	0.381626000	0.198279000
C	2.874393000	-3.010545000	-1.503210000
H	2.821431000	-2.090213000	-0.910560000
C	4.604348000	-4.664978000	2.995355000
H	4.756077000	-3.584879000	3.088037000
C	3.437537000	-1.261131000	5.830641000
H	3.153262000	-0.545763000	6.610161000
H	2.524780000	-1.648995000	5.368098000
H	3.951331000	-2.095545000	6.319792000
C	5.668757000	-0.131463000	5.426630000
H	6.343214000	0.295465000	4.676984000
H	5.482063000	0.638023000	6.183386000
H	6.185283000	-0.962217000	5.917955000
C	3.653507000	-5.084331000	4.118062000
H	2.691712000	-4.567723000	4.044855000
H	3.467614000	-6.163754000	4.098833000
H	4.095413000	-4.842015000	5.090408000
C	5.973310000	-5.335294000	3.132089000
H	5.889702000	-6.425330000	3.065642000
H	6.662817000	-5.005707000	2.347855000
H	6.418948000	-5.095103000	4.102694000
C	4.025579000	-2.859232000	-2.501830000
H	4.135368000	-3.767423000	-3.104244000
H	3.841594000	-2.020635000	-3.181671000
H	4.976701000	-2.679031000	-1.991797000
C	1.536640000	-3.160527000	-2.225306000
H	0.719056000	-3.307803000	-1.514040000
H	1.325654000	-2.260544000	-2.812560000
H	1.541519000	-4.003852000	-2.923574000
C	1.224305000	1.963100000	0.046921000
H	1.138054000	3.045248000	0.188961000
H	1.071106000	1.769082000	-1.020020000
H	0.417031000	1.481473000	0.606125000
C	3.718615000	2.173416000	-0.249629000
H	4.697843000	1.754360000	0.000197000
H	3.586902000	2.102555000	-1.334473000
H	3.727963000	3.234121000	0.023360000
H	0.468487000	-0.928887000	-0.230306000
C	-0.024493000	-1.464659000	0.553558000
C	-0.974534000	-1.935436000	1.187881000
C	-2.142829000	-2.484321000	1.786472000
C	-2.900811000	-3.428940000	1.075506000
H	-2.572922000	-3.737565000	0.087841000
C	-4.055182000	-3.955934000	1.636386000
H	-4.637682000	-4.686495000	1.083003000
C	-4.464612000	-3.548857000	2.905269000
H	-5.367852000	-3.964189000	3.342629000

C	-3.710929000	-2.618385000	3.615944000
H	-4.018921000	-2.314029000	4.611438000
C	-2.549633000	-2.089015000	3.069254000
H	-1.935708000	-1.393977000	3.629221000

3a / $AuC_{35}N_2H_{41}$

-1602.05964445 Nimag=0

C	-1.036965000	-2.828795000	2.828946000
N	0.192530000	-2.197789000	2.815875000
C	0.151053000	-1.044545000	2.105887000
N	-1.131126000	-0.966534000	1.674922000
C	-1.876714000	-2.047563000	2.105526000
Au	1.660286000	0.260255000	1.760671000
H	-1.192567000	-3.761702000	3.346363000
H	-2.920504000	-2.154191000	1.857776000
C	5.107264000	3.235957000	0.953751000
C	4.905676000	4.366064000	0.142336000
C	5.942752000	5.257390000	-0.100079000
C	7.201075000	5.043659000	0.459069000
C	7.413766000	3.927207000	1.265285000
C	6.381233000	3.031738000	1.511831000
H	3.923724000	4.528209000	-0.290931000
H	5.768517000	6.125554000	-0.729921000
H	8.010412000	5.742409000	0.267840000
H	8.392014000	3.753200000	1.705190000
H	6.541994000	2.160576000	2.139105000
C	4.046931000	2.320497000	1.203857000
C	3.132747000	1.531665000	1.419016000
C	1.372683000	-2.686133000	3.463524000
C	1.614169000	-2.296355000	4.787344000
C	2.242194000	-3.505541000	2.732265000
C	2.778619000	-2.772738000	5.390690000
C	3.392618000	-3.955243000	3.381587000
C	3.657293000	-3.595271000	4.696826000
H	3.005195000	-2.484484000	6.412843000
H	4.095193000	-4.585396000	2.844296000
H	4.560990000	-3.951469000	5.182667000
C	-1.631760000	0.108931000	0.872773000
C	-1.551897000	-0.008174000	-0.520961000
C	-2.150108000	1.237230000	1.521303000
C	-2.031968000	1.059877000	-1.279777000
C	-2.616807000	2.277583000	0.716902000
C	-2.560979000	2.189527000	-0.668302000
H	-1.978464000	1.009867000	-2.363261000
H	-3.017371000	3.172716000	1.183410000
H	-2.924653000	3.012441000	-1.276692000
C	0.692597000	-1.349974000	5.528823000
H	-0.212305000	-1.216459000	4.926204000
C	1.989727000	-3.859223000	1.281185000
H	0.996268000	-3.486964000	1.009208000
C	-0.923061000	-1.210595000	-1.194366000
H	-0.730809000	-1.967444000	-0.426303000
C	-2.163501000	1.365584000	3.030558000
H	-1.858057000	0.403436000	3.455523000
C	1.352129000	0.024216000	5.676088000
H	0.667612000	0.727112000	6.162712000
H	2.259769000	-0.041680000	6.285609000
H	1.632404000	0.432951000	4.699988000
C	0.260158000	-1.912792000	6.883018000
H	-0.453166000	-1.235526000	7.363221000
H	-0.216113000	-2.892393000	6.776469000
H	1.110968000	-2.026495000	7.562619000
C	1.989179000	-5.371760000	1.055957000
H	1.749115000	-5.599128000	0.012459000
H	2.969200000	-5.810444000	1.270185000
H	1.252976000	-5.871358000	1.693381000
C	3.004977000	-3.155855000	0.376365000
H	2.978520000	-2.071591000	0.524541000
H	4.023123000	-3.499767000	0.587835000
H	2.788936000	-3.366839000	-0.676307000
C	-1.855444000	-1.838412000	-2.230912000
H	-1.398294000	-2.737992000	-2.655089000
H	-2.816190000	-2.118807000	-1.787978000
H	-2.056922000	-1.151880000	-3.059648000
C	0.426380000	-0.829356000	-1.809452000
H	0.908587000	-1.709046000	-2.248797000
H	0.298541000	-0.082930000	-2.600762000
H	1.097482000	-0.407102000	-1.054704000
C	-1.141649000	2.411450000	3.484841000
H	-1.111314000	2.466415000	4.578180000
H	-0.138653000	2.164376000	3.122571000
H	-1.401810000	3.404650000	3.103423000
C	-3.562059000	1.677833000	3.564176000
H	-4.289122000	0.923222000	3.248248000
H	-3.551829000	1.706609000	4.658369000
H	-3.918100000	2.652268000	3.214156000

phenylacetylene / C_8H_6

-308.038633709 Nimag=0

C	0.008032000	0.000000000	-0.704503000
C	0.008032000	0.000000000	0.504916000
H	0.008032000	0.000000000	1.571043000
C	0.008032000	0.000000000	-2.130969000
C	1.218139000	0.000000000	-2.840380000
C	-1.202075000	0.000000000	-2.840380000
C	1.213402000	0.000000000	-4.228963000
C	-1.197338000	0.000000000	-4.228963000
C	0.008032000	0.000000000	-4.926674000
H	2.153303000	0.000000000	-2.290222000
H	-2.137239000	0.000000000	-2.290222000
H	2.155139000	0.000000000	-4.769552000
H	-2.139075000	0.000000000	-4.769552000
H	0.008032000	0.000000000	-6.012525000

[AuCl(IPr)(η²-phenylacetylene)] / $AuC_{35}N_2H_{42}Cl$

-2062.71678891 Nimag=0

C	-0.871639000	-5.670731000	3.400879000
N	-0.747112000	-4.478224000	4.093124000
C	-1.331207000	-3.458917000	3.422400000
N	-1.823278000	-4.029679000	2.298381000
C	-1.553287000	-5.387049000	2.265843000
Au	-1.353131000	-1.430992000	3.864197000
Cl	0.745031000	-1.089451000	2.579279000
H	-0.475631000	-6.596057000	3.786595000

H	-1.871243000	-6.011951000	1.447445000
C	-1.489972000	1.784452000	4.551854000
C	-2.198137000	2.809258000	5.199992000
C	-1.728550000	4.114248000	5.157423000
C	-0.551739000	4.411297000	4.470264000
C	0.152810000	3.397362000	3.826658000
C	-0.308469000	2.086347000	3.863452000
H	-3.113130000	2.568274000	5.732948000
H	-2.280129000	4.903034000	5.660773000
H	-0.186230000	5.433758000	4.438354000
H	1.069386000	3.626185000	3.291044000
H	0.229762000	1.282779000	3.366473000
C	-1.991611000	0.434280000	4.603676000
C	-2.836217000	-0.452609000	4.945997000
H	-3.741294000	-0.793786000	5.413885000
C	-0.224389000	-4.371294000	5.423338000
C	-1.108942000	-4.597913000	6.486704000
C	-0.598209000	-4.491457000	7.781132000
C	0.736943000	-4.175147000	7.993900000
C	1.588956000	-3.960735000	6.917114000
C	1.129111000	-4.052774000	5.602394000
H	-1.256781000	-4.653165000	8.629819000
H	1.117889000	-4.092846000	9.007831000
H	2.628770000	-3.710009000	7.098417000
C	2.059899000	-3.861993000	4.423930000
H	1.459674000	-3.520243000	3.574927000
H	2.642196000	-1.840166000	4.955389000
C	3.111388000	-2.782687000	4.663845000
H	3.661524000	-2.599965000	3.736735000
H	3.839416000	-3.075341000	5.429165000
H	1.976065000	-5.960143000	3.803511000
C	2.718150000	-5.194962000	4.052474000
H	3.325071000	-5.575053000	4.881996000
H	3.371942000	-5.066317000	3.183885000
C	-2.571821000	-4.928470000	6.267698000
C	-3.465421000	-3.797946000	6.780162000
H	-3.372833000	-3.679095000	7.864945000
H	-4.516917000	-4.006080000	6.553051000
H	-3.184767000	-2.851074000	6.312042000
H	-2.745923000	-5.016531000	5.190740000
C	-2.946769000	-6.270455000	6.897841000
H	-2.825954000	-6.250642000	7.985926000
H	-2.322718000	-7.080422000	6.507963000
H	-3.993071000	-6.512428000	6.684419000
C	-2.595899000	-3.329916000	1.314002000
C	-1.982448000	-2.969003000	0.107902000
C	-2.779958000	-2.332974000	-0.846656000
C	-4.115212000	-2.054913000	-0.593753000
C	-4.686525000	-2.399115000	0.626175000
C	-3.939892000	-3.044587000	1.610617000
H	-2.340346000	-2.040636000	-1.794798000
H	-4.715647000	-1.554643000	-1.348142000
H	-5.727137000	-2.158088000	0.815931000
C	-4.562128000	-3.445236000	2.934706000
H	-3.771097000	-3.408747000	3.690193000
H	-5.294784000	-1.447729000	3.387085000
C	-5.651288000	-2.481944000	3.399387000
H	-5.952807000	-2.731347000	4.422039000
H	-6.550129000	-2.542558000	2.776514000
H	-4.303096000	-5.591903000	2.616605000
C	-5.093039000	-4.880824000	2.875322000
H	-5.886128000	-4.969239000	2.124872000
H	-5.508009000	-5.177278000	3.845003000
C	-0.522996000	-3.261786000	-0.173657000
C	0.192824000	-2.073584000	-0.814037000
H	-0.182759000	-1.862781000	-1.821440000
H	1.260868000	-2.294543000	-0.902222000
H	0.088944000	-1.181315000	-0.193242000
H	-0.028725000	-3.443275000	0.786308000
C	-0.384231000	-4.513085000	-1.046566000
H	-0.868133000	-4.363170000	-2.018155000
H	-0.841261000	-5.392713000	-0.582740000
H	0.671965000	-4.737697000	-1.226712000

[Au(IPr)(η²-phenylacetylene)]⁺ / $AuC_{35}N_2H_{42}$

-1602.47796814 Nimag=0

C	-0.978433000	-3.839875000	4.000348000
N	-0.769345000	-2.629509000	4.629935000
C	-0.899292000	-1.610904000	3.758081000
N	-1.192273000	-2.184773000	2.573056000
C	-1.246775000	-3.558757000	2.698640000
Au	-0.710627000	0.355637000	4.125408000
H	-0.918021000	-4.775450000	4.533164000
H	-1.467262000	-4.198194000	1.858752000
C	0.456263000	2.769097000	2.419641000
C	1.787549000	3.214987000	2.387880000
C	2.399851000	3.445185000	1.164544000
C	1.696560000	3.229139000	-0.020321000
C	0.378824000	2.774931000	0.012234000
C	-0.247727000	2.538716000	1.226818000
H	2.320824000	3.380850000	3.318111000
H	3.426063000	3.796236000	1.133399000
H	2.179789000	3.415599000	-0.974504000
H	-0.162488000	2.600701000	-0.911304000
H	-1.267274000	2.167503000	1.262263000
C	-0.174438000	2.543739000	3.678431000
C	-0.689452000	2.415484000	4.798604000
H	-1.120805000	2.701201000	5.738815000
C	-1.417112000	-1.446445000	1.362572000
C	-0.335374000	-1.258825000	0.489650000
C	-0.582328000	-0.535935000	-0.677933000
C	-1.845932000	-0.023801000	-0.949464000
C	-2.890882000	-0.215319000	-0.054232000
C	-2.701548000	-0.937311000	1.126599000
H	0.226618000	-0.370766000	-1.382212000
H	-2.019500000	0.526253000	-1.869973000
H	-3.873170000	0.189532000	-0.278812000
C	-3.852849000	-1.140723000	2.090390000
H	-3.494941000	-1.745151000	2.930802000
H	-3.512647000	0.724406000	3.165507000
C	-4.329752000	0.196754000	2.661389000
H	-5.131721000	0.037370000	3.388607000
H	-4.718717000	0.850518000	1.874087000
H	-4.665120000	-2.872049000	1.040404000
C	-5.001282000	-1.906857000	1.430245000
H	-5.432430000	-1.342478000	0.597496000
H	-5.800658000	-2.090518000	2.154308000

C	1.057559000	-1.762844000	0.811018000
C	1.923810000	-0.616085000	1.342902000
H	2.024545000	0.177895000	0.595843000
H	2.925871000	-0.978218000	1.593840000
H	1.486642000	-0.171332000	2.242582000
H	0.973941000	-2.509535000	1.608797000
C	1.722187000	-2.448255000	-0.382666000
H	1.934022000	-1.741929000	-1.191335000
H	1.094855000	-3.246804000	-0.788780000
H	2.677400000	-2.885739000	-0.078334000
C	-0.460328000	-2.443428000	6.019799000
C	-1.526320000	-2.324516000	6.922771000
C	-1.199568000	-2.100482000	8.260707000
C	0.126585000	-2.004151000	8.666103000
C	1.157099000	-2.129955000	7.742990000
C	0.887528000	-2.353186000	6.391523000
H	-1.993162000	-1.999551000	8.994382000
H	0.358581000	-1.831827000	9.712714000
H	2.188079000	-2.053308000	8.074971000
C	2.019394000	-2.464769000	5.390167000
H	1.589719000	-2.703546000	4.410911000
H	2.066893000	-0.329347000	4.957553000
C	2.754749000	-1.129064000	5.253121000
H	3.542127000	-1.201513000	4.496337000
H	3.222618000	-0.836526000	6.198607000
H	2.460028000	-4.553444000	5.839069000
C	2.982418000	-3.596104000	5.754931000
H	3.483676000	-3.404579000	6.708738000
H	3.757886000	-3.695851000	4.989526000
C	-2.973606000	-2.385603000	6.476253000
C	-3.580799000	-0.979630000	6.444220000
H	-3.579448000	-0.531651000	7.443389000
H	-4.616164000	-1.014843000	6.090571000
H	-3.014684000	-0.319031000	5.777661000
H	-2.999202000	-2.777784000	5.453186000
C	-3.808574000	-3.328712000	7.342912000
H	-3.899998000	-2.962059000	8.369841000
H	-3.370100000	-4.329872000	7.381866000
H	-4.820992000	-3.414452000	6.937479000

[Au(IPr)(η²-phenylethynyl)] / $AuC_{35}N_2H_{41}$
-1602.02365823

C	-0.978433000	-3.839875000	4.000348000
N	-0.769345000	-2.629509000	4.629935000
C	-0.899292000	-1.610904000	3.758081000
N	-1.192273000	-2.184773000	2.573056000
C	-1.246775000	-3.558757000	2.698640000
Au	-0.710627000	0.355637000	4.125408000
H	-0.918021000	-4.775450000	4.533164000
H	-1.467262000	-4.198194000	1.858752000
C	0.456263000	2.769097000	2.419641000
C	1.787549000	3.214987000	2.387880000
C	2.399851000	3.445185000	1.164544000
C	1.696560000	3.229139000	-0.020321000
C	0.378824000	2.774931000	0.012234000
C	-0.247727000	2.538716000	1.226818000
H	2.320824000	3.380850000	3.318111000
H	3.426063000	3.796236000	1.133399000
H	2.179789000	3.415599000	-0.974504000
H	-0.162488000	2.600701000	-0.911304000
H	-1.267274000	2.167503000	1.262263000
C	-0.174438000	2.543739000	3.678431000
C	-0.689452000	2.415484000	4.798604000
C	-1.417112000	-1.446445000	1.362572000
C	-0.335374000	-1.258825000	0.489650000
C	-0.582328000	-0.535935000	-0.677933000
C	-1.845932000	-0.023801000	-0.949464000
C	-2.890882000	-0.215319000	-0.054232000
C	-2.701548000	-0.937311000	1.126599000
H	0.226618000	-0.370766000	-1.382212000
H	-2.019500000	0.526253000	-1.869973000
H	-3.873170000	0.189532000	-0.278812000
C	-3.852849000	-1.140723000	2.090390000
H	-3.494941000	-1.745151000	2.930802000
H	-3.512647000	0.724406000	3.165507000
C	-4.329752000	0.196754000	2.661389000
H	-5.131721000	0.037370000	3.388607000
H	-4.718717000	0.850518000	1.874087000
H	-4.665120000	-2.872049000	1.040404000
C	-5.001282000	-1.906857000	1.430245000
H	-5.432430000	-1.342478000	0.597496000
H	-5.800658000	-2.090518000	2.154308000
C	1.057559000	-1.762844000	0.811018000
C	1.923810000	-0.616085000	1.342902000
H	2.024545000	0.177895000	0.595843000
H	2.925871000	-0.978218000	1.593840000
H	1.486642000	-0.171332000	2.242582000
H	0.973941000	-2.509535000	1.608797000
C	1.722187000	-2.448255000	-0.382666000
H	1.934022000	-1.741929000	-1.191335000
H	1.094855000	-3.246804000	-0.788780000
H	2.677400000	-2.885739000	-0.078334000
C	-0.460328000	-2.443428000	6.019799000
C	-1.526320000	-2.324516000	6.922771000
C	-1.199568000	-2.100482000	8.260707000
C	0.126585000	-2.004151000	8.666103000
C	1.157099000	-2.129955000	7.742990000
C	0.887528000	-2.353186000	6.391523000
H	-1.993162000	-1.999551000	8.994382000
H	0.358581000	-1.831827000	9.712714000
H	2.188079000	-2.053308000	8.074971000
C	2.019394000	-2.464769000	5.390167000
H	1.589719000	-2.703546000	4.410911000
H	2.066893000	-0.329347000	4.957553000
C	2.754749000	-1.129064000	5.253121000
H	3.542127000	-1.201513000	4.496337000
H	3.222618000	-0.836526000	6.198607000
H	2.460028000	-4.553444000	5.839069000
C	2.982418000	-3.596104000	5.754931000
H	3.483676000	-3.404579000	6.708738000
H	3.757886000	-3.695851000	4.989526000
C	-2.973606000	-2.385603000	6.476253000
C	-3.580799000	-0.979630000	6.444220000
H	-3.579448000	-0.531651000	7.443389000
H	-4.616164000	-1.014843000	6.090571000
H	-3.014684000	-0.319031000	5.777661000
H	-2.999202000	-2.777784000	5.453186000

C	-3.808574000	-3.328712000	7.342912000
H	-3.899998000	-2.962059000	8.369841000
H	-3.370100000	-4.329872000	7.381866000
H	-4.820992000	-3.414452000	6.937479000

$[1a\cdot Cbz]^{-}_{‡}$ / $AuC_{39}N_3H_{44}Cl$

-2271.02202932 Nimag=1, v=-4.9429

N	2.938822000	0.136164000	0.703936000
C	2.415806000	-0.932017000	0.047541000
C	1.424620000	-0.569394000	-0.937003000
C	2.332848000	1.216830000	0.135642000
C	2.560353000	2.579405000	0.413718000
C	1.875110000	3.540598000	-0.312127000
C	0.954069000	3.191125000	-1.321245000
C	0.710414000	1.853668000	-1.610761000
C	1.385942000	0.862467000	-0.892514000
H	3.295108000	2.855313000	1.165429000
H	2.062270000	4.593354000	-0.106232000
H	0.443792000	3.972410000	-1.881208000
H	0.008962000	1.581871000	-2.399712000
C	2.717824000	-2.296148000	0.235584000
C	2.030387000	-3.252913000	-0.494353000
C	1.040563000	-2.895107000	-1.432093000
C	0.745505000	-1.555092000	-1.658231000
H	3.485373000	-2.579364000	0.952132000
H	2.259590000	-4.306646000	-0.343017000
H	0.517435000	-3.670657000	-1.987006000
H	-0.009771000	-1.277940000	-2.393529000
C	-0.352227000	0.835818000	5.871597000
N	0.389175000	1.272077000	4.789641000
C	1.716596000	1.084299000	4.998459000
N	1.782157000	0.503723000	6.225336000
C	0.525855000	0.343408000	6.778507000
Au	3.306984000	1.774413000	4.034078000
Cl	5.234649000	2.827604000	3.295609000
H	-1.428520000	0.897336000	5.876140000
H	0.383122000	-0.108831000	7.746437000
C	3.001323000	0.037103000	6.808121000
C	3.676826000	0.864463000	7.713395000
C	4.860562000	0.377263000	8.268272000
C	5.350791000	-0.873619000	7.915123000
C	4.670769000	-1.659149000	6.993130000
C	3.478625000	-1.221298000	6.414299000
H	5.414806000	0.996701000	8.967873000
H	6.280188000	-1.232076000	8.349041000
H	5.077303000	-2.623469000	6.702385000
C	2.776217000	-2.066165000	5.370875000
H	1.824966000	-1.584945000	5.123402000
H	3.754022000	-1.137826000	3.650087000
C	3.597418000	-2.131867000	4.080218000
H	3.073616000	-2.731481000	3.329925000
H	4.577923000	-2.586666000	4.262016000
H	1.854786000	-3.419286000	6.817051000
C	2.452460000	-3.464161000	5.900320000
H	3.362610000	-4.032935000	6.120299000
H	1.887973000	-4.025000000	5.148621000
C	3.189334000	2.259540000	8.043073000
C	4.181874000	3.308470000	7.535153000
H	5.147694000	3.216989000	8.044397000
H	3.796857000	4.316998000	7.721933000
H	4.353622000	3.196490000	6.459976000
H	2.246296000	2.420288000	7.510721000
C	2.911957000	2.420204000	9.538501000
H	3.824927000	2.288120000	10.129538000
H	2.178426000	1.687232000	9.890434000
H	2.523135000	3.422047000	9.749326000
C	-0.183120000	1.676790000	3.537612000
C	-0.137009000	3.024707000	3.163681000
C	-0.662741000	3.355015000	1.915206000
C	-1.192844000	2.383226000	1.079500000
C	-1.225576000	1.055723000	1.481703000
C	-0.733128000	0.671579000	2.727751000
H	-0.618741000	4.384340000	1.574271000
H	-1.532697000	2.655384000	0.087042000
H	-1.597973000	0.297207000	0.800513000
C	-0.757578000	-0.787951000	3.137009000
H	-0.466259000	-0.857668000	4.190162000
H	-2.890908000	-0.816657000	3.617775000
C	-2.162357000	-1.382512000	3.026088000
H	-2.162171000	-2.419506000	3.379092000
H	-2.508685000	-1.391237000	1.987736000
H	1.249855000	-1.133713000	2.382034000
C	0.259165000	-1.591494000	2.329934000
H	-0.005355000	-1.631840000	1.269089000
H	0.318542000	-2.621171000	2.701861000
C	0.422640000	4.104048000	4.067439000
C	-0.712828000	4.963427000	4.630644000
H	-1.249234000	5.476530000	3.824626000
H	-0.319779000	5.725639000	5.312968000
H	-1.440171000	4.354139000	5.178027000
H	0.922166000	3.617167000	4.911402000
C	1.472305000	4.960930000	3.360594000
H	1.041890000	5.512181000	2.517931000
H	2.288262000	4.342850000	2.977681000
H	1.894615000	5.691149000	4.059558000

4a / $AuC_{39}N_3H_{44}$

-1810.92346965 Nimag=0

N	1.428486000	-0.616637000	-3.877543000
C	2.281892000	-0.871493000	-2.858895000
N	2.758580000	0.342712000	-2.497926000
C	2.211515000	1.344947000	-3.277644000
C	1.370968000	0.737395000	-4.152620000
Au	2.737480000	-2.626105000	-2.054338000
N	3.209356000	-4.393608000	-1.218292000
H	0.743601000	1.133452000	-4.934781000
H	2.471308000	2.381808000	-3.137401000
C	2.769843000	-5.637660000	-1.614443000
C	3.315027000	-6.650462000	-0.777426000
C	4.035104000	-4.580828000	-0.131188000
C	4.719056000	-3.618110000	0.619301000
C	5.498746000	-4.049240000	1.683178000
C	5.606031000	-5.412137000	2.006818000
C	4.928942000	-6.369919000	1.263610000
C	4.136769000	-5.963316000	0.187387000
H	4.638102000	-2.562322000	0.368978000

H	6.038038000	-3.316394000	2.277968000
H	6.224877000	-5.716464000	2.845978000
H	5.014002000	-7.423926000	1.516350000
C	2.993781000	-7.989608000	-1.010798000
C	2.143547000	-8.309546000	-2.060925000
C	1.610206000	-7.301288000	-2.881108000
C	1.912927000	-5.963347000	-2.671378000
H	3.404814000	-8.771963000	-0.377542000
H	1.886632000	-9.347424000	-2.252127000
H	0.946069000	-7.574601000	-3.697071000
H	1.498388000	-5.182830000	-3.306132000
C	3.713890000	0.510883000	-1.443282000
C	3.245073000	0.595974000	-0.125712000
C	4.200927000	0.704594000	0.885915000
C	5.557681000	0.716649000	0.589189000
C	5.989629000	0.618635000	-0.727876000
C	5.075515000	0.510348000	-1.776271000
H	3.875591000	0.765242000	1.920239000
H	6.285409000	0.792013000	1.391759000
H	7.053379000	0.608751000	-0.944895000
C	5.554313000	0.323605000	-3.201473000
H	4.691233000	0.434332000	-3.867120000
H	6.192896000	2.392569000	-3.471474000
C	6.581885000	1.379124000	-3.610067000
H	6.849683000	1.256033000	-4.664107000
H	7.504626000	1.291600000	-3.027602000
H	5.350370000	-1.845450000	-3.127379000
C	6.102105000	-1.094375000	-3.390230000
H	6.977770000	-1.261994000	-2.754317000
H	6.402777000	-1.254184000	-4.431133000
C	1.771507000	0.536228000	0.219554000
C	1.312774000	1.813447000	0.925665000
H	1.825120000	1.944673000	1.884421000
H	0.237837000	1.771049000	1.128096000
H	1.511980000	2.700822000	0.316704000
H	1.206096000	0.454139000	-0.714744000
C	1.459730000	-0.709510000	1.052417000
H	1.976470000	-0.682409000	2.017339000
H	1.771451000	-1.619559000	0.530414000
H	0.384769000	-0.776518000	1.248940000
C	0.693284000	-1.650249000	-4.543685000
C	1.313076000	-2.337179000	-5.595609000
C	0.593983000	-3.374806000	-6.191389000
C	-0.678466000	-3.709803000	-5.746790000
C	-1.260416000	-3.014766000	-4.693643000
C	-0.584970000	-1.968522000	-4.064596000
H	1.044855000	-3.935463000	-7.004862000
H	-1.217710000	-4.526181000	-6.218120000
H	-2.247895000	-3.298928000	-4.343012000
C	-1.192716000	-1.266183000	-2.867591000
H	-0.582374000	-0.383932000	-2.645505000
H	-2.651394000	-0.127079000	-4.023496000
C	-2.614586000	-0.777446000	-3.144143000
H	-2.993103000	-0.214313000	-2.285381000
H	-3.302551000	-1.611633000	-3.315075000
H	-0.117786000	-2.498653000	-1.426314000
C	-1.143271000	-2.180512000	-1.639653000
H	-1.746068000	-3.080783000	-1.799123000
H	-1.535235000	-1.661225000	-0.758681000
C	2.719264000	-2.017606000	-6.059115000
C	2.746010000	-1.623995000	-7.537037000
H	2.422092000	-2.451379000	-8.176863000
H	3.762254000	-1.351620000	-7.839131000
H	2.089318000	-0.771323000	-7.735957000
H	3.081039000	-1.159342000	-5.482922000
C	3.660802000	-3.190020000	-5.772626000
H	3.365835000	-4.081927000	-6.335165000
H	3.655271000	-3.446947000	-4.708650000
H	4.686021000	-2.934768000	-6.059764000

Cbz^- / $C_{12}NH_8$

-516.331209846 Nimag=0

N	1.392296000	0.970912000	0.000000000
C	0.093957000	1.372814000	0.000000000
C	-0.849500000	0.280683000	0.000000000
C	1.320656000	-0.386329000	0.000000000
C	2.387967000	-1.307555000	0.000000000
C	2.117369000	-2.666349000	0.000000000
C	0.795355000	-3.155394000	0.000000000
C	-0.275058000	-2.269303000	0.000000000
C	-0.030266000	-0.894159000	0.000000000
H	3.411029000	-0.937964000	0.000000000
H	2.943991000	-3.375780000	0.000000000
H	0.616570000	-4.228566000	0.000000000
H	-1.297598000	-2.646589000	0.000000000
C	-0.401576000	2.692773000	0.000000000
C	-1.770136000	2.908551000	0.000000000
C	-2.685981000	1.837056000	0.000000000
C	-2.224492000	0.526343000	0.000000000
H	0.298904000	3.524991000	0.000000000
H	-2.150072000	3.929454000	0.000000000
H	-3.754801000	2.040241000	0.000000000
H	-2.932013000	-0.302724000	0.000000000

CbzH / $C_{12}NH_9$

-516.908901260 Nimag=0

N	1.352580000	0.943217000	0.000000000
C	0.056566000	1.414426000	0.000000000
C	-0.824588000	0.305666000	0.000000000
C	1.346770000	-0.435796000	0.000000000
C	2.415496000	-1.329695000	0.000000000
C	2.118671000	-2.686253000	0.000000000
C	0.793425000	-3.144791000	0.000000000
C	-0.266833000	-2.249240000	0.000000000
C	0.001786000	-0.879417000	0.000000000
H	3.443662000	-0.980129000	0.000000000
H	2.931689000	-3.406173000	0.000000000
H	0.598104000	-4.212505000	0.000000000
H	-1.292352000	-2.607465000	0.000000000
C	-0.412834000	2.726266000	0.000000000
C	-1.788364000	2.916663000	0.000000000
C	-2.676693000	1.831581000	0.000000000
C	-2.202809000	0.527120000	0.000000000
H	0.270617000	3.570200000	0.000000000
H	-2.182850000	3.928425000	0.000000000
H	-3.746109000	2.017355000	0.000000000
H	-2.893470000	-0.311332000	0.000000000

H	2.176691000	1.517885000	0.000000000