Evidence for Genuine Hydrogen Bonding in Gold(I) Complexes

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Supplementary Information

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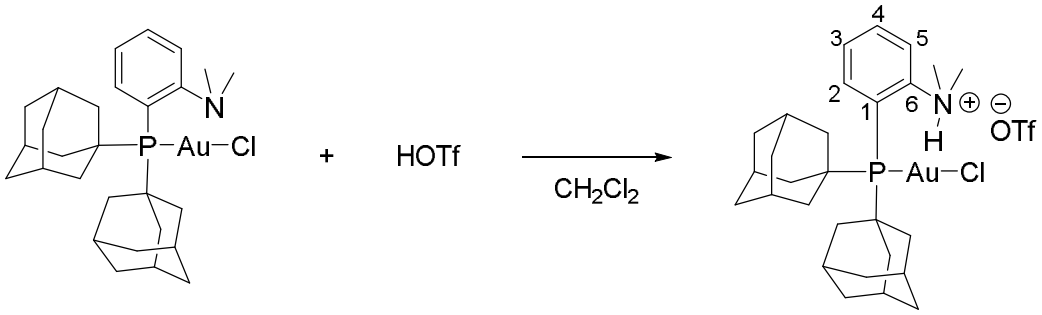
1. Materials and Methods

Unless otherwise stated, all reactions and manipulations were carried out under an atmosphere of dry argon using standard Schlenk techniques or in a glovebox under an inert atmosphere. Dry, oxygen-free solvents were employed. Solution ^{1}H, ^{13}C, ^{31}P, ^{11}B and ^{19}F NMR spectra were recorded on Bruker Avance II 300, Avance III HD 400 or Avance III HD 500 spectrometers at 298K unless otherwise stated. Chemical shifts are expressed with a positive sign, in parts per million, calibrated to residual ^{1}H and ^{13}C solvent signals. External $BF_3.OEt_2$, 85% H_3PO_4 and $CFCl_3$ were used as reference for ^{11}B, ^{31}P and ^{19}F NMR respectively. The following abbreviations and their combinations are used: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. The ^{1}H and ^{13}C resonance signals were assigned by means of J-MOD and 2D COSY, HSQC, HMBC experiments. Mass spectra were recorded on a Waters UPLC Xevo G2 Q TOF apparatus. MALDI were recorded on a Waters Micromass MALDI micro MX™. IR analyses were performed on Thermoscientific IS50 with a CaF_2 tank. All starting materials were purchased from Aldrich and used as received unless otherwise stated. Elemental analyses were recorded on an analyser PERKIN ELMER 2400 série II.

2. Experimental Procedures and Analytical Data

Synthesis of the cationic gold MeDalPhos complex 2

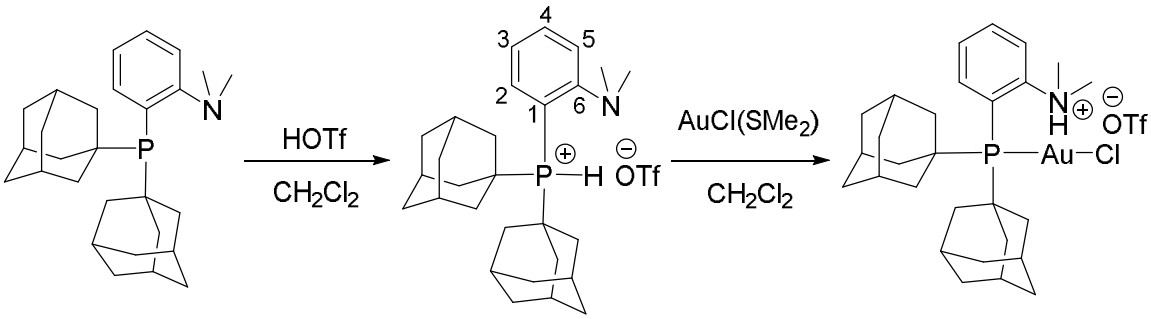
Method A (gold first): In a glovebox, a dried Schlenk was charged with complex **1** (30 mg, 0.046 mmol) in dichloromethane (1 mL). Outside the glovebox, the Schlenk was cooled to -80°C (Acetone/N_2 cold bath) and 0.17 mL dichloromethane solution of trifluoromethane sulfonic acid (0.28 M, 0.046 mmol) was added dropwise. The Schlenk was allowed to warm to room temperature and the reaction mixture was stirred for 1 hour. The product was precipitated by addition of pentane (5 mL). The gold complex **2** was obtained as a white powder (31 mg, 85%) after filtration and drying under *vacuum*. Crystals suitable for XRD analysis were obtained from a dichloromethane/pentane solution at -30°C.



1 **2**

$^{31}P\{^1H\}$ NMR (162 MHz, CD_2Cl_2): ŭ 45.6 (s). **^1H NMR** (500 MHz, CD_2Cl_2): ŭ 10.88 (bs, 1H, NH), 8.43-8.36 (m, 1H, H_5), 8.06-8.00 (pseudo t, 1H, H_4), 7.93-7.87 (pseudo t, 1H, H_2), 7.83-7.77 (pseudo t, 1H, H_3), 3.48 (d, J_{H-H} = 5.0 Hz, 6H, $N(CH_3)_2$), 2.33-2.05 (m, 18H, H_{Ad}), 1.74 (s, 12H, H_{Ad}). **^{13}C NMR** (126 MHz, CD_2Cl_2): ŭ 146.6 (d, $^2J_{C-P}$ = 3.5 Hz, C_6), 136.4 (d, $^4J_{C-P}$ = 1.8 Hz, C_4), 136.2 (d, $^2J_{C-P}$ = 1.4 Hz, C_2), 131.0 (d, $^3J_{C-P}$ = 6.5 Hz, C_3), 124.8 (d, $^3J_{C-P}$ = 3.9 Hz, C_5), 115.2 (d, J_{C-P} = 36.9 Hz, C_1), 48.6 (s, $N(CH_3)_2$), 45.3 (d, J_{C-P} = 21.0 Hz, C_{qtAd}), 42.9 (s, CH_{2Ad}), 36.1 (d, $^2J_{C-P}$ = 1.6 Hz, CH_{2Ad}), 29.1 (d, $^3J_{C-P}$ = 10.2 Hz, CH_{Ad}). **$^{19}F\{^1H\}$ NMR** (282 MHz, CD_2Cl_2): ŭ - 78.99 (s). **^{15}N NMR** (51 MHz, CD_2Cl_2): ŭ 49.1 (d, J_{P-N} = 7.1 Hz, J_{H-N} = 69.5 Hz). **MALDI:** calculated for $[M^+]$ = $C_{28}H_{41}NClPAu^+$: 654.2331. Found: 654.2506. **Elemental Analysis**: calculated for $C_{29}H_{41}NClF_3O_3AuPS$: C 43.32, H 5.14, N 1.74. Found: C 43.56, H 4.92, N 1.72. **Mp:** 208°C (decomposition)

Method B (proton first): In a glovebox, a dried Schlenk was charged with MeDalPhos **3** (80 mg, 0.19 mmol) in dichloromethane (4 mL). Outside the glovebox, the Schlenk was cooled to -80°C (Acetone/N_2 cold bath) and 0.7 mL of dichloromethane solution of trifluoromethane sulfonic acid (0.28 M, 0.19 mmol) was added dropwise. The Schlenk was allowed to warm to room temperature and the reaction mixture was stirred for 1 hour. The product was precipitated by addition of pentane (5 mL). The protonated ligand was obtained as a white powder (80 mg, 74 %) after filtration and drying under *vacuum*. Crystals suitable for XRD analysis were obtained from a dichloromethane/pentane solution at -30°C.



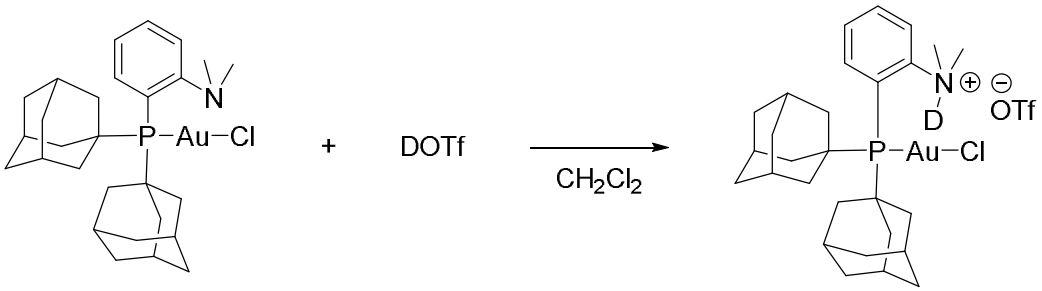
3 **4** **2**

^{31}P NMR (121 MHz, CD_2Cl_2): ŭ 17.6 (d, J_{P-H} = 485.3 Hz). **^{1}H NMR** (500 MHz, CD_2Cl_2): ŭ 7.83-7.78 (m, 1H, H_4), 7.66-7.64 (m, 1H, H_2), 7.63-7.60 (m, 1H, H_5), 7.52-7.46 (m, 1H, H_3), 6.80 (d, J_{P-H} = 485.3 Hz, 1H, PH), 2.70 (s, 6H, $N(CH_3)_2$), 2.22-2.05 (m, 18H, H_{Ad}), 1.84-1.76 (m, 12H, H_{Ad}). **^{13}C NMR** (126 MHz, CD_2Cl_2): ŭ 160.4 (s, C_6), 136.5 (d, $^{4}J_{C-P}$ = 2.3 Hz, C_4), 133.7 (d, $^{2}J_{C-P}$ = 8.0 Hz, C_2), 126.7 (d, $^{3}J_{C-P}$ = 11.5 Hz, C_3), 125.3 (d, $^{3}J_{C-P}$ = 6.3 Hz, C_5), 111.5 (d, J_{C-P} = 74.7 Hz, C_1), 46.5 (s, $N(CH_3)_2$), 39.4 (d, $^{2}J_{C-P}$ = 3.2 Hz, CH_{2Ad}), 39.3 (d, J_{C-P} = 32 Hz, C_{qtAd}), 35.8 (d, $^{4}J_{C-P}$ = 1.8 Hz, CH_{2Ad}), 28.7 (d, $^{3}J_{C-P}$ = 9.9 Hz, CH_{Ad}). **^{19}F NMR** (282 MHz, CD_2Cl_2): ŭ -78.86 (s). **HRMS (ESI+):** calculated for $[L^+]$ = $C_{28}H_{41}NP^+$: 422.2979. Found: 422.2977. **Elemental Analysis:** calculated for $C_{29}H_{41}F_3NO_3PS$: C 60.93, H 7.23, N 2.45. Found: C 59.05, H 6.92, N 2.30. **Mp:** 216 °C

In a glovebox, a dried Schlenk was charged with phosphonium **4** (40 mg, 0.07 mmol) and $AuCl(SMe_2)$ (21 mg, 0.07 mmol) in dichloromethane (1.5 mL). The reaction mixture was stirred for 1 hour. The product was precipitated by addition of pentane (5 mL). The gold complex **2** was obtained as a white powder (46 mg, 80 %) after filtration and drying under *vacuum*.

Synthesis of the cationic gold MeDalPhos complex 2-D

In a glovebox, a screw cap NMR tube was charged with complex **1** (10 mg, 0.015 mmol) and dichloromethane (0.6 mL). DOTf (1.3 εL, 0.015 mmol) was carefully added. The tube was gently shaken. ^{31}P and ^{1}H NMR analyses show the formation of the desired complex **2-D** with 93% deuteration of the ammonium moiety. The crude mixture was diluted with dichloromethane and directly analyzed by IR.



1 **2-D**

^{31}P{^{1}H} NMR (121 MHz, CH_2Cl_2): ŭ 45.7 (s, **2-D**), 45.6 (s, **2**) **IR:** з(N-D) = 2124 cm^{-1}.

Synthesis of the cationic gold MorDalPhos complex 6-OTf

In a glovebox, a dried Schlenk was charged with complex **5** (48 mg, 0.07 mmol) in dichloromethane (1 mL). Outside the glovebox, the Schlenk was cooled to -80°C (Acetone/N_2 cold bath) and 0.25 mL dichloromethane solution of trifluoromethane sulfonic acid (0.28 M, 0.07 mmol) was added dropwise. The Schlenk was allowed to warm to room temperature and the reaction mixture was stirred for 1 hour. The product was precipitated by addition of pentane (8 mL). The gold complex **6-OTf** was obtained as a white powder (37 mg, 62 %) after filtration and drying under *vacuum*.

$^{31}P\{^1H\}$ NMR (202 MHz, CD_2Cl_2): ŭ 44.4 (s). **^1H NMR** (500 MHz, CD_2Cl_2): ŭ 11.02 (s, 1H, NH), 8.33-8.28 (m, 1H, H_2), 8.09-8.04 (m, 1H, H_4), 7.96-7.91 (m, 1H, H_3), 7.86-7.81 (m, 1H, H_5), 4.69-4.61 (m, 2H, H_8), 4.31-4.23 (m, 4H, Hô$_{8,}$ H_7), 3.53-3.48 (m, 2H, Hô$_7$), 2.30-2.24 (m, 6H, H_{Ad}), 2.18-2.09 (m, 12H, H_{Ad}), 1.79-1.71 (m, 12H, H_{Ad}).

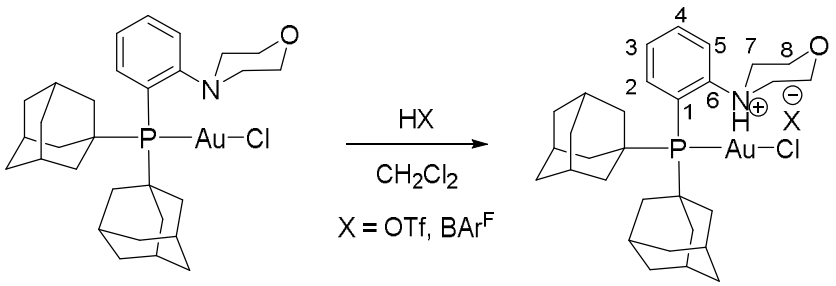
Synthesis of the cationic gold MorDalPhos complex 6-BAr^F_4

Synthesis of $H(Et_2O)_2BAr^F_4$ (BAr^F_4 = $B(3,5\text{-}(F_3C)_2C_6H_3)_4$)

Under argon, a solution of $NaBAr^F_4$ (1.00 g, 1.13 mmol) in diethyl ether (3 mL) was transferred via cannula to a 100 mL Schlenk containing a solution of HCl in diethyl ether (2 M, 3 mL, 6 mmol) at -30 °C. The solution was stirred for 4 hours. After filtration, the solvent was evaporated under *vacuum*. The solid was triturated in cold pentane. The product was obtained as a white powder (710 mg, 62 %) after filtration and drying under *vacuum*. Analytical data are consistent with those previously reported (*Organometallics* **1992**, *11*, 3920-3922).

^1H NMR (300 MHz, CD_2Cl_2): ŭ 11.44 (bs, 1H, H), 7.72 (s, 8H, $H_{BArF4,ortho}$), 7.58 (s, 4H, $H_{BArF4,para}$), 3.75 (q, 8H, CH_2), 1.27 (t, 12H, CH_3)

In a glovebox, a dried Schlenk was charged with complex **5** (42 mg, 0.06 mmol) and dichloromethane (1 mL). Another dried Schlenk was charged with $H(Et_2O)_2BAr^F_4$ (61 mg, 0.06 mmol) and dichloromethane (1 mL). Outside the glovebox, both Schlenk were cooled to -80°C (Acetone/N_2 cold bath) and the solution of $H(Et_2O)_2BAr^F_4$ was added to the solution of complex **5** via a cannula. The Schlenk was rinsed with 1 mL of dichloromethane. The reaction mixture was allowed to warm to room temperature and stirred for 1 hour. The product was precipitated by addition of pentane (8 mL). The gold complex **6-BAr^F_4** was obtained as a white powder (77 mg, 82 %) after filtration and drying under *vacuum*. Crystals suitable for XRD analysis were obtained from a dichloromethane/pentane solution at -30°C.



5 **6-OTf** **6-BAr$^F_4$**

^{31}P{^{1}H} NMR (202 MHz, CD_2Cl_2): ŭ 44.3 (s). **^{1}H NMR** (500 MHz, CD_2Cl_2): ŭ 11.37 (s, 1H, NH), 8.00-7.96 (m, 1H, H_2), 7.95-7.91 (m, 1H, H_4), 7.85-7.80 (m, 1H, H_3), 7.72 (s, 8H, $H_{BArF4,ortho}$), 7.71-7.67 (m, 1H, H_5), 7.56 (s, 4H, $H_{BArF4,para}$), 4.75-4.68 (m, 2H, H_8), 4.29-4.24 (m, 2H, Hô$_8$), 3.90-3.82 (m, 2H, H_7), 3.55-3.51 (m, 2H, Hô$_7$), 2.27-2.24 (m, 6H, H_{Ad}), 2.13-2.09 (m, 12H, H_{Ad}), 1.80-1.70 (m, 12H, H_{Ad}). **^{13}C NMR** (126 MHz, CD_2Cl_2): ŭ 162.2 (q, J_{C-B} = 49.9 Hz, C_{BArF4}), 143.9 (d, $^2J_{C-P}$ = 3.5 Hz, C_6), 136.7 (d, $^2J_{C-P}$ = 1.6 Hz, C_2), 135.6 (d, $^4J_{C-P}$ = 1.7 Hz, C_4), 134.7 (s, o-C_{BArF4}), 131.2 (d, $^3J_{C-P}$ = 6.6 Hz, C_3), 128.3 (qq, $^2J_{C-F}$ = 31.6 Hz, $^4J_{C-F}$ = 2.8 Hz, m-C_{BArF4}), 124.6 (q, J_{C-F} = 272.2 Hz, CF_3), 123.3 (d, $^3J_{C-P}$ = 3.9 Hz, C_5), 117.9 (sept, $^3J_{C-F}$ = 4.1 Hz, p-C_{BArF4}), 116.0 (d, $^2J_{C-P}$ = 34.7 Hz, C_1), 63.7 (s, C_8), 57.7 (s, C_7), 45.4 (d, $^2J_{C-P}$ = 19.9 Hz, C_{qtAd}), 42.7 (s, CH_{2Ad}), 35.6 (d, $^2J_{C-P}$ = 1.2 Hz, CH_{2Ad}), 28.7 (d, $^2J_{C-P}$ = 9.7 Hz, CH_{Ad}). **^{15}N NMR** (51 MHz, CD_2Cl_2): ŭ 60.0 ppm (d, J_{P-N} = 7.1 Hz, J_{H-N} = 68.3 Hz). **^{19}F{^{1}H} NMR** (470 MHz, CD_2Cl_2): ŭ -62.85 (s). **^{11}B{^{1}H} NMR** (96 Hz, CD_2Cl_2): ŭ -6.6 ppm (s). **MALDI:** calculated for [M^+] = $C_{30}H_{43}NOPClAu^+$: 696.2436. Found: 696.2870. **Elemental Analysis:** calculated for $C_{31}H_{43}AuClF_3NO_4PS$: C 44.00, H 5.12, N 1.66. Found: C 43.08, H 4.84, N 1.56. **Mp:** 190°C (decomposition)

3. NMR Spectra

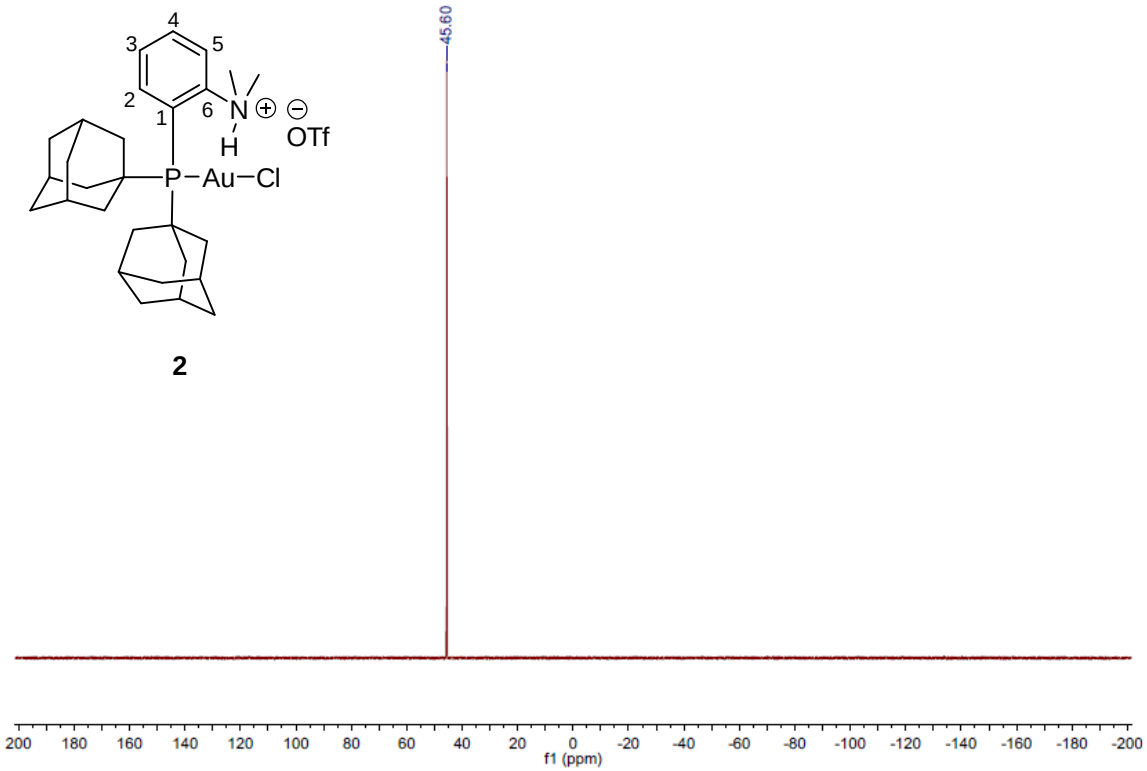


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Figure S1. $^{31}P\{^{1}H\}$ NMR spectrum of (**2**) in CD_2Cl_2.

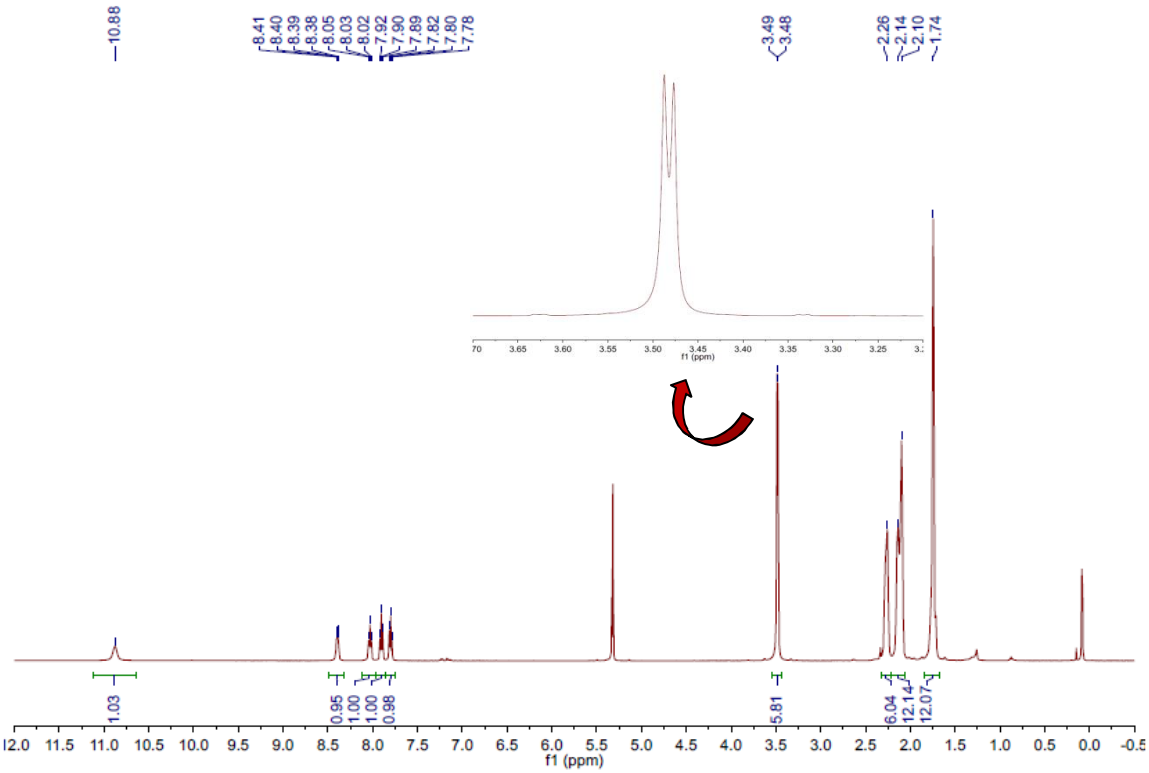

Figure S2. ^{1}H NMR spectrum of (**2**) in CD_2Cl_2.

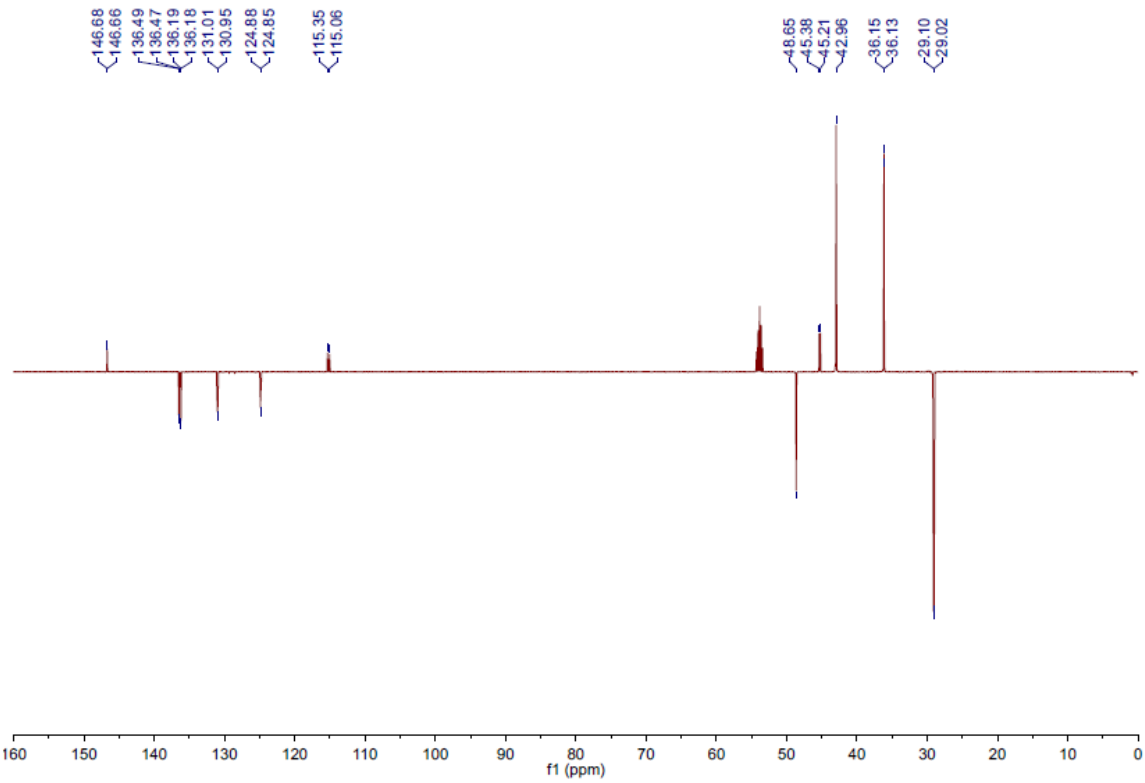

Figure S3. $^{13}C_{jmod}$ NMR spectrum of (**2**) in CD_2Cl_2.

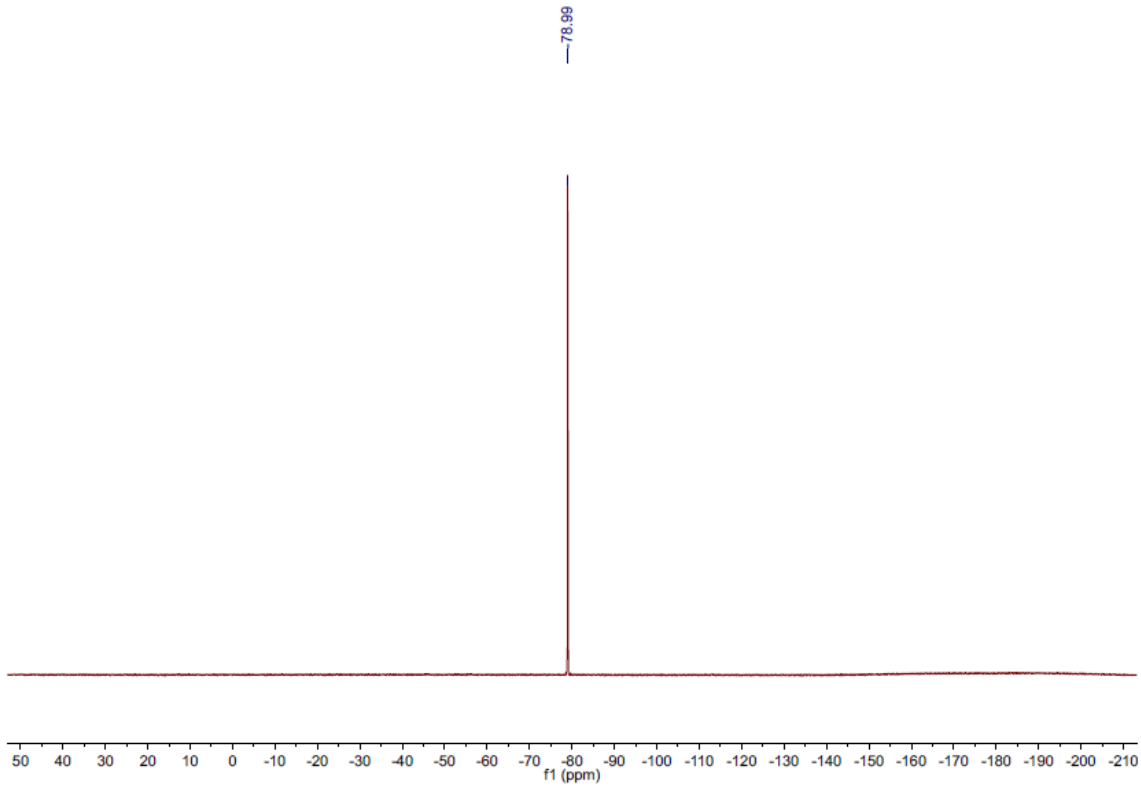

Figure S4. ^{19}F NMR spectrum of (**2**) in CD_2Cl_2.

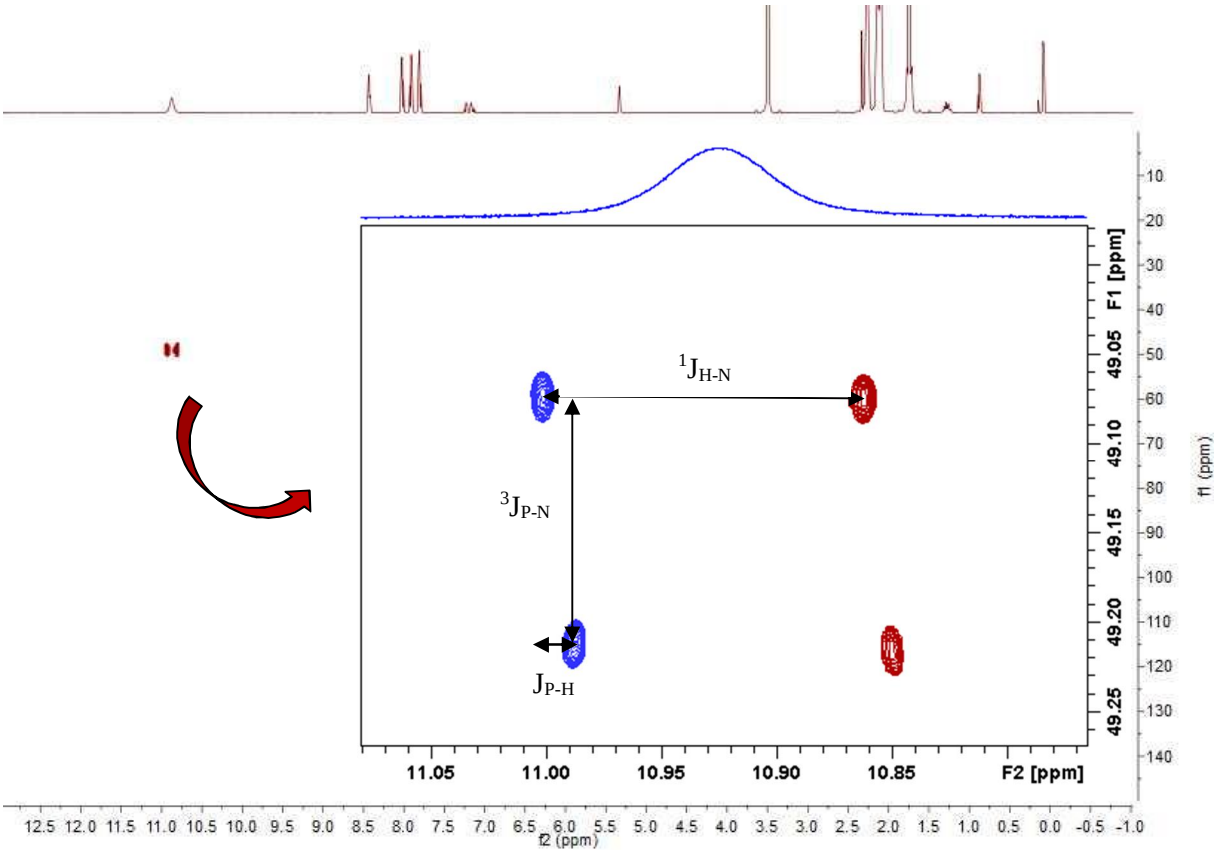

Figure S5. No refocused HSQC ^{1}H-^{15}N NMR spectrum of (**2**) in CD_2Cl_2. HOBS observation scheme has been used. To determine $^1J_{1H\text{-}15N}$, no ^{15}N decoupling has been applied during acquisition. High resolution is achieved in the indirect dimension because of ^{15}N small spectral width (1 ppm). [1,2,3]

[1] Castañar, L.; Nolis, P.; Virgili, A.; Parella, T. *Chem. Eur. J.* **2013**, *19*, 17283ï 17286.
[2] Castañar, L.; Saurí, J.; Nolis, P.; Virgili, A.; Parella, T. *J. Magn. Reson.* **2014**, *238*, 63ï 69.
[3] Marcó, N.; Fredi, A.; Parella, T. *Chem. Commun.* **2015**, *51*, 3262ï 3265.

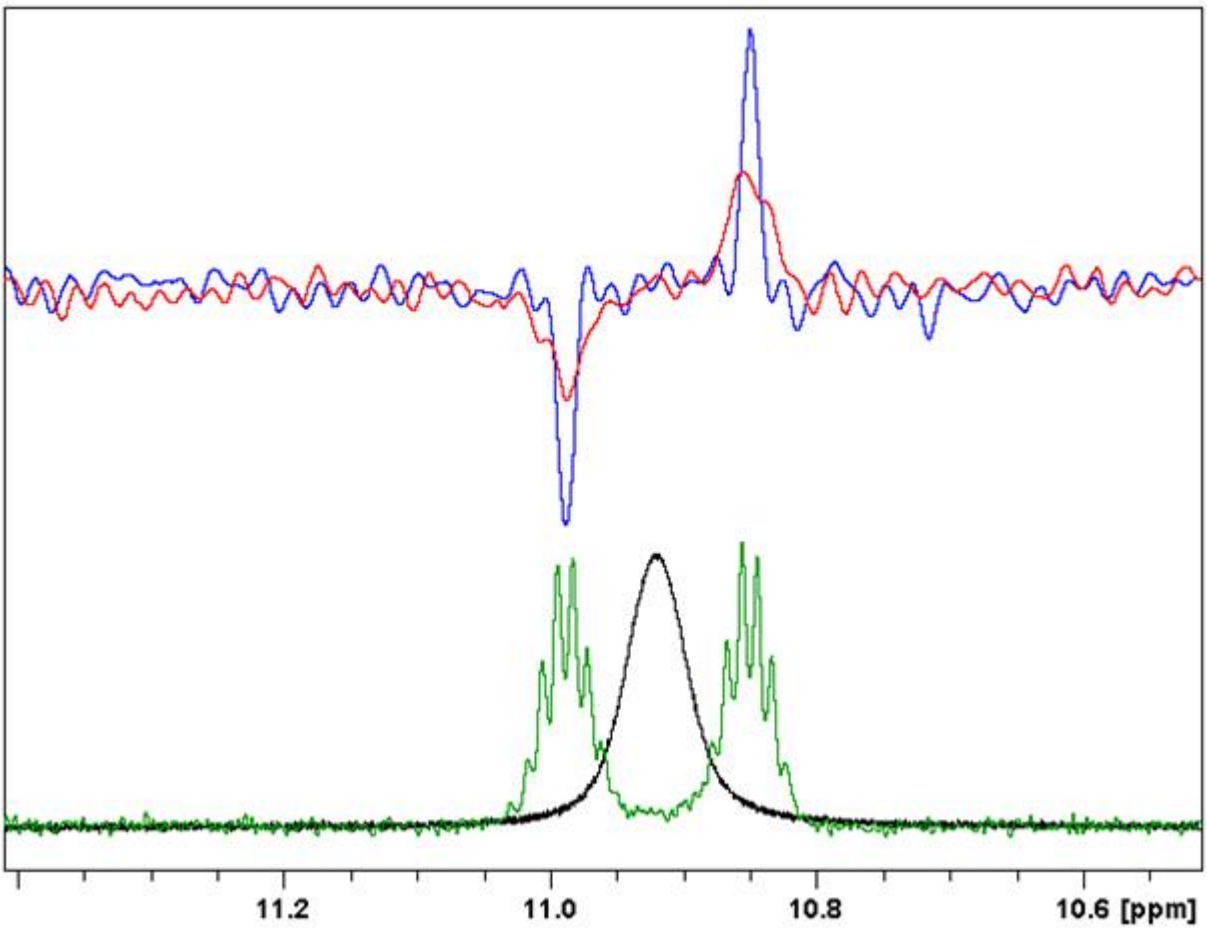

Figure S6. HOBS and $^{14}N/^{15}N$ isotopic effect: row extraction of no refocused ^{1}H-^{15}N HSQC with (blue line) and without (red line) HOBS detection scheme. All parameters are the same apart from those used during detection. Sensitivity increase and enhanced resolution is observed thanks to $J_{1H\text{-}1H}$ decoupling. This advantage cannot be used for ^{1}H bounded to ^{14}N because the preferential broadening mechanism is ^{14}N quadrupolar relaxation effect on nearby nuclei. Indeed, in classical 1D ^{1}H spectrum (black line), the amine ^{1}H signal shows no multiplicity unlike in 1D ^{15}N edited ^{1}H spectrum (green line).

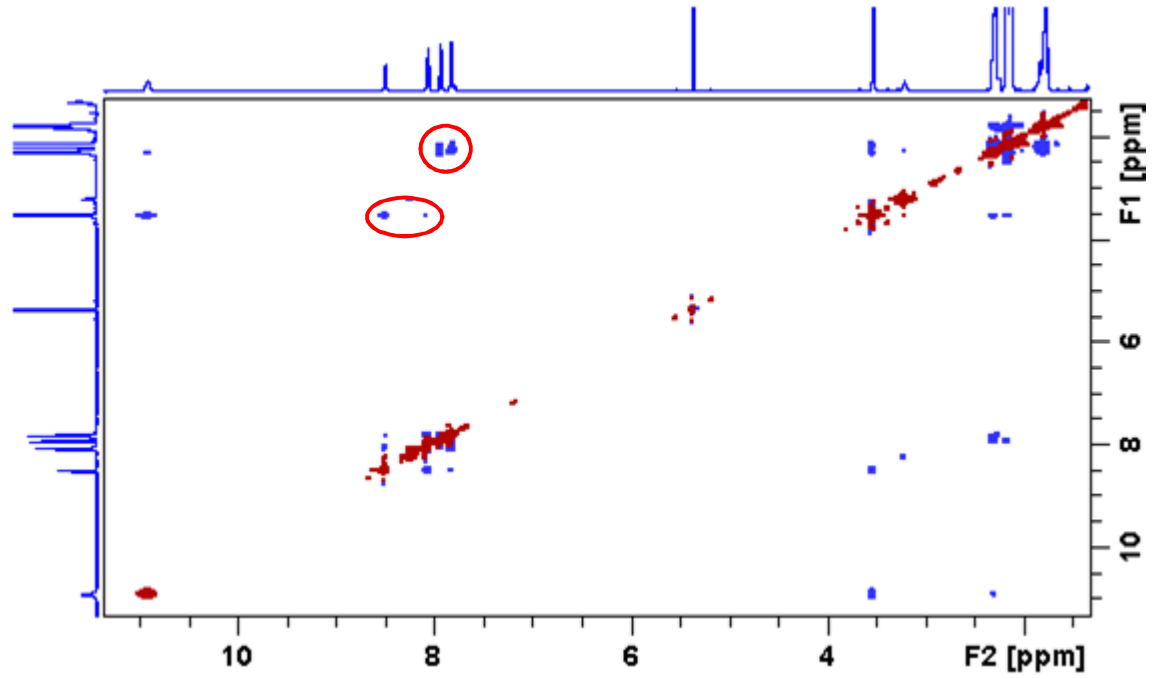

Figure S7. NOESY ^{1}H-^{1}H NMR spectrum of (**2**) in CD_2Cl_2 (mixing time = 1s). Positive and negative levels are plotted in red and blue, respectively.

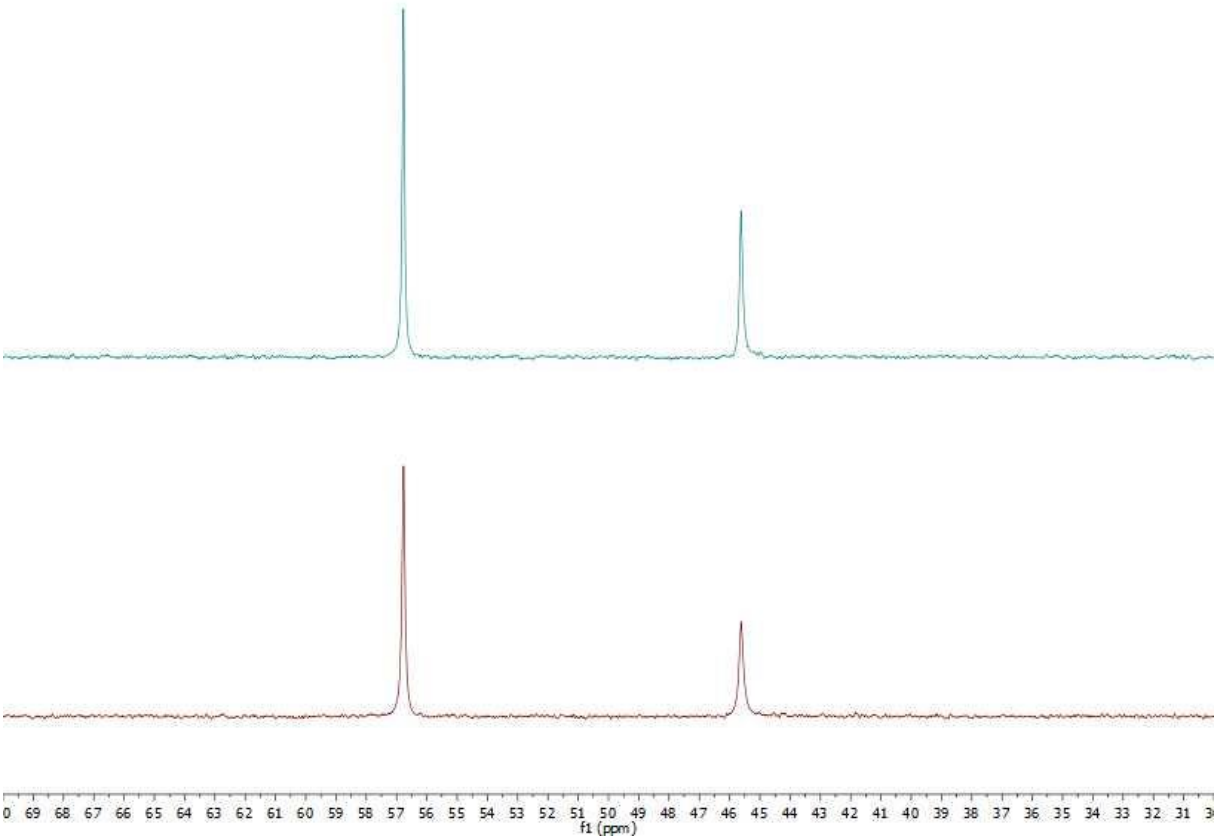

Figure S8. ^{31}P NMR spectra of a 2:1 mixture of (**1**) and (**2**) in CD_2Cl_2 at 25°C (blue) and 45°C (red).

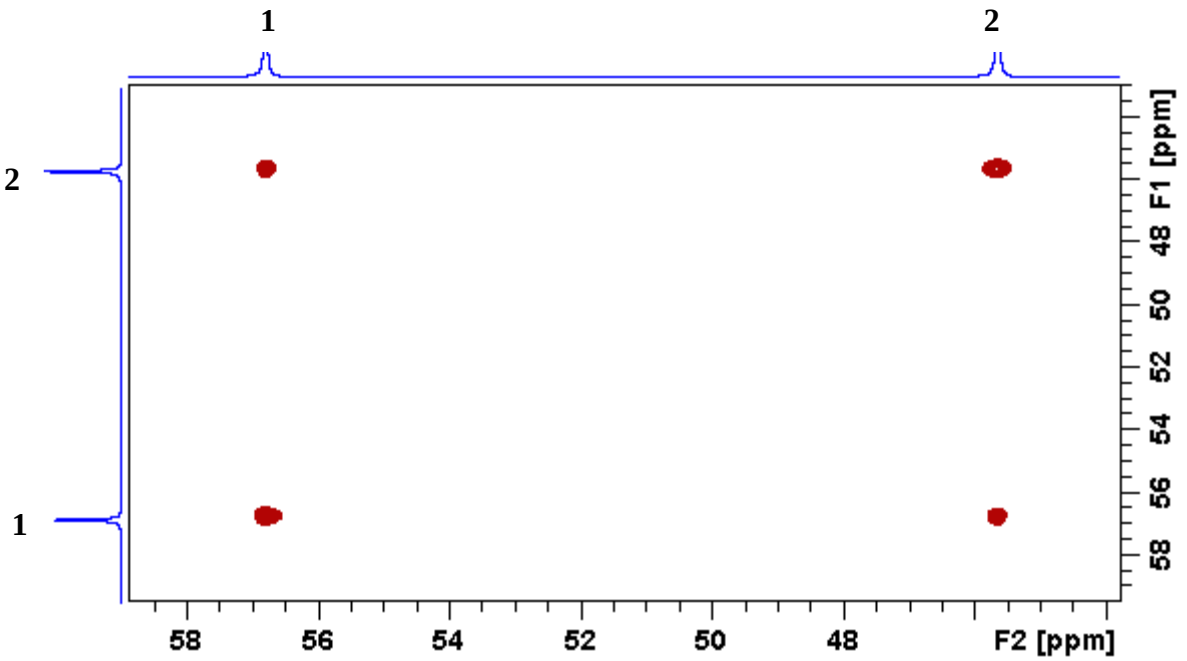

Figure S9 : EXSY ^{31}P-^{31}P NMR spectrum of a 1:1 mixture of (**1**) and (**2**) in CD_2Cl_2 at 25°C (mixing time = 50 ms).

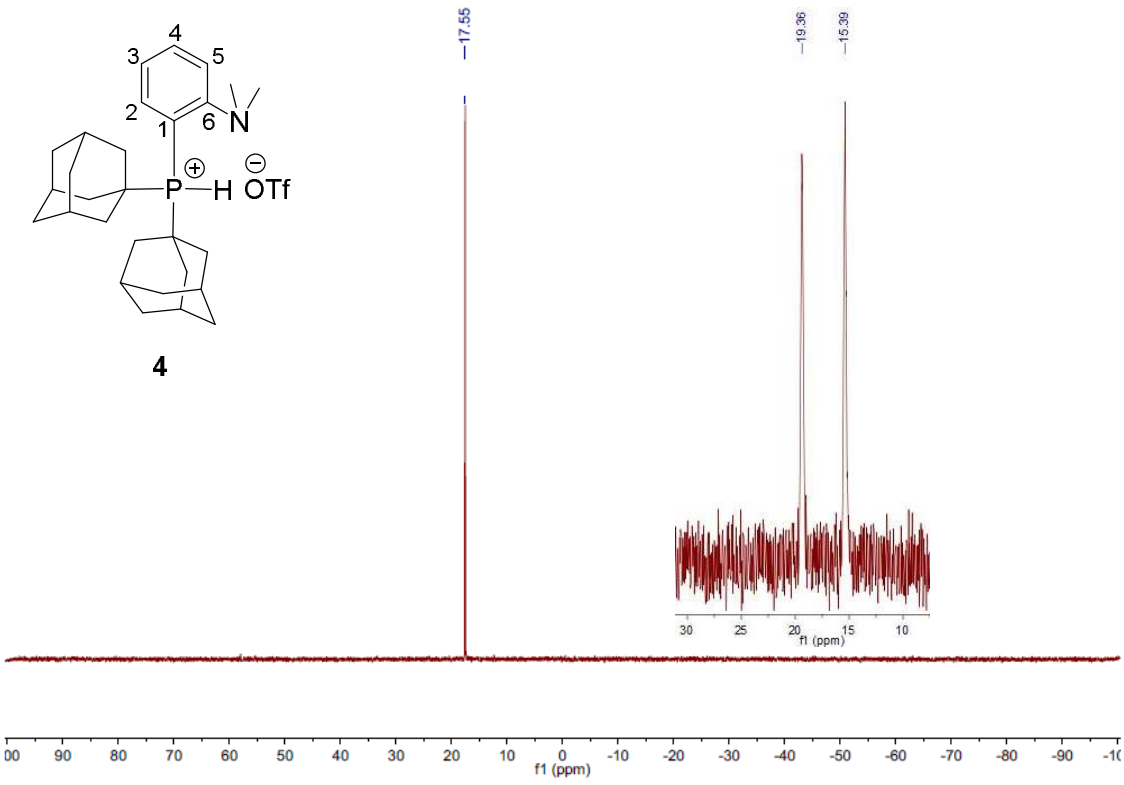

Figure S10. $^{31}P\{^1H\}$ NMR spectrum (inset: ^{31}P NMR spectrum) of (**4**) in CD_2Cl_2.

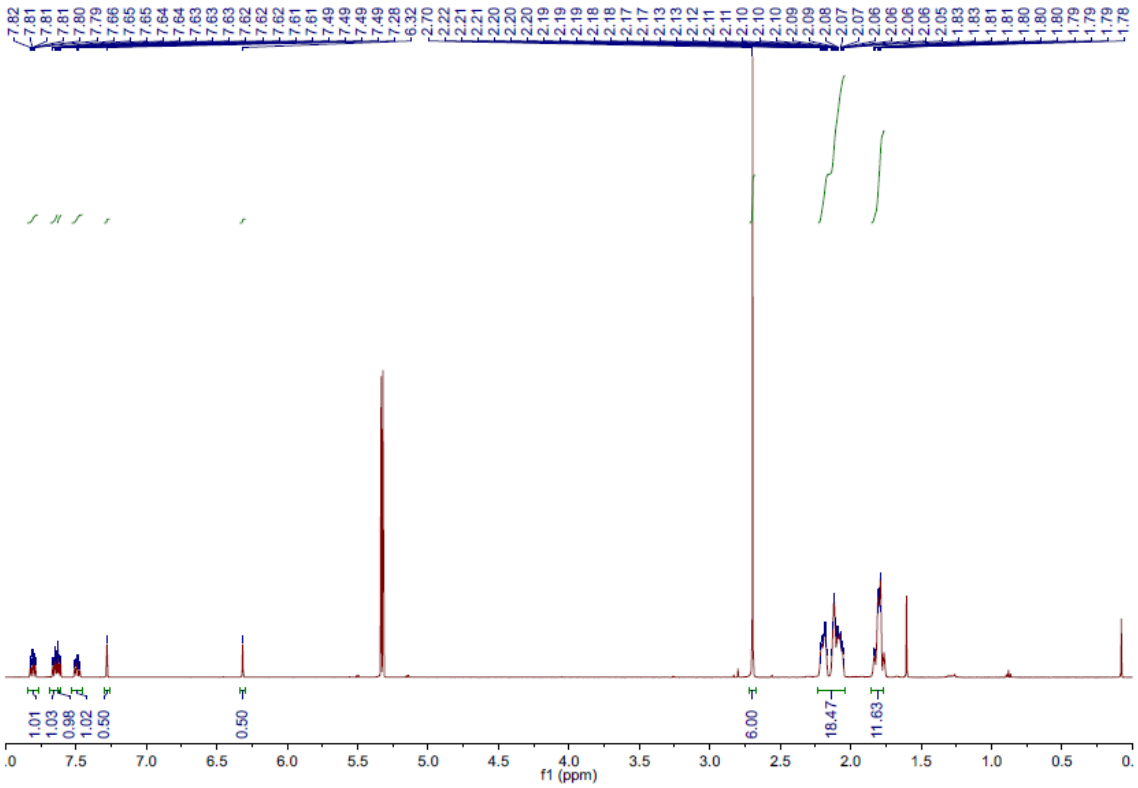

Figure S11. ^{1}H NMR spectrum of (**4**) in CD_2Cl_2.

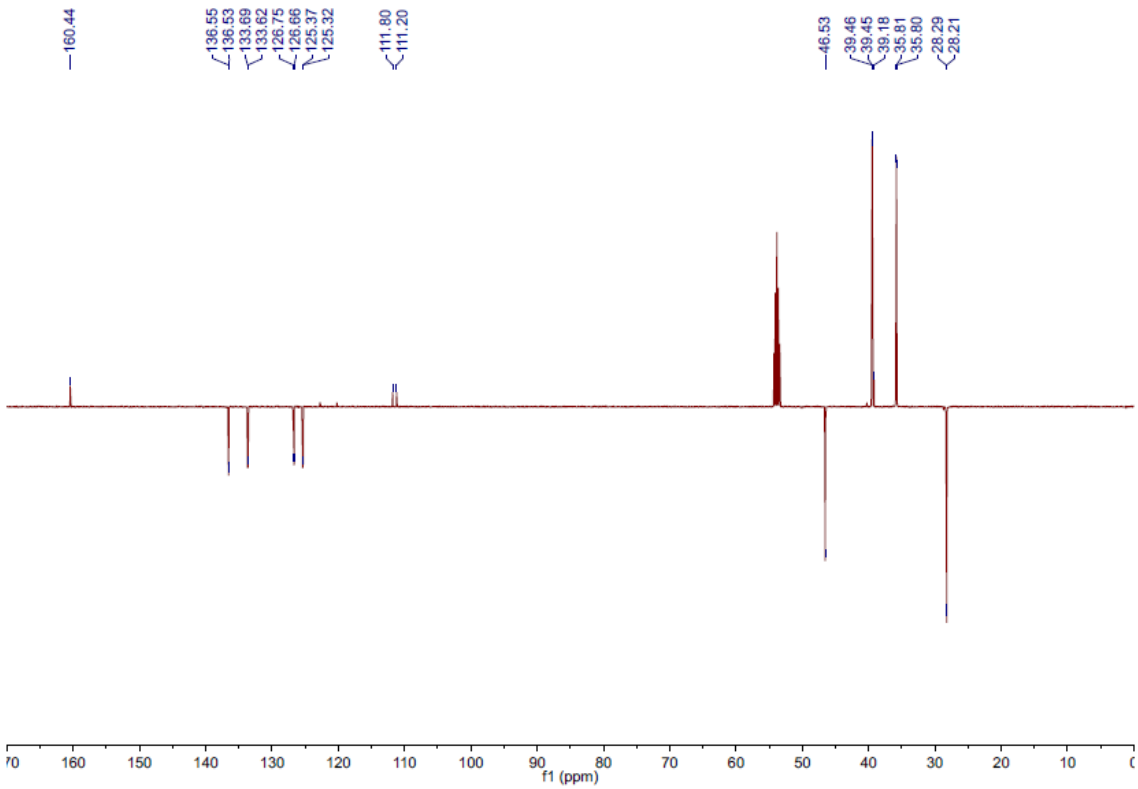

Figure S12. $^{13}C_{jmod}$ NMR spectrum of (**4**) in CD_2Cl_2.

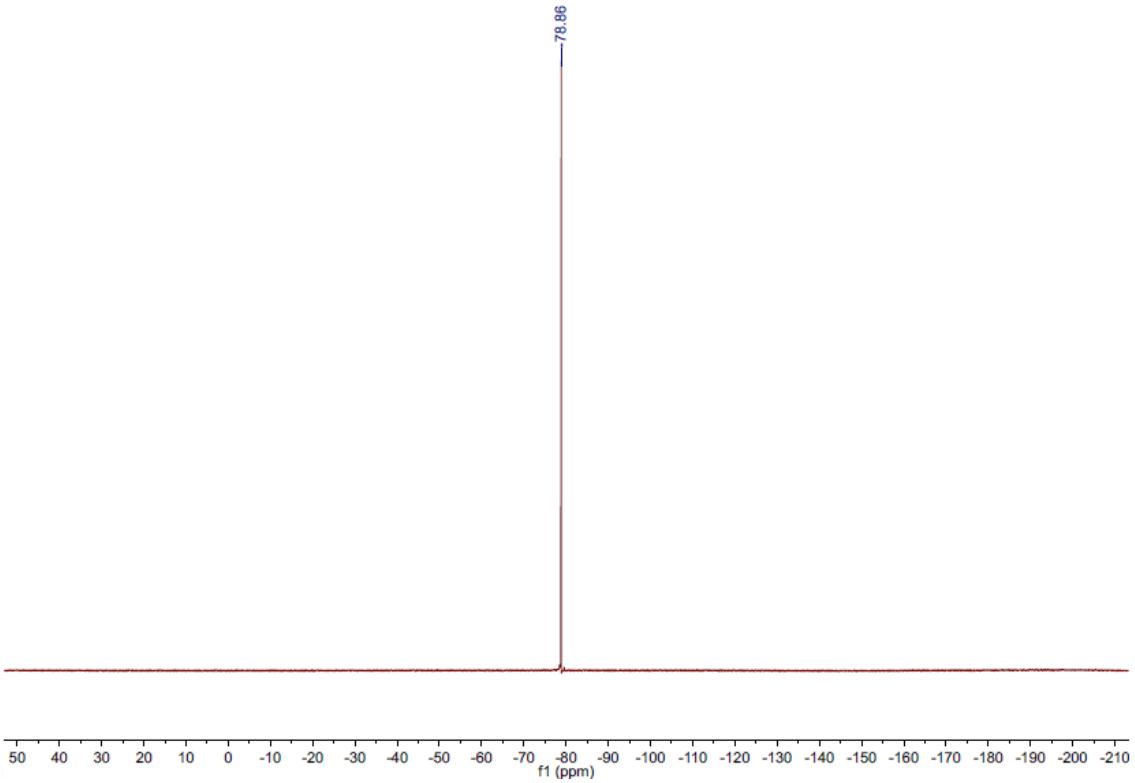

Figure S13. ^{19}F NMR spectrum of (**4**) in CD_2Cl_2.

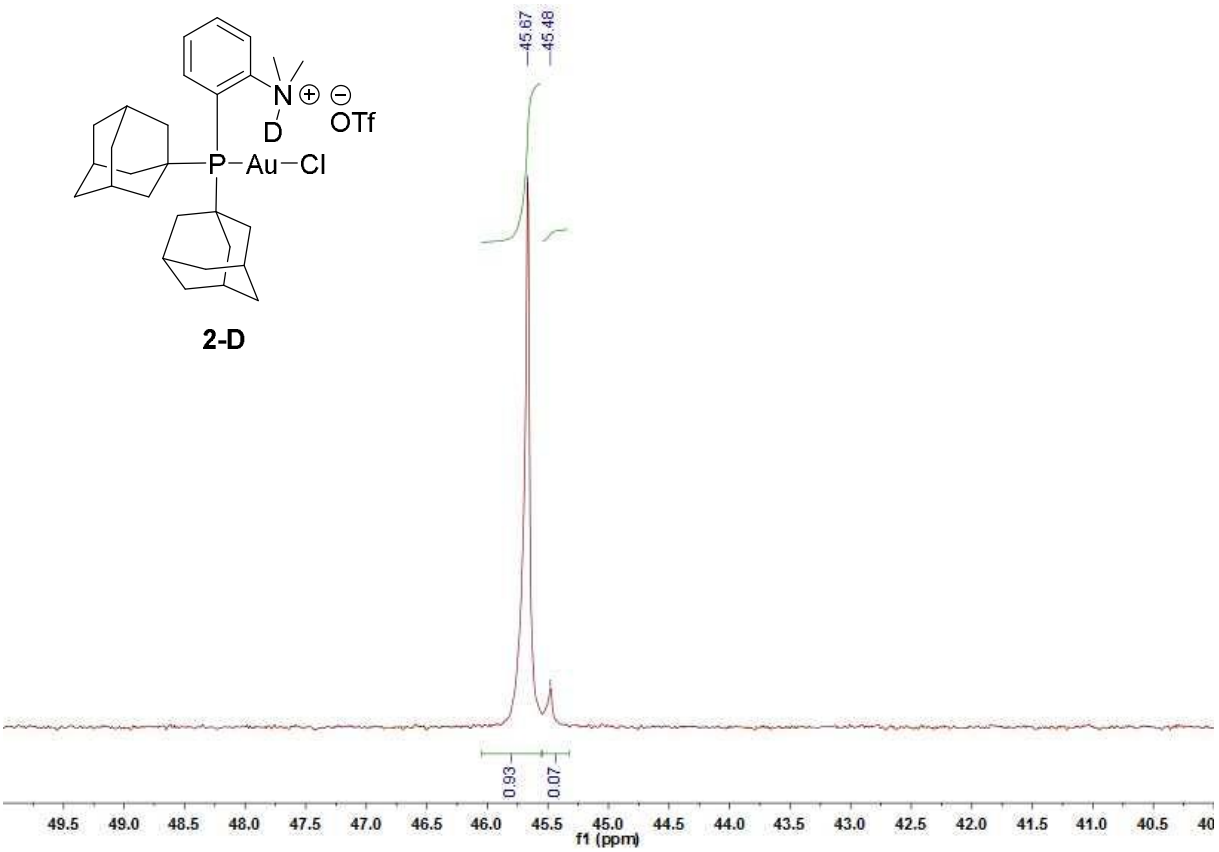

Figure S14. $^{31}P\{^1H\}$ NMR spectrum of (**2-D**) and (**2**).

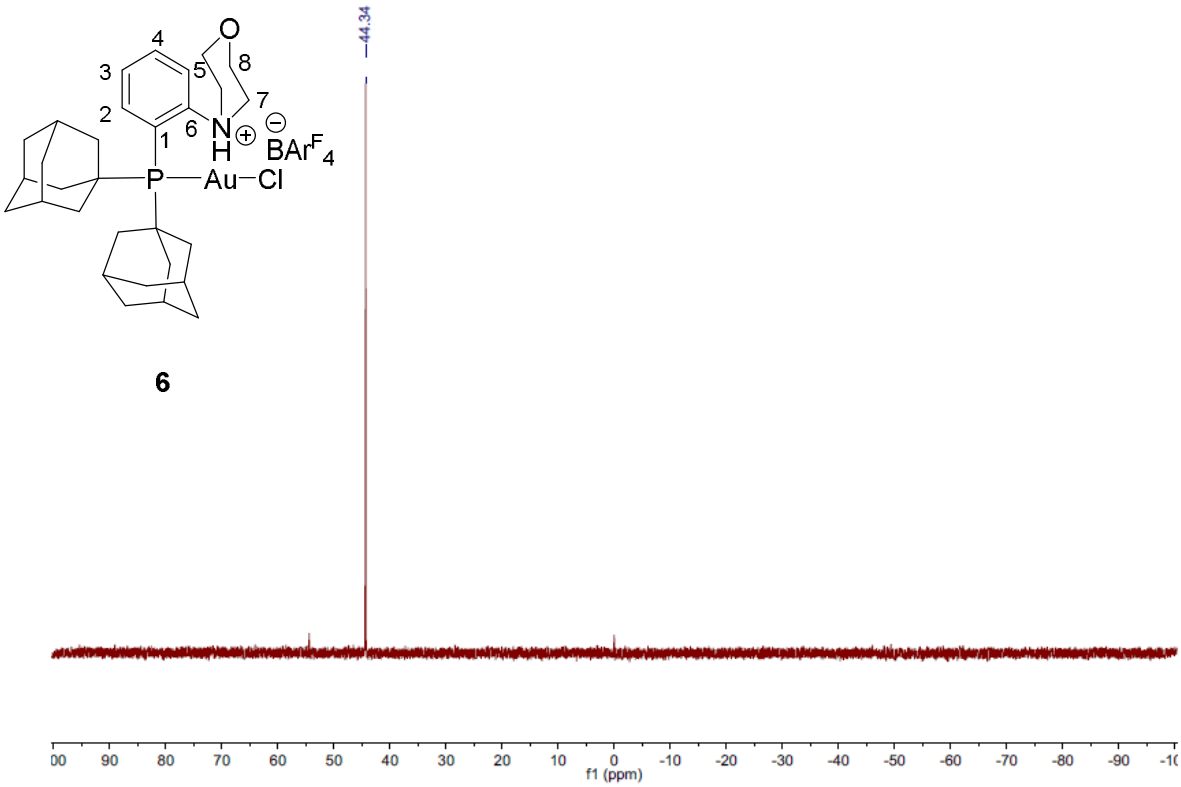

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Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum of (**6-BAr$^{F}_{4}$**) in CD_2Cl_2.

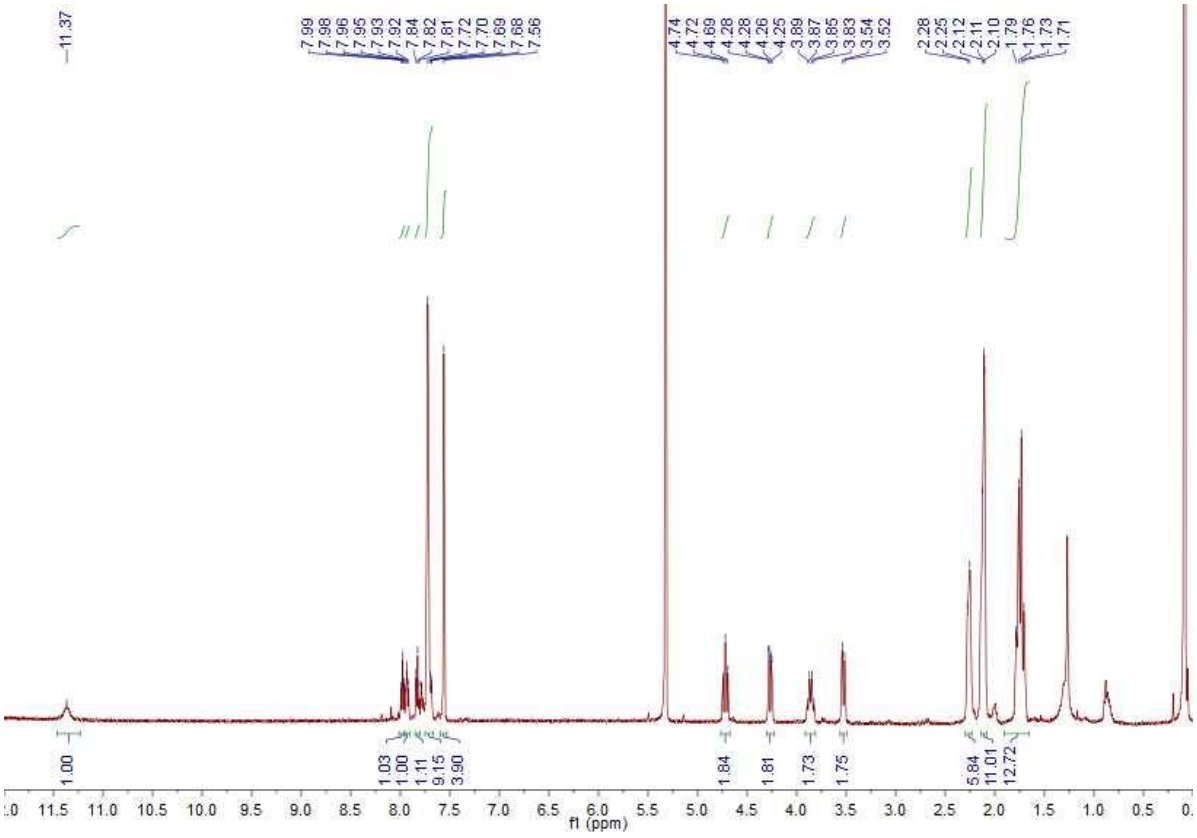

Figure S16. ^{1}H NMR spectrum of (**6-BAr$^{F}_{4}$**) in CD_2Cl_2.

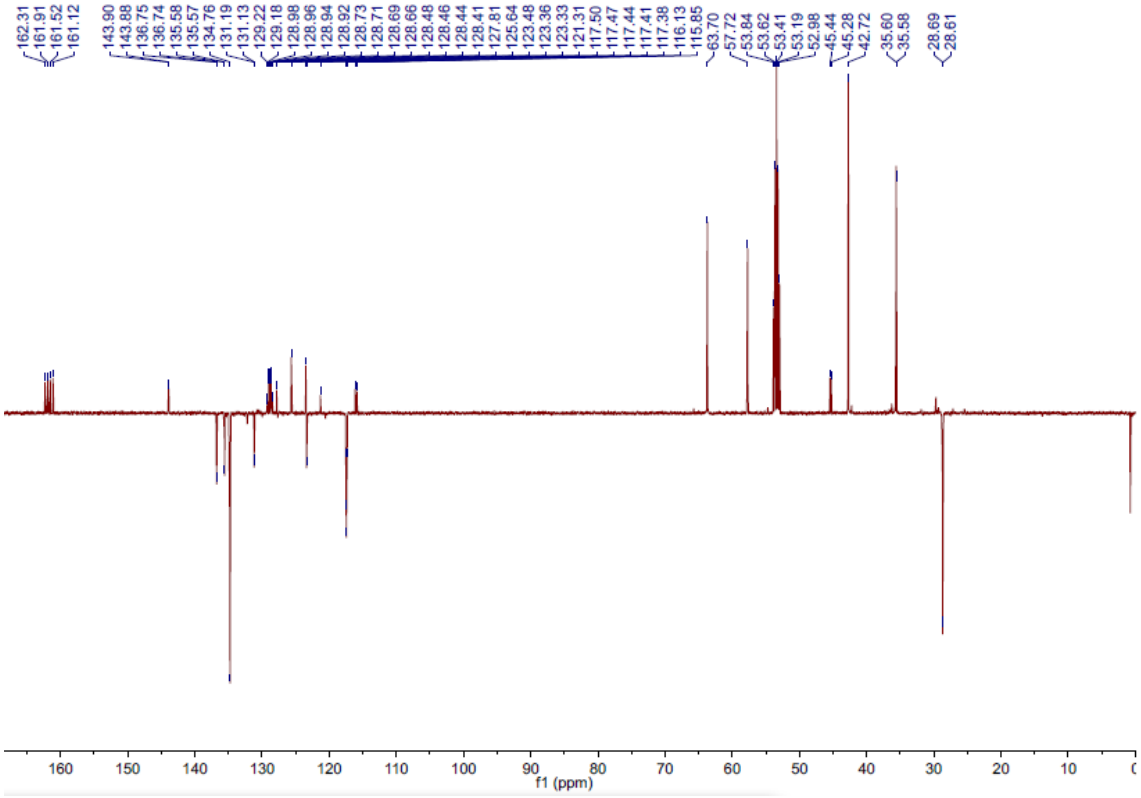

Figure S17. $^{13}C_{jmod}$ NMR spectrum of (**6-BAr$^{F}_{4}$**) in CD_2Cl_2.

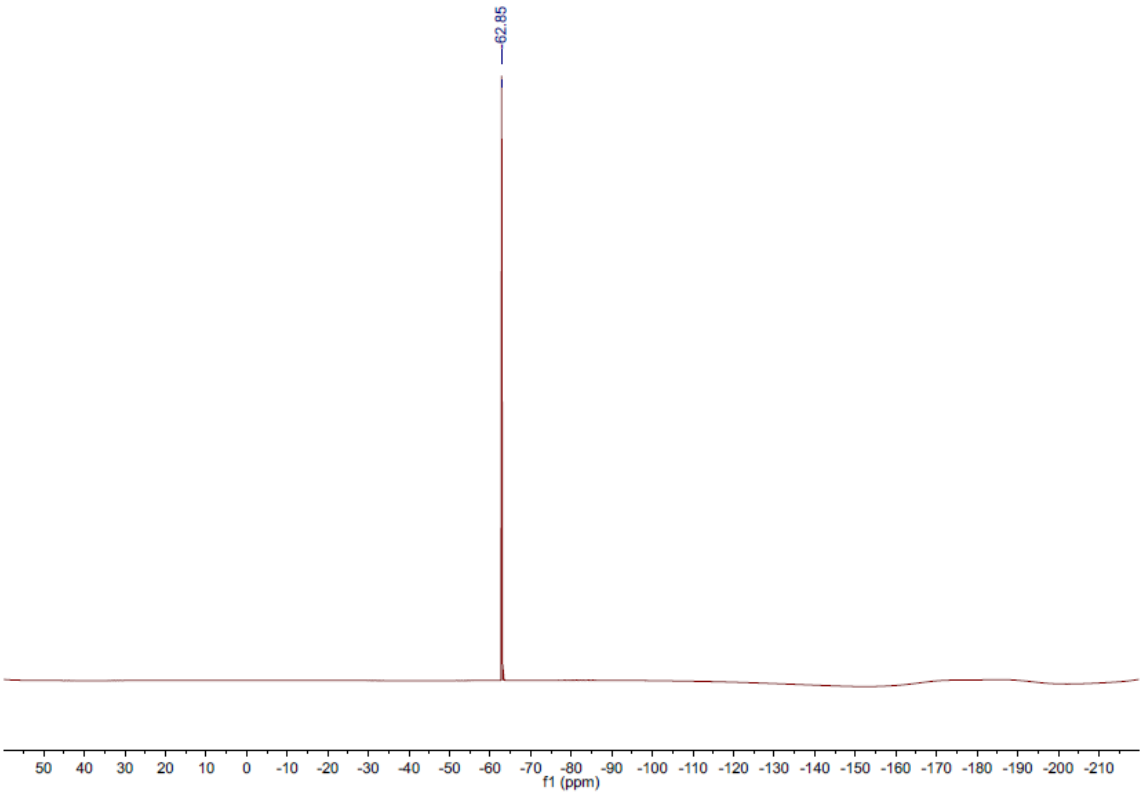

Figure S18. ^{19}F NMR spectrum of (**6-BAr$^{F}_{4}$**) in CD_2Cl_2.

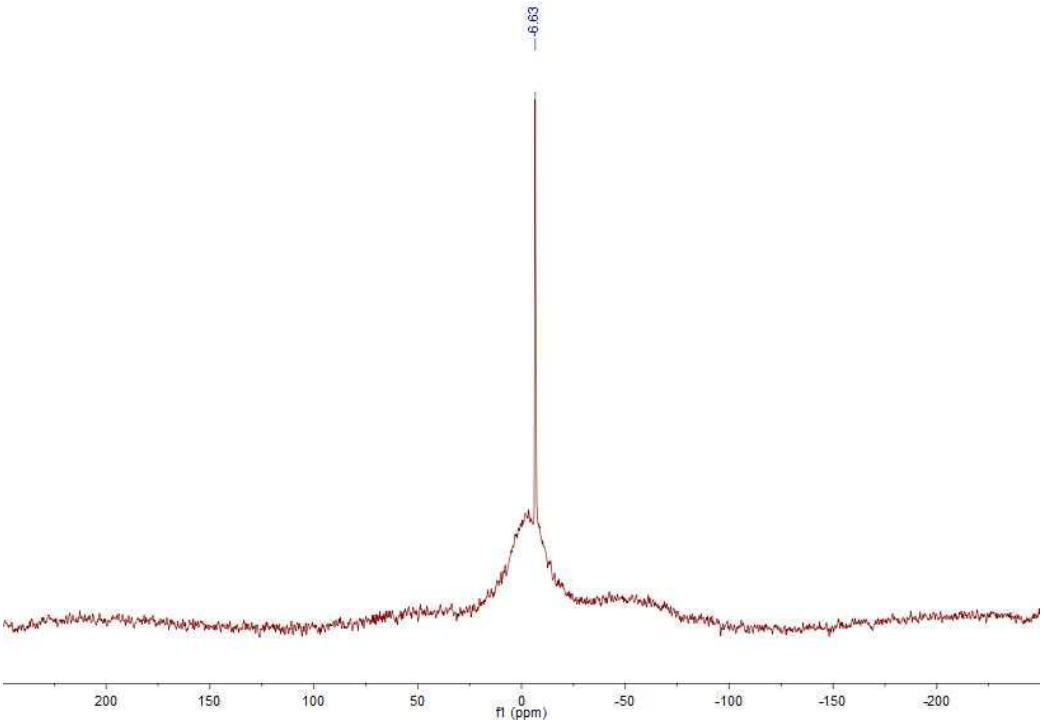

Figure S19. $^{11}B\{^{1}H\}$ NMR spectrum of (**6-BAr$^{F}_{4}$**) in CD_2Cl_2.

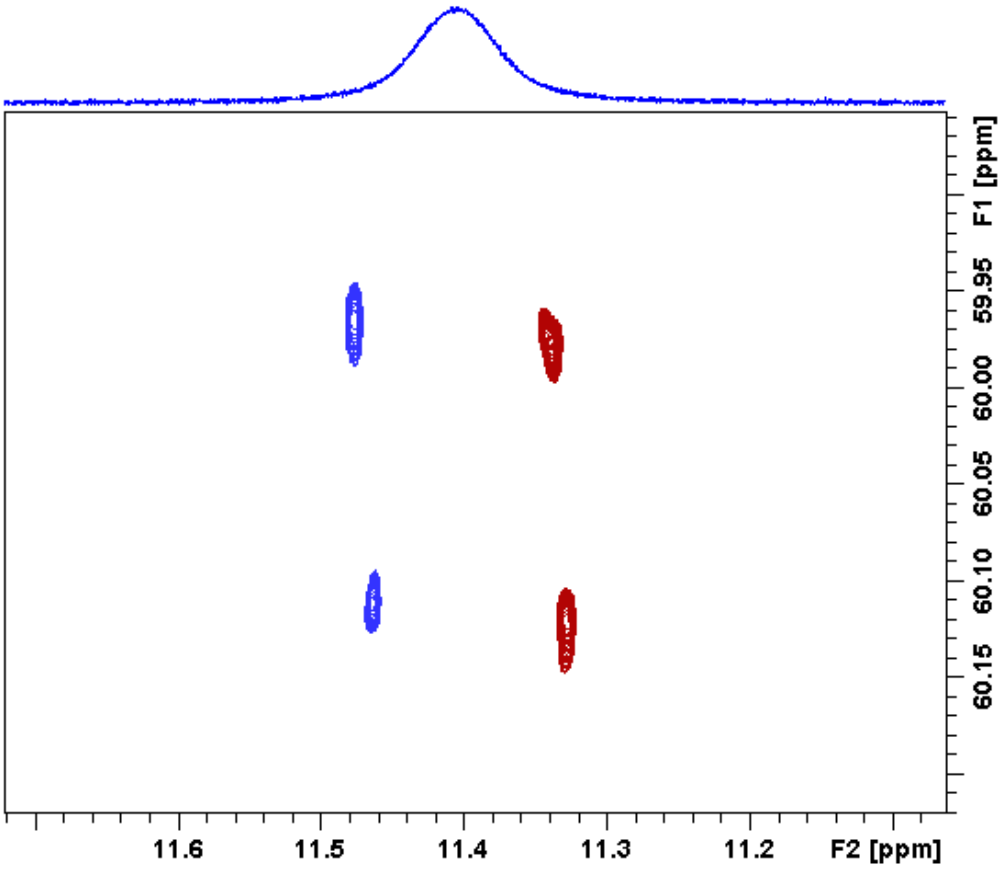

Figure S20. No refocused HSQC ^{1}H-^{15}N NMR spectrum of (**6-BAr$^{F}_{4}$**) in CD_2Cl_2 (HOBS observation scheme).

4. Selected Crystallographic Data

Crystallographic data were collected at low temperature (193(2) K) on a Bruker-AXS APEX II Quazar diffractometer equipped with a 30W air-cooled microfocus or on a Bruker-AXS PHOTON100 D8 VENTURE diffractometer, using MoKŭ radiation (ə = 0.71073 Å). Phi- and omega-scans were used. An empirical absorption correction was performed with SADABS.[4] The structures were solved by direct intrinsic phasing method (SHELXT),[5] and refined using the least-squares method on F^2.[6] All H atoms on carbon atoms were refined isotropically at calculated positions using a riding model. The N-bound and P-bound H atoms were located in a difference Fourier maps and refined freely for **2** and **4**. For **6-BAr$^F_4$**, the standard N-H distance was fixed.

CCDC 1868951 (**2**), 1868952 (**4**) and 1868953 (**6-BAr$^F_4$**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

Table S1. Crystal Data, Data Collection, and Structure Refinement.

ID	(**2**)	(**4**)	(**6-BAr$^F_4$**)
formula	$C_{28}H_{41}AuClNP$, CF_3O_3S, CH_2Cl_2	$C_{28}H_{41}NP$, CF_3O_3S, CH_2Cl_2	$C_{30}H_{43}AuClNOP$, $C_{32}H_{12}BF_{24}$, CH_2Cl_2
M_r	889.00	656.58	1645.20
crystal system	orthorhombic	orthorhombic	monoclinic
space group	*Pbca*	*Pna*2$_1$	*P*2$_1$/*c*
a (Å)	16.2991 (11)	20.1177 (11)	10.0805 (8)
b (Å)	14.3181 (11)	10.9433 (6)	30.253 (3)
c (Å)	28.507 (2)	14.4201 (10)	21.381 (2)
Ŭ (°)	90	90	90
ɓ (°)	90	90	97.816 (4)
ɔ (°)	90	90	90
V (Å^3)	6652.7 (8)	3174.6 (3)	6459.9 (10)
Z	8	4	4
ρ_{calc} (g cm^{-3})	1.775	1.374	1.692
μ (mm^{-1})	4.824	0.371	2.539
F(000)	3536	1384	3264
crystal size (mm^3)	0.180 x 0.160 x 0.140	0.200 x 0.060 x 0.060	0.140 x 0.060 x 0.040
T/K	193 (2)	193 (2)	193 (2)
measd reflns	234119	25042	68767
Unique reflns (Rint)	10598 (0.0417)	5538 (0.0619)	13005 (0.0993)
reflns used for refinement	10598	5538	13005
refined parameters	394	376	1000
GOF on F^2	1.079	1.067	1.038
R_1[a] [I>2ů(I)]	0.0250	0.0508	0.0629
wR_2[b] [all data]	0.0564	0.1363	0.1646

[a] $R_1 = Ǽ||F_o| - |F_c||/ Ǽ |F_o|$. [b] $wR_2 = [Ǽ[w(F_o^2 - F_c^2)^2] / Ǽ [w(F_o^2)^2]]^{1/2}$

[4] Bruker, *SADABS*, Bruker AXS Inc., Madison, Wisconsin, USA.
[5] G. M. Sheldrick *Acta Cryst*. **2015**, A71, 3–8.
[6] G. M. Sheldrick *Acta Cryst*. **2015**, C71, 3–8.

5. Computational Details

All calculations were performed using the Gaussian 09 package[7] and the B3PW91 hybrid functional[8] on the real experimental systems. The gold atom was described with the relativistic electron core potential SDD and associated basis set,[9] augmented by a set of f-orbital polarization functions.[10] The 6-31G** basis set were employed for all other atoms. Optimizations were carried out without any symmetry restrictions taking into solvent effect (DCM: CH_2Cl_2) by means of the continuum standard solvation SMD model.[11] All stationary points involved were fully optimized. All total energies and Gibbs free energies have been zero-point energy (ZPE) and temperature corrected using unscaled density functional frequencies.

Electrostatic Potential Surface (ESP) map has been plotted with chemcraft program.[12]

^{1}H NMR chemical shifts were evaluated by employing the direct implementation of the Gauge Including Atomic Orbitals (GIAO),[13] with the IGLOII[14] basis set on H, C, P, and N atoms, using as reference the corresponding $SiMe_4$ shielding constant calculated at the same level of theory.

Natural Bond Orbital[15] (NBO, 5.9 version)[16] and NCIPLOT[17] calculations were used to analyse the bonding situation of the different gold complexes. The optimized structure of complexes **2**, **6**, **7** and **8** was also subjected to an Atoms-In Molecules analysis (QTAIM analysis)[18] using AIMAll software.[19]

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[7] Gaussian 09, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, 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, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, 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. Cross, V. Bakken, 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. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**.

[8] a) A. D. Becke *J. Chem. Phys.* **1993**, *98*, 5648; b) J. P. Perdew, in *Electronic Structure of Solids 91*, Ed. P. Ziesche and H. Eschrig, Akademie Verlag, Berlin, **1991**, 11.

[9] a) D. Andrae, U. Häussermann, M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta* **1990**, *77*, 123; b) M. Dolg, *Modern Methods and Algorithm of Quantum Chemistry, Vol. 1* (Ed.: J. Grotendorst), John von Neuman Institute for Computing, Jülich (Germany), **2000**, 479.

[10] A. W. Ehlers, M. Biihme, S. Dapprich, A. Gobbi, A. Hijllwarth, V. Jonas, K. F. Kiihler, R. Stegmann, A. Veldkamp, G. Frenking, *Chem. Phys. Letters* **1993**, *208*, 111.

[11] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378.

[12] Chemcraft graphical software for visualization of quantum chemistry computations. https://www.chemcraftprog.com

[13] a) F. London, *J. Phys. Radium* **1937**, *8*, 397; b) R. McWeeny, *Phys. Rev.* **1962**, *126*, 1028; c) R. Ditchfield, *Mol. Phys.* **1974**, *27*, 789; d) K. Wolinski, J. F. Hilton, Pulay, P. *J. Am. Chem. Soc.* **1990**, *112*, 8251; e) J. R. Cheeseman, G. W. Trucks, T. A. Keith, Frisch, M. J. *J. Chem. Phys.* **1996**, *104*, 5497.

[14] W. Kutzelnigg, U. Fleischer, M. Schindler, *The IGLO-Method: Ab Initio Calculation and Interpretation of NMR Chemical Shifts and Magnetic Susceptibilities*, Springer-Verlag, Heidelberg, **1990**, vol. 23.

[15] a) E. Reed, L. A. Curtiss, F. Weinhold, *Chem. Rev.* **1988**, *88*, 899; b) J. P. Foster, F. Weinhold, *J. Am. Chem. Soc.* **1980**, *102*, 7211; c) A. E. Reed, F. Weinhold, *J. Chem. Phys.* **1985**, *83*, 1736.

[16] NBO 5.0 program, E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, F. Weinhold, Theoretical Chemistry Institute, University of Wisconsin, Madison, **2001**.

[17] a) E. R. Johnson, S. Keinan, P. Mori-Sanchez, J. Contreras-Garcia, A. J. Cohen, W. Yang, *J. Am. Chem. Soc.* **2010**, *132*, 6498; b) J. Contreras-Garcia, E. R. Johnson, S. Keinan, R. Chaudret, J. P. Piquemal, D. N. Beratan, W. Yang. *J. Chem. Theory Comput.* **2011**, *7*, 625.

[18] a) R. F. W. Bader, *Chem. Rev.* **1991**, *91*, 893; b) R. F. W. Bader, *Acc. Chem. Res.* **1985**, *18*, 9.

[19] AIMAll (Version 10.10.11), Todd A. Keith, **2010** (aim.tkgristmill.com).

Natural Localized Molecular Orbital (NLMO) were plotted with Molekel 4.3[20] and all the geometrical structures with Gaussview 5.0[21] and CYLview.[22] NCIPLOT were drawn with VMD software.[23]

In order to analyze the impact of the relativistic effects on the geometrical parameters of complex **2**, structural optimization and frequency calculations were performed with the ADF-2017[24] program developed by Baerends *et al.*. BP86 functional[2a,25] was used. The MOs were expanded in a large uncontracted set of Slater-type orbitals (STOs) containing diffuse functions, TZ2P.[26] Auxiliary sets of s, p, d, f, and g STOs were used to fit the molecular densities and to represent the Coulomb and exchange potentials accurately in each SCF cycle. Scalar relativistic effects or spin-orbit coupling effects were incorporated by applying the zeroth-order regular approximation (ZORA) to the Dirac equation.[27] Finally, we considered the solvent effect using Conductor like Screening Model (COSMO) of solvation implemented in ADF.[28] The results were compared to those calculated with Gaussian 09 program at the SMD-BP86/SDD+f(Au),6-31G**(other atoms) level of theory.

[20] MOLEKEL 4.3, P. Flükiger, H. P. Lüthi, S. Portmann, J. Weber, Swiss Center for Scientific Computing, Manno (Switzerland), **2000-2002**.
[21] GaussView, Version 5, R. Dennington, T. Keith, J. Millam, *Semichem Inc.*, Shawnee Mission, KS, **2009**.
[22] C. Y. Legault, CYLview, 1.0b, Université de Sherbrooke, **2009** (http://www.cylview.org).
[23] W. Humphrey, A. Dalke, K. Schulten, "VMD - Visual Molecular Dynamics", *J. Molec. Graphics* **1996**, *14*, 33-38. http://www.ks.uiuc.edu/Research/vmd/
[24] E. J. Baerends, T. Ziegler, J. Autschbach, D. Bashford, A. Bérces, F.M. Bickelhaupt, C. Bo, P.M. Boerrigter, L. Cavallo, D.P. Chong, L. Deng, R.M. Dickson, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, C. Fonseca Guerra, M. Franchini, A. Ghysels, A. Giammona, S.J.A. van Gisbergen, A.W. Götz, J.A. Groeneveld, O.V. Gritsenko, M. Grüning, S. Gusarov, F.E. Harris, P. van den Hoek, C.R. Jacob, H. Jacobsen, L. Jensen, J.W. Kaminski, G. van Kessel, F. Kootstra, A. Kovalenko, M.V. Krykunov, E. van Lenthe, D.A. McCormack, A. Michalak, M. Mitoraj, S.M. Morton, J. Neugebauer, V.P. Nicu, L. Noodleman, V.P. Osinga, S. Patchkovskii, M. Pavanello, P.H.T. Philipsen, D. Post, C.C. Pye, W. Ravenek, J.I. Rodríguez, P. Ros, P.R.T. Schipper, H. van Schoot, G. Schreckenbach, J.S. Seldenthuis, M. Seth, J.G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E.M. van Wezenbeek, G. Wiesenekker, S.K. Wolff, T.K. Woo, A.L. Yakovle, ADF2017, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands,http://www.scm.com.
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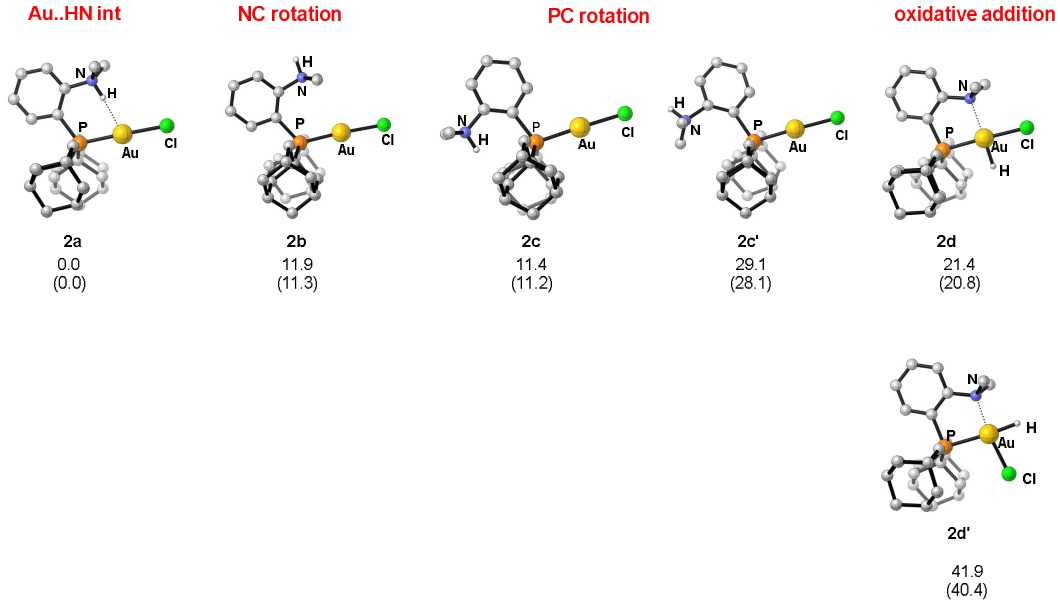
[28] a) A. Klamtn G. Schüürmann, *J. Chem. Soc. Perkin Trans 2* **1993**, 799; b) A. Klamt, *J. Phys. Chem.* **1995**, *99*, 2224; c) A. Klamt, V. Jones, *J. Phys. Chem.* **1996**, *105*, 9972.

6. Computational Results

Table S2. Optimized geometries of the different forms of the cationic complex **2** at the SMD(DCM)-B3PW91/SDD+f(Au)/6-31G**(other atoms) level of theory, without taking into account the TfO counter-anion. Distances in Å, bond angles in ° and relative energies in kcal/mol (ΔG values and ΔE values into brackets). Spectroscopic data computed for the three conformers **2a-c**.



	2a	2b	2c	2d
P-Au	2.303	2.304	2.305	2.295
Au-Cl	2.338	2.344	2.339	2.382
N-H	1.046	1.024	1.025	/
Au-H	2.134	/	/	1.544
P-Au-Cl	178.53	176.51	178.14	176.55
N-H-Au	174.18	/	/	/
ν_{NH} **(cm^{-1})**	3032.3	3457.3	3445.9	/
$\Delta\nu_{NH}$[a]	-443.3	-18.3	-29.7	/
ν_{ND}	2089.4	2544.5	2489.2	/
δ^1H (NH) NMR (ppm)	11.94	5.64	6.31	/

[a] difference with $HNMe_2Ph^+$

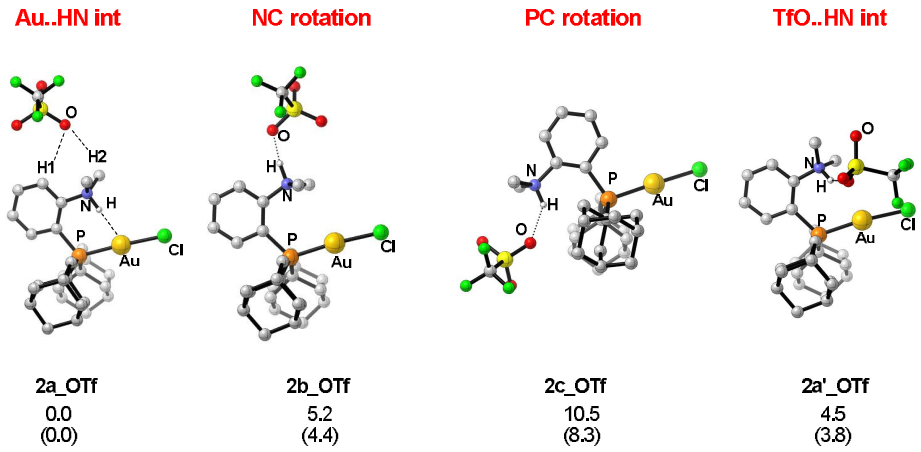
Table S3. Investigations of the relativistic effects on the geometry of complex **2** in its form **2a**, with AuÄHï N contact. ADF calculations were performed with and without ZORA effect on **2a**, without taking into account the TfO counter-anion, and compared with Gaussian 09 calculations. Solvent effects (DCM) were taken into account via SMD (Gaussian) or COSMO (ADF) models. Distances in Å and bond angles in °.

	Au-H	**N-H**	**P-Au-Cl**	**N-H-Au**	**Au-Cl**	**Au-P**
Gaussian						
BP86[a]	2.101	1.065	178.37	178.78	2.348	2.307
B3PW91[a]	2.134	1.046	178.53	174.18	2.338	2.303
ADF						
BP86[b]	2.277	1.049	176.48	174.23	2.461	2.529
ZORA (relativistic scalar)-BP86[c]	2.078	1.063	178.48	174.95	2.317	2.297
ZORA (spin orbit)-BP86[d]	2.099	1.060	178.32	175.79	2.314	2.294

[a] Gaussian 09, optimization in solvent with SMD model (DCM) using SDD+f(Au)/6- 31G** basis set.
[b] ADF 2017, optimization in solvent using COSMO (DCM) model with TZ2P basis set.
[c] ADF 2017 optimization in solvent using COSMO (DCM) model with TZ2P basis set and by taking into account relativistic effects using ZORA with scalar correction.
[d] ADF 2017 optimization in solvent using COSMO (DCM) model with TZ2P basis set and by taking into account relativistic effects using ZORA with spin-orbit coupling.

The geometrical structures computed for **2a** using Gaussian 09 program with the two functionals, B3PW91 and BP86, are very similar. These structures are also similar close to that obtained upon optimization using the ADF program with BP86 functional taking into account zero-order regular approximation (ZORA).

Table S4. Optimized geometries of the different forms of the cationic complex **2** at the SMD(DCM)-B3PW91/SDD+f(Au)/6-31G**(other atoms) level of theory, taking into account the TfO counter-anion. Distances in Å, bond angles in ° and relative energies in kcal/mol (ΔG values and ΔE values into brackets).



	2a_OTf	2b_OTf	2c_OTf	2aô_OTf
P-Au	2.301	2.303	2.325	2.294
Au-Cl	2.343	2.344	2.344	2.347
N-H	1.043	1.056	1.034	1.038
Au-H	2.161	/	/	2.658
H-O_{OTf}	2.288/2.340	1.670	2.008	2.018
P-Au-Cl	177.30	175.18	178.12	171.42
N-H-Au	172.80	/	/	127.87

Figure S21. Optimized geometries of the different forms of the protonated ligand **4** at the SMD(DCM)-B3PW91/6-31G** level of theory, without taking into account the TfO counter-anion. Protonation of P (**4-PH**) or N (**4-NH**), and transition state for the proton transfer. Distances in Å and relative energies in kcal/mol (ΔG values and ΔE values into brackets).

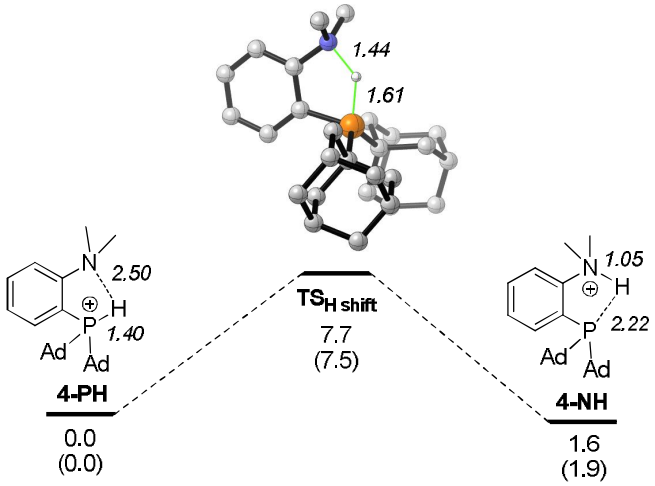
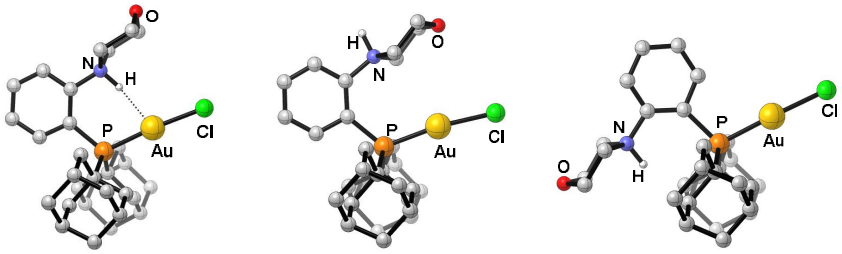


Table S5. Optimized geometries of the different forms of the cationic complex **6** at the SMD(DCM)-B3PW91/SDD+f(Au)/6-31G**(other atoms) level of theory, without taking into account the TfO/BAr^F_4 counter-anion. Distances in Å, bond angles in ° and relative energies in kcal/mol (ΔG values and ΔE values into brackets). Spectroscopic data computed for the three conformers **6a-c**.



6a
0.0
(0.0)

6b
9.1
(9.0)

6c
12.8
(12.1)

	6a	**6b**	**6c**
P-Au	2.298	2.302	2.308
Au-Cl	2.338	2.343	2.339
N-H	1.045	1.028	1.026
Au-H	2.218	/	/
P-Au-Cl	175.15	172.47	178.18
N-H-Au	170.07	/	/
ν_{NH} (cm^{-1})	3078.4	3406.4	3489.9
$\Delta\nu_{NH}$[a]	-365.3	-37.4	46.1
δ^1H (NH) NMR (ppm)	11.23	5.04	5.81

[a] difference with HNmorpholine$^+$

Table S6. NBO analyses for complexes **2** (forms **2a**, **2b** and **2c**), **2a-OTf** and **6a**. Stabilizing energy ΔE(2) and percentage of main atoms in the Natural Localized Molecular Orbital (NLMO) accounting for the Au···H–N interaction, populations of LP(Au) and σ^*_{NH} NBO orbitals. Wiberg Bond index (WBI). NPA charges of the NR_2H and PAuCl fragments (q_X).

	2a	**2b**	**2c**	**2a-OTf**	**6a**
LP(Au)→σ*$_{NH}$ ΔE(2)[a]	12.8	/	/	12.3	8.9
NLMO LP(Au)	95.9% Au 0.7% N 2.5% H	97.7% Au	97.6% Au	96.6% Au 0.6% N 2.0% H	97.1% Au 0.4% N 1.5% H
pop (LP(Au)[b]	1.92	1.95	1.95	1.93	1.94
pop (σ*$_{NH}$)[b]	0.12	0.02	0.03	0.10	0.09
WBI (Au···H)	0.12	/	/	0.10	0.08
WBI (N-H)	0.61	0.73	0.71	0.65	0.64
NPA charges					
q_{NR2H}	0.605	0.656	0.675	0.595	1.274
q_{PAuCl}	0.765	0.713	0.651	0.754	0.720

[a] Stabilizing energy ΔE(2) in kcal/mol for the Au→NH donor-acceptor interaction

[b] Population of the occupied d_{Au} orbital and vacant σ^*_{NH} orbital involved in the Au→NH interaction

Figure S22. Electrostatic potential surface (ESP) maps of complex **2** (forms **2a** and **2b**) computed at SMD(DCM)-B3PW91/SDD+f(Au)/6-31G**(other atoms) level of theory and plotted over the range 0.1 (red) to 0.3 au (blue). The isosurfaces are drawn at 0.002 e.au^{-3}. Side views (left) and front views (right).

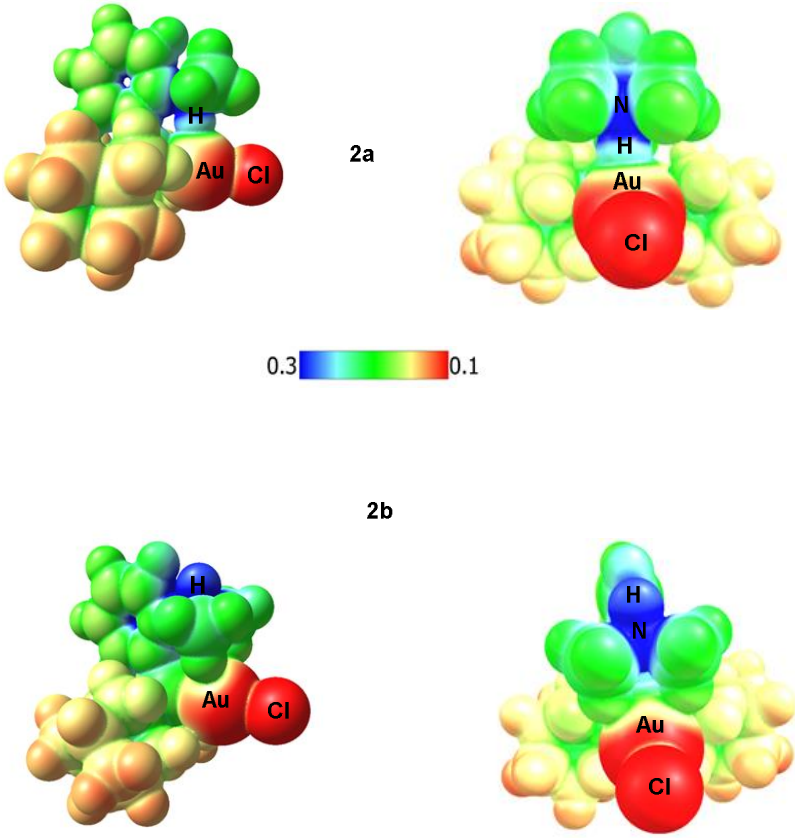


Figure S23. Superposition plot (cutoff: 0.08) of the donor LP(Au) and acceptor σ*(NH) NBO orbitals involved in the Au···H–N interaction in complexes **2a** and **6a**. Participation of each atom in percent in the associated NLMO. Stabilizing interaction ΔE(2) for the Au→NH donor-acceptor interaction in kcal/mol. Calculations performed at the SMD(DCM)-B3PW91/SDD+f(Au)/6-31G**(other atoms) level of theory.

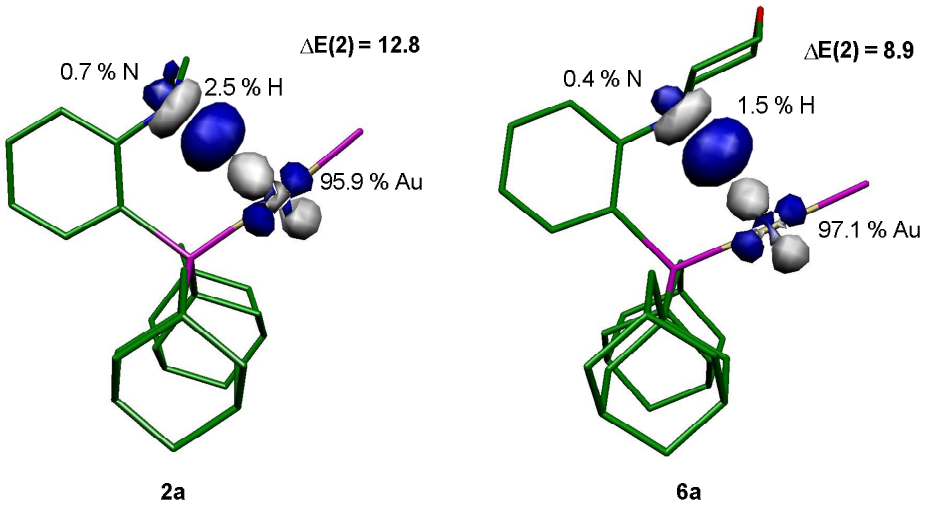


Table S7. AIM analysis of complexes **2** and **6** (forms **2a**, **2a-OTf** and **6a** with Au···H–N interaction).

	2a	**2a-OTf**	**6a**
		Au···H	
ρ(r)[a]	0.039	0.037	0.033
$\nabla^2\rho(r)$[b]	0.068	0.070	0.061
Bond index $\delta_{H\text{-}Au}$[c]	0.165	0.153	0.147
		N-H	
ρ(r)[a]	0.319	0.324	0.320
$\nabla^2\rho(r)$[b]	-1.68	-1.70	-1.69
Bond index $\delta_{H\text{-}N}$[c]	0.598	0.627	0.613

[a] $\rho(r_c)$ density in e.bohr^{-3}

[b] $\nabla^2\rho(r_c)$ Laplacian of density in e.bohr^{-5}

[c] δ delocalization index, often called bond order, as introduced by Bader.

Figure S24. Contour line diagrams of the Laplacian distribution $\nabla^2\rho(r_c)$ in the plane containing the three atoms N, H and Au, with charge accumulation ($\nabla^2\rho(r)<0$) in blue lines and charge depletion ($\nabla^2\rho(r)>0$) in red.

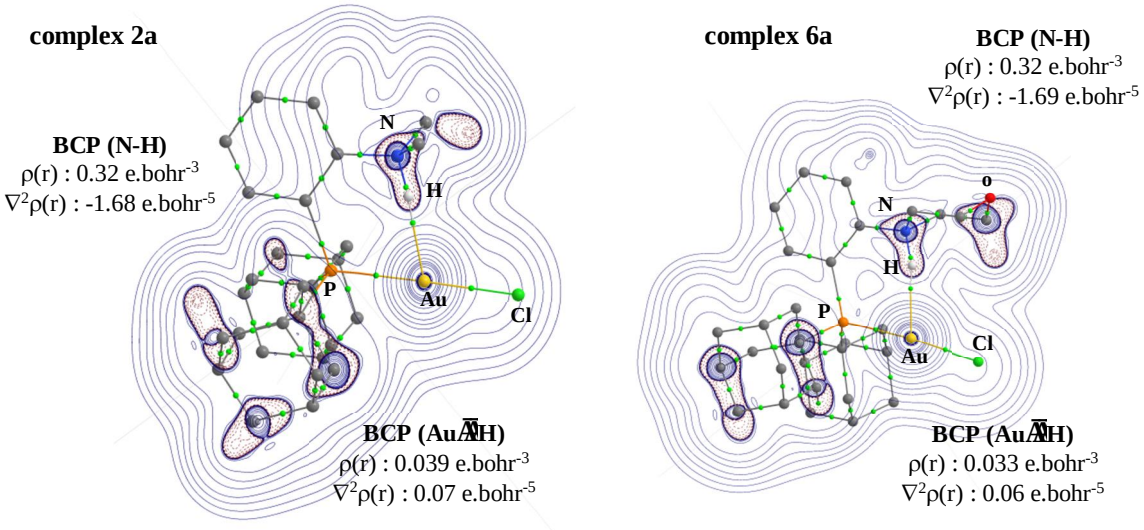


Figure S25. Contour plots of the reduced density gradient isosurfaces representing the noncovalent interactions in complexes **2** and **6** (forms **2a** and **6a** with Au···H–N contact). NCI surfaces correspond to s = 0.5 au and a color scale of -0.05 < sign (λ_2)ρ < 0.05 au for SCF densities. Density ρ(r) in e.bohr^{-3} and eigenvalue λ_2 of the electron density Hessian. Calculations have been performed at the SMD(DCM)-B3PW91/SDD+f(Au)/6-31G**(other atoms) level of theory. Side views (left) and front views (right).

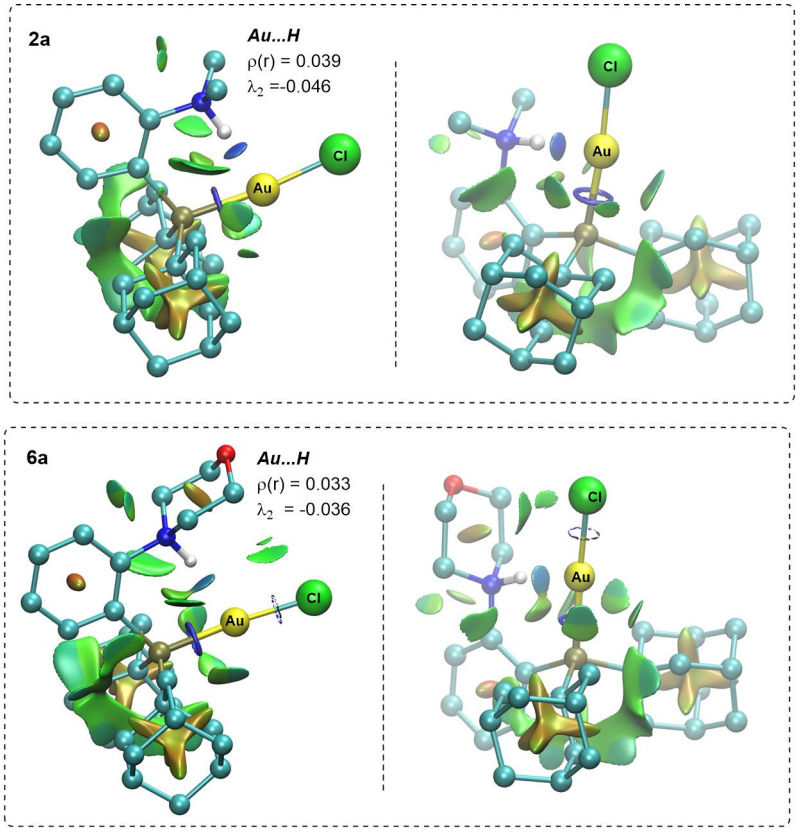
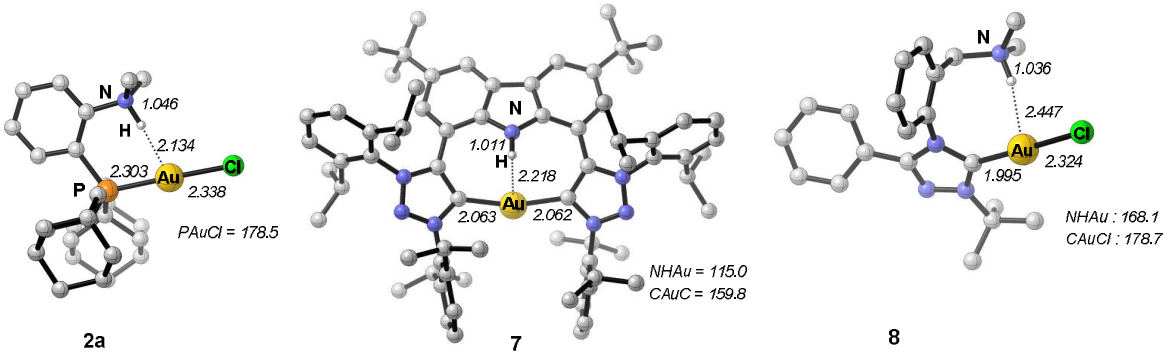


Table S8. Comparison of complex **2** (form **2a** with AuÄHï N contact) with the two recently reported complexes **7** and **8**.[29] Calculations performed at the SMD(DCM)-B3PW91/SDD+f(Au)/6-31G**(other atoms) level of theory on the naked cations. Optimized geometries with main features (distances in Å, angles in °). NBO and AIM analyses.

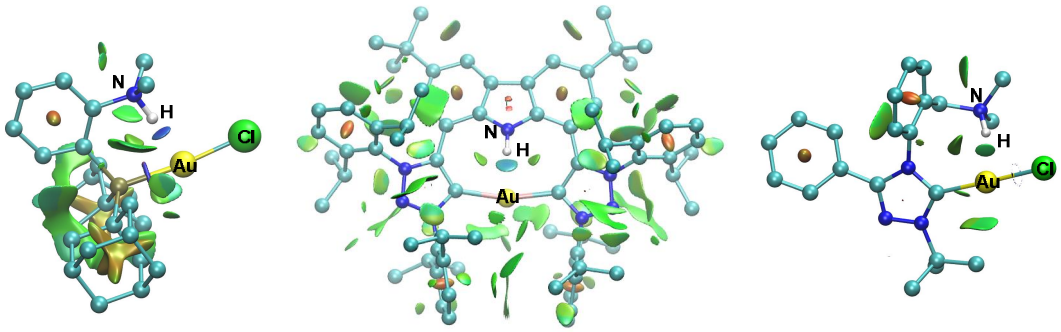


complex	2a	7	8
		NBO	
ΔE(2)[a] LP(Au)→σ*$_{NH}$	12.8	3.8	2.1
NLMO LP(Au)	95.9% Au 0.7% N 2.5% H	98.4% Au 0.4% N 0.2% H	96.1% Au 0.6% N 0.2% H
WBI (AuÄH)[b] **WBI (N-H)**	0.12 0.61	0.03 0.73	0.08 0.65
		AIM	
		AuÄH	
ρ(r)[c] **$\nabla^2\rho(r)$[d]** **Bond index $\delta_{H\text{-}Au}$[e]**	0.039 0.068 0.165	0.034 0.112 0.089	0.021 0.042 0.110
		NÄH	
ρ(r)[c] **$\nabla^2\rho(r)$[d]** **Bond index $\delta_{H\text{-}N}$[e]**	0.319 -1.680 0.598	0.340 -1.830 0.681	0.328 -1.777 0.636

[a] Stabilizing energy ΔE(2) in kcal/mol for the Au→NH donor-acceptor interaction;
[b] Wiberg Bond Index; [c] $\rho(r_c)$ density in e.bohr^{-3}; [d] $\nabla^2\rho(r_c)$ Laplacian of density in e.bohr^{-5};
[e] δ delocalization index, often called bond order, as introduced by Bader.

[29] a) G. Kleinhans, M. M. Hansmann, G. Guisado-Barrios, D. C. Liles, G. Bertrand, D. I. Bezuidenhout, *J. Am. Chem. Soc.* **2016**, *138*, 15873. b) E. Andris, P. C. Andrikopoulos, J. Schulz, J. Turek, A. RŢğiļka, J. Roithova, L. Rulíģek, *J. Am. Chem. Soc.* **2018**, *140*, 216.

Figure S26. NCI plots for complexes **2** (form **2a** with Au···H–N contact), **7** and **8**.



2a **7** **8**

7. Z-matrices and Energies in au

2a

Sum of electronic and zero-point Energies= -2082.729375
Sum of electronic and thermal Enthalpies = -2082.698949
Sum of electronic and thermal Free Energies = -2082.788876

C	-0.05439	-0.43617	2.04719
C	0.28974	0.46011	3.07735
H	0.62077	1.45895	2.82690
C	0.22639	0.11579	4.42291
H	0.50523	0.84636	5.17580
C	-0.19130	-1.15769	4.79255
H	-0.24891	-1.44372	5.83793
C	-0.53469	-2.07378	3.80632
H	-0.85516	-3.07088	4.09029
C	-0.46455	-1.72121	2.46044
C	-2.26357	-3.20910	1.61260
H	-2.40509	-3.73933	2.55388
H	-2.47880	-3.87192	0.77370
H	-2.90143	-2.32675	1.57154
C	0.10120	-3.94176	1.50897
H	1.12060	-3.57233	1.40365
H	-0.15765	-4.58507	0.66717
H	-0.01301	-4.48649	2.44568
C	1.89952	0.73317	0.04403
C	2.80865	-0.32091	0.71736
H	2.57454	-1.32115	0.32731
H	2.63540	-0.33953	1.79889
C	4.28816	0.00963	0.44599
H	4.90633	-0.74874	0.94246
C	2.19204	0.72155	-1.47936
H	1.96354	-0.26803	-1.89648
H	1.55522	1.44559	-1.99815
C	3.73111	2.44986	0.32406
H	3.94786	3.44367	0.73487
C	4.00062	2.44032	-1.18549
H	5.05142	2.68818	-1.38313
H	3.39013	3.20410	-1.68503
C	3.67224	1.04959	-1.74387
H	3.83752	1.03266	-2.82820
C	2.24540	2.13551	0.59081
H	1.61888	2.89181	0.10643
H	2.06342	2.19586	1.66824
C	4.55696	-0.00405	-1.06469
H	5.61556	0.20929	-1.26049
H	4.34626	-0.99913	-1.47819
C	4.61169	1.39898	1.01490
H	4.43982	1.41427	2.09953
H	5.67190	1.63321	0.85454
C	-1.22767	1.54695	0.11759
C	-3.57259	2.43232	-1.46235
H	-4.38933	3.13409	-1.67446
H	-3.62867	1.63492	-2.21521
C	-2.33046	3.68338	0.88857
H	-2.27275	4.47934	1.64148
C	-1.07848	2.15999	-1.29355
H	-0.11815	2.68111	-1.37944
H	-1.09067	1.36379	-2.05082
C	-3.73707	1.84428	-0.05350
H	-4.69335	1.31134	0.01836
C	-1.19738	2.67504	1.17030
H	-1.34173	2.25864	2.17259
H	-0.23478	3.19559	1.16072
C	-2.22184	3.15516	-1.55649
H	-2.09192	3.57111	-2.56318
C	-3.68598	2.97097	0.98662
H	-3.82745	2.56322	1.99630
H	-4.50106	3.68416	0.80931
C	-2.60219	0.83991	0.21268
H	-2.65931	0.02794	-0.52366
H	-2.72430	0.39545	1.20889
C	-2.16314	4.28107	-0.51510
H	-2.95670	5.01459	-0.70710
H	-1.20686	4.81537	-0.58996
Au	-0.40359	-1.37564	-1.32194
Cl	-0.92230	-2.91705	-3.00168
N	-0.83651	-2.77463	1.49625
P	0.08701	0.18592	0.29812
H	-0.74509	-2.35637	0.54232

2b

Sum of electronic and zero-point Energies= -2082.711304
Sum of electronic and thermal Enthalpies = -2082.681012
Sum of electronic and thermal Free Energies = -2082.769836

C	-0.09614	0.00998	2.16077
C	-0.29976	1.22913	2.83887
H	-0.39426	2.13988	2.26501
C	-0.39158	1.34279	4.22192
H	-0.55063	2.31894	4.66923
C	-0.27809	0.20760	5.01045
H	-0.34341	0.26115	6.09229
C	-0.07937	-1.01639	4.38662
H	0.00615	-1.91284	4.99711
C	0.00863	-1.12625	2.99754
C	1.53675	-2.83604	1.95460
H	1.61607	-2.33413	0.99231
H	1.60246	-3.91610	1.81894
H	2.30867	-2.48996	2.64184
C	-0.96147	-3.14868	1.85437
H	-1.85635	-2.95981	2.44717
H	-0.77271	-4.21996	1.77781
H	-1.05073	-2.71148	0.86058
C	1.49753	1.26764	-0.06789
C	2.73127	0.38391	0.24128
H	2.76115	0.15016	1.31355
H	2.66103	-0.56721	-0.30290
C	4.02470	1.11021	-0.16809
H	4.87483	0.45541	0.06074
C	1.48255	1.59344	-1.57978
H	1.37088	0.66921	-2.16230
H	0.62803	2.23641	-1.81774
C	2.93885	3.31122	0.30481
H	3.00506	4.24460	0.87772
C	2.90142	3.62308	-1.19680
H	2.05149	4.27883	-1.42783
H	3.81170	4.16069	-1.49201
C	2.78327	2.30968	-1.98177
H	2.74106	2.52030	-3.05754
C	1.64688	2.58205	0.72730
H	0.78643	3.23826	0.56331
H	1.70642	2.37045	1.79964
C	3.98732	1.40899	-1.67357
H	3.91581	0.47333	-2.24365
H	4.91700	1.90433	-1.98192
C	4.15068	2.42283	0.61610
H	4.20246	2.21763	1.69364
H	5.07897	2.94004	0.34120
C	-1.72535	0.95906	-0.20223
C	-4.41268	0.39692	-1.35519
H	-5.41468	0.71319	-1.67273
H	-4.33980	-0.68146	-1.54915
C	-3.28506	2.93991	-0.41058
H	-3.36396	4.01728	-0.21871
C	-1.94552	0.68020	-1.71206
H	-1.18103	1.18609	-2.31073
H	-1.84957	-0.39567	-1.90882
C	-4.21914	0.68153	0.13992
H	-4.97074	0.13598	0.72424
C	-1.88118	2.47794	0.02883
H	-1.75555	2.73321	1.08436
H	-1.12266	3.02803	-0.53840
C	-3.34205	1.15293	-2.15248
H	-3.45231	0.93775	-3.22259
C	-4.35158	2.18900	0.39913
H	-4.23525	2.40103	1.47038
H	-5.35310	2.53337	0.11096
C	-2.82352	0.20703	0.58675
H	-2.70985	0.38420	1.66199
H	-2.73050	-0.87423	0.41862
C	-3.48030	2.66068	-1.90542
H	-4.46989	3.00835	-2.22932
H	-2.73627	3.21222	-2.49512
N	0.20455	-2.53762	2.57246
P	-0.03602	0.19117	0.29476
Au	0.22994	-1.69578	-0.99983
Cl	0.50685	-3.53065	-2.43144
H	0.23219	-3.04668	3.46083

2c

Sum of electronic and zero-point Energies= -2082.711584
Sum of electronic and thermal Enthalpies = -2082.681156
Sum of electronic and thermal Free Energies = -2082.770699

C	-0.46578	0.85296	1.81279
C	0.15100	0.20604	2.90377
H	0.80395	-0.63808	2.70091
C	-0.03435	0.58647	4.22804
H	0.47568	0.04148	5.01625
C	-0.87496	1.64943	4.52564
H	-1.04736	1.95954	5.55127
C	-1.49981	2.32537	3.48482
H	-2.15094	3.16041	3.72199
C	-1.29383	1.94630	2.15926
C	-1.59241	4.23565	1.21964
H	-2.04852	4.69584	2.09364
H	-1.95337	4.72283	0.31365
H	-0.50869	4.30141	1.28923
C	-3.49936	2.68399	1.23802
H	-3.78791	1.63572	1.21209
H	-3.91432	3.22012	0.38396
H	-3.83608	3.14587	2.16494
C	1.12889	1.22270	-0.78813
C	2.36436	1.46291	0.11468
H	2.06050	1.96675	1.04090
H	2.81061	0.50053	0.39834
C	3.40500	2.32102	-0.62770
H	4.26302	2.47487	0.03828
C	1.58901	0.50452	-2.07765
H	2.01034	-0.47793	-1.82644
H	0.73405	0.33662	-2.74310
C	1.57771	3.44111	-1.91700
H	1.11527	4.40090	-2.17917
C	2.01784	2.70790	-3.19145
H	1.15863	2.55263	-3.85770
H	2.74527	3.31843	-3.74149
C	2.64076	1.35820	-2.80897
H	2.94989	0.82139	-3.71407
C	0.53761	2.59458	-1.15625
H	-0.36811	2.49015	-1.76208
H	0.28045	3.12881	-0.23666
C	3.85530	1.58695	-1.89831
H	4.31979	0.62715	-1.63748
H	4.61350	2.17946	-2.42636
C	2.79205	3.67585	-1.00895
H	2.49083	4.22531	-0.10682
H	3.53684	4.29347	-1.52701
C	-1.58985	-0.49855	-0.76692
C	-3.46299	-2.76056	-1.26458
H	-4.35538	-3.18950	-1.73797
H	-3.01299	-3.54917	-0.64768
C	-3.51424	-0.02555	-2.33992
H	-3.96938	0.75684	-2.95981
C	-1.21398	-1.71500	-1.65683
H	-0.48353	-1.42331	-2.41848
H	-0.74446	-2.49264	-1.04119
C	-3.85428	-1.56374	-0.38839
H	-4.55547	-1.88581	0.39140
C	-2.25074	0.55760	-1.67801
H	-2.53643	1.45861	-1.12306
H	-1.54749	0.87109	-2.45718
C	-2.46822	-2.29417	-2.33587
H	-2.15830	-3.14609	-2.95340
C	-4.50493	-0.47754	-1.25858
H	-4.80587	0.37726	-0.63794
H	-5.41734	-0.86816	-1.72650
C	-2.59914	-0.99351	0.29508
H	-2.88332	-0.17538	0.96357
H	-2.12986	-1.76546	0.91944
C	-3.12198	-1.22171	-3.21624
H	-4.01072	-1.63119	-3.71311
H	-2.42938	-0.90165	-4.00570
N	-2.00152	2.78905	1.15922
P	-0.01473	0.04737	0.16199
Au	1.22217	-1.85009	0.58849
Cl	2.49354	-3.78049	0.94744
H	-1.73566	2.45671	0.22688

2cô

Sum of electronic and zero-point Energies= -2082.684661
Sum of electronic and thermal Enthalpies = -2082.654733
Sum of electronic and thermal Free Energies = -2082.742465

C	-0.17508	-1.27300	1.69968
C	-0.85428	-0.50423	2.67410
H	-1.08665	0.52874	2.43388
C	-1.25628	-0.96120	3.92331
H	-1.77464	-0.28451	4.59534
C	-0.98275	-2.26832	4.28719
H	-1.27537	-2.66799	5.25261
C	-0.30513	-3.06674	3.37842
H	-0.06938	-4.08891	3.66578
C	0.09479	-2.60675	2.11861
C	2.35148	-3.52682	1.54277
H	2.67765	-2.67523	0.95732
H	2.81524	-4.44204	1.17355
H	2.59267	-3.37542	2.59475
C	0.40940	-4.12592	0.07268
H	-0.62796	-4.44485	0.15658
H	1.03544	-4.96891	-0.22210
H	0.51035	-3.31973	-0.64221
C	-1.53335	-0.60628	-0.96102
C	-2.77688	-0.33133	-0.07832
H	-2.79419	-1.01625	0.77747
H	-2.73133	0.69056	0.32063
C	-4.06508	-0.50854	-0.90150
H	-4.92084	-0.31261	-0.24364
C	-1.55023	0.37597	-2.15407
H	-1.45488	1.40882	-1.79444
H	-0.70376	0.17279	-2.81730
C	-2.92096	-2.20939	-2.33360
H	-2.95296	-3.23900	-2.71180
C	-2.91882	-1.22261	-3.50804
H	-2.06271	-1.41845	-4.16731
H	-3.82627	-1.35665	-4.11061
C	-2.84996	0.21074	-2.96329
H	-2.82842	0.92569	-3.79500
C	-1.63535	-2.04229	-1.49726
H	-0.76184	-2.28954	-2.11204
H	-1.67440	-2.74255	-0.65855
C	-4.06576	0.48566	-2.06860
H	-4.03308	1.51538	-1.68934
H	-4.99216	0.38507	-2.64874
C	-4.14100	-1.94317	-1.44162
H	-4.16852	-2.66045	-0.61026
H	-5.06576	-2.08123	-2.01641
C	1.71850	-0.20220	-0.71055
C	4.18481	1.43799	-1.07755
H	5.19979	1.57984	-1.47052
H	3.91788	2.35290	-0.53290
C	3.56921	-1.26278	-2.06566
H	3.84467	-2.17484	-2.60995
C	1.77583	1.01469	-1.67647
H	1.09066	0.87026	-2.51520
H	1.46509	1.92846	-1.15385
C	4.14650	0.23098	-0.13189
H	4.83592	0.39103	0.70638
C	2.13842	-1.44198	-1.51827
H	2.11926	-2.33970	-0.90099
H	1.44027	-1.60056	-2.34850
C	3.20180	1.19835	-2.23003
H	3.19219	2.06761	-2.89903
C	4.54417	-1.03815	-0.89897
H	4.54324	-1.90572	-0.22587
H	5.56723	-0.93680	-1.28328
C	2.72411	0.07772	0.43437
H	2.70136	-0.71894	1.18462
H	2.43248	1.00192	0.95146
C	3.61318	-0.05644	-3.01001
H	4.62345	0.06609	-3.42110
H	2.93564	-0.21503	-3.85936
N	0.86557	-3.68769	1.42448
P	-0.00580	-0.20477	0.12198
Au	-0.27738	2.01453	0.74939
Cl	-0.53601	4.27251	1.30913
H	0.66975	-4.50797	2.00536

2d

Sum of electronic and zero-point Energies= -2082.696152
Sum of electronic and thermal Enthalpies = -2082.666306
Sum of electronic and thermal Free Energies = -2082.754739

C	-0.04866	-0.42089	1.93148
C	0.20354	0.32815	3.09363
H	0.48808	1.37126	3.01605
C	0.10498	-0.25238	4.35245
H	0.30463	0.34265	5.23831
C	-0.24748	-1.59519	4.46573
H	-0.32995	-2.06139	5.44298
C	-0.48921	-2.35228	3.32456
H	-0.75332	-3.39925	3.43083
C	-0.38786	-1.77847	2.05468
C	-2.00636	-3.18706	0.90592
H	-2.14226	-3.83977	1.77375
H	-2.16504	-3.76761	-0.00422
H	-2.72878	-2.37030	0.94759
C	0.36160	-3.74198	0.83252
H	1.37301	-3.33225	0.83167
H	0.19877	-4.31453	-0.08244
H	0.23628	-4.40364	1.69511
C	1.88988	0.85625	-0.02106
C	2.79184	-0.24126	0.59172
H	2.55529	-1.21453	0.14084
H	2.61554	-0.32433	1.66939
C	4.27157	0.10330	0.34233
H	4.88632	-0.68652	0.79100
C	2.17435	0.93102	-1.54080
H	1.94470	-0.03396	-2.00718
H	1.53843	1.68433	-2.01677
C	3.71568	2.54615	0.37698
H	3.93315	3.51230	0.84855
C	3.98116	2.63017	-1.13183
H	5.03114	2.89106	-1.31494
H	3.36947	3.42336	-1.58144
C	3.65541	1.27699	-1.77860
H	3.82265	1.33063	-2.86131
C	2.22926	2.21899	0.62283
H	1.60679	3.00734	0.18675
H	2.03526	2.19512	1.70081
C	4.54045	0.18336	-1.16621
H	5.59894	0.40889	-1.34789
H	4.33044	-0.78411	-1.64114
C	4.59633	1.45325	0.99861
H	4.42654	1.39908	2.08206
H	5.65605	1.69674	0.85081
C	-1.25330	1.64423	0.06376
C	-3.58946	2.58156	-1.48747
H	-4.41443	3.28224	-1.66780
H	-3.62672	1.82793	-2.28501
C	-2.39140	3.71659	0.94341
H	-2.35276	4.46852	1.74111
C	-1.09265	2.33540	-1.30751
H	-0.14004	2.87450	-1.34988
H	-1.08799	1.58810	-2.11125
C	-3.75999	1.91182	-0.11657
H	-4.70864	1.36221	-0.08500
C	-1.24564	2.71359	1.18217
H	-1.38955	2.23794	2.15766
H	-0.29026	3.24663	1.20684
C	-2.24899	3.32808	-1.52530
H	-2.11262	3.80094	-2.50538
C	-3.73523	2.97784	0.98728
H	-3.87907	2.51031	1.97017
H	-4.55979	3.68750	0.84322
C	-2.61516	0.90645	0.10538
H	-2.65531	0.13772	-0.67767
H	-2.74195	0.40579	1.07344
C	-2.21729	4.39476	-0.42186
H	-3.01976	5.12599	-0.58157
H	-1.26838	4.94613	-0.45485
Au	-0.41999	-1.48408	-1.02360
Cl	-0.95874	-3.28782	-2.48264
N	-0.62568	-2.62658	0.87427
P	0.09482	0.33843	0.27315
H	-0.27433	-0.59851	-2.28020

2dô

Sum of electronic and zero-point Energies= -2082.665007
Sum of electronic and thermal Enthalpies = -2082.635468
Sum of electronic and thermal Free Energies = -2082.722120

C	-0.01625	-0.73768	1.84436
C	0.13282	-0.12410	3.10039
H	0.31239	0.94278	3.15386
C	0.06336	-0.85739	4.27804
H	0.18235	-0.35776	5.23451
C	-0.15965	-2.23055	4.21926
H	-0.22195	-2.81899	5.12953
C	-0.29413	-2.86212	2.98837
H	-0.45372	-3.93470	2.96618
C	-0.21711	-2.12433	1.80332
C	-1.58694	-3.66167	0.48087
H	-1.61463	-4.36865	1.31263
H	-1.62586	-4.21102	-0.45878
H	-2.43293	-2.97744	0.54748
C	0.85752	-3.80948	0.42064
H	1.77969	-3.22835	0.42549
H	0.77469	-4.37089	-0.50966
H	0.85287	-4.49883	1.26841
C	1.77239	1.01774	0.16393
C	2.80111	-0.02238	0.66762
H	2.70501	-0.95232	0.08960
H	2.61646	-0.26722	1.71931
C	4.22888	0.53395	0.51632
H	4.93318	-0.22018	0.88908
C	2.07976	1.31007	-1.32452
H	1.98998	0.38831	-1.90887
H	1.35947	2.02389	-1.73680
C	3.35980	2.86412	0.82190
H	3.44302	3.78575	1.41116
C	3.64165	3.16435	-0.65676
H	4.65187	3.57798	-0.77166
H	2.93964	3.92210	-1.02923
C	3.50607	1.86963	-1.47006
H	3.68650	2.07587	-2.53222
C	1.92466	2.32240	0.97465
H	1.21439	3.07455	0.61588
H	1.71633	2.14891	2.03578
C	4.51574	0.83221	-0.96133
H	5.53927	1.21098	-1.07726
H	4.44331	-0.08935	-1.55400
C	4.36290	1.82377	1.33914
H	4.18052	1.61660	2.40199
H	5.38514	2.21534	1.25944
C	-1.43246	1.38759	0.27029
C	-3.82944	2.27809	-1.22007
H	-4.73498	2.88979	-1.32336
H	-3.74392	1.67329	-2.13241
C	-2.85710	3.12431	1.42086
H	-2.94163	3.72910	2.33241
C	-1.32951	2.31630	-0.96000
H	-0.45392	2.96750	-0.86535
H	-1.20233	1.72356	-1.87323
C	-3.94887	1.36868	0.01137
H	-4.81949	0.70955	-0.09436
C	-1.59761	2.24312	1.54482
H	-1.70625	1.59668	2.42193
H	-0.71939	2.87649	1.70489
C	-2.59791	3.18159	-1.06809
H	-2.50023	3.82764	-1.94921
C	-4.09431	2.22810	1.27460
H	-4.20476	1.58734	2.15960
H	-5.00081	2.84330	1.20769
C	-2.68786	0.49272	0.12403
H	-2.60278	-0.13949	-0.76962
H	-2.77436	-0.17243	0.99307
C	-2.73627	4.04111	0.19597
H	-3.62239	4.68444	0.12059
H	-1.86601	4.70257	0.30026
Au	-0.27206	-1.66725	-1.21394
Cl	-0.31192	-0.61584	-3.28254
N	-0.31085	-2.87273	0.52175
P	0.05531	0.21676	0.28175
H	-0.48974	-2.96741	-2.08808

4-NH

Sum of electronic and zero-point Energies= -1486.647440
Sum of electronic and thermal Enthalpies = -1486.620983
Sum of electronic and thermal Free Energies = -1486.700439

C	0.07179	1.72050	0.58630
C	-0.02905	1.67152	1.98734
H	-0.14621	0.71381	2.48002
C	0.01096	2.82655	2.76426
H	-0.07144	2.75042	3.84455
C	0.15523	4.07444	2.16063
H	0.18789	4.97771	2.76207
C	0.25344	4.16506	0.77582
H	0.35911	5.13392	0.29664
C	0.20910	2.99985	0.01755
C	1.59754	3.66595	-1.92745
H	1.66606	4.71339	-1.63379
H	1.62739	3.57869	-3.01419
H	2.40794	3.09256	-1.47907
C	-0.86594	3.82199	-2.05685
H	-1.78289	3.33537	-1.72576
H	-0.77504	3.76026	-3.14200
H	-0.85213	4.86366	-1.73670
C	-1.64173	-0.61922	-0.18044
C	-2.73471	0.47415	-0.11901
H	-2.70005	1.08876	-1.02963
H	-2.55429	1.14180	0.73126
C	-4.12769	-0.16481	0.02143
H	-4.87702	0.63581	0.07004
C	-1.95250	-1.52556	-1.40006
H	-1.91365	-0.93172	-2.32270
H	-1.19740	-2.31259	-1.49410
C	-3.11001	-2.10424	1.24182
H	-3.13439	-2.69922	2.16377
C	-3.38622	-3.00914	0.03247
H	-4.36885	-3.48794	0.13583
H	-2.64004	-3.81346	-0.01651
C	-3.34223	-2.16915	-1.25217
H	-3.52392	-2.81262	-2.12245
C	-1.71116	-1.47194	1.10070
H	-0.95571	-2.26502	1.06470
H	-1.50045	-0.85957	1.98449
C	-4.41004	-1.06989	-1.18634
H	-5.40894	-1.51671	-1.09650
H	-4.40395	-0.48004	-2.11281
C	-4.17307	-0.99778	1.31057
H	-3.99258	-0.35481	2.18248
H	-5.16958	-1.44026	1.43855
C	1.54686	-0.75977	-0.13675
C	3.93969	-2.05302	-1.33334
H	4.87869	-2.61631	-1.25380
H	3.77572	-1.84983	-2.40009
C	3.14183	-1.85709	1.48971
H	3.31171	-2.06301	2.55427
C	1.46145	-2.09641	-0.90723
H	0.63962	-2.70379	-0.51078
H	1.24791	-1.90920	-1.96823
C	4.05035	-0.73422	-0.55483
H	4.87172	-0.13017	-0.96151
C	1.83124	-1.05534	1.34920
H	1.92621	-0.11665	1.90603
H	1.00597	-1.61984	1.79566
C	2.77774	-2.88124	-0.76747
H	2.68512	-3.82186	-1.32522
C	4.30818	-1.03151	0.92891
H	4.41290	-0.09388	1.49118
H	5.25081	-1.58282	1.04323
C	2.73699	0.05393	-0.70356
H	2.56180	0.28029	-1.76381
H	2.81726	1.01256	-0.17298
C	3.03079	-3.17915	0.71715
H	3.95440	-3.76137	0.83303
H	2.21321	-3.78873	1.12481
N	0.29740	3.10841	-1.45278
P	0.00064	0.26123	-0.56212
H	0.24262	2.10841	-1.76874

4-PH

Sum of electronic and zero-point Energies= -1486.650515
Sum of electronic and thermal Enthalpies = -1486.624065
Sum of electronic and thermal Free Energies = -1486.703046

C	0.33796	1.75316	0.57344
C	0.12909	1.76992	1.96116
H	-0.30943	0.90868	2.45543
C	0.49540	2.87622	2.72102
H	0.33292	2.87377	3.79435
C	1.07889	3.97471	2.09341
H	1.37376	4.84265	2.67675
C	1.27879	3.97357	0.71549
H	1.72358	4.84145	0.23873
C	0.91214	2.87463	-0.07166
C	2.36614	3.46791	-1.93193
H	2.35827	4.56918	-1.89117
H	2.53774	3.17877	-2.97391
H	3.20451	3.10219	-1.33393
C	-0.01964	3.35265	-2.24771
H	-0.94224	2.85786	-1.93443
H	0.14105	3.13869	-3.30925
H	-0.16211	4.43974	-2.13129
C	-1.80950	-0.31422	-0.14233
C	-2.69071	0.94653	0.02821
H	-2.54894	1.62407	-0.82292
H	-2.40470	1.49378	0.93226
C	-4.16998	0.53284	0.12206
H	-4.77057	1.44178	0.24892
C	-2.23926	-1.04274	-1.44123
H	-2.09683	-0.38037	-2.30464
H	-1.62437	-1.93350	-1.60666
C	-3.50184	-1.65081	1.15308
H	-3.62837	-2.31514	2.01633
C	-3.91466	-2.38230	-0.13194
H	-4.96493	-2.69281	-0.06511
H	-3.31644	-3.29450	-0.25681
C	-3.72049	-1.45002	-1.33648
H	-3.99832	-1.97149	-2.26043
C	-2.01659	-1.25317	1.06496
H	-1.40258	-2.15311	0.95321
H	-1.71291	-0.75667	1.99370
C	-4.58681	-0.19449	-1.16256
H	-5.64683	-0.47307	-1.10918
H	-4.47108	0.46974	-2.02892
C	-4.36450	-0.39327	1.33109
H	-4.08960	0.12933	2.25668
H	-5.42129	-0.67442	1.42213
C	1.34509	-0.99436	-0.10258
C	3.54150	-2.55642	-1.31266
H	4.39215	-3.24546	-1.23724
H	3.42078	-2.30878	-2.37538
C	2.74568	-2.32180	1.50968
H	2.87252	-2.57363	2.56953
C	1.07130	-2.27692	-0.91752
H	0.16606	-2.77358	-0.55223
H	0.91213	-2.02828	-1.97445
C	3.81894	-1.28465	-0.50072
H	4.71521	-0.78370	-0.88620
C	1.55501	-1.35293	1.38448
H	1.75784	-0.44667	1.96641
H	0.65584	-1.82029	1.79950
C	2.27104	-3.23327	-0.77788
H	2.05738	-4.13844	-1.35927
C	4.01649	-1.64411	0.97859
H	4.23726	-0.74073	1.56219
H	4.87631	-2.31692	1.08986
C	2.63047	-0.31781	-0.64406
H	2.49877	-0.04660	-1.69861
H	2.83486	0.60423	-0.08781
C	2.46341	-3.59662	0.70183
H	3.29808	-4.30095	0.80881
H	1.56697	-4.09933	1.08809
N	1.12201	2.85343	-1.48056
P	-0.03212	0.24065	-0.35387
H	0.06490	0.59540	-1.70445

TS_{Hshift} (proton shift 4-PH→4-NH)
Sum of electronic and zero-point Energies= -1486.638577
Sum of electronic and thermal Enthalpies = -1486.612435
Sum of electronic and thermal Free Energies = -1486.690715

C	0.02332	1.77383	0.67116
C	-0.03869	1.84472	2.06858
H	-0.09661	0.93409	2.65493
C	-0.03134	3.08027	2.71131
H	-0.08035	3.12433	3.79532
C	0.03648	4.25810	1.96643
H	0.04245	5.22033	2.47013
C	0.09445	4.20994	0.57521
H	0.14357	5.12837	-0.00250
C	0.08643	2.97542	-0.06959
C	1.38491	3.35997	-2.10849
H	1.44656	4.45271	-2.04608
H	1.41568	3.06248	-3.15970
H	2.23718	2.92411	-1.58598
C	-1.05187	3.41660	-2.18918
H	-1.95442	2.96969	-1.76866
H	-0.99322	3.17408	-3.25330
H	-1.10324	4.50531	-2.07300
C	-1.62647	-0.63211	-0.13909
C	-2.75632	0.42082	-0.04882
H	-2.75105	1.05404	-0.94510
H	-2.59766	1.07408	0.81628
C	-4.11971	-0.28283	0.07967
H	-4.89987	0.48567	0.14690
C	-1.88965	-1.51655	-1.38301
H	-1.88052	-0.89731	-2.28921
H	-1.10327	-2.26839	-1.49619
C	-3.01817	-2.20207	1.25522
H	-3.01369	-2.81898	2.16246
C	-3.25352	-3.08974	0.02392
H	-4.21351	-3.61353	0.11750
H	-2.47289	-3.85917	-0.04286
C	-3.25124	-2.22095	-1.24276
H	-3.40717	-2.85210	-2.12644
C	-1.64949	-1.50702	1.13036
H	-0.85886	-2.26428	1.08008
H	-1.46145	-0.89078	2.01846
C	-4.36489	-1.16986	-1.14919
H	-5.34256	-1.66227	-1.06820
H	-4.38668	-0.55819	-2.06084
C	-4.12844	-1.14586	1.34948
H	-3.97778	-0.51677	2.23678
H	-5.10376	-1.63585	1.46455
C	1.58409	-0.68980	-0.10094
C	3.99294	-1.89335	-1.33666
H	4.95011	-2.42640	-1.27055
H	3.80981	-1.69064	-2.40017
C	3.22841	-1.73941	1.49879
H	3.41856	-1.94536	2.55948
C	1.52182	-2.02029	-0.88339
H	0.72317	-2.65495	-0.48384
H	1.29507	-1.82926	-1.94040
C	4.07071	-0.57628	-0.55212
H	4.86415	0.05848	-0.96618
C	1.89044	-0.98223	1.38386
H	1.95586	-0.04323	1.94442
H	1.08941	-1.57987	1.83127
C	2.86556	-2.76138	-0.76072
H	2.79460	-3.70087	-1.32274
C	4.35792	-0.87156	0.92660
H	4.43831	0.06622	1.49216
H	5.31959	-1.39148	1.02487
C	2.73196	0.17225	-0.68068
H	2.53613	0.39640	-1.73700
H	2.78864	1.12809	-0.14433
C	3.14625	-3.05948	0.71902
H	4.08841	-3.61373	0.81862
H	2.35328	-3.69599	1.13374
N	0.13309	2.86145	-1.51556
P	-0.00199	0.28617	-0.38255
H	0.07078	1.42130	-1.52746

6a
Sum of electronic and zero-point Energies= -2235.263730
Sum of electronic and thermal Enthalpies = -2235.232161
Sum of electronic and thermal Free Energies = -2235.324061

C	0.27683	-0.05716	1.98467
C	-0.60278	-0.03323	3.08424
H	-1.66661	0.05322	2.91013
C	-0.16587	-0.11716	4.40092
H	-0.89146	-0.09663	5.20821
C	1.19312	-0.22768	4.66999
H	1.55678	-0.29503	5.69028
C	2.09438	-0.25147	3.61356
H	3.15530	-0.33617	3.82483
C	1.64821	-0.16725	2.29495
C	-1.29362	1.76012	0.18457
C	-0.13030	2.78218	0.17536
H	0.41437	2.73650	1.12730
H	0.57875	2.53593	-0.62636
C	-0.67515	4.20549	-0.04365
H	0.17202	4.90257	-0.04593
C	-2.04465	1.84461	-1.16340
H	-1.37356	1.56184	-1.98577
H	-2.88556	1.14225	-1.16884
C	-2.80868	3.56463	1.09132
H	-3.50105	3.80016	1.90897
C	-3.54923	3.62688	-0.25138
H	-4.39769	2.93000	-0.25091
H	-3.95918	4.63303	-0.40723
C	-2.57476	3.27230	-1.38308
H	-3.09600	3.30097	-2.34786
C	-2.25793	2.14355	1.32720
H	-3.09029	1.43592	1.39204
H	-1.73162	2.13138	2.28699
C	-1.40583	4.26661	-1.39264
H	-0.71298	4.02768	-2.21019
H	-1.77814	5.28314	-1.57274
C	-1.64795	4.56700	1.08757
H	-1.12877	4.54952	2.05509
H	-2.02902	5.58630	0.94473
C	-1.67865	-1.46107	0.16094
C	-2.07411	-4.19302	-0.94446
H	-2.66831	-5.10712	-1.07109
H	-1.13641	-4.33871	-1.49692
C	-3.87007	-2.58032	0.73343
H	-4.80955	-2.44068	1.28239
C	-1.97689	-1.71833	-1.33890
H	-2.49778	-0.86270	-1.78030
H	-1.03606	-1.84711	-1.88942
C	-1.78400	-3.95779	0.54363
H	-1.22789	-4.80949	0.95473
C	-3.02419	-1.30190	0.89758
H	-2.87139	-1.12129	1.96526
H	-3.57410	-0.44650	0.48986
C	-2.83670	-2.98528	-1.50406
H	-3.02864	-3.12812	-2.57459
C	-3.10568	-3.78275	1.30586
H	-2.90884	-3.63330	2.37580
H	-3.71416	-4.69143	1.21439
C	-0.92534	-2.69129	0.71845
H	-0.70147	-2.55320	1.78198
H	0.03182	-2.81188	0.19186
C	-4.16322	-2.81515	-0.75313
H	-4.78531	-3.71052	-0.87902
H	-4.72811	-1.96939	-1.16688
P	-0.49651	0.03629	0.29626
Au	0.95277	-0.12465	-1.47984
Cl	2.27121	-0.33265	-3.39990
C	3.65655	0.96821	1.36727
C	3.46137	-1.50791	1.24308
H	2.23817	-0.12141	0.32828
C	4.73475	0.85573	0.30343
H	4.09757	0.93555	2.36432
H	3.06963	1.88151	1.25448
C	4.55438	-1.45715	0.18923
H	3.88627	-1.64890	2.23762
H	2.73915	-2.30013	1.03670
H	5.45641	1.66245	0.45545
H	4.30203	0.96930	-0.70223
H	5.14098	-2.37685	0.25679
H	4.11756	-1.40170	-0.81913
N	2.70317	-0.20002	1.26123
O	5.43439	-0.37018	0.40935

6b

Sum of electronic and zero-point Energies= -2235.247604
Sum of electronic and thermal Enthalpies = -2235.215625
Sum of electronic and thermal Free Energies = -2235.309504

C	0.17904	-0.12059	2.08772
C	-0.86908	0.00051	3.02210
H	-1.87099	0.17546	2.65803
C	-0.70101	-0.09427	4.39872
H	-1.56161	0.00753	5.05219
C	0.56628	-0.31734	4.91585
H	0.73640	-0.39601	5.98465
C	1.63044	-0.44198	4.03387
H	2.62500	-0.62046	4.43556
C	1.45628	-0.34874	2.65056
C	-1.00471	1.85376	0.15806
C	0.26091	2.74538	0.18624
H	0.75351	2.66308	1.16364
H	0.97510	2.40429	-0.57457
C	-0.11359	4.21407	-0.08466
H	0.80429	4.81458	-0.06124
C	-1.67854	1.99363	-1.22685
H	-1.00173	1.62749	-2.01051
H	-2.58709	1.38326	-1.26748
C	-2.35257	3.83674	0.95930
H	-3.04949	4.16482	1.74063
C	-3.02214	3.94891	-0.41654
H	-3.94136	3.34847	-0.44195
H	-3.31282	4.98951	-0.61016
C	-2.04288	3.46451	-1.49446
H	-2.51440	3.52756	-2.48302
C	-1.97254	2.36895	1.24394
H	-2.88038	1.75850	1.28169
H	-1.49699	2.32033	2.22901
C	-0.77353	4.32610	-1.46652
H	-0.07565	3.99751	-2.24776
H	-1.02442	5.37324	-1.67960
C	-1.08856	4.70574	0.99310
H	-0.61873	4.65200	1.98424
H	-1.34791	5.75738	0.81567
C	-1.76682	-1.28930	0.08213
C	-2.38533	-3.98020	-1.03244
H	-3.07464	-4.81299	-1.22235
H	-1.41392	-4.26173	-1.45997
C	-4.14562	-2.10276	0.37926
H	-5.11875	-1.82538	0.80351
C	-1.91450	-1.55201	-1.44003
H	-2.25353	-0.64748	-1.95560
H	-0.93959	-1.82021	-1.86679
C	-2.25275	-3.74161	0.47759
H	-1.86985	-4.64663	0.96582
C	-3.16523	-0.94207	0.63971
H	-3.13344	-0.76671	1.71815
H	-3.54813	-0.03163	0.16732
C	-2.90544	-2.70084	-1.69998
H	-2.97696	-2.84865	-2.78466
C	-3.62545	-3.37574	1.06131
H	-3.54773	-3.21989	2.14565
H	-4.33175	-4.20118	0.90534
C	-1.26035	-2.59307	0.74219
H	-1.14707	-2.45602	1.82301
H	-0.27276	-2.85718	0.33937
C	-4.28178	-2.33947	-1.12869
H	-4.99704	-3.14937	-1.32187
H	-4.67346	-1.43952	-1.62092
P	-0.40017	0.05013	0.31423
Au	1.07036	-0.23695	-1.43336
Cl	2.32846	-0.46718	-3.39609
C	2.87571	-1.79453	1.11657
C	3.25643	0.67039	1.16142
H	3.42487	-0.64495	2.68314
C	4.32510	-1.92867	0.67815
H	2.20190	-1.71375	0.26162
H	2.57520	-2.62430	1.75952
C	4.68486	0.37566	0.73560
H	2.60436	0.81659	0.29766
H	3.20639	1.53136	1.83079
H	4.41314	-2.79695	0.02121
H	4.97183	-2.09496	1.55553
H	5.04974	1.20547	0.12602
H	5.33246	0.28868	1.62457
N	2.73945	-0.52597	1.92652
O	4.76461	-0.79841	-0.04928

6c

Sum of electronic and zero-point Energies= -2235.244402
Sum of electronic and thermal Enthalpies = -2235.213287
Sum of electronic and thermal Free Energies = -2235.303639

C	0.66866	-0.04838	1.77376
C	-0.18692	0.00436	2.89397
H	-1.25790	0.03226	2.71672
C	0.25728	0.03318	4.21078
H	-0.46763	0.07167	5.01800
C	1.61876	0.02490	4.47175
H	1.99960	0.06251	5.48717
C	2.50482	-0.03641	3.40384
H	3.56844	-0.04181	3.61508
C	2.05185	-0.08722	2.08508
C	-0.10488	-1.64545	-0.75805
C	-0.73838	-2.73862	0.13922
H	-0.18897	-2.81276	1.08691
H	-1.77309	-2.46642	0.38407
C	-0.71988	-4.09654	-0.58591
H	-1.17513	-4.84535	0.07373
C	-0.90268	-1.55992	-2.07874
H	-1.93663	-1.25304	-1.87274
H	-0.45921	-0.80789	-2.74043
C	1.35668	-3.42283	-1.80660
H	2.39893	-3.68540	-2.02696
C	0.55991	-3.31170	-3.11295
H	1.01473	-2.56274	-3.77497
H	0.58593	-4.27001	-3.64689
C	-0.89051	-2.92373	-2.79157
H	-1.46553	-2.83141	-3.72103
C	1.34206	-2.06910	-1.06749
H	1.85398	-1.31361	-1.67546
H	1.88385	-2.19188	-0.12349
C	-1.52600	-3.98863	-1.88773
H	-2.56797	-3.72321	-1.66684
H	-1.54261	-4.95819	-2.40174
C	0.72706	-4.49498	-0.90757
H	1.30690	-4.60307	0.01906
H	0.74679	-5.46809	-1.41445
C	0.15641	1.56367	-0.82714
C	-0.55126	4.38759	-1.44582
H	-0.36028	5.34104	-1.95485
H	-1.46504	4.51585	-0.85110
C	1.70513	2.77488	-2.41745
H	2.61701	2.65672	-3.01623
C	-1.03362	1.94298	-1.74813
H	-1.22027	1.15431	-2.48298
H	-1.94709	2.05173	-1.15026
C	0.62956	4.03228	-0.53226
H	0.76944	4.81809	0.22016
C	1.41480	1.43912	-1.70637
H	2.28582	1.16713	-1.10149
H	1.27582	0.64972	-2.45264
C	-0.74335	3.26803	-2.47618
H	-1.60213	3.49755	-3.11886
C	1.90454	3.88459	-1.37578
H	2.76031	3.64849	-0.72833
H	2.13651	4.83277	-1.87703
C	0.33924	2.70791	0.19738
H	1.15851	2.48032	0.88892
H	-0.57056	2.80843	0.80437
C	0.52348	3.12702	-3.33013
H	0.72538	4.06436	-3.86407
H	0.38634	2.34667	-4.09021
P	-0.31504	-0.00033	0.15793
Au	-2.56251	0.17507	0.65284
Cl	-4.85505	0.34929	1.08160
C	4.02704	1.05575	1.03209
C	4.03519	-1.39533	1.27526
H	2.72718	-0.28110	0.14758
C	5.10268	0.88044	-0.02724
H	4.46798	1.16457	2.02286
H	3.39198	1.91602	0.81748
C	5.09726	-1.42906	0.19148
H	4.49952	-1.29912	2.25576
H	3.40408	-2.28431	1.25838
H	5.76052	1.75259	0.00343
H	4.65084	0.82799	-1.03063
H	5.75132	-2.28397	0.38017
H	4.63776	-1.56211	-0.80051
N	3.14495	-0.17811	1.07935
O	5.89630	-0.26307	0.21872

7

Sum of electronic and zero-point Energies= -3315.010357

Sum of electronic and thermal Enthalpies = -3314.927081

Sum of electronic and thermal Free Energies = -3315.129970

N	-4.05878	-0.06130	0.46097
C	-2.83352	0.40499	0.03187
C	-2.04197	-0.74448	-0.18800
N	-2.89883	-1.76205	0.13878
N	-4.09944	-1.37565	0.52589
C	-2.51344	1.83561	-0.14490
C	-1.21469	2.32725	0.09195
C	-0.82156	3.62511	-0.31245
C	-1.77469	4.51711	-0.80572
C	-3.09913	4.10197	-0.97050
C	-3.42769	2.76180	-0.67232
C	0.62598	3.66376	-0.20963
C	1.02789	2.37979	0.23251
N	-0.10081	1.66867	0.55132
C	2.36416	1.94409	0.12853
C	3.29181	2.93192	-0.24721
C	2.94104	4.26664	-0.54041
C	1.58724	4.61199	-0.55745
Au	-0.01522	-0.90546	-0.52566
C	2.01227	-0.62047	-0.30039
C	2.72839	0.51121	0.15407
N	3.99175	0.04772	0.46590
N	4.13693	-1.23305	0.19470
N	2.96165	-1.60786	-0.27001
H	4.32846	2.64020	-0.37167
H	1.27226	5.60032	-0.87393
H	-4.42884	2.41638	-0.90459
H	-1.46802	5.51689	-1.09264
H	-0.10319	0.74181	0.95382
C	4.03330	5.26807	-0.94918
C	5.17778	5.26105	0.08067
H	4.81758	5.54506	1.07575
H	5.65801	4.28181	0.16593
H	5.95099	5.97933	-0.21485
C	3.49400	6.70328	-1.03940
H	4.31663	7.38539	-1.27963
H	2.74109	6.81636	-1.82661
H	3.05315	7.03457	-0.09246
C	4.58270	4.87133	-2.33250
H	5.38124	5.55639	-2.64085
H	4.99375	3.85684	-2.32618
H	3.79375	4.90639	-3.09225
C	-4.17935	5.03897	-1.53650
C	-5.39277	5.06805	-0.58880
H	-6.15711	5.75025	-0.97842
H	-5.85723	4.08355	-0.47889
H	-5.10641	5.41712	0.40940
C	-3.66895	6.47869	-1.69140
H	-3.32208	6.89408	-0.73861
H	-2.85124	6.55315	-2.41627
H	-4.48267	7.11606	-2.05342
C	-4.62423	4.53430	-2.92220
H	-5.40810	5.18321	-3.33019
H	-3.78711	4.53033	-3.62949
H	-5.02739	3.51771	-2.87441
C	-5.26156	0.64758	0.84981
C	-6.38946	0.54543	0.01099
C	-5.26043	1.36466	2.05998
C	-7.54422	1.22259	0.41670
C	-6.44391	2.02692	2.40496
C	-7.57183	1.96049	1.59546
H	-8.43626	1.16395	-0.19953
H	-6.48301	2.58882	3.33341
H	-8.48007	2.48012	1.88823
C	-2.60829	-3.17714	0.17295
C	-2.64703	-3.90458	-1.02872
C	-2.32216	-3.75806	1.42272
C	-2.33369	-5.26643	-0.95568
C	-2.02225	-5.12439	1.43291
C	-2.01796	-5.86888	0.25734
H	-2.35213	-5.86364	-1.86279
H	-1.80065	-5.61191	2.37819
H	-1.78121	-6.92900	0.28942
C	5.12003	0.70489	1.09213
C	4.98933	1.12965	2.42841
C	6.31710	0.82457	0.35550
C	6.10938	1.72832	3.01595
C	7.40233	1.42157	1.00557
C	7.30088	1.87594	2.31626
H	6.04820	2.06548	4.04663
H	8.34396	1.52706	0.47538
H	8.15873	2.33781	2.79730
C	2.83472	-2.93999	-0.81657
C	2.75410	-3.05665	-2.21776
C	2.81781	-4.04446	0.05594
C	2.57431	-4.34372	-2.73653
C	2.65321	-5.30593	-0.52604
C	2.51719	-5.45449	-1.90271
H	2.49748	-4.47457	-3.81196
H	2.62892	-6.18483	0.11015
H	2.38197	-6.44500	-2.32876
C	-2.38609	-2.98733	2.73244
H	-2.56735	-1.93184	2.50633
C	-3.56436	-3.48577	3.58215
H	-4.51438	-3.38442	3.04798
H	-3.44101	-4.54094	3.84994
H	-3.63096	-2.91257	4.51302
C	-1.07449	-3.05921	3.52243
H	-0.84209	-4.08316	3.83245
H	-0.23185	-2.68112	2.93516
H	-1.15402	-2.45211	4.43105
C	-3.05992	-3.29464	-2.35778
H	-3.19365	-2.21744	-2.21631
C	-1.98462	-3.48725	-3.43283
H	-2.27856	-2.97856	-4.35759
H	-1.02292	-3.07868	-3.11025
H	-1.83905	-4.54670	-3.67006
C	-4.40505	-3.87306	-2.81941
H	-4.73875	-3.37147	-3.73447
H	-4.32231	-4.94378	-3.03654
H	-5.17945	-3.74419	-2.05712
C	-4.07737	1.40939	3.01420
H	-3.23103	0.89950	2.54366
C	-3.63515	2.84668	3.31799
H	-2.73114	2.83930	3.93648
H	-3.41578	3.40353	2.40241
H	-4.40505	3.39641	3.86992
C	-4.40901	0.65495	4.30999
H	-4.72611	-0.37227	4.10675
H	-3.53046	0.62021	4.96383
H	-5.21592	1.15213	4.85963
C	-6.41838	-0.28616	-1.26284
H	-5.39680	-0.60021	-1.49846
C	-6.93488	0.50627	-2.46916
H	-6.34500	1.41251	-2.63767
H	-6.86972	-0.10958	-3.37254
H	-7.98235	0.80164	-2.34913
C	-7.25900	-1.55417	-1.04690
H	-7.26199	-2.16678	-1.95452
H	-6.86806	-2.15938	-0.22331
H	-8.29877	-1.29868	-0.81370
C	3.00833	-3.91310	1.55945
H	2.74516	-2.88795	1.84522
C	4.48140	-4.14353	1.93653
H	4.80016	-5.15118	1.64602
H	5.14263	-3.42386	1.44716
H	4.61555	-4.04972	3.01998
C	2.11087	-4.86302	2.36064
H	1.06922	-4.81839	2.03160
H	2.44701	-5.90248	2.27956
H	2.14507	-4.59712	3.42251
C	2.91315	-1.88001	-3.17219
H	3.18609	-0.99504	-2.58961
C	1.60920	-1.55138	-3.90899
H	1.75663	-0.68873	-4.56867
H	1.27777	-2.39229	-4.52805
H	0.80783	-1.30453	-3.20264
C	4.05348	-2.12989	-4.17022
H	3.82156	-2.95552	-4.85135
H	4.21795	-1.23519	-4.78053
H	4.99142	-2.36805	-3.65855
C	6.48959	0.30595	-1.06580
H	5.49834	0.10258	-1.48327
C	7.27445	-1.01543	-1.05906
H	6.76835	-1.78166	-0.46562
H	7.38887	-1.39492	-2.08031
H	8.27752	-0.86974	-0.64234
C	7.17308	1.32190	-1.98934
H	8.21483	1.50093	-1.70394
H	7.17926	0.94047	-3.01593
H	6.65517	2.28548	-1.99378
C	3.73932	0.92246	3.27230
H	2.96389	0.46921	2.64850
C	4.02130	-0.05408	4.42381
H	3.10416	-0.24408	4.99230
H	4.39648	-1.01378	4.05453
H	4.76460	0.35255	5.11818

C	3.18173	2.24946	3.80331
H	2.24527	2.07442	4.34435
H	3.87870	2.72769	4.49956
H	2.97824	2.95465	2.99191

8

Sum of electronic and zero-point Energies= -1630.651224
Sum of electronic and thermal Enthalpies = -1630.623188
Sum of electronic and thermal Free Energies = -1630.709360

C	-3.93100	-0.78323	0.51326
C	-3.50400	0.47374	0.06432
C	-4.45541	1.41123	-0.36867
C	-5.80832	1.09045	-0.35832
C	-6.22803	-0.16511	0.08280
C	-5.28752	-1.09709	0.51942
C	-2.09306	0.87966	0.06602
N	-0.97927	0.09301	-0.17293
C	0.13537	0.89379	-0.12486
N	-0.35596	2.10792	0.15957
N	-1.71105	2.11036	0.28282
C	-0.97376	-1.27542	-0.62275
C	-1.28382	-1.51020	-1.96074
C	-1.32345	-2.81470	-2.44539
C	-1.06614	-3.88018	-1.58632
C	-0.76243	-3.63716	-0.24933
C	-0.69404	-2.33407	0.25921
Au	1.98641	0.22838	-0.45610
Cl	4.12326	-0.59438	-0.85122
C	0.31137	3.43719	0.37459
C	0.03365	3.85006	1.82348
C	-0.40263	-2.10778	1.71824
N	1.07151	-1.99878	2.03849
C	1.81438	-3.27693	1.85382
C	-0.32291	4.42371	-0.61100
C	1.81260	3.35700	0.12976
C	1.27218	-1.45942	3.41281
H	1.47173	-1.31366	1.37222
H	-1.49718	-0.66947	-2.61288
H	-7.28502	-0.41570	0.08686
H	-0.85541	-1.18095	2.07238
H	-0.78308	-2.93255	2.32448
H	-1.11087	-4.90141	-1.95190
H	2.34244	-1.35546	3.59090
H	0.83708	-2.15817	4.12873
H	0.78338	-0.48785	3.48722
H	-4.12524	2.38401	-0.71941
H	-3.21461	-1.51240	0.87383
H	-0.58515	-4.47269	0.42189
H	-6.53538	1.82070	-0.70142
H	-5.60897	-2.07265	0.87244
H	-1.56508	-2.99347	-3.48851
H	-1.03931	3.92649	2.01671
H	0.48728	4.82721	2.01195
H	0.46783	3.13021	2.52506
H	-0.15184	4.10653	-1.64465
H	0.13614	5.40666	-0.47353
H	-1.39818	4.51976	-0.44493
H	2.31321	2.68098	0.82853
H	2.22519	4.35894	0.28142
H	2.04877	3.04983	-0.89312
H	2.86338	-3.09856	2.09146
H	1.39619	-4.02324	2.53077
H	1.72612	-3.60132	0.81826

2a_OTf

Sum of electronic and zero-point Energies= -3044.035350
Sum of electronic and thermal Enthalpies = -3043.995761
Sum of electronic and thermal Free Energies = -3044.109477

C	0.12552	-0.31774	-1.17760
C	0.07518	-0.41386	-2.58132
H	-0.87532	-0.30569	-3.08667
C	1.20685	-0.64486	-3.35577
H	1.11203	-0.71118	-4.43535
C	2.44700	-0.78385	-2.74254
H	3.34722	-0.95572	-3.32334
C	2.53983	-0.69821	-1.35898
H	3.50975	-0.80846	-0.88089
C	1.39967	-0.47144	-0.59339
C	2.48908	0.73289	1.28085
H	3.51061	0.52809	0.95792
H	2.44695	0.80271	2.36876
H	2.11065	1.64859	0.82824
C	2.09510	-1.70292	1.44012
H	1.43162	-2.50129	1.10899
H	2.06755	-1.61365	2.52695
H	3.11770	-1.87880	1.10501
C	-2.68778	-1.38261	-0.79191
C	-1.90698	-2.71638	-0.72664
H	-1.44800	-2.83058	0.26504
H	-1.09912	-2.72357	-1.46653
C	-2.85616	-3.89826	-0.99934
H	-2.27173	-4.82560	-0.95428
C	-3.81675	-1.43590	0.26999
H	-3.37994	-1.55069	1.27073
H	-4.38882	-0.50277	0.27289
C	-4.27534	-2.43012	-2.45233
H	-4.71028	-2.30422	-3.45167
C	-5.39029	-2.45967	-1.39977
H	-6.07663	-3.29221	-1.60114
H	-5.98098	-1.53536	-1.44727
C	-4.76228	-2.61804	-0.00897
H	-5.54662	-2.61663	0.75818
C	-3.33898	-1.23497	-2.18371
H	-3.91390	-0.30353	-2.23367
H	-2.58265	-1.20192	-2.97363
C	-3.96984	-3.92994	0.05596
H	-4.63562	-4.78325	-0.12640
H	-3.54076	-4.06393	1.05767
C	-3.47530	-3.73926	-2.39556
H	-2.68858	-3.73732	-3.16165
H	-4.13392	-4.59001	-2.61314
C	-1.97983	1.77233	-0.78038
C	-2.73638	4.44606	0.25271
H	-3.02172	5.49597	0.10770
H	-2.71339	4.26552	1.33563
C	-2.42040	3.54323	-2.52559
H	-2.44390	3.72411	-3.60748
C	-3.37618	2.05341	-0.18007
H	-4.12454	1.40414	-0.64820
H	-3.37287	1.83392	0.89624
C	-1.35154	4.18831	-0.35791
H	-0.60575	4.83281	0.12389
C	-2.00742	2.07539	-2.29335
H	-1.01547	1.91822	-2.72901
H	-2.70667	1.41113	-2.81067
C	-3.76530	3.52334	-0.41510
H	-4.75637	3.69146	0.02427
C	-1.39254	4.47238	-1.86571
H	-0.40048	4.31586	-2.30924
H	-1.66298	5.52139	-2.04342
C	-0.95143	2.72149	-0.11767
H	-0.90278	2.52519	0.96172
H	0.04783	2.53874	-0.53362
C	-3.80885	3.79901	-1.92426
H	-4.11326	4.83707	-2.11000
H	-4.55609	3.15411	-2.40561
Au	-1.35387	-0.02017	2.00182
Cl	-1.33791	-0.02087	4.34458
N	1.61054	-0.40688	0.86548
P	-1.47461	0.00783	-0.29619
H	0.67894	-0.23263	1.30128
C	7.33108	0.57200	-0.06094
F	8.33169	0.75786	-0.93239
F	6.55594	1.66749	-0.08203
F	7.86122	0.46658	1.16531
O	5.86156	-0.65261	-1.85548
O	5.29039	-0.94208	0.54975
O	7.32879	-2.03468	-0.38025
S	6.35064	-0.93901	-0.49190

2aô_OTf

Sum of electronic and zero-point Energies= -3044.029339
Sum of electronic and thermal Enthalpies = -3043.989881
Sum of electronic and thermal Free Energies = -3044.102324

C	1.04508	-0.14671	2.13208
C	2.03588	0.46708	2.92284
H	2.74519	1.13597	2.45586
C	2.16035	0.25185	4.29030
H	2.94748	0.75419	4.84399
C	1.28128	-0.61333	4.92683
H	1.36364	-0.81455	5.99026
C	0.27351	-1.22129	4.18852
H	-0.41600	-1.88445	4.69627
C	0.13703	-0.98217	2.82136
C	-2.22051	-1.80482	3.00818
H	-2.06978	-2.58987	3.74715
H	-3.04765	-2.06033	2.34957
H	-2.41822	-0.84887	3.48948
C	-0.58646	-3.03028	1.65137
H	0.25327	-2.91423	0.96738
H	-1.43720	-3.46715	1.12745
H	-0.30603	-3.64258	2.50897
C	2.94619	-0.34969	-0.20662
C	3.26841	-1.67655	0.51965
H	2.48945	-2.41917	0.29878
H	3.28226	-1.52758	1.60461
C	4.63882	-2.21345	0.06522
H	4.84052	-3.14539	0.60828
C	2.94815	-0.63415	-1.73208
H	2.17620	-1.37686	-1.96970
H	2.70405	0.27327	-2.29382
C	5.42768	0.12562	-0.36489
H	6.19284	0.87560	-0.12758
C	5.40942	-0.14034	-1.87465
H	6.38814	-0.51289	-2.20415
H	5.21795	0.79152	-2.42289
C	4.31807	-1.17220	-2.18384
H	4.27143	-1.35555	-3.26455
C	4.06077	0.67829	0.08542
H	3.85740	1.61533	-0.44248
H	4.12042	0.90765	1.15309
C	4.61840	-2.48265	-1.44493
H	5.58658	-2.88622	-1.76873
H	3.85752	-3.23658	-1.68662
C	5.72637	-1.17836	0.38765
H	5.76393	-0.99181	1.46919
H	6.71099	-1.56386	0.09306
C	0.79673	2.03462	0.06324
C	-0.83924	3.99499	-1.44457
H	-1.14824	5.02177	-1.68065
H	-1.42443	3.32547	-2.08849
C	1.17599	4.46279	0.64190
H	1.76115	5.13169	1.28587
C	1.07439	2.36955	-1.41979
H	2.13913	2.24672	-1.64573
H	0.51868	1.67768	-2.06688
C	-1.12071	3.68678	0.03296
H	-2.19332	3.78898	0.23741
C	1.58027	3.01048	0.96593
H	1.35253	2.81150	2.01867
H	2.66016	2.89529	0.83160
C	0.65977	3.81913	-1.72232
H	0.87082	4.02548	-2.77931
C	-0.32142	4.65063	0.91982
H	-0.53714	4.45850	1.97932
H	-0.61642	5.68795	0.71363
C	-0.71174	2.23525	0.34317
H	-1.30897	1.54385	-0.26091
H	-0.92956	2.00903	1.39443
C	1.46906	4.77312	-0.83252
H	1.20419	5.81477	-1.05621
H	2.54253	4.66344	-1.03812
Au	-0.23260	-0.99956	-1.08443
Cl	-1.37803	-2.25062	-2.70641
N	-0.99228	-1.67839	2.15499
P	1.16241	0.18396	0.29988
H	-1.31018	-1.11537	1.34286
O	-5.16033	-0.97030	1.56499
S	-4.43918	0.02431	0.74724
O	-2.97612	-0.22060	0.63700
O	-4.80578	1.43267	0.97408
C	-5.03386	-0.31367	-0.97442
F	-4.35739	0.42196	-1.86885
F	-6.33515	-0.01806	-1.09261
F	-4.87240	-1.60537	-1.29116

2b_OTf

Sum of electronic and zero-point Energies= -3044.028390
Sum of electronic and thermal Enthalpies = -3043.989085
Sum of electronic and thermal Free Energies = -3044.101186

C	0.07555	-0.25084	1.65974
C	0.64657	-0.31160	2.94629
H	1.71762	-0.21002	3.04569
C	-0.08653	-0.50531	4.11161
H	0.42576	-0.54234	5.06805
C	-1.46341	-0.65013	4.03112
H	-2.06749	-0.80264	4.91994
C	-2.06994	-0.60553	2.78239
H	-3.14639	-0.72745	2.71107
C	-1.33058	-0.41417	1.61178
C	-1.98939	-1.58121	-0.51492
H	-1.03986	-1.48877	-1.04142
H	-2.81650	-1.56972	-1.22648
H	-2.02034	-2.49382	0.08063
C	-2.28295	0.89456	-0.30322
H	-2.51619	1.66246	0.43442
H	-3.09194	0.81301	-1.03061
H	-1.34288	1.11128	-0.81020
C	2.52312	-1.52543	0.44476
C	1.63248	-2.77385	0.64654
H	0.87752	-2.82676	-0.14840
H	1.09996	-2.71070	1.60162
C	2.49180	-4.05091	0.63095
H	1.82994	-4.91253	0.78330
C	3.26106	-1.67777	-0.91013
H	2.53008	-1.72608	-1.72719
H	3.89711	-0.80745	-1.10080
C	4.43387	-2.76144	1.54902
H	5.16618	-2.69538	2.36355
C	5.15971	-2.88730	0.20418
H	5.78627	-3.78860	0.19582
H	5.82690	-2.02883	0.05063
C	4.11796	-2.95589	-0.91974
H	4.62108	-3.02192	-1.89249
C	3.58390	-1.47448	1.56550
H	4.23765	-0.60604	1.43122
H	3.11529	-1.38869	2.55009
C	3.21353	-4.17823	-0.71681
H	3.81016	-5.09953	-0.73946
H	2.48313	-4.24758	-1.53370
C	3.52582	-3.98085	1.76395
H	3.01804	-3.90870	2.73509
H	4.12728	-4.89888	1.78283
C	2.16331	1.68897	0.65124
C	2.86100	4.29603	-0.58297
H	3.28782	5.30638	-0.53819
H	2.49622	4.14496	-1.60757
C	3.29370	3.36792	2.16830
H	3.65702	3.51723	3.19292
C	3.34256	1.83965	-0.33926
H	4.12440	1.10541	-0.11501
H	2.99688	1.64791	-1.36412
C	1.70180	4.17020	0.41625
H	0.91942	4.90002	0.17312
C	2.67060	1.95967	2.08322
H	1.83935	1.91070	2.79374
H	3.41100	1.21172	2.38446
C	3.93747	3.25554	-0.24531
H	4.76413	3.32925	-0.96310
C	2.22178	4.41511	1.83872
H	1.39771	4.35387	2.56197
H	2.64378	5.42556	1.91614
C	1.09555	2.75896	0.31426
H	0.71805	2.60084	-0.70463
H	0.24317	2.66624	0.99962
C	4.45907	3.49114	1.17840
H	4.91343	4.48753	1.25465
H	5.24318	2.76122	1.42047
Au	0.66239	0.11883	-1.88448
Cl	0.14598	0.30594	-4.16344
N	-2.18789	-0.41825	0.40468
P	1.34913	-0.00718	0.30991
H	-3.17119	-0.57374	0.75572
O	-4.77272	-0.89436	1.10323
S	-5.78742	-0.87863	0.00016
O	-6.79500	-1.94071	0.09575
O	-5.19230	-0.64320	-1.32882
C	-6.72226	0.67925	0.35526
F	-7.67992	0.86974	-0.55765
F	-5.89992	1.73652	0.33007
F	-7.29448	0.62259	1.56281

2c_OTf

Sum of electronic and zero-point Energies= -3044.014459
Sum of electronic and thermal Enthalpies = -3043.974957
Sum of electronic and thermal Free Energies = -3044.087392

C	-0.75308	-0.08269	2.06692
C	-1.91025	0.21607	2.81945
H	-2.79438	0.55365	2.28647
C	-1.99556	0.09295	4.20055
H	-2.92455	0.34330	4.70353
C	-0.89686	-0.36586	4.91121
H	-0.93426	-0.49898	5.98769
C	0.27330	-0.64723	4.22007
H	1.13378	-0.99356	4.78181
C	0.36421	-0.48982	2.83528
C	2.10288	-2.22394	2.46177
H	2.26217	-2.42930	3.51964
H	3.02923	-2.38143	1.90645
H	1.29892	-2.84914	2.07723
C	2.77314	0.09365	2.92709
H	2.50827	1.13653	2.76246
H	3.72166	-0.14393	2.45027
H	2.82348	-0.11733	3.99300
C	-0.75459	-1.56104	-0.69020
C	-1.46163	-2.64176	0.16426
H	-2.50271	-2.34690	0.35408
H	-0.96992	-2.73889	1.14015
C	-1.42716	-3.99999	-0.56155
H	-1.93375	-4.73976	0.07107
C	-1.47832	-1.47372	-2.06008
H	-2.52412	-1.17184	-1.91557
H	-1.00771	-0.71529	-2.69448
C	0.72941	-3.36334	-1.65971
H	1.77990	-3.63890	-1.81312
C	0.01588	-3.25218	-3.01258
H	0.05417	-4.21474	-3.53920
H	0.52309	-2.51591	-3.64958
C	-1.44072	-2.83533	-2.77569
H	-1.96165	-2.72991	-3.73559
C	0.69838	-1.99757	-0.94230
H	1.23176	-1.26246	-1.54627
H	1.24310	-2.09214	-0.00144
C	-2.15032	-3.88495	-1.91009
H	-2.15178	-4.85726	-2.41959
H	-3.19933	-3.60022	-1.75500
C	0.03049	-4.42084	-0.79544
H	0.55228	-4.53439	0.16418
H	0.06439	-5.39783	-1.29489
C	-0.16401	1.68201	-0.44403
C	0.21104	4.62206	-0.21767
H	0.64024	5.57364	-0.55733
H	-0.39882	4.84193	0.66882
C	1.30567	2.74939	-2.20101
H	1.91337	2.52794	-3.08745
C	-1.27551	2.69553	-0.81408
H	-1.92585	2.26705	-1.58709
H	-1.90770	2.89458	0.06087
C	1.33291	3.63751	0.13704
H	1.95852	4.05642	0.93556
C	0.70389	1.42296	-1.69339
H	1.52013	0.73796	-1.44978
H	0.10459	0.97325	-2.49178
C	-0.66343	4.01178	-1.32079
H	-1.48214	4.69784	-1.57205
C	2.18938	3.36382	-1.10711
H	3.01353	2.68386	-0.86229
H	2.63786	4.29908	-1.46718
C	0.72930	2.31258	0.64362
H	0.15675	2.49273	1.56142
H	1.55069	1.63035	0.88192
C	0.18528	3.73015	-2.56762
H	0.61314	4.66449	-2.95392
H	-0.44304	3.30963	-3.36420
Au	-3.36327	0.38662	-0.04744
Cl	-5.67283	0.62757	-0.36986
N	1.72075	-0.78072	2.30069
P	-1.06969	0.10373	0.21015
H	1.78954	-0.57700	1.28901
O	3.23932	-0.23963	-0.05882
S	4.55272	-0.90543	-0.29289
O	4.69984	-1.53878	-1.61090
O	5.02624	-1.69104	0.86671
C	5.72172	0.53079	-0.34336
F	6.98070	0.11079	-0.50783
F	5.65866	1.23011	0.79830
F	5.42002	1.35656	-1.35406