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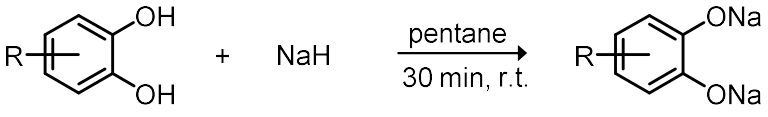
1. Materials and Methods

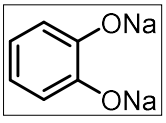
All reactions and manipulations were carried out under an atmosphere of dry argon using standard Schlenk techniques or in a glovebox under an inert atmosphere unless stated otherwise. All reagents were purchased from commercial sources and used without further purification. Dry, oxygen-free solvents were employed. Solution ^{1}H, ^{13}C, ^{31}P and ^{11}B NMR spectra were recorded on a Bruker Avance 300, 400 or 500 spectrometer at 298 K unless otherwise stated. Chemical shifts (δ) are expressed with a positive sign, in parts per million. ^{1}H and ^{13}C chemical shifts are referenced internally to residual protio (^{1}H) or deutero (^{13}C) solvent, while ^{31}P and ^{11}B chemical shifts are relative to 85% H_3PO_4 and BF_3-OEt_2 respectively. The following abbreviations and their combination are used: br, broad; s, singlet; d, doublet; t, triplet; m, multiplet. The ^{1}H and ^{13}C resonance signals were attributed by means of 2D HSQC, HMBC and NOESY experiments. Mass spectra were recorded on a Waters UPLC Xevo G2 QTOF apparatus. X-Band EPR data were recorded using an ELEXYS 500 EPR spectrometer from Brüker. Measurements were performed with different modulation amplitudes and number of scans (from 8 to 32). VT UV-vis experiments were performed with an Optistat DN optical cryostat, using a PerkinElmer Lambda 750 UV-Vis spectrometer. *i*PrPAuI_2 (**1**) and *closo*-carboranyl diphosphine (**5**) were prepared according to previously reported procedures.[1-2] 3,5-di-*tert*-butyl-*o*-benzoquinone (**4b**) and *o*-chloranil (**4d**) are commercially available.

2. Preparation of sodium catecholates

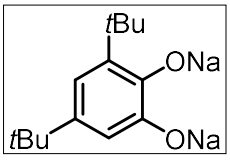
Sodium catecholates (**2a-d**) were prepared by an alternative method to that reported in the literature.[3-4] NaH (10 mmol) was suspended in pentane (10 ml), the corresponding catechol (5 mmol, 0.5 equiv.) was added in one portion and the mixture was stirred for 30 minutes at room temperature, after which a large amount of white precipitate appeared. The volatiles were evaporated *in vacuo* and the resulting off white solid was placed inside the glovebox. All the catecholates were obtained in quantitative yields, and used without further purification.



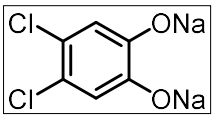
2a-d



2a. **^{1}H NMR** (300 MHz, MeOD): δ (ppm) 6.62-6.68 (m, CH_{cat}, 2H), 6.40-6.46 (m, CH_{cat}, 2H).



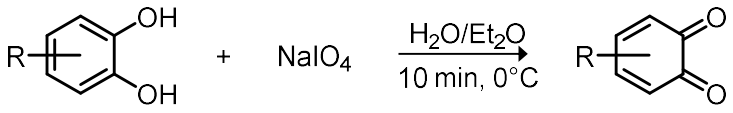
2b. **^{1}H NMR** (300 MHz, MeOD): δ (ppm) 6.66(d, $^{4}J_{HH}$ = 2.3 Hz, CH_{cat}, 1H), 6.42(d, $^{4}J_{HH}$ = 2.3 Hz, CH_{cat}, 1H), 1.38 (s, C(CH_3)$_3$, 9H), 1.25 (s, C(CH_3)$_3$, 9H).



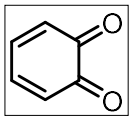
2c. **^{1}H NMR** (300 MHz, MeOD): δ (ppm) 6.87 (s, CH_{cat}, 2H).

3. Preparation of 1,2-benzoquinones

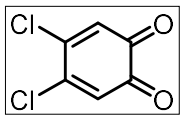
Non-commercial 1,2-benzoquinones **4a** and **4c** were prepared by a previously reported method.[5] To a solution of the corresponding catechol (1 mmol) in a mixture of H_2O/Et_2O (1/1) in an ice bath (0 °C) was added in one portion $NaIO_4$ (1.2 mmol, 1.2 equiv.). The mixture was stirred for 10 minutes and the ethereal phase was transferred *via* cannula to a Schlenk with anhydrous magnesium sulphate under argon in an ice bath (0 °C) and stirred for 30 min. After this time, the heterogenous mixture was filtered with a cannula and transferred to a Schlenk in an ice bath (0° C) where the volatiles were evaporated *in vacuo*. The resulting solid was transferred to a vial and stored in the glovebox freezer. The formation of the target compounds was verified by ^{1}H NMR and they were used without further purification.



4a or **4c**



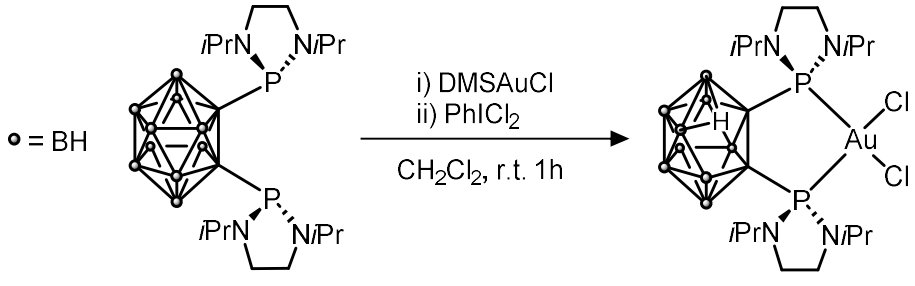
4a. Obtained as an intense red crystalline material (71 %). **^{1}H NMR** (300 MHz, CD_2Cl_2): δ (ppm) 6.97-7.01 (m, CH_{cat}, 2H), 6.30-6.34 (m, CH_{cat}, 2H).



4c. Obtained as an orange solid (65 %). **^{1}H NMR** (300 MHz, CD_2Cl_2): δ (ppm) 6.68 (s, CH_{cat}, 2H).

4. Preparation of *nido*-P^PAuCl$_2$ precursor (6)

Over a solution of **5** (0.34 mmol) in CH_2Cl_2 (50 ml) DMSAuCl (0.34 mmol, 1 equiv.) was added under air. After 30 minutes dichloro(phenyl)-λ^3-iodane (0.40 mmol, 1.2 equiv.) was added in several portions and the mixture stirred for 1 hour. After this time, the solvent was evaporated and the remaining solid was washed with EtOH (3 x 10 ml) and dried *in vacuo* to give **6** as an off-white solid (89%). X-Ray quality crystals were obtained from a CD_2Cl_2 solution at room temperature.

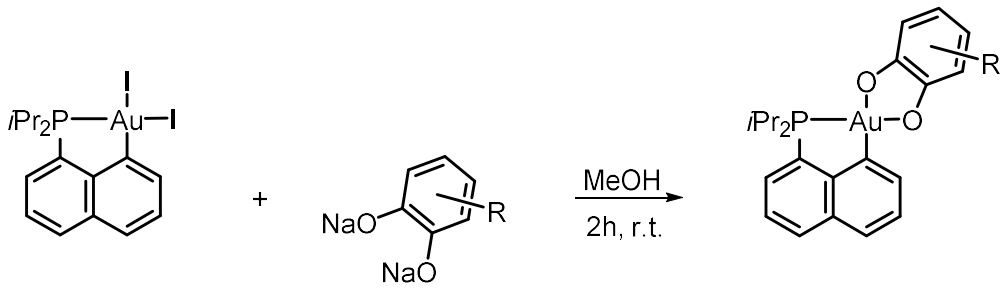


5 **6**

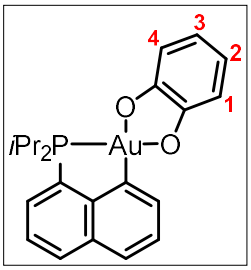
^{1}H NMR (500 MHz, CD_2Cl_2): δ (ppm) 3.66-3.78 (m, 2xC*H*$(CH_3)_2$ & 2xN(CH_2)$_2$N, 6H), 3.39-3.50 (m, 2xC*H*$(CH_3)_2$ & 2xN(CH_2)$_2$N, 6H), 1.47 (d, $^{3}J_{HH}$ = 6.7 Hz, CH(CH_3)$_2$, 12H), 1.42 (d, $^{3}J_{HH}$ = 6.7 Hz, 2xCH(CH_3)$_2$, 6H), 1.33 (d, $^{3}J_{HH}$ = 6.7 Hz, CH(CH_3)$_2$, 6H), 0.25-3.00 (bs, ~9H, BH), -2.67 (bs, BHB, 1H). **^{13}C{^{1}H} NMR** (125.8 MHz, CD_2Cl_2): δ (ppm) 56.6 (bs, 2x$C_{carborane}$), 48.1 (d, $^{3}J_{CP}$ = 7 Hz, 2xC*H*$(CH_3)_2$), 47.2 (d, $^{3}J_{CP}$ = 7 Hz, 2xC*H*$(CH_3)_2$), 42.3 (d, $^{2}J_{CP}$ = 5 Hz, 2xN(CH_2CH_2)N), 41.3 (d, $^{2}J_{CP}$ = 5 Hz, 2xN(CH_2CH_2)N), 21.1 (s, CH(CH_3)$_2$), 21.0 (d, $^{3}J_{CP}$ = 7 Hz, CH(CH_3)$_2$), 20.6 (d, $^{3}J_{CP}$ = 7 Hz, CH(CH_3)$_2$), 20.2 (s, CH(CH_3)$_2$).). **^{31}P NMR** (202.5 MHz. CD_2Cl_2): δ (ppm) 116.1 (s). **^{11}B NMR** (160.5 MHz): δ (ppm) -8.5, -15.4, -19.7, -26.9, -33.1. **HRMS** (ESI) calcd. for $[M-H]^-$ = $C_{18}H_{45}AuB_9Cl_2N_4P_2$: 744.3058, found 744.3051.

5. Preparation of P^C catecholate complexes (3a-d)

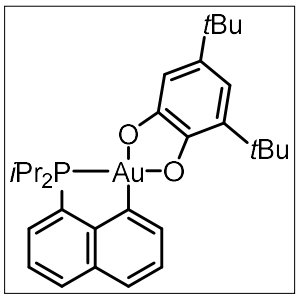
A mixture of **1** (0.3 mmol) and the corresponding sodium catecholate (**2a-d**) (0.45 mmol, 1.5 equiv.) in MeOH (2 ml) was stirred vigorously for 2 hours at room temperature, under argon atmosphere. After this time the supernatant was removed by cannula filtration and the precipitate was washed with MeOH (3 x 2 ml). The remaining solid was dried *in vacuo* for 1 hour.



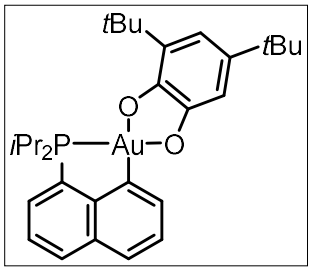
1 **2a-d** **3a-d**



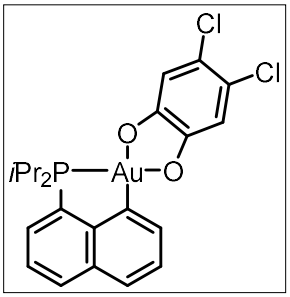
3a. Obtained as an orange powder (76 %). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ (ppm) 8.43 (dd, $^{3}J_{HH}$ = 7.6 Hz, $^{4}J_{HH}$ = 1.6 Hz, CH_{Naphth}, 1H), 8.07 (dd, $^{3}J_{HH}$ = 8.1 Hz, $^{5}J_{HP}$ = 2.9 Hz, CH_{Naphth}, 1H), 7.85 (dd, $^{3}J_{HH}$ = 8.2 Hz, $^{4}J_{HH}$ = 2.5 Hz, CH_{Naphth}, 1H), 7.71-7.77 (m, CH_{Naphth}, 1H), 7.54-7.67 (m, CH_{Naphth}, 2H), 6.72-6.75 (m, H_1, 1H), 6.58-6.61 (m, H_2, 1H), 6.50-6.47 (m, H_{2-3}, 2H), 2.96-3.09 (m, 2xC*H*$(CH_3)_2$, 2H), 1.45 (dd, $^{3}J_{HP}$ = 19.1 Hz, $^{3}J_{HH}$ = 7.1 Hz, CH(CH_3)$_2$, 6H), 1.32 (dd, $^{3}J_{HP}$ = 18.1 Hz, $^{3}J_{HH}$ = 7.1 Hz, CH(CH_3)$_2$, 6H),. **^{13}C{^{1}H} NMR** (125.8 MHz, CD_2Cl_2): δ (ppm) 163.0 (d, $^{3}J_{CP}$ = 5 Hz, OC_{Cat}), 160.3 (d, $^{3}J_{CP}$ = 5 Hz, OC_{Cat}), 148.2 (d, $^{2}J_{CP}$ = 24 Hz, $C_{q-\ Naphth}$), 140.1 (s, $C_{q-\ Naphth}$), 134.5 (d, $^{3}J_{CP}$ = 14 Hz, $C_{q-Naphth}$), 133.5 (d, $^{3}J_{CP}$ = 3 Hz, CH_{Naphth}), 130.7 (d, $^{3}J_{CP}$ = 3 Hz, CH_{Naphth}), 130.3 (s, CH_{Naphth}), 128.6 (s, CH_{Naphth}), 127.3 (s, CH_{Naphth}), 130.3 (s, CH_{Naphth}), 126.7 (d, $^{3}J_{CP}$ = 10 Hz, CH_{Naphth}), 125.2 (d, $^{1}J_{CP}$ = 59 Hz, $C_{q-Naphth}$), 117.9 (s, 2xCH_{cat}). 117.3 (d, $^{4}J_{CP}$ = 4 Hz, CH_{Cat}), 115.9 (d, $^{4}J_{CP}$ = 5 Hz, CH_{Cat}), 26.4 (d, $^{1}J_{CP}$ = 32 Hz, 2x*C*H$(CH_3)_2$), 17.9 (s, CH(CH_3)$_2$), 17.8 (s, CH(CH_3)$_2$).**^{31}P NMR** (202.5 MHz, CD_2Cl_2): δ (ppm) 88.7. **HRMS** (DCI) calcd. for $[M]^+$ = $C_{22}H_{24}O_2PAu$: 548.1180, found 548.1186. X-Ray quality crystals were obtained from a dichloromethane solution of **3a** at room temperature.



3b-1. After the reaction, a mixture of **3b-1** and **3b-2** (86/14) was obtained. By successive methanol washings (6 x 2 mL), **3b-1** could be obtained in a pure form as an orange powder (68 %). ^{1}H NMR (500 MHz, CD_2Cl_2): δ (ppm) 8.55 (d, $^{3}J_{HH}$ = 7.1 Hz, CH_{Naphth}, 1H), 8.06 (dd, $^{3}J_{HH}$ = 8.1 Hz, $^{5}J_{HP}$ = 2.9 Hz, CH_{Naphth}, 1H), 7.84 (dd, $^{3}J_{HH}$ = 8.1 Hz, $^{4}J_{HH}$ = 2.5 Hz, CH_{Naphth}, 1H), 7.70-7.76 (m, CH_{Naphth}, 1H), 7.56-7.66 (m, CH_{Naphth}, 2H), 6.55 (s, $CH_{cat,}$ 2H), 2.95-3.07 (m, C*H*(CH_3)$_2$, 2H), 1.56 (s, C(C*H*$_3$)$_{3,}$ 9H), 1.45 (dd, $^{3}J_{HP}$ = 19.3 Hz, $^{3}J_{HH}$ = 7.1 Hz, CH(C*H*$_3$), 6H), 1.27-1.36 (m, CH(C*H*$_3$)$_2$ & C(C*H*$_3$)$_3$, 15H).**^{13}C{^{1}H} NMR** (125.8 MHz, CD_2Cl_2): δ (ppm) 162.3 (d, $^{3}J_{CP}$ = 5 Hz, O*C*$_{Cat}$), 156.1 (d, $^{3}J_{CP}$ = 4 Hz, O*C*$_{Cat}$), 148.3 (d, $^{2}J_{CP}$ = 24 Hz, $C_{q\text{-}Naphth}$), 141.1 (s, $C_{q\text{-}Naphth}$), 139.8 ($C_{q\text{-}Cat}$), 135.6 (d, $^{4}J_{CP}$ = 5 Hz, $C_{q\text{-}Cat}$), 134.5 (d, $^{3}J_{CP}$ = 13 Hz, $C_{q\text{-}Naphth}$), 133.4 (d, $^{4}J_{CP}$ = 3 Hz, CH_{Naphth}), 130.8 (d, $^{4}J_{CP}$ = 1 Hz, CH_{Naphth}), 130.7 (d, $^{3}J_{CP}$ = 3 Hz, CH_{Naphth}), 128.6 (s, CH_{Naphth}), 127.0 (s, CH_{Naphth}), 126.6 (d, $^{2}J_{CP}$ = 10 Hz, CH_{Naphth}), 125.6 (d, $^{1}J_{CP}$ = 58 Hz, $C_{q\text{-}Naphth}$), 113.0 (s, CH_{Cat}), 111.3 (s, CH_{Cat}), 34.9 (s, *C*(CH_3)$_3$), 34.3 (s, *C*(CH_3)$_3$), 32.3 (s, C(*C*H$_3$)$_3$), 30.0 (s, C(*C*H$_3$)$_3$), 26.3 (d, $^{1}J_{CP}$ = 32 Hz, 2x*C*H(CH_3)$_2$), 17.9 (d, $^{2}J_{CP}$ = 1 Hz, CH(*C*H$_3$)$_2$), 17.8 (s, CH(*C*H$_3$)$_2$). **^{31}P NMR** (202.5 MHz, CD_2Cl_2): δ (ppm) 85.6. **HRMS** (DCI) calcd. for $[M]^+$ = $C_{30}H_{40}AuO_2P$: 660.2432, found 660.2414. The position of *t*Bu groups could be assigned based on ^{1}H-^{1}H NOESY experiments, which showed an interaction between the methyl protons and the *o*-Au-Ar proton, see Figure S14).

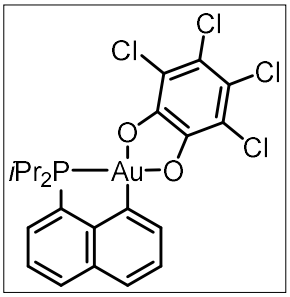


3b-2. From the reaction mixture (**3b-1**/**3b-2**=86/14), **3b-2** could not be obtained in a pure form. **3b-2** could be only characterized by ^{1}H and ^{31}P NMR as a minor product in mixture with **3b-1**. **^{1}H NMR** (500 MHz, CD_2Cl_2): δ (ppm) Most of the signals are totally overlapped with the ones of **3b-1,** the exceptions to this are: 8.45 (d, $^{3}J_{HH}$ = 7.1 Hz, CH_{Naphth}, 1H), 6.75 (d, $^{4}J_{HH}$ = 2.2 Hz, CH_{cat}. 1H), 6.60 (d, $^{4}J_{HH}$ = 2.2 Hz, $CH_{cat,}$ 1H). **^{31}P NMR** (202.5 MHz, CD_2Cl_2): δ (ppm) 87.8. X-ray quality crystals of **3b-2** were obtained in the isomerization experiments, from CD_2Cl_2 at room temperature.



3c. Obtained as an orange powder (81 %). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ (ppm) 8.33 (dd, $^{3}J_{HH}$ = 7.3 Hz, $^{4}J_{HH}$ = 2.3 Hz, CH_{Naphth}, 1H), 8.08 (dd, $^{3}J_{HH}$ = 8.1 Hz, $^{5}J_{HP}$ = 3.0 Hz, CH_{Naphth}, 1H), 7.86 (dd, $^{3}J_{HH}$ = 8.1 Hz, $^{4}J_{HH}$ = 2.9 Hz, CH_{Naphth}, 1H), 7.72-7.75 (m, CH_{Naphth}, 1H), 7.67-7.63 (m, CH_{Naphth}, 1H), 7.56 (t, $^{3}J_{HH}$ = 7.9 Hz, CH_{Naphth}, 1H), 6.78 (s, CH_{Cat}, 1H), 6.65 (s, CH_{Cat}, 1H), 2.94-3.05 (m, 2xC*H*(CH_3)$_2$, 2H), 1.43 (dd, $^{3}J_{HP}$ = 19.4 Hz, $^{3}J_{HH}$ = 7.1 Hz, CH(C*H*$_3$), 6H), 1.31 (dd, $^{3}J_{HP}$ = 19.3 Hz, $^{3}J_{HH}$ = 7.1 Hz, CH(C*H*$_3$), 6H). **^{13}C{^{1}H} NMR** (125.8 MHz, CD_2Cl_2): δ (ppm) 163.3 (d, $^{3}J_{CP}$ = 5 Hz, O*C*$_{Cat}$), 160.4 (d, $^{3}J_{CP}$ = 5 Hz, O*C*$_{Cat}$), 147.9 (d, $^{2}J_{CP}$ = 23 Hz, $C_{q\text{-}Naphth}$), 139.5 (s, $C_{q\text{-}Naphth}$), 134.5 (d, $^{3}J_{CP}$ = 14 Hz, $C_{q\text{-}Naphth}$), 133.7 (d, $^{3}J_{CP}$ = 3 Hz, CH_{Naphth}), 130.9 (d, $^{3}J_{CP}$ = 3 Hz, CH_{Naphth}), 130.2 (d, $^{4}J_{CP}$ = 1 Hz, CH_{Naphth}), 128.7 (s, CH_{Naphth}), 127.6 (s, CH_{Naphth}), 127.0 (d, $^{3}J_{CP}$ = 10 Hz, CH_{Naphth}), 124.6 (d, $^{1}J_{CP}$ = 60 Hz, $C_{q\text{-}Naphth}$), 118.9 (s, $C_{q\text{-}Cat}$), 118.3 (d, $^{5}J_{CP}$ = 1 Hz, $C_{q\text{-}Cat}$), 117.0 (s, CH_{Cat}), 115.7 (d, $^{4}J_{CP}$ = 7 Hz, CH_{Cat}), 26.7 (d, $^{1}J_{CP}$ = 32 Hz, 2x*C*H(CH_3)$_2$), 17.9 (d, $^{2}J_{CP}$ = 2 Hz, CH(*C*H$_3$)$_2$), 17.8 (s,

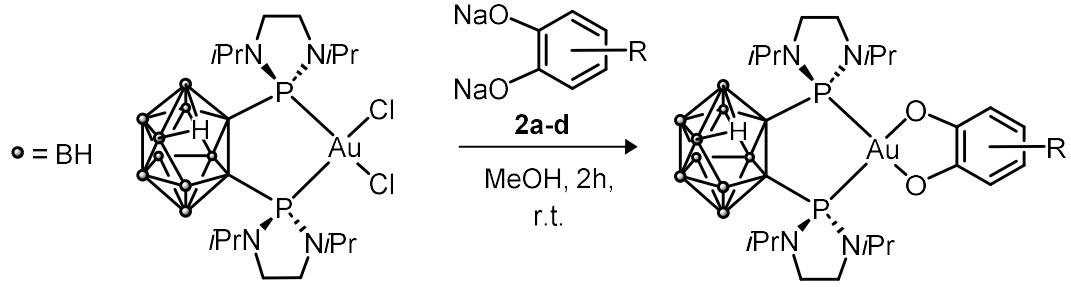
$CH(CH_3)_2$).**^{31}P NMR** (202.5 MHz, CD_2Cl_2): δ (ppm) 92.0. **HRMS** (DCI) calcd. for $[M]^+$ = $C_{22}H_{22}O_2PCl_2Au$: 616.0400, found 616.0425. X-Ray quality crystals were obtained from a dichloromethane solution of **3c** at room temperature.

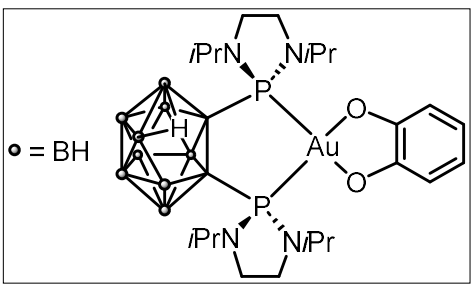


3d. Obtained as an orange powder (66 %). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ (ppm) 8.39 (dd, $^3J_{HH}$ = 7.2 Hz, $^4J_{HH}$ = 2.1 Hz, CH_{Naphth}, 1H), 8.10 (dd, $^3J_{HH}$ = 8.3 Hz, $^5J_{HP}$ = 3.0 Hz, CH_{Naphth}, 1H), 7.89 (dd, $^3J_{HH}$ = 8.1 Hz, $^4J_{HH}$ = 2.5 Hz, CH_{Naphth}, 1H), 7.74-7.77 (m, CH_{Naphth}, 1H), 7.65-7.69 (m, CH_{Naphth}, 1H), 7.60 (t, $^3J_{HH}$ = 7.9 Hz, CH_{Naphth}, 1H), 3.01-3.08 (m, 2x$CH(CH_3)_2$, 2H), 1.48 (dd, $^3J_{HP}$ = 19.6 Hz, $^3J_{HH}$ = 7.1 Hz, $CH(CH_3)$, 6H), 1.34 (dd, $^3J_{HP}$ = 19.6 Hz, $^3J_{HH}$ = 7.1 Hz, $CH(CH_3)$, 6H). **^{13}C{^{1}H} NMR** (125.8 MHz, CD_2Cl_2): δ (ppm) 159.1 (d, $^3J_{CP}$ = 4 Hz, OC_{Cat}), 156.2 (d, $^3J_{CP}$ = 4 Hz, OC_{Cat}), 147.8 (d, $^2J_{CP}$ = 22 Hz, $C_{q\text{-}Naphth}$), 139.0 (s, $C_{q\text{-}Naphth}$), 134.6 (d, $^3J_{CP}$ = 14 Hz, $C_{q\text{-}Naphth}$), 133.9 (d, $^3J_{CP}$ = 3 Hz, CH_{Naphth}), 131.1 (d, $^3J_{CP}$ = 3 Hz, CH_{Naphth}), 130.2 (d, $^4J_{CP}$ = 1 Hz, CH_{Naphth}), 128.9 (s, CH_{Naphth}), 127.9 (s, CH_{Naphth}), 127.1 (d, $^3J_{CP}$ = 11 Hz, CH_{Naphth}), 124.1 (d, $^1J_{CP}$ = 59 Hz, $C_{q\text{-}Naphth}$), 119.1 (s, $C_{q\text{-}Cat}$), 118.8 (s, $C_{q\text{-}Cat}$), 118.6 (s, $C_{q\text{-}Cat}$), 117.6 (d, $^4J_{CP}$ = 5 Hz, $C_{q\text{-}Cat}$), 26.8 (d, $^1J_{CP}$ = 32 Hz, 2x$CH(CH_3)_2$), 17.9 (d, $^2J_{CP}$ = 2 Hz, $CH(CH_3)_2$), 17.7 (s, $CH(CH_3)_2$).**^{31}P NMR** (202.5 MHz, CD_2Cl_2): δ (ppm) 95.6. **HRMS** (DCI) calcd. for $[M]^+$ = $C_{22}H_{20}O_2PCl_4Au$: 683.9621, found 683.9639. X-Ray quality crystals were obtained from a dichloromethane solution of **3d** at room temperature.

6. Preparation of P^P catecholate complexes (7a-d)

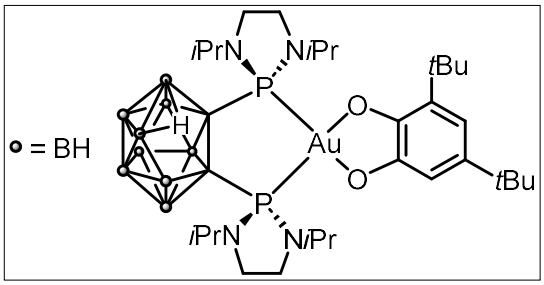
A mixture of **6** (0.3 mmol) and the corresponding sodium catecholate (**2a-d**) (1.5 equiv., 0.45 mmol) were suspended in MeOH (2 ml) and stirred vigorously for 2 hours at room temperature, under argon atmosphere. After this time, the supernatant was removed by cannula filtration and the precipitate was washed with MeOH (3 x 2 ml). The remaining solid was dried *in vacuo* for 1 hour.



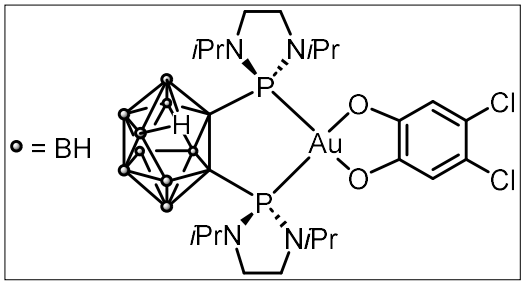


7a. Obtained using as a dark brown powder (74 %). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ (ppm) 6.54 (m, CH_{cat}, 2H), 6.42 (m, CH_{cat}, 2H), 3.65-3.72 (m, 2x$CH(CH_3)_2$, 2H), 3.28-3.60 (m, 2x$CH(CH_3)_2$ & 2x$N(CH_2)_2N$, 10H), 1.46 (d, $^3J_{HH}$ = 6.6 Hz, $CH(CH_3)_2$, 6H), 1.35 (d, $^3J_{HH}$ = 6.6 Hz, 2x$CH(CH_3)_2$, 12H), 1.32 (d, $^3J_{HH}$ = 6.6 Hz, $CH(CH_3)_2$, 6H), 0.91-3.00 (bs, ~9H, BH), -2.71 (bs, BHB, 1H).**^{13}C{^{1}H}**

NMR (125.8 MHz, CD_2Cl_2): δ (ppm) 160.1 (dd, $^3J_{CP}$ = 7Hz, $^3J_{CP}$ = 5Hz, 2xO-C_{cat}), 117.7 (s, 2xCH$_{cat}$), 116.8 (d, $^4J_{CP}$ = 4Hz, 2xCH$_{cat}$), 57.9 (d, $^1J_{CP}$ = 48 Hz, 2x$C_{carborane}$), 48.7 (d, $^3J_{CP}$ = 8 Hz, 2xC*H*(CH_3)$_2$), 47.2 (d, $^3J_{CP}$ = 8 Hz, 2xC*H*(CH_3)$_2$), 41.7 (d, $^2J_{CP}$ = 6 Hz, 2xN(*C*H_2CH_2)N), 41.3 (d, $^2J_{CP}$ = 7 Hz, 2xN(*C*H_2CH_2)N), 21.4 (s, CH(*C*H_3)$_2$), 21.3 (d, $^3J_{CP}$ = 7 Hz, CH(*C*H_3)$_2$), 20.9 (d, $^3J_{CP}$ = 7 Hz, CH(*C*H_3)$_2$), 20.4 (s, CH(*C*H_3)$_2$).**^{31}P NMR** (202.5 MHz, CD_2Cl_2): δ (ppm) 107.1 (s). **^{11}B NMR** (160.5 MHz, CD_2Cl_2): δ (ppm) -8.6 (s), -15.2 (s), -19.9 (s), -26.9 (s), -32.8 (s). **HRMS** (ESI) calcd. for [M-H]$^-$ = $C_{24}H_{49}AuB_9N_4O_2P_2$: 782.3898, found 782.3887. X-Ray quality crystals were obtained by cooling down (4 °C) a saturated solution of **7a** in dichloromethane.

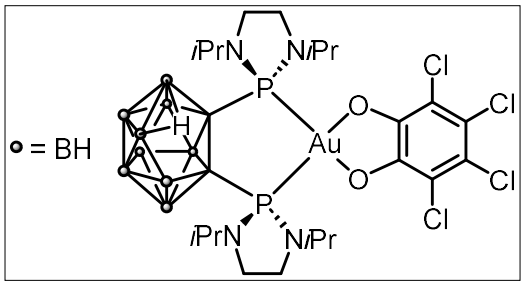


7b. Obtained as a dark brown powder (72 %). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ (ppm) 6.52-5.54 (m, 2xC*H*$_{cat}$, 2H), 3.65-3.79 (m, 2xC*H*(CH_3)$_2$, 2H), 3.29-3.59 (m, 2xC*H*(CH_3)$_2$ & 2xN(CH_2)$_2$N, 10H), 1.47 (d, $^3J_{HH}$ = 6.6 Hz, CH(CH_3)$_2$, 3H), 1.45 (d, $^3J_{HH}$ = 6.6 Hz, CH(CH_3)$_2$, 3H), 1.31-1.38 (m, 3xCH(CH_3)$_2$ & C(C*H*)$_3$, 27H), 1.25 (s, C(C*H*)$_3$, 9H), 0.91-3.01 (bs, ~9H, BH), -2.66 (bs, BHB, 1H). **^{13}C{^{1}H} NMR** (125.8 MHz, CD_2Cl_2): δ (ppm) 159.6 (dd, $^3J_{CP}$ = 6Hz, $^3J_{CP}$ = 4Hz, O-C_{cat}), 155.5 (dd, $^3J_{CP}$ = 6Hz, $^3J_{CP}$ = 4Hz, O-C_{cat}), 139.8 (d, $^5J_{CP}$ = 1Hz, $C_{q\text{-}cat}$), 136.5 (d, $^4J_{CP}$ = 4Hz, $C_{q\text{-}cat}$), 112.6 (d, $^4J_{CP}$ = 1Hz, CH$_{cat}$), 112.3 (s, CH$_{cat}$), 58.9 (d, $^1J_{CP}$ = 48 Hz, $C_{carborane}$), 56.5 (d, $^1J_{CP}$ = 48 Hz, $C_{carborane}$), 48.9 (d, $^3J_{CP}$ = 9 Hz, C*H*(CH_3)$_2$), 47.7 (d, $^2J_{CP}$ = 8 Hz, C*H*(CH_3)$_2$), 47.2 (d, $^2J_{CP}$ = 9 Hz, N(*C*H_2CH_2)N), 47.1 (d, $^2J_{CP}$ = 9 Hz, N(CH_2*C*H_2)N), 41.7 (d, $^2J_{CP}$ = 6 Hz, 2xN(*C*H_2CH_2)N), 41.5 (d, $^2J_{CP}$ = 8 Hz, *C*H(CH_3)$_2$), 40.9 (d, $^2J_{CP}$ = 8 Hz, *C*H(CH_3)$_2$), 35.0 (s, *C*(CH_3)$_3$), 34.2 (s, *C*(CH_3)$_3$), 32.2 (s, C(*C*H_3)$_3$), 30.3 (s, C(*C*H_3)$_3$), 21.9 (s, CH(CH_3)$_2$), 21.4 (s, CH(CH_3)$_2$), 21.3 (d, $^3J_{CP}$ = 7 Hz, CH(*C*H_3)$_2$), 21.2 (d, $^3J_{CP}$ = 7 Hz, CH(*C*H_3)$_2$), 21.1 (d, $^3J_{CP}$ = 8 Hz, CH(*C*H_3)$_2$), 21.2 (s, CH(*C*H_3)$_2$), 20.7 (d, $^3J_{CP}$ = 7 Hz, CH(*C*H_3)$_2$), 20.5 (s, CH(*C*H_3)$_2$). **^{31}P NMR** (202.5 MHz, CD_2Cl_2): δ (ppm) 107.4 (s), 104.9 (s). **^{11}B NMR** (160.5 MHz, CD_2Cl_2): δ (ppm) -8.2 (s), -14.0 (s), -16.3 (s), -19.6 (s), -27.1 (s), -32.7 (s). **HRMS** (ESI) calcd. for [M-H]$^-$ = $C_{32}H_{65}AuB_9N_4O_2P_2$: 894.5151, found 894.5144. X-Ray quality crystals were obtained by cooling down (4 °C) a saturated solution of **7b** in dichloromethane.



7c. Obtained as an orange powder (69 %). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ (ppm) 6.60 (s, C*H*$_{cat}$, 2H), 3.65-3.72 (m, 2xC*H*(CH_3)$_2$, 2H), 3.30-3.57 (m, 2xC*H*(CH_3)$_2$ & 2xN(CH_2)$_2$N, 10H), 1.45 (d, $^3J_{HH}$ = 6.5 Hz, CH(CH_3)$_2$, 6H), 1.32 (m, 3xCH(CH_3)$_2$, 18H), 0.91-3.00 (bs, ~9H, BH), -2.73 (bs, BHB, 1H). **^{13}C{^{1}H} NMR** (125.8 MHz, CD_2Cl_2): δ (ppm) 161.1 (dd, $^3J_{CP}$ = 7Hz, $^3J_{CP}$ = 4Hz, 2xO-C_{cat}), 119.8 (s, 2xC-Cl$_{cat}$), 117.5 (s, d, $^3J_{CP}$ = 4Hz, 2xCH$_{cat}$), 58.3 (bs, 2x$C_{carborane}$), 49.7 (d, $^3J_{CP}$ = 7 Hz, 2xC*H*(CH_3)$_2$), 48.2 (d, $^3J_{CP}$ = 7 Hz, 2xC*H*(CH_3)$_2$), 42.8 (d, $^2J_{CP}$ = 6 Hz, 2xN(*C*H_2CH_2)N), 42.3 (d, $^2J_{CP}$ = 7 Hz, 2xN(*C*H_2CH_2)N), 22.3 (s, CH(*C*H_3)$_2$), 22.2 (d, $^3J_{CP}$ = 6 Hz, CH(*C*H_3)$_2$), 21.8 (d, $^3J_{CP}$ = 7 Hz, CH(*C*H_3)$_2$), 21.3 (s, CH(*C*H_3)$_2$). **^{31}P NMR** (202.5 MHz, CD_2Cl_2): δ (ppm) 106.7 (s). **^{11}B NMR** (160.5 MHz,

CD_2Cl_2): δ (ppm) -8.6 (s), -15.1 (s), -19.9 (s), -26.8 (s), -32.7 (s). **HRMS** (ESI) calcd. for $[M-H]^-$ = $C_{24}H_{47}AuB_9Cl_2N_4O_2P_2$: 852.3093, found 852.3084.



7d. Obtained as an orange powder (80 %). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ (ppm) 3.60-3.78 (m, 2xC*H*$(CH_3)_2$ & 2xN(C*H*$_2)_2$N, 6H), 3.38-3.49 (m, 2xC*H*$(CH_3)_2$ & 2xN(C*H*$_2)_2$N, 6H), 1.50 (d, $^3J_{HH}$ = 6.5 Hz, CH(C*H*$_3)_2$, 6H), 1.36 (d, $^3J_{HH}$ = 6.7 Hz, 2xCH(C*H*$_3)_2$, 12H), 1.35 (d, $^3J_{HH}$ = 6.7 Hz, CH(C*H*$_3)_2$, 6H), 0.91-3.00 (bs, ~9H, BH), -2.67 (bs, BHB, 1H). **^{13}C{^{1}H} NMR** (125.8 MHz, CD_2Cl_2): δ (ppm) 155.8 (dd, $^3J_{CP}$ = 7Hz, $^3J_{CP}$ = 5Hz, 2xO-C_{cat}), 119.0 (s, 2xCH$_{-cat}$), 118.9 (s, 2xCH$_{-cat}$), 56.4 (bs, 2x$C_{carborane}$), 48.7 (d, $^3J_{CP}$ = 8 Hz, 2xC*H*$(CH_3)_2$), 47.4 (d, $^3J_{CP}$ = 8 Hz, 2xC*H*$(CH_3)_2$), 41.9 (d, $^2J_{CP}$ = 6 Hz, 2xN(*C*H_2CH_2)N), 41.2 (d, $^2J_{CP}$ = 7 Hz, 2xN(*C*H_2CH_2)N), 21.5 (s, CH(*C*$H_3)_2$), 21.3 (d, $^3J_{CP}$ = 7 Hz, CH(*C*$H_3)_2$), 20.9 (d, $^3J_{CP}$ = 7 Hz, CH(*C*$H_3)_2$), 20.4 (s, CH(*C*$H_3)_2$). **^{31}P NMR** (202.5 MHz, CD_2Cl_2): δ (ppm) 106.2 (s). **^{11}B NMR** (160.5 MHz, CD_2Cl_2): δ (ppm) -8.3 (s), -14.9 (s), -20.2 (s), -26.6 (s), -32.6 (s). **HRMS** (ESI) calcd. for $[M-H]^-$ = $C_{24}H_{45}AuB_9Cl_4N_4O_2P_2$: 920.2301, found 920.2307.

7. NMR spectra

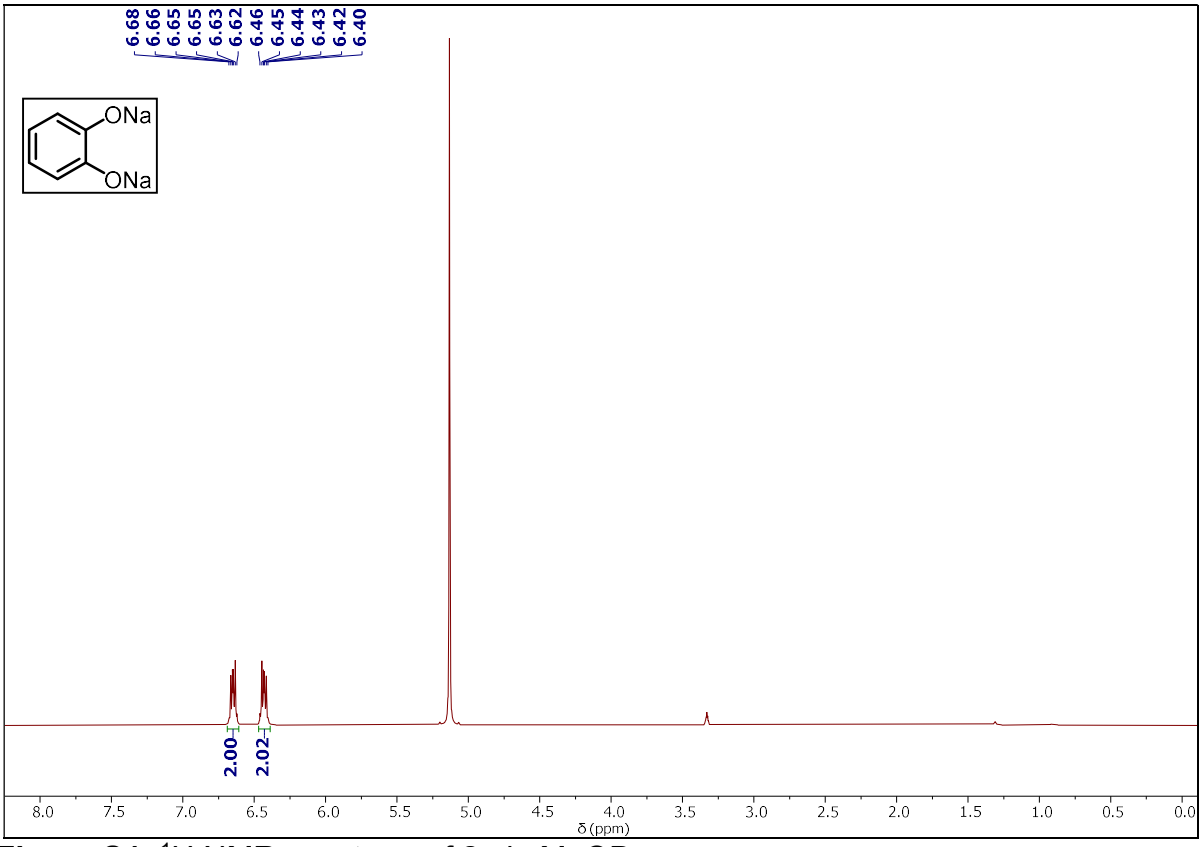


Figure S1. ^{1}H NMR spectrum of **2a** in MeOD.

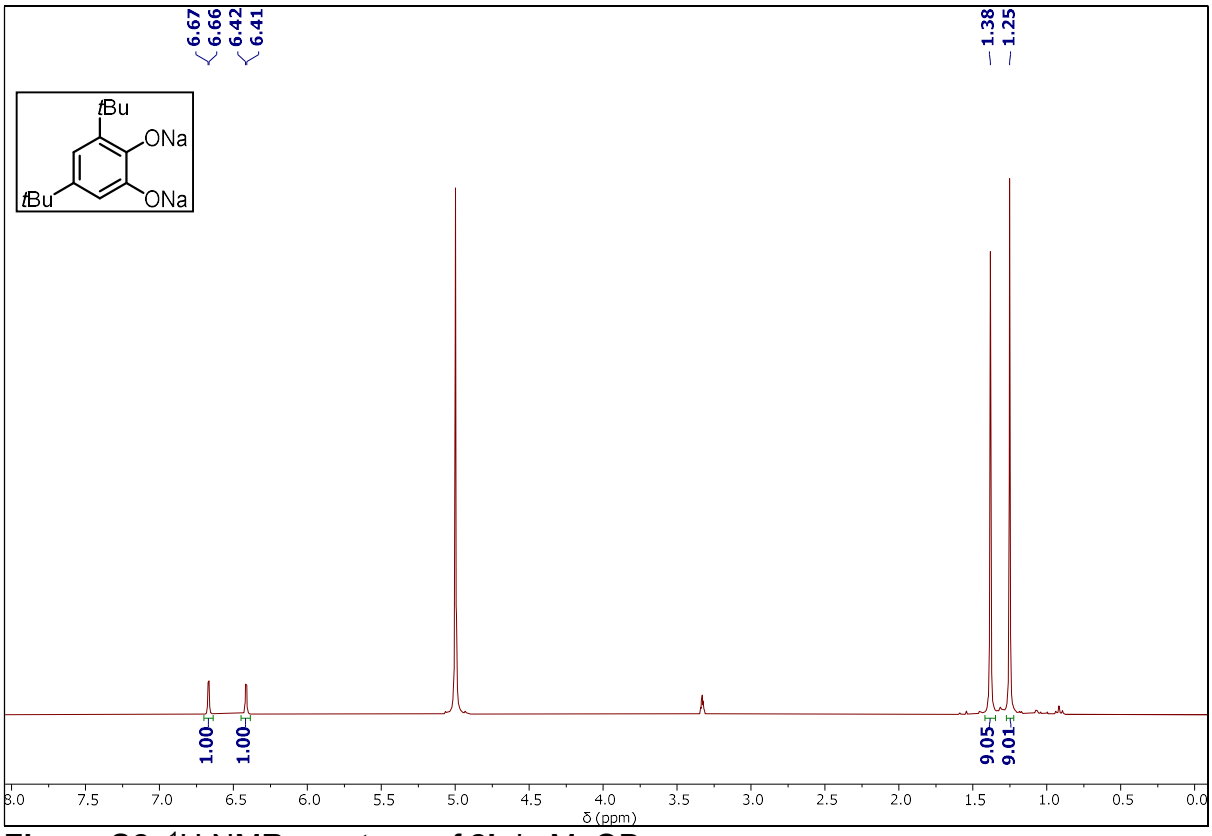


Figure S2. ^{1}H NMR spectrum of **2b** in MeOD.

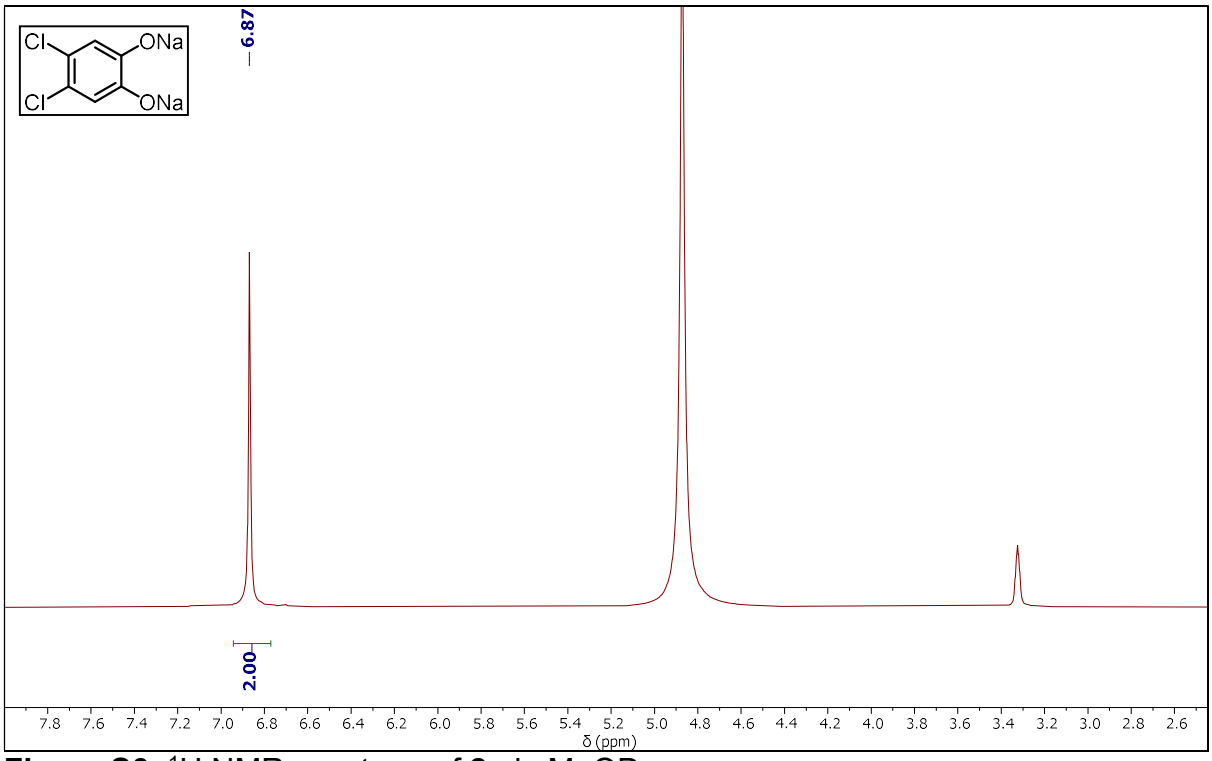


Figure S3. ^{1}H NMR spectrum of **2c** in MeOD.

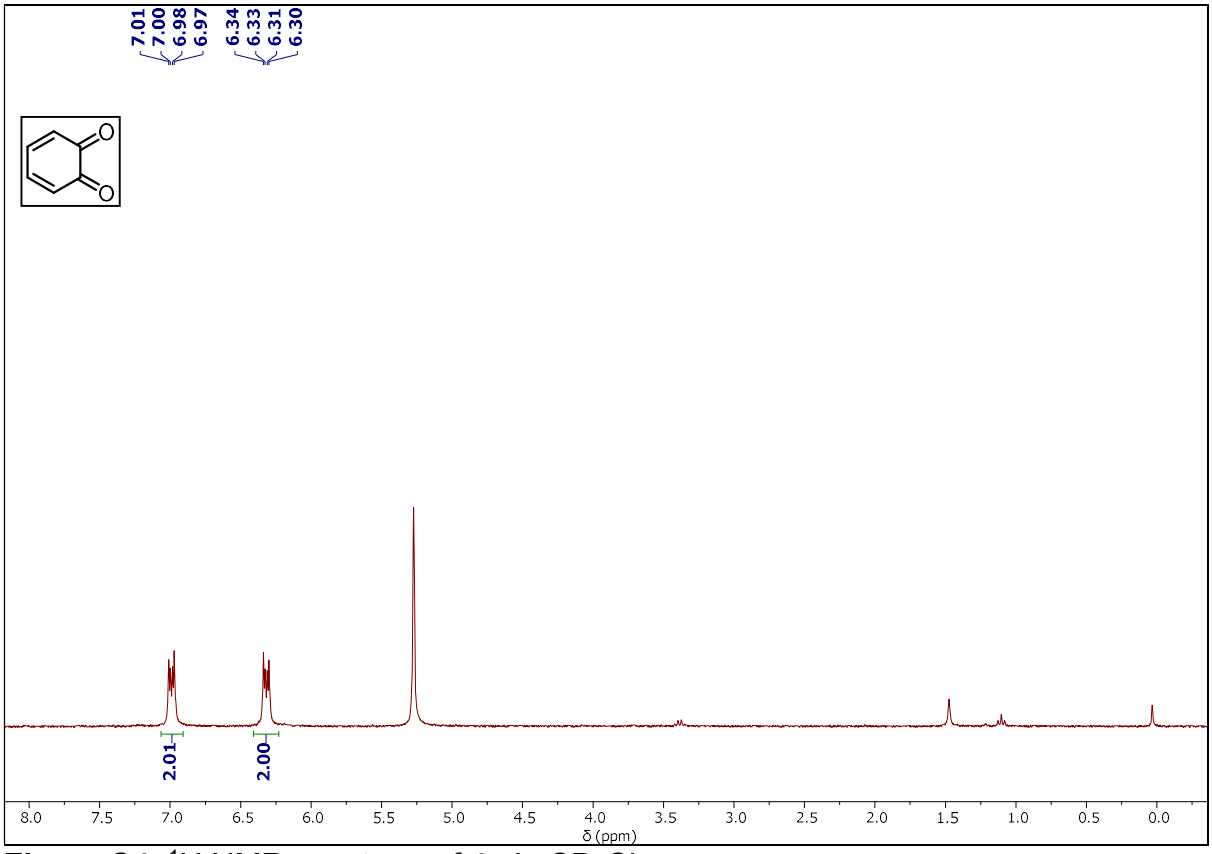


Figure S4. ^{1}H NMR spectrum of **4a** in CD_2Cl_2.

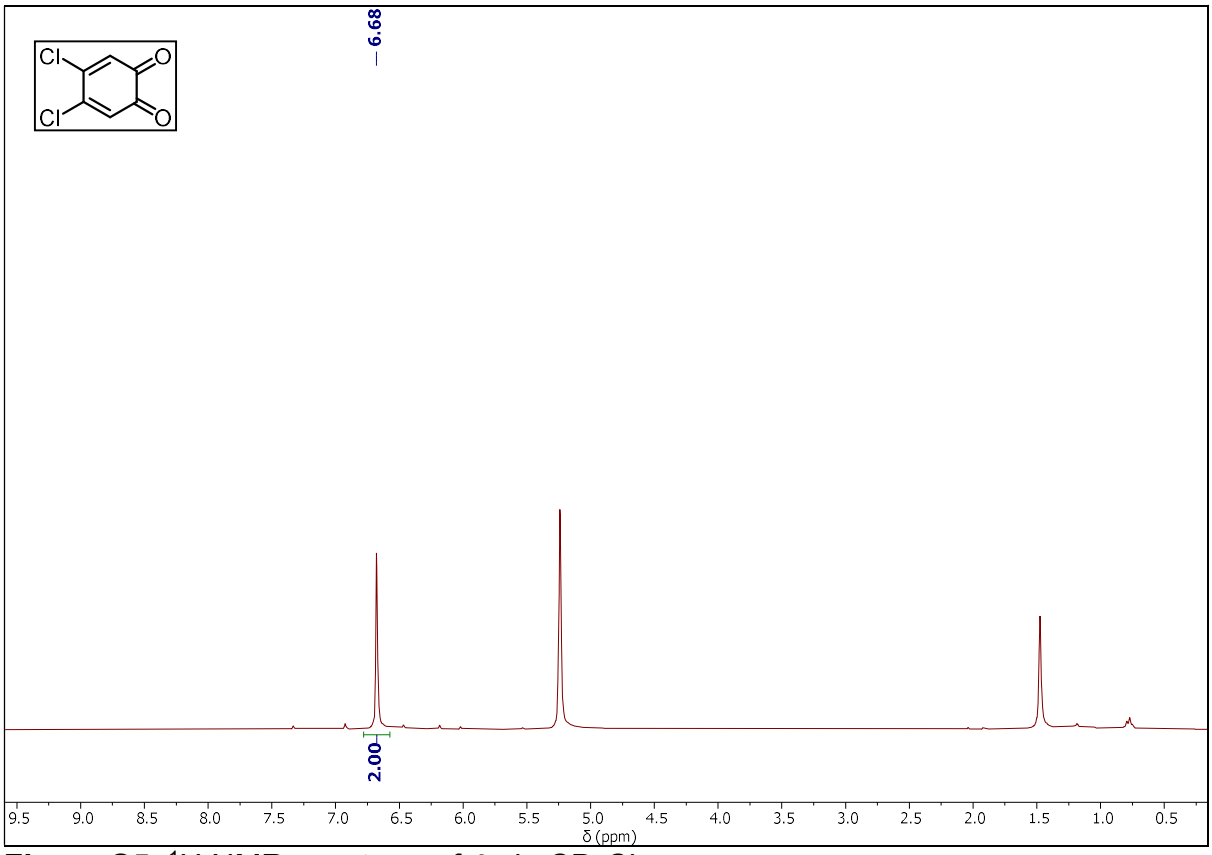


Figure S5. ^{1}H NMR spectrum of **4c** in CD_2Cl_2.

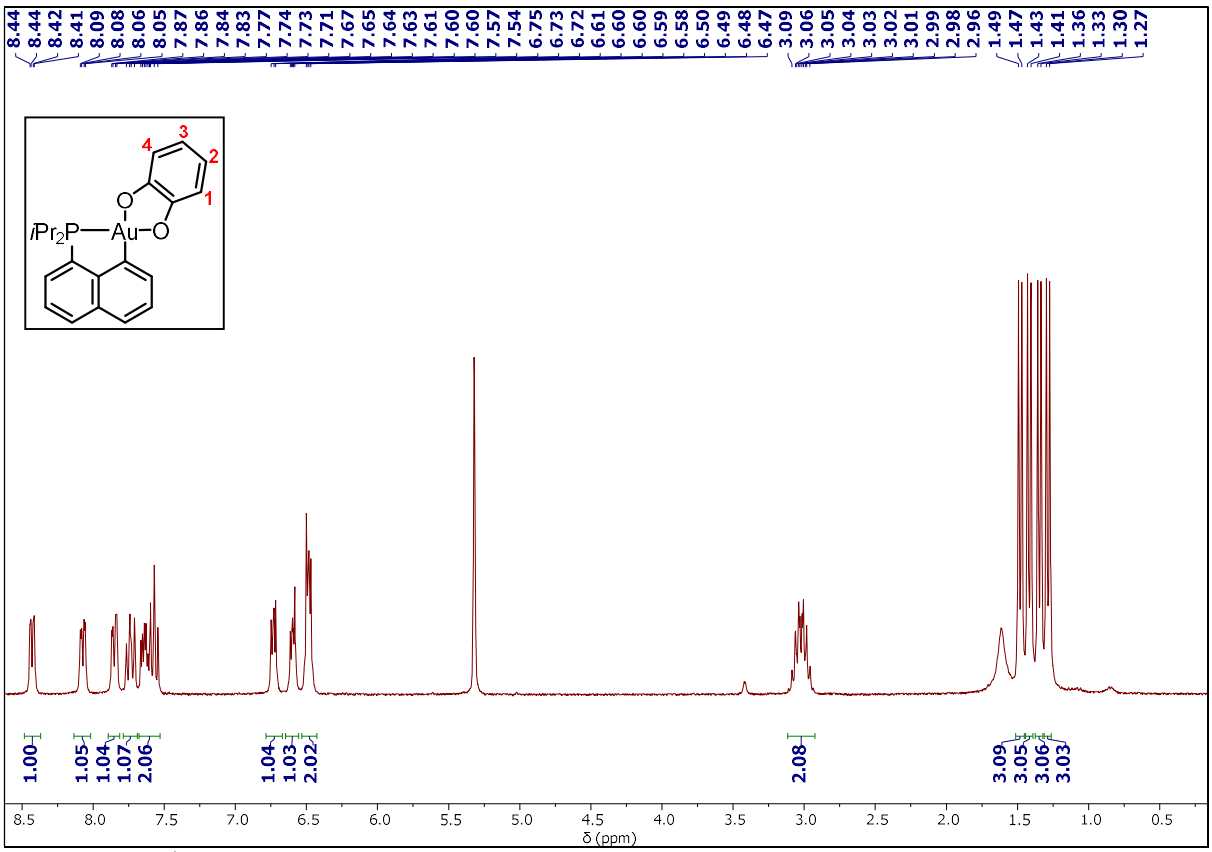


Figure S6. ^{1}H NMR spectrum of **3a** in CD_2Cl_2.

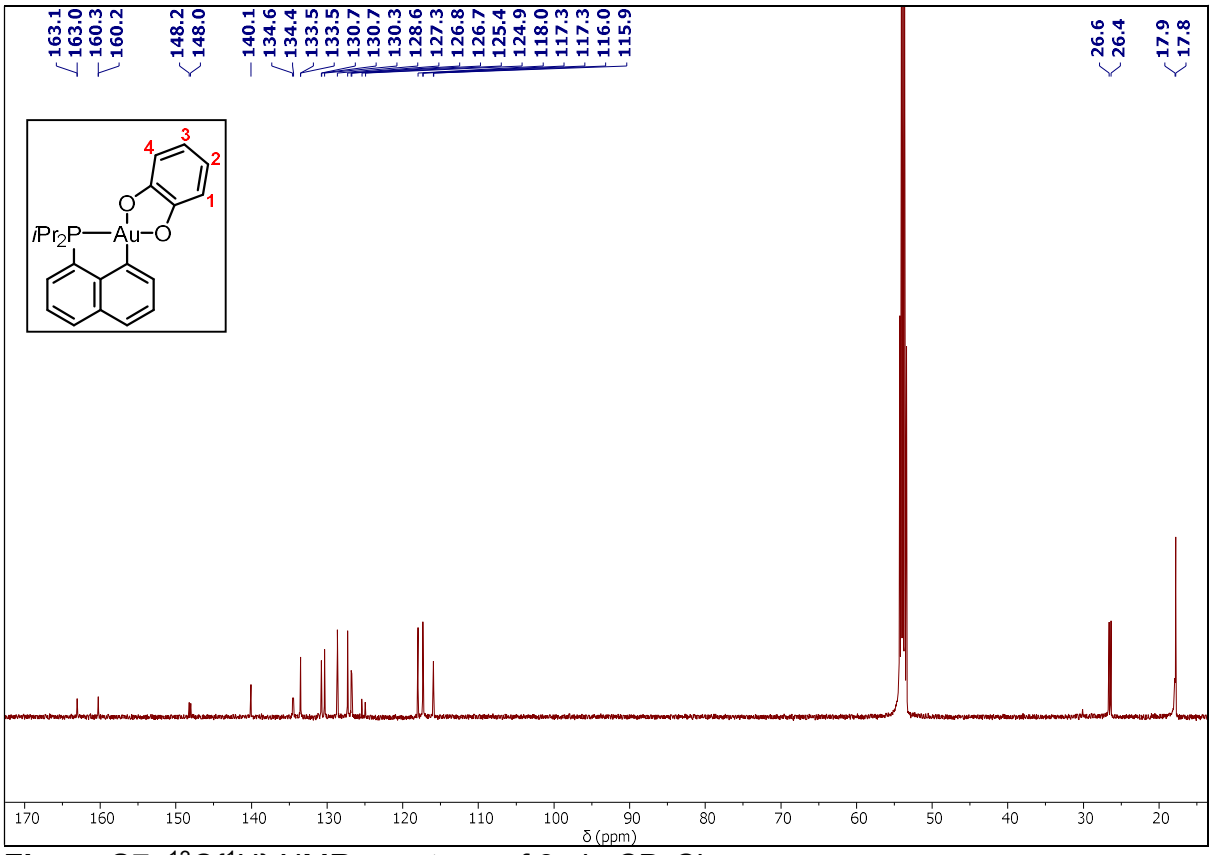


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of **3a** in CD_2Cl_2.

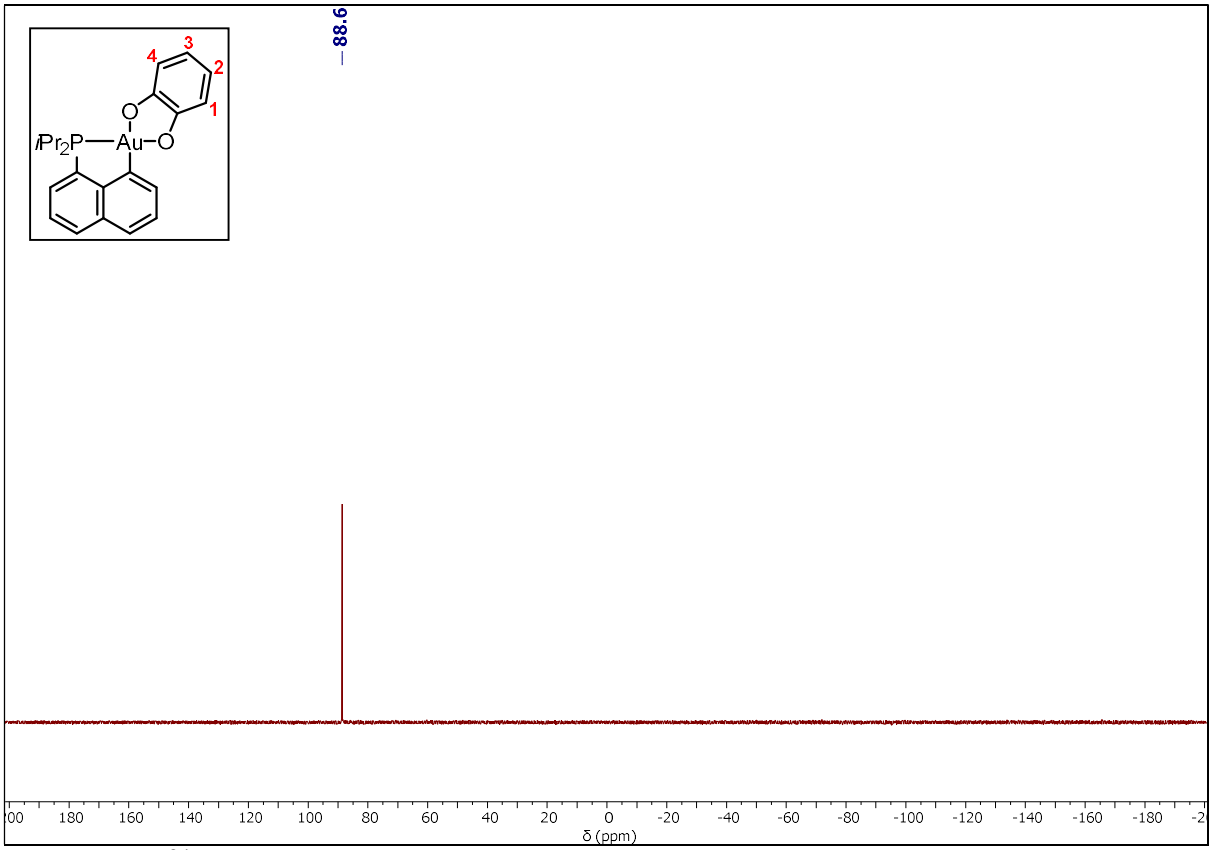


Figure S8. ^{31}P NMR spectrum of **3a** in CD_2Cl_2.

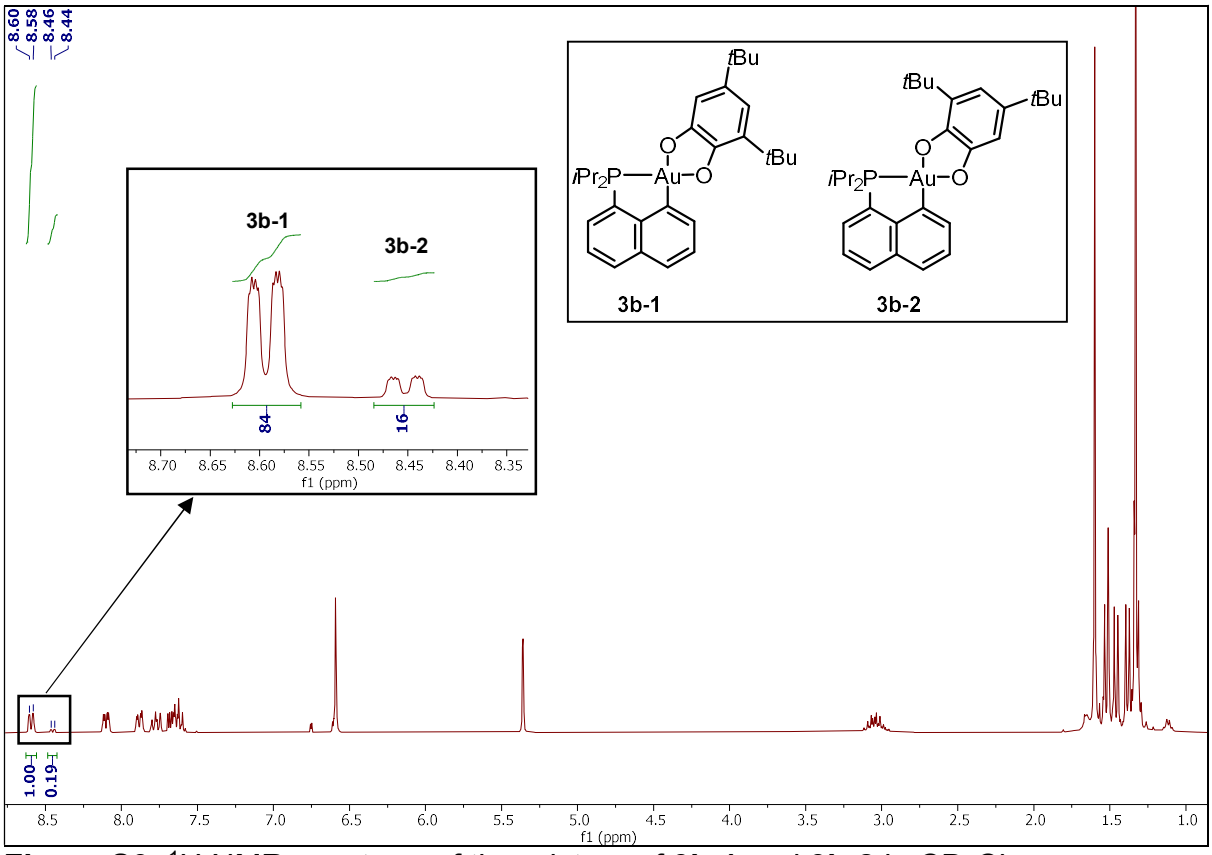


Figure S9. ^{1}H NMR spectrum of the mixture of **3b-1** and **3b-2** in CD_2Cl_2.

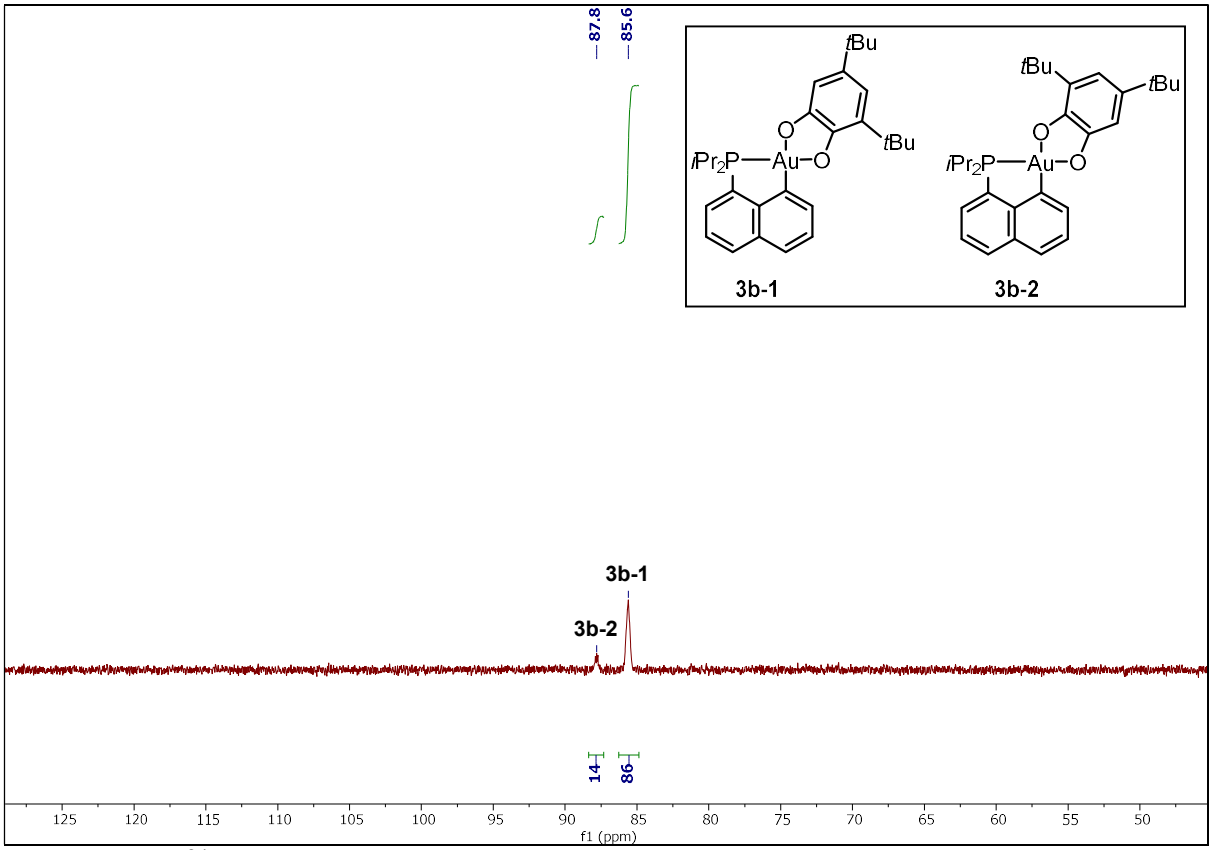


Figure S10. ^{31}P NMR spectrum of the mixture of **3b-1** and **3b-2** in CD_2Cl_2.

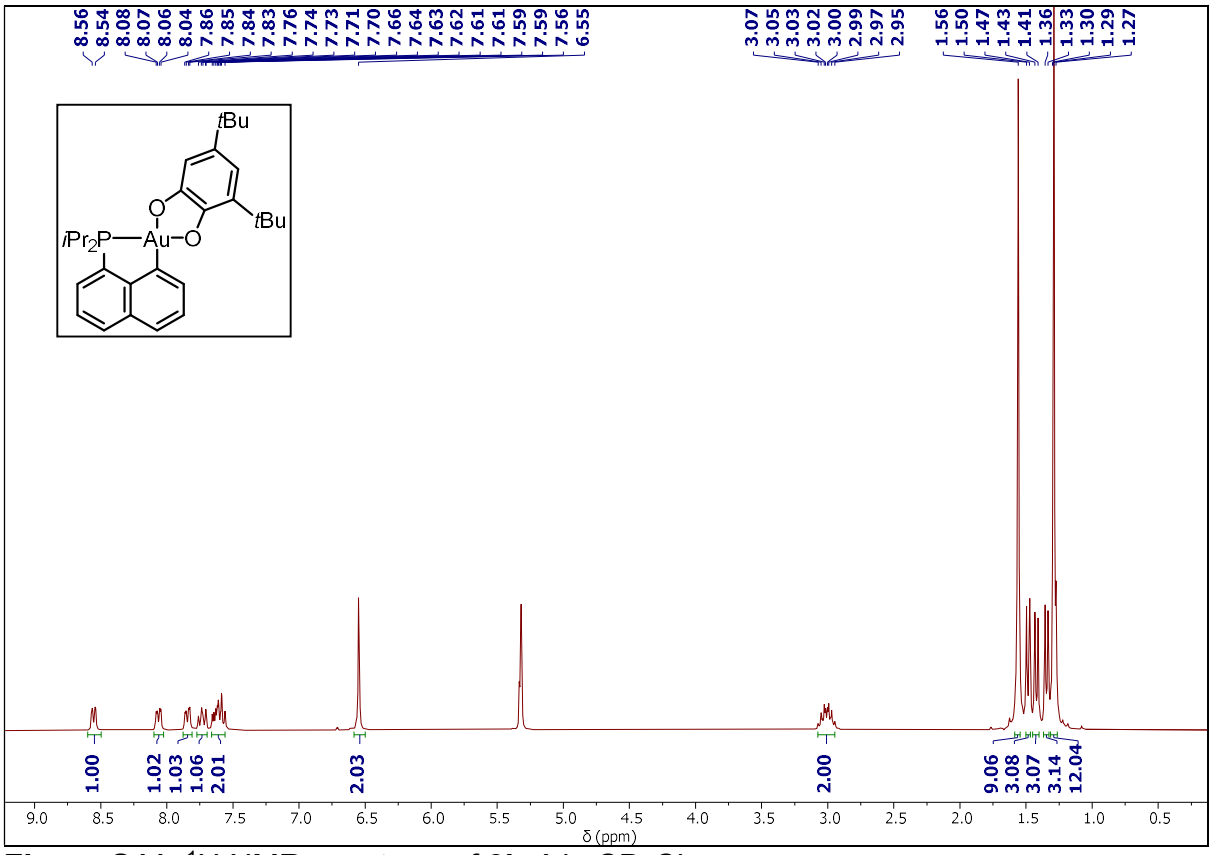


Figure S11. ^{1}H NMR spectrum of **3b-1** in CD_2Cl_2.

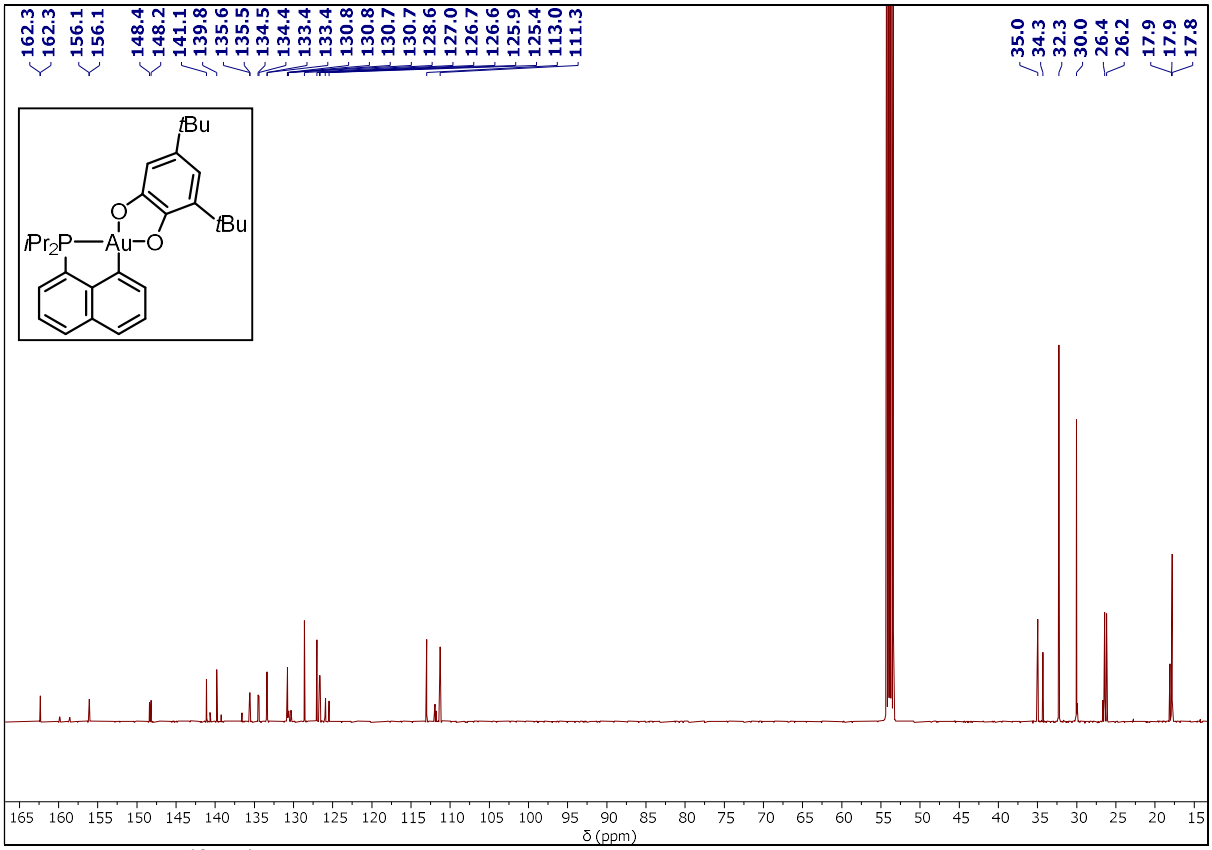


Figure S12. ^{13}C{^{1}H} NMR spectrum of **3b-1** in CD_2Cl_2.

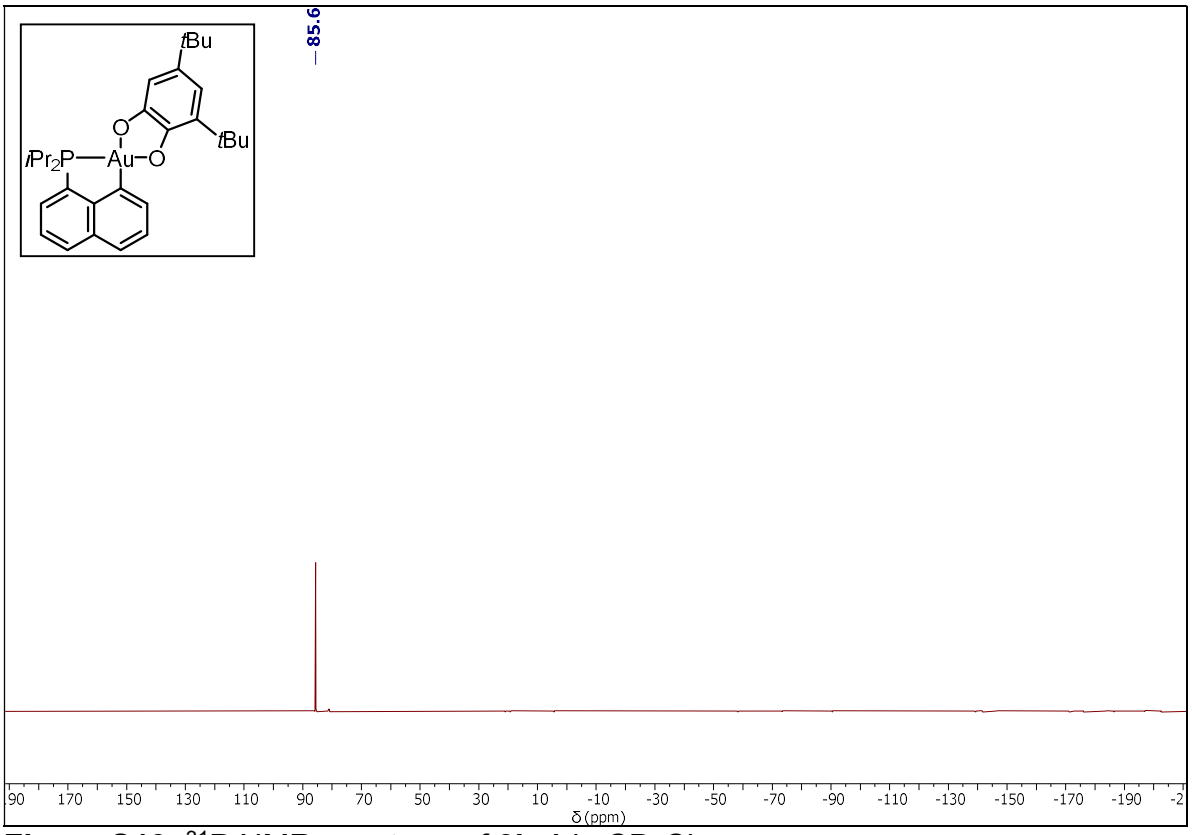


Figure S13. ^{31}P NMR spectrum of **3b-1** in CD_2Cl_2.

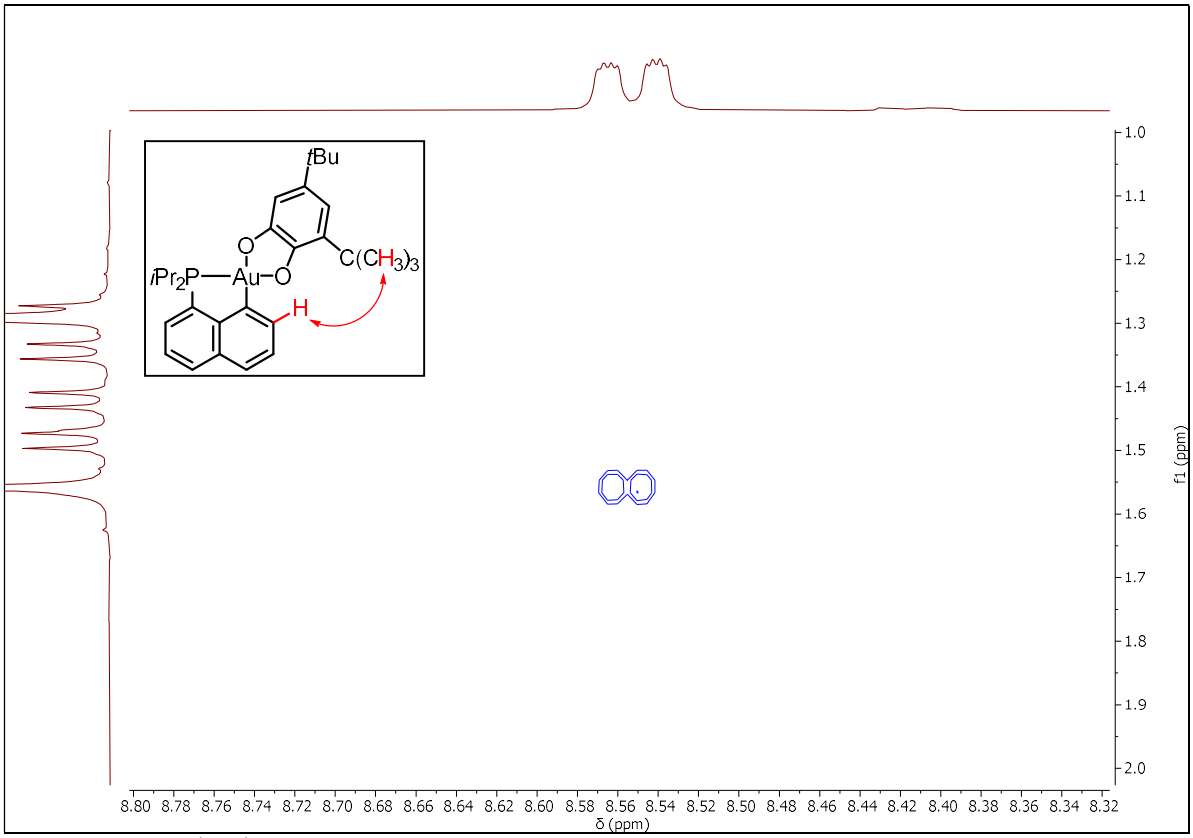


Figure S14. ^{1}H-^{1}H NOESY NMR of **3b-1** in CD_2Cl_2 highlighting the *o*-C*H*-*t*Bu NOE signal.

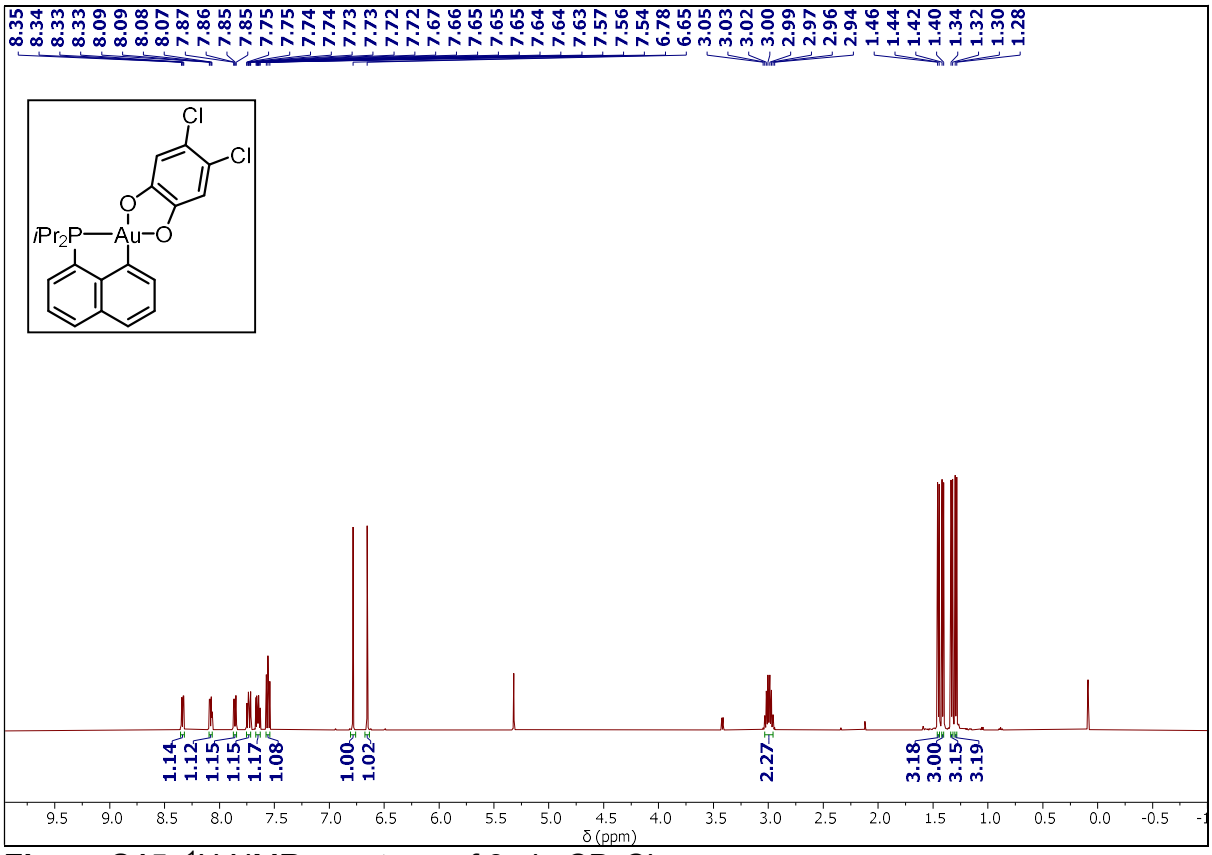


Figure S15. ^{1}H NMR spectrum of **3c** in CD_2Cl_2.

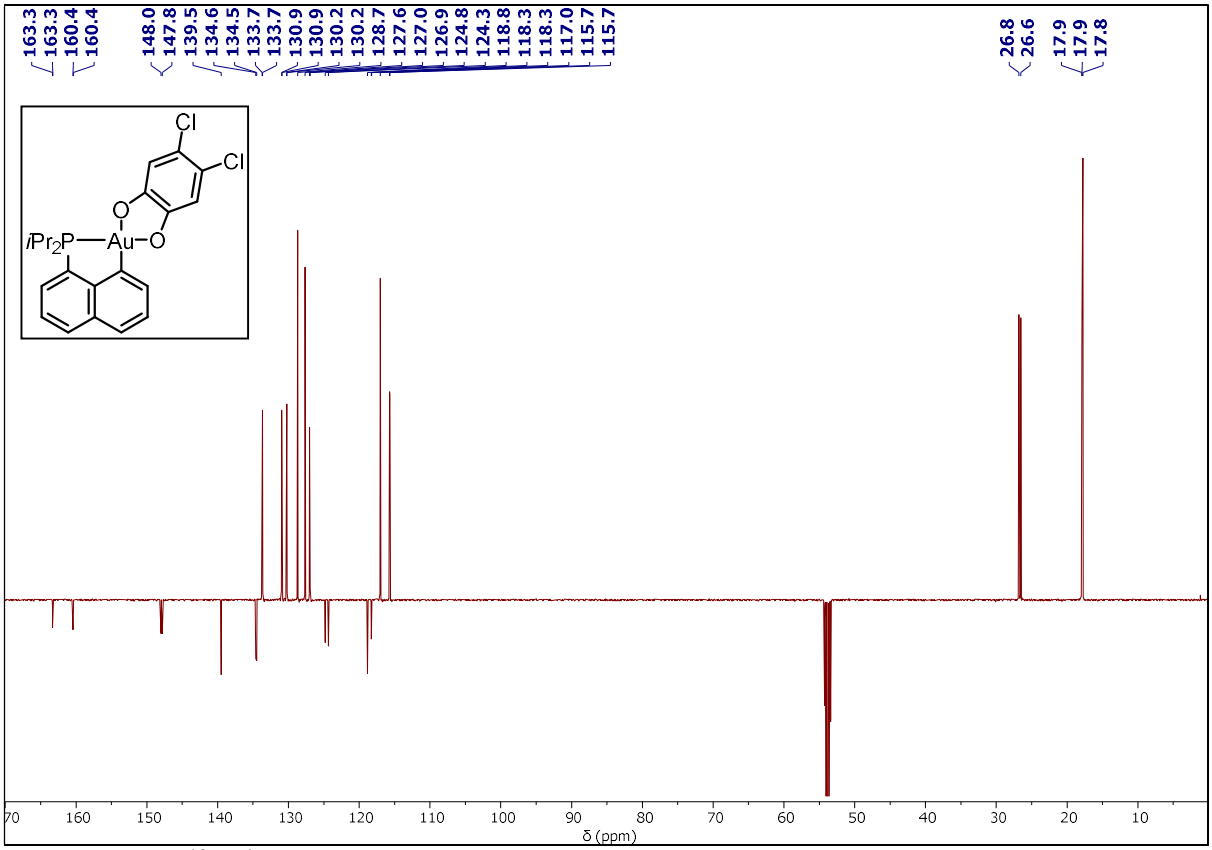


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of **3c** in CD_2Cl_2.

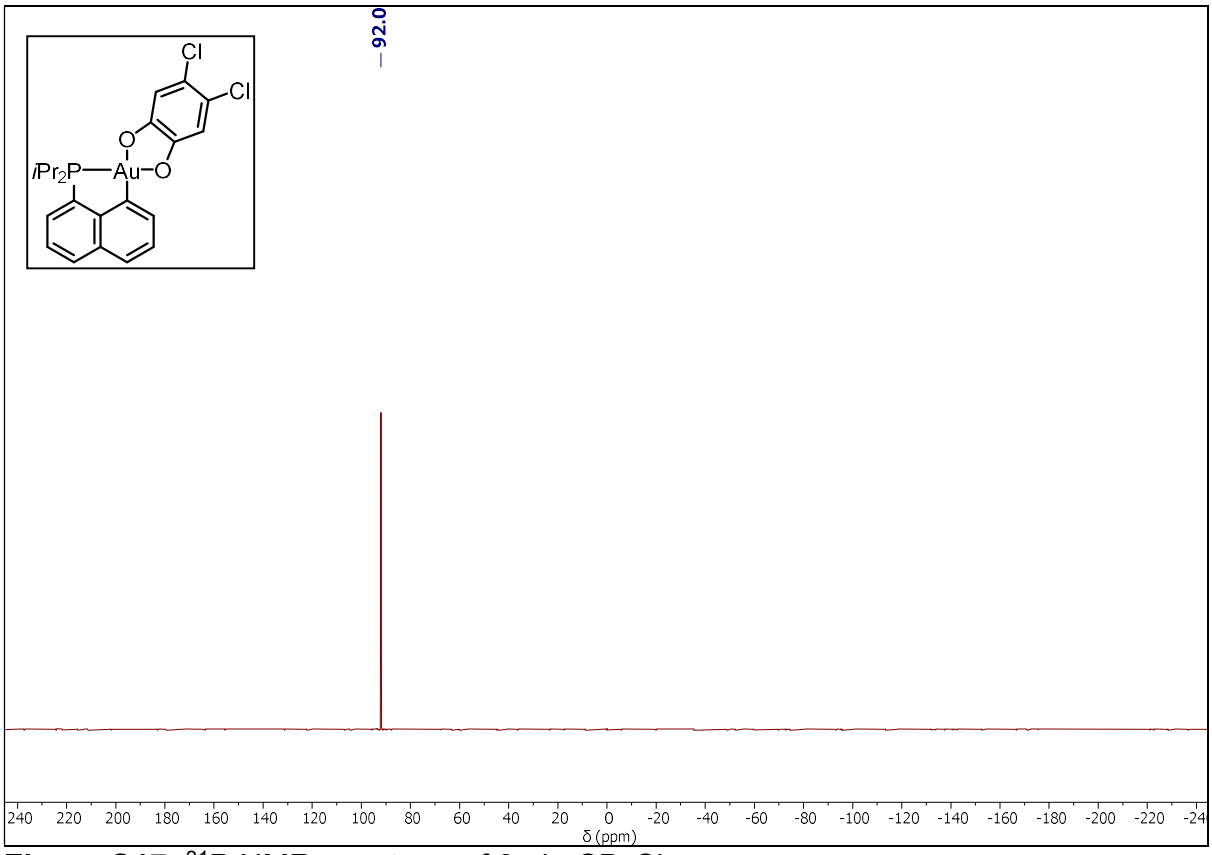


Figure S17. ^{31}P NMR spectrum of **3c** in CD_2Cl_2.

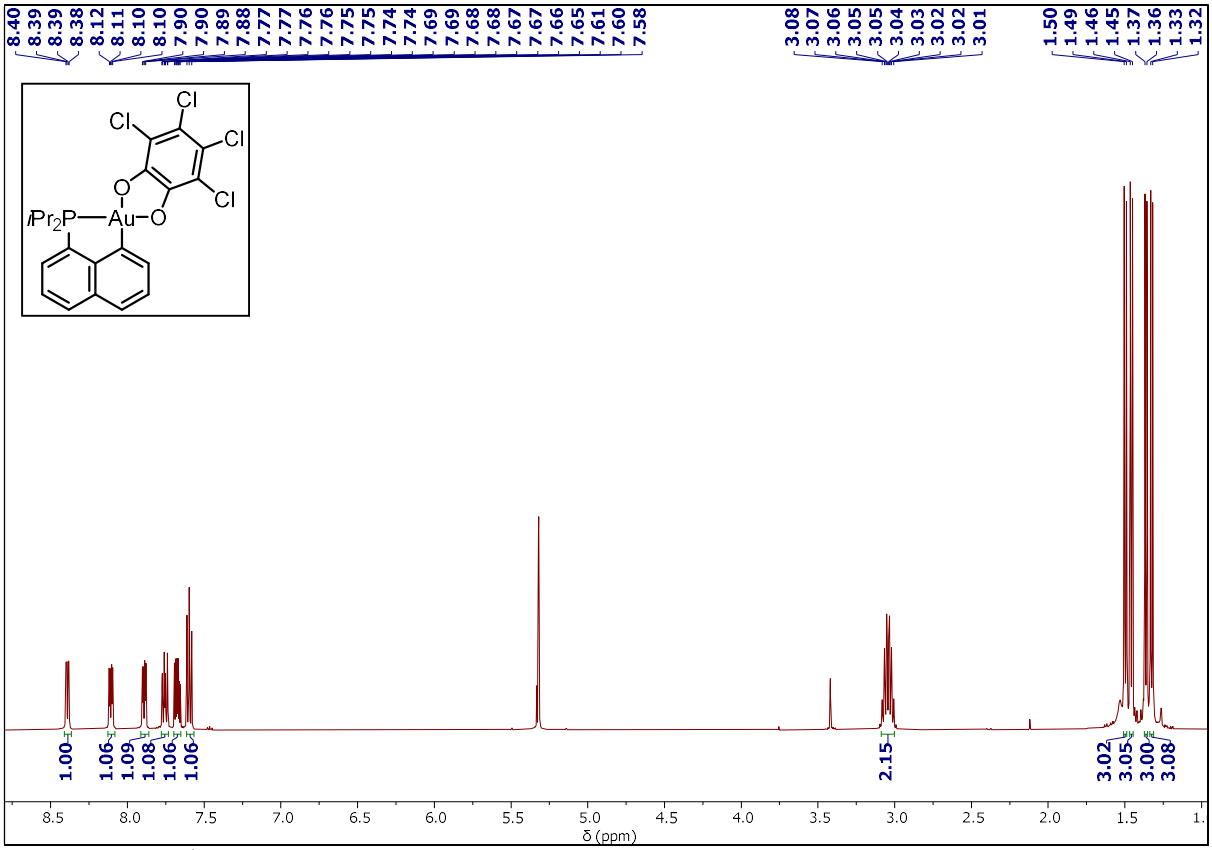


Figure S18. ^{1}H NMR spectrum of **3d** in CD_2Cl_2.

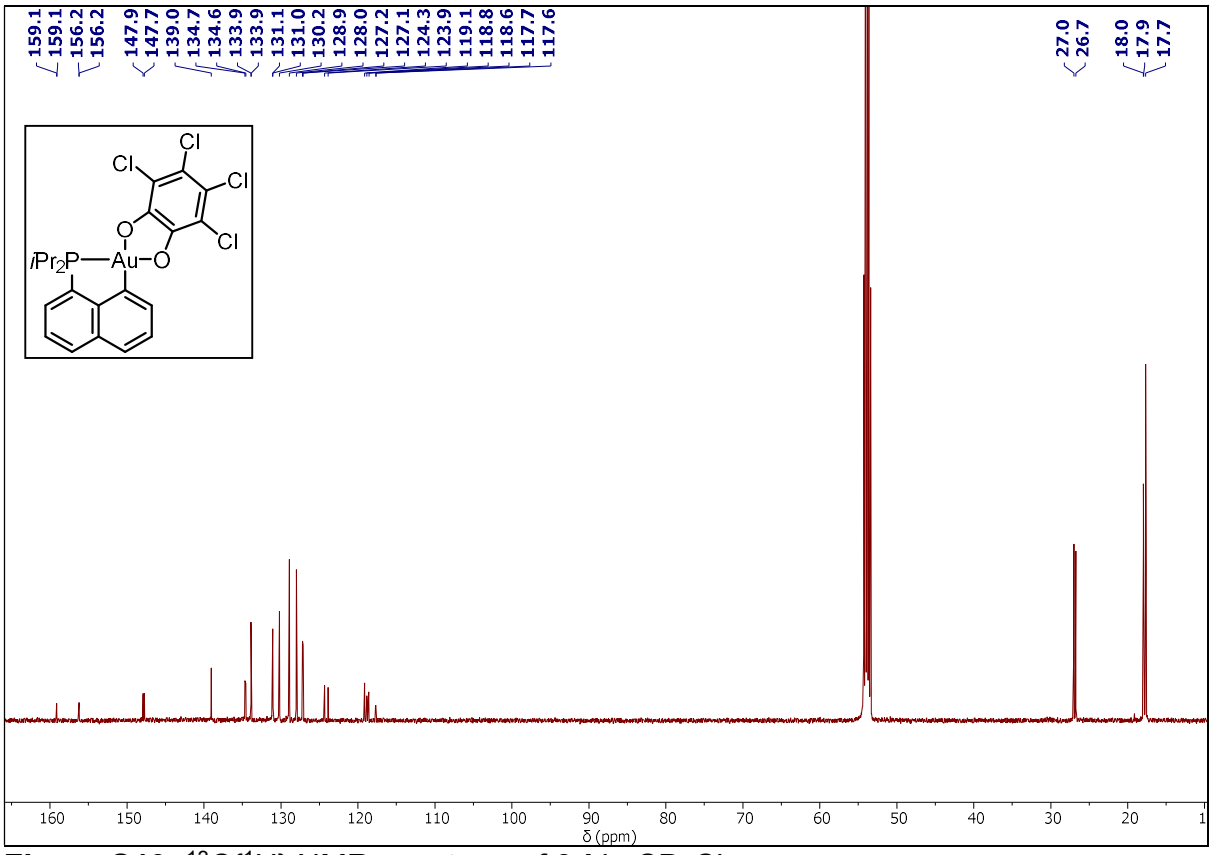


Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum of **3d** in CD_2Cl_2.

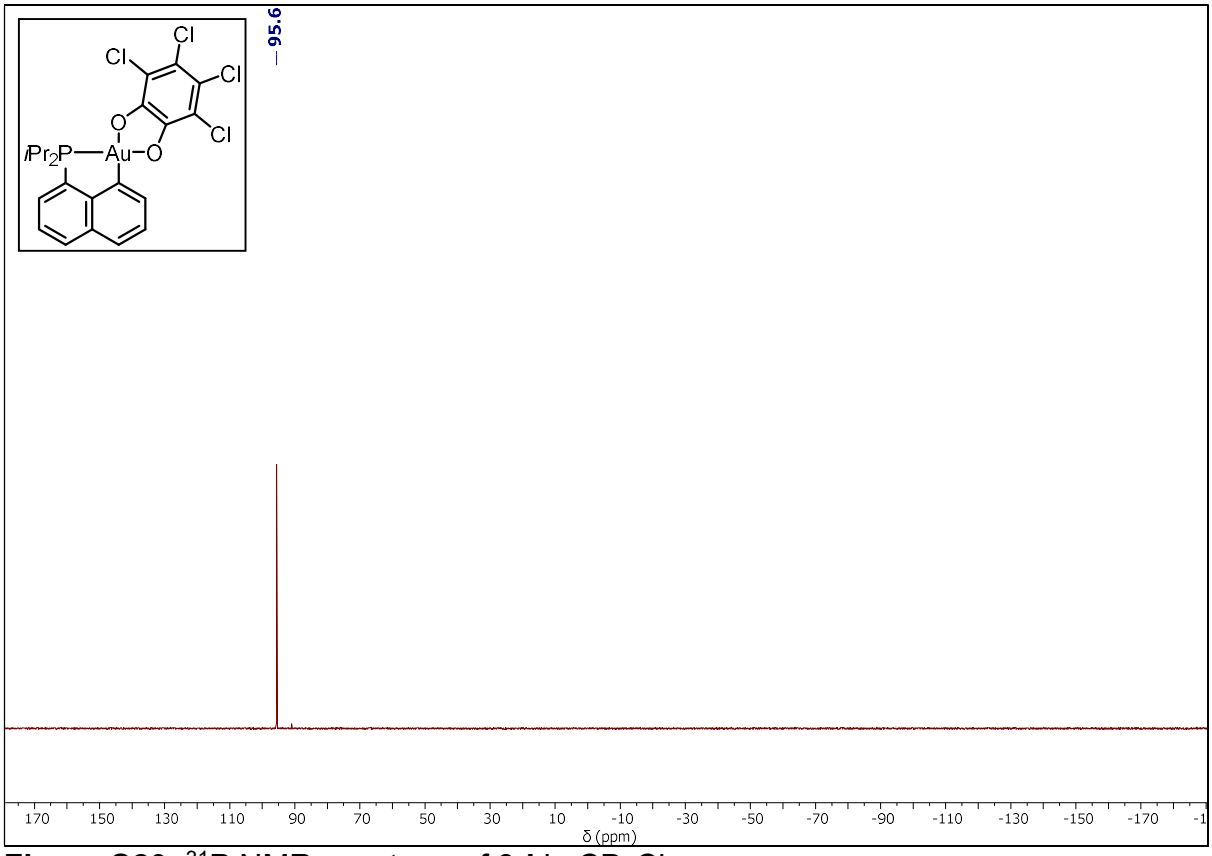


Figure S20. ^{31}P NMR spectrum of **3d** in CD_2Cl_2.

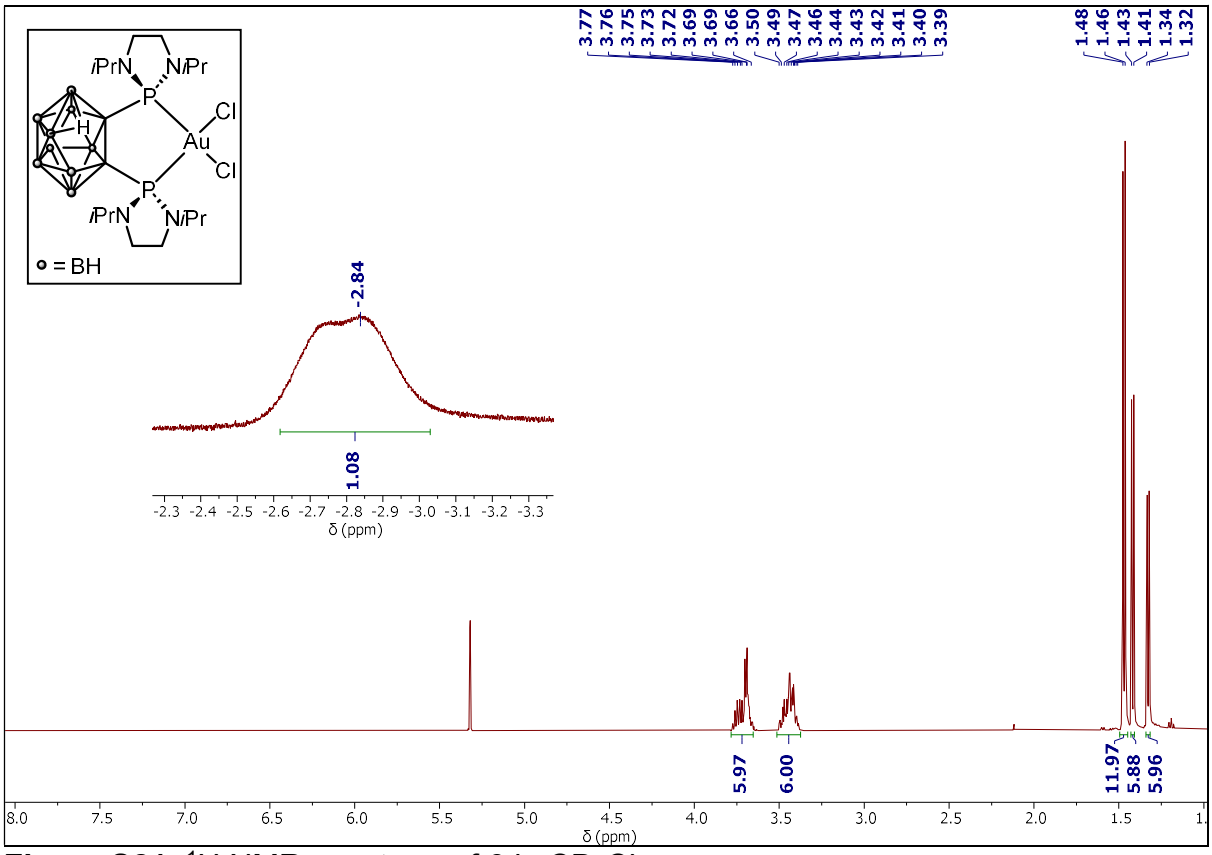


Figure S21. ^{1}H NMR spectrum of **6** in CD_2Cl_2.

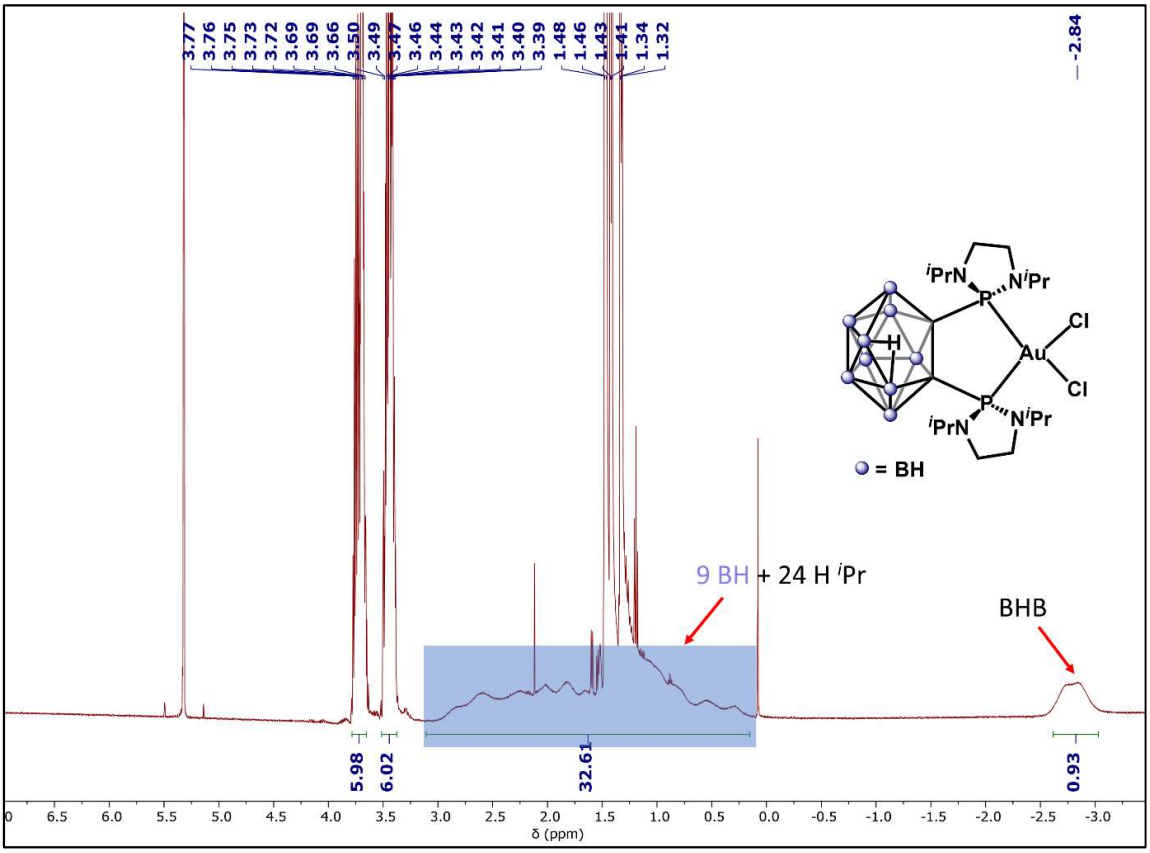


Figure S22. ^{1}H NMR spectrum of **6** in CD_2Cl_2 with zoom on the baseline depicting the BH and the BHB regions.

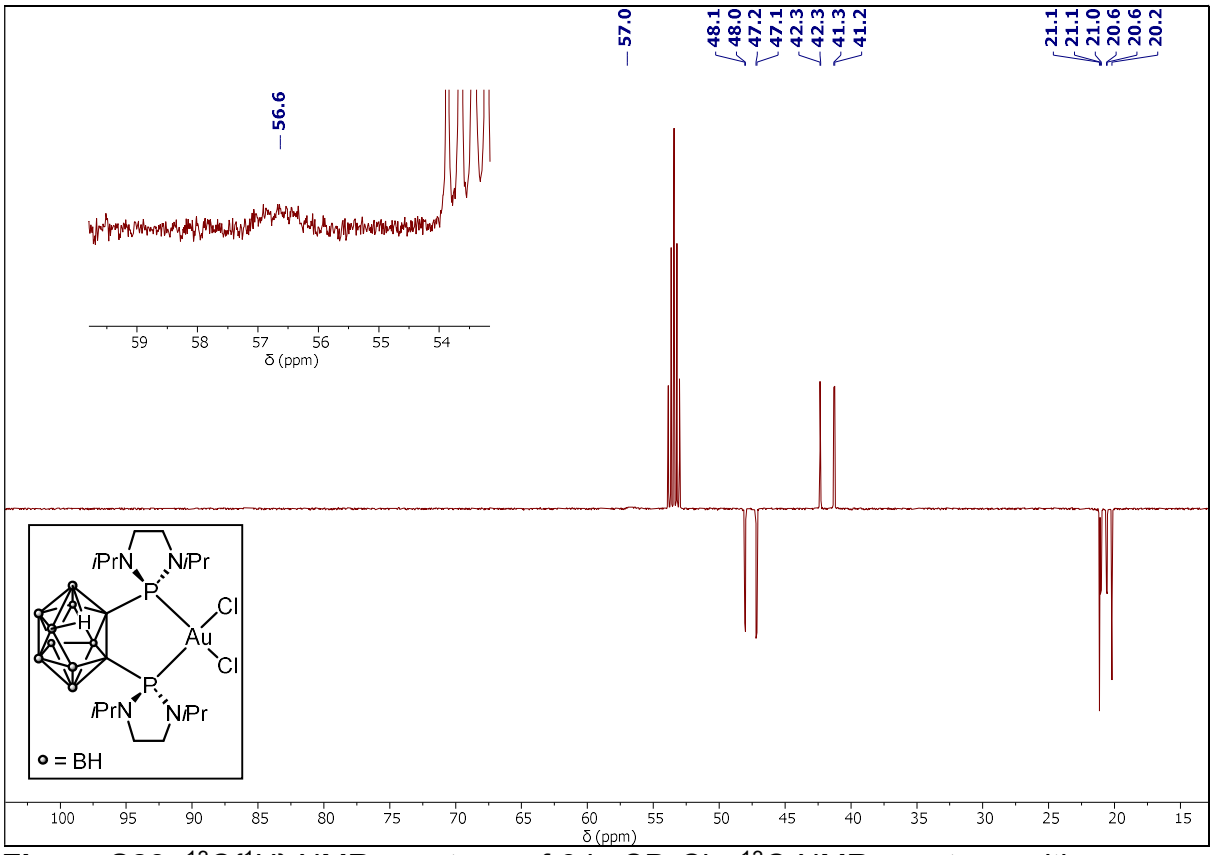


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of **6** in CD_2Cl_2. ^{13}C NMR spectrum with zoom on the baseline depicting the $C_{carborane}$ signals.

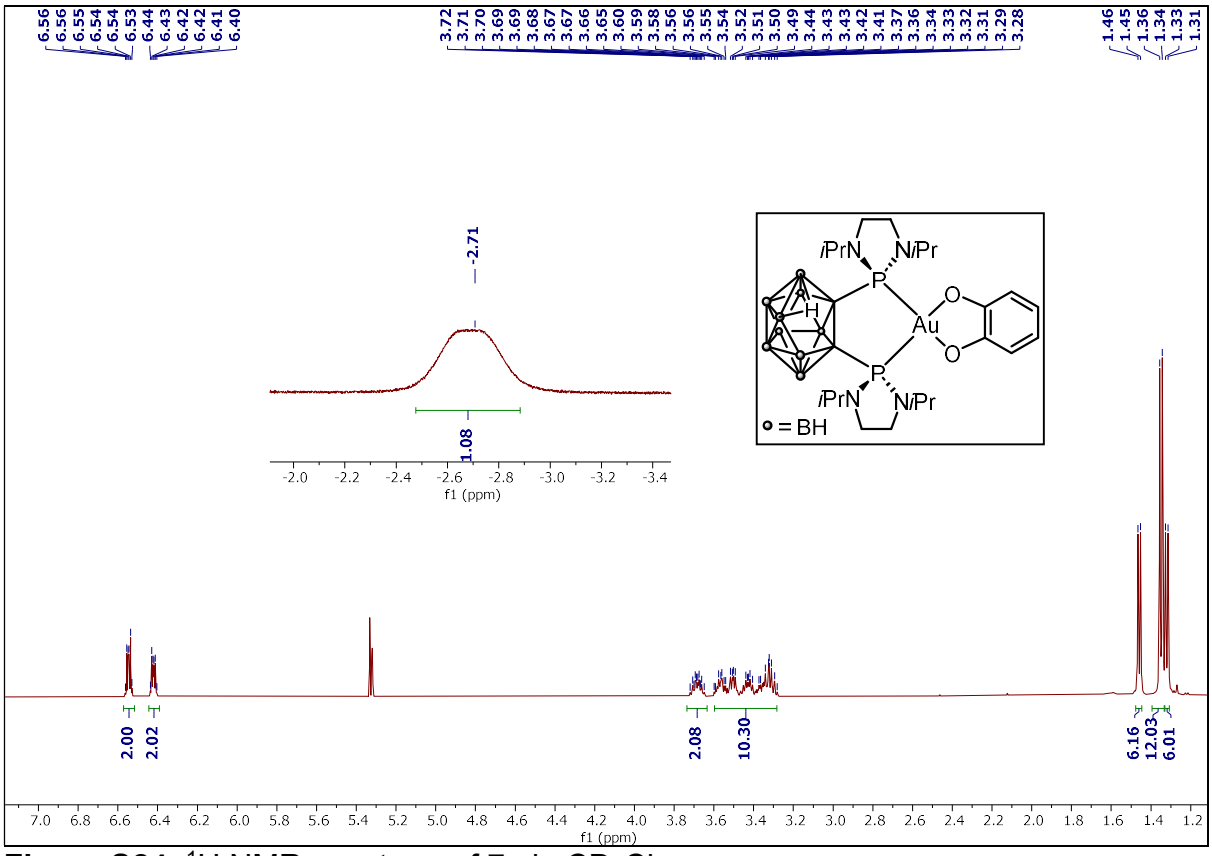


Figure S24. ^{1}H NMR spectrum of **7a** in CD_2Cl_2.

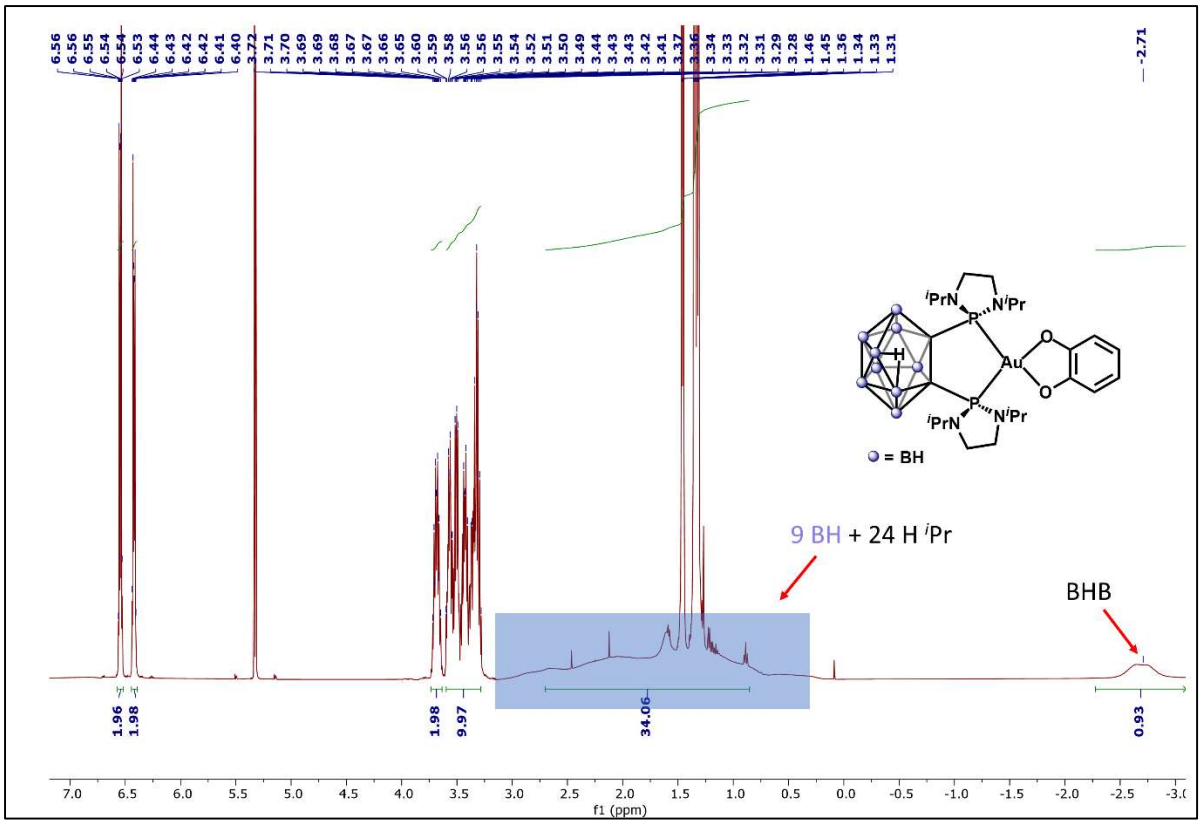


Figure S25. ^{1}H NMR spectrum of **7a** in CD_2Cl_2 with zoom on the baseline depicting the BH and the BHB regions.

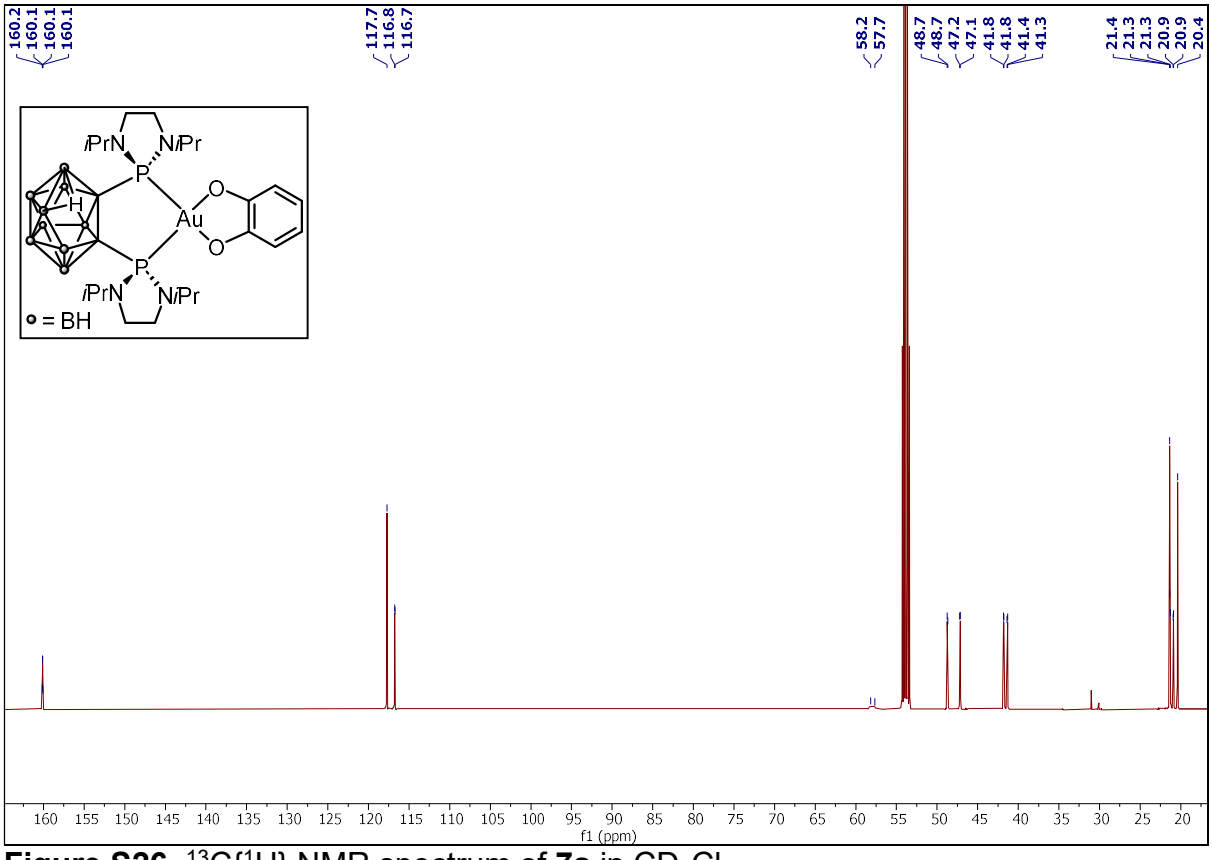


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of **7a** in CD_2Cl_2.

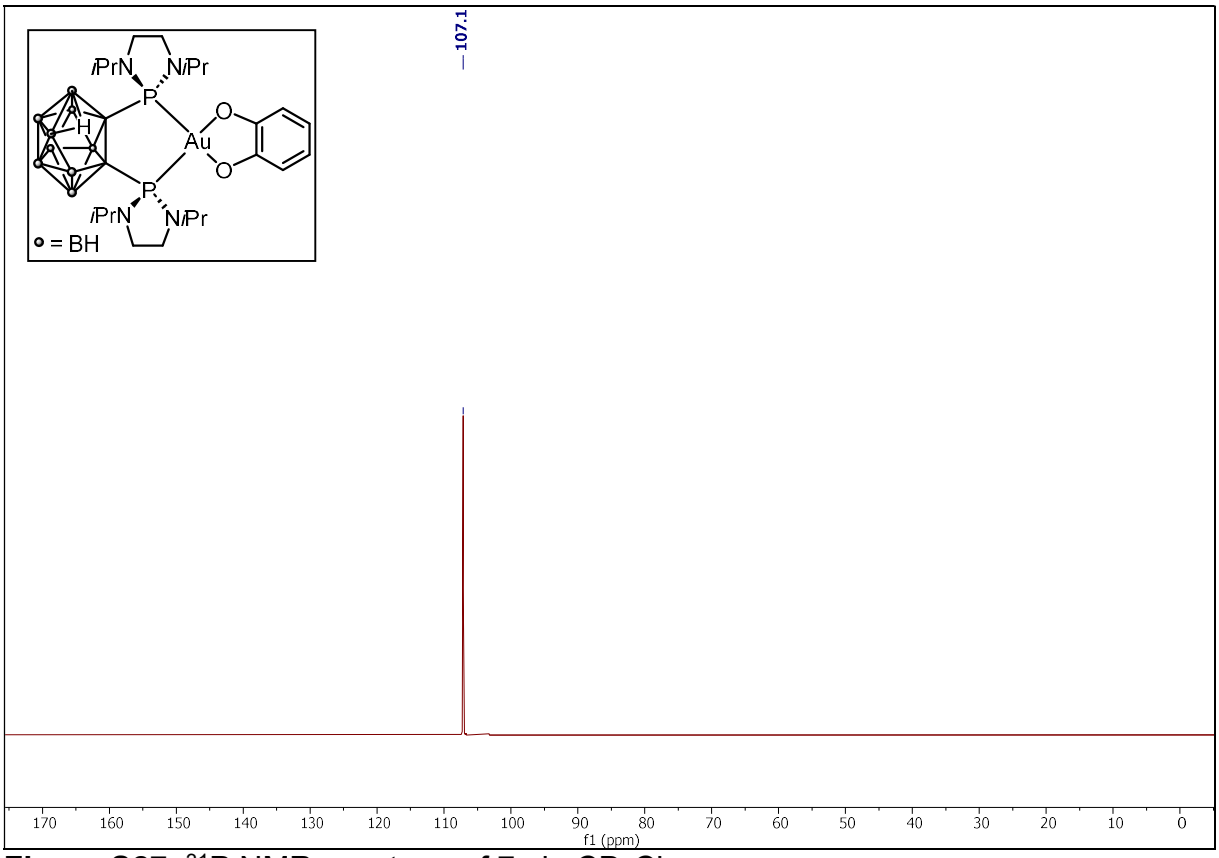


Figure S27. ^{31}P NMR spectrum of **7a** in CD_2Cl_2.

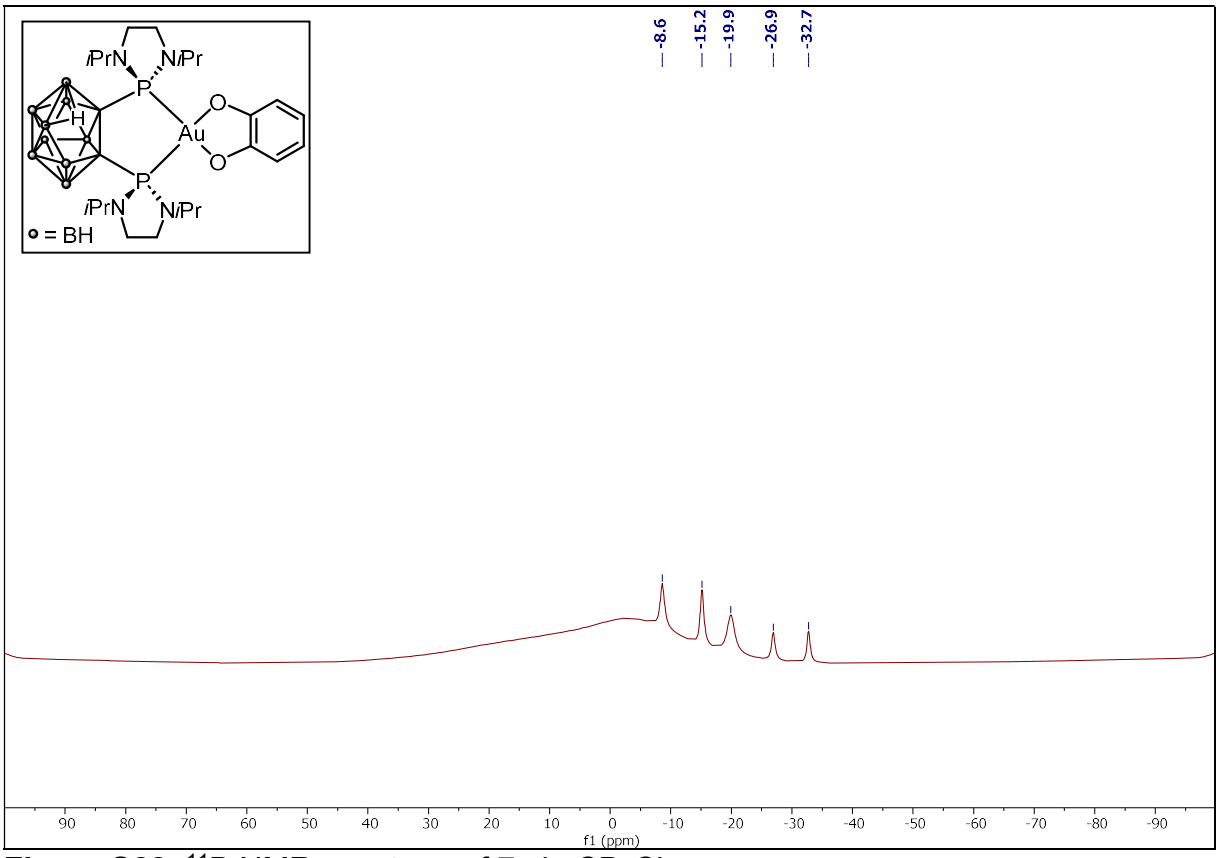


Figure S28. ^{11}B NMR spectrum of **7a** in CD_2Cl_2.

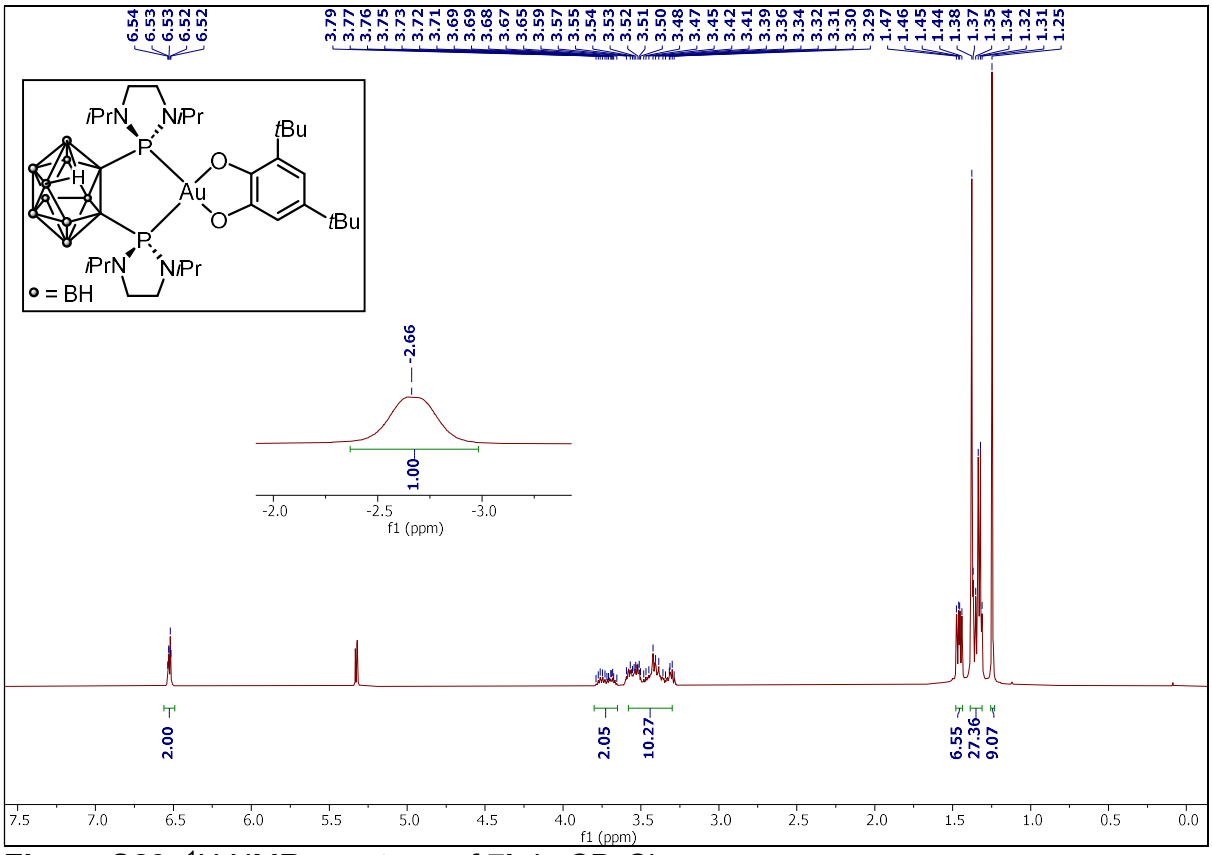


Figure S29. ^{1}H NMR spectrum of **7b** in CD_2Cl_2.

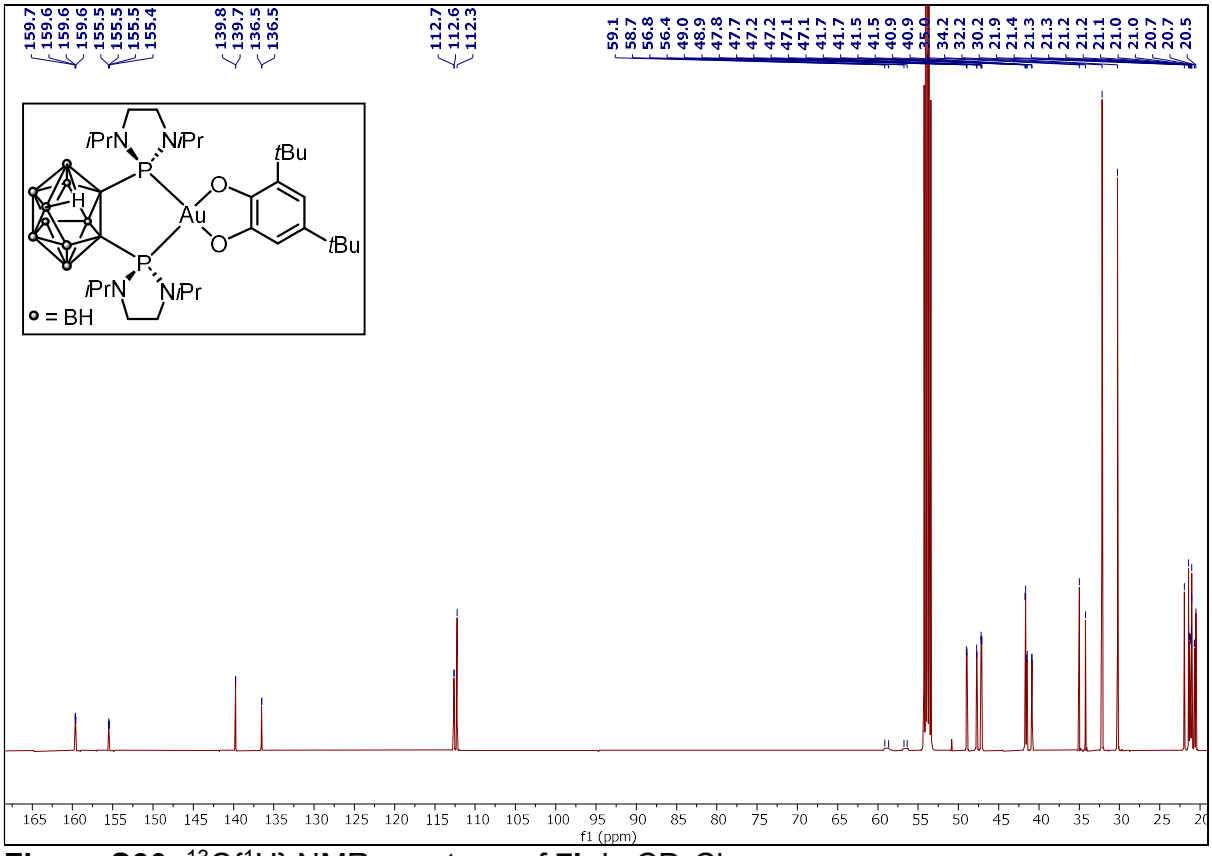


Figure S30. $^{13}C\{^{1}H\}$ NMR spectrum of **7b** in CD_2Cl_2.

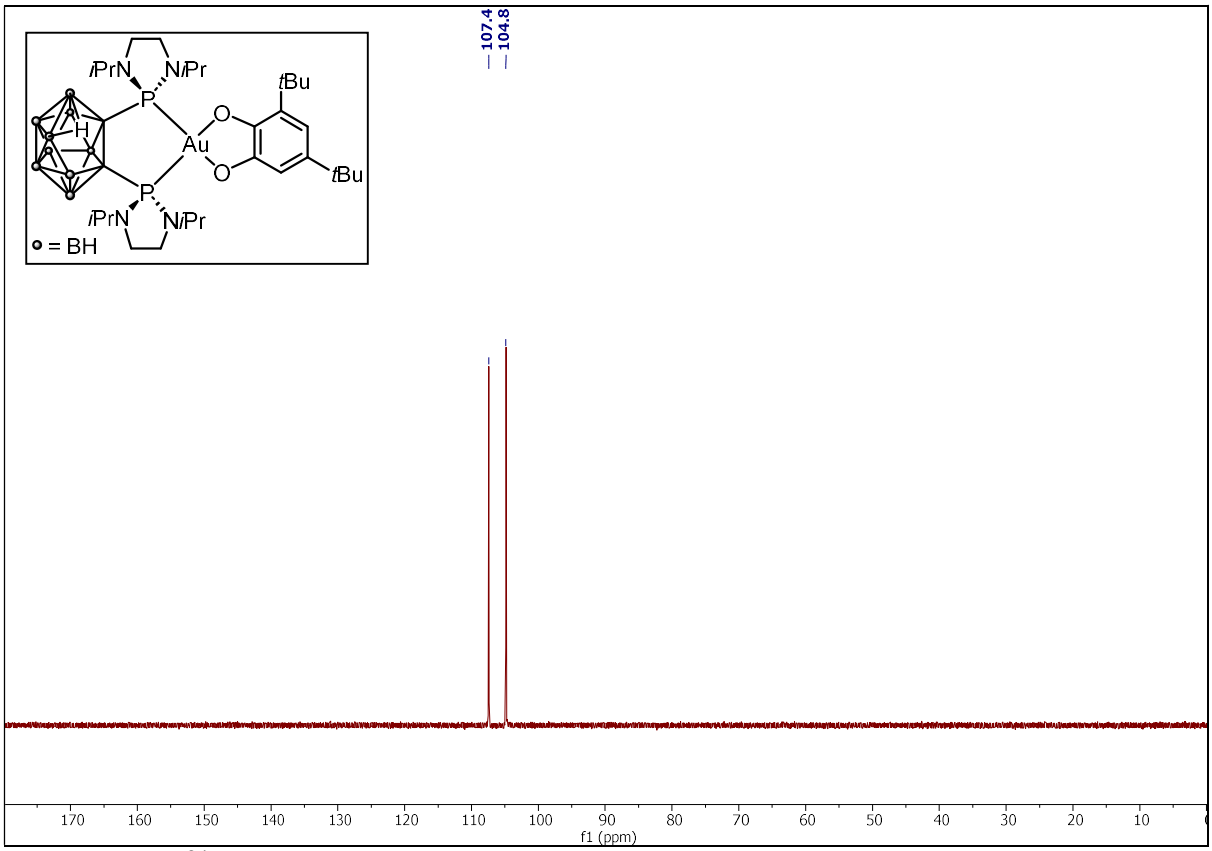


Figure S31. ^{31}P NMR spectrum of **7b** in CD_2Cl_2.

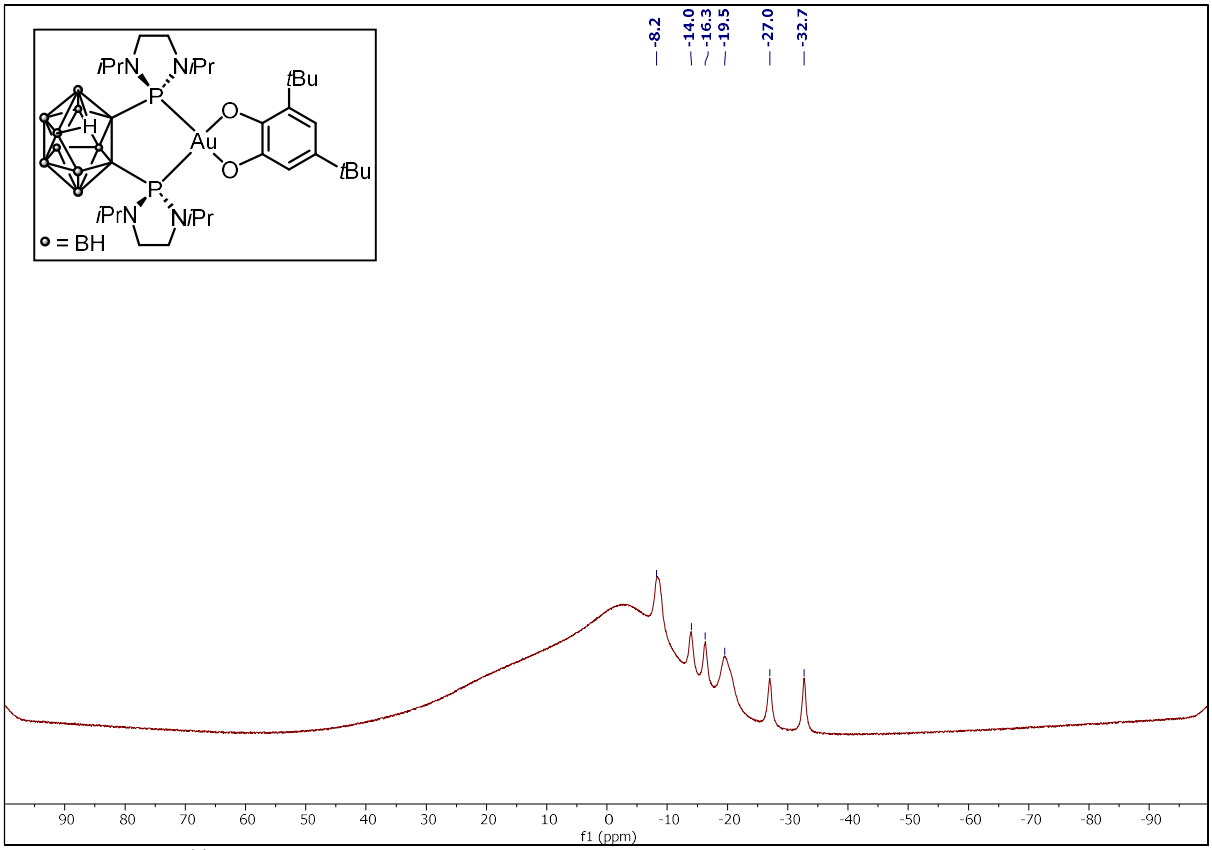


Figure S32. ^{11}B NMR spectrum of **7b** in CD_2Cl_2.

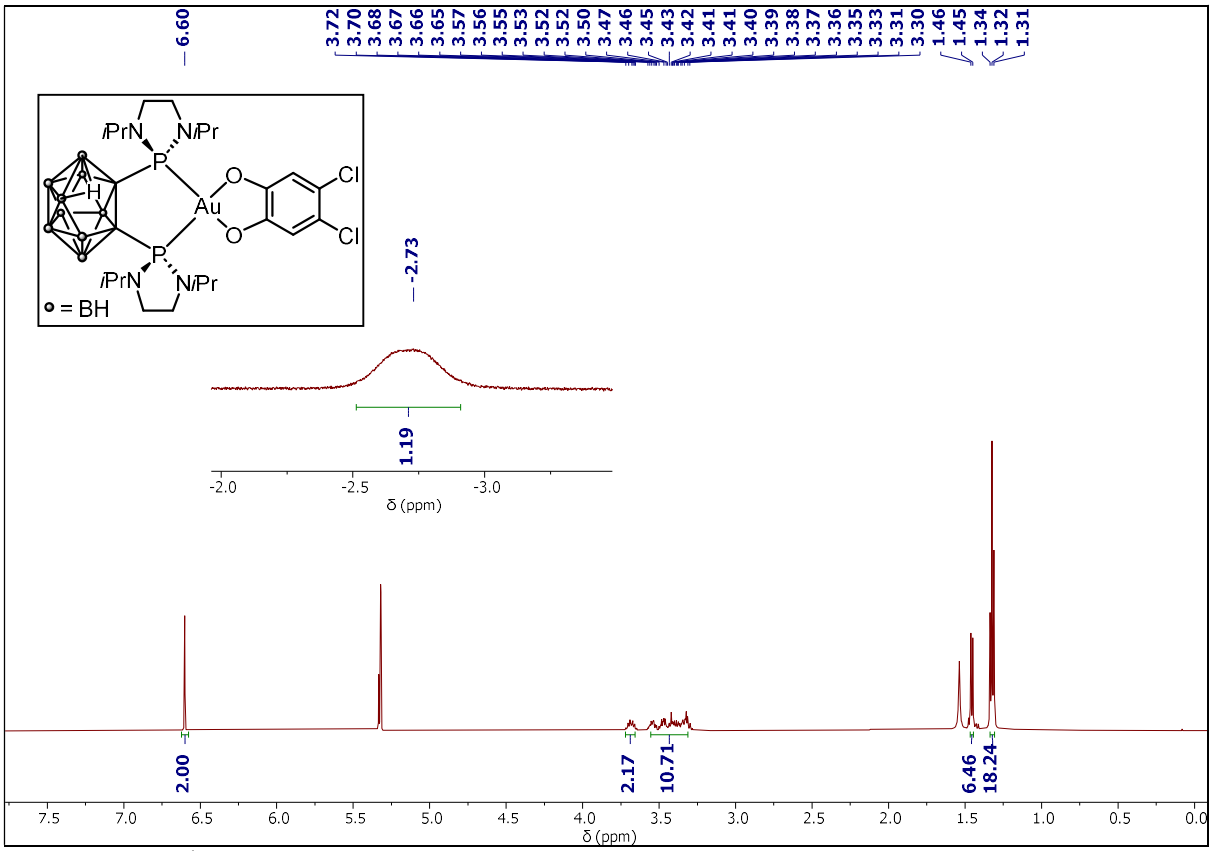


Figure S33. ^{1}H NMR spectrum of **7c** in CD_2Cl_2.

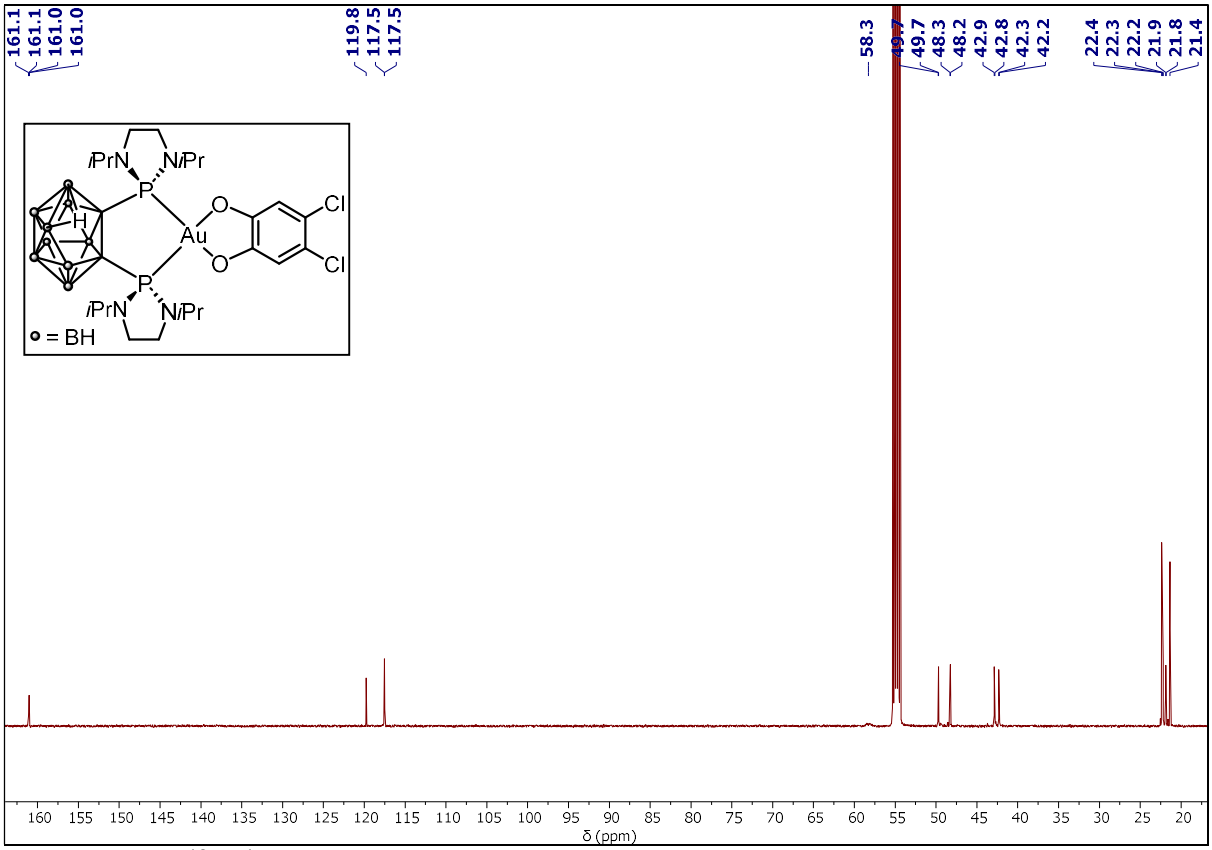


Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum of **7c** in CD_2Cl_2.

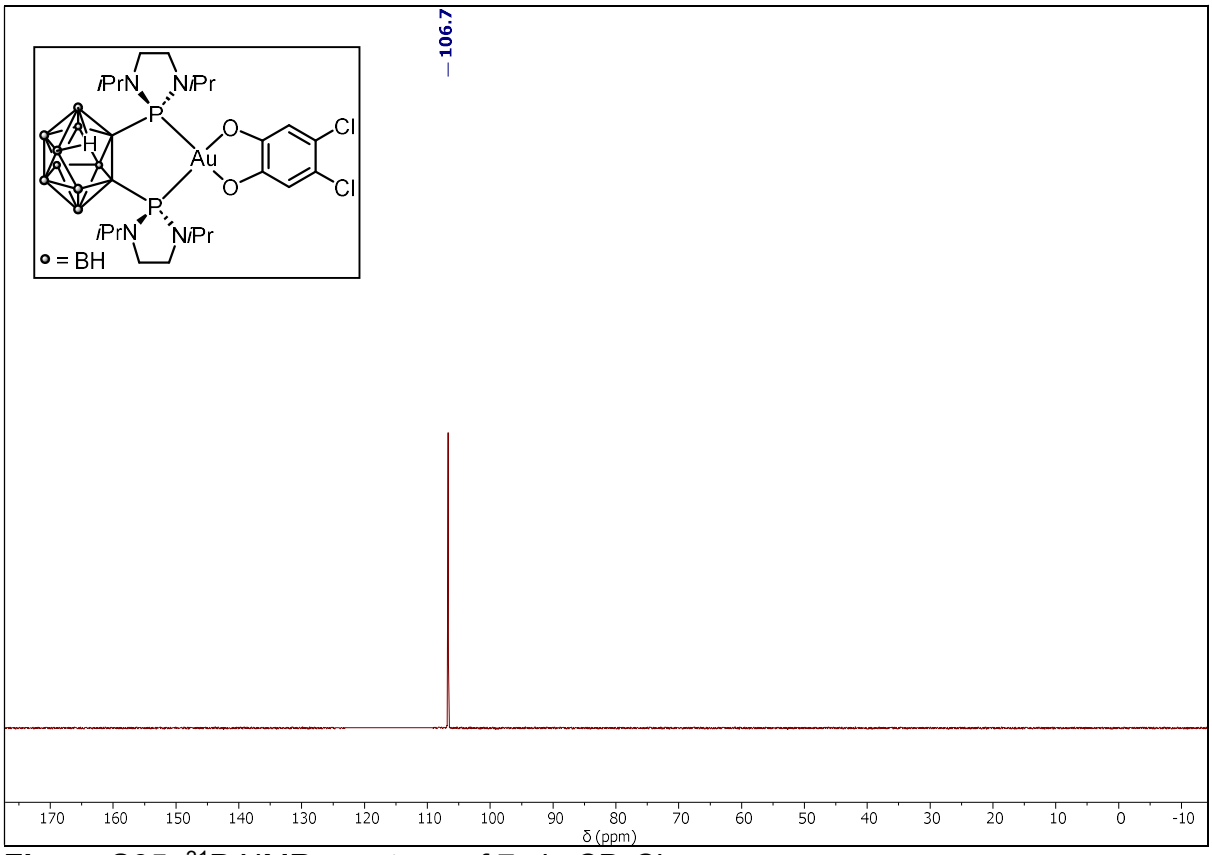


Figure S35. ^{31}P NMR spectrum of **7c** in CD_2Cl_2.

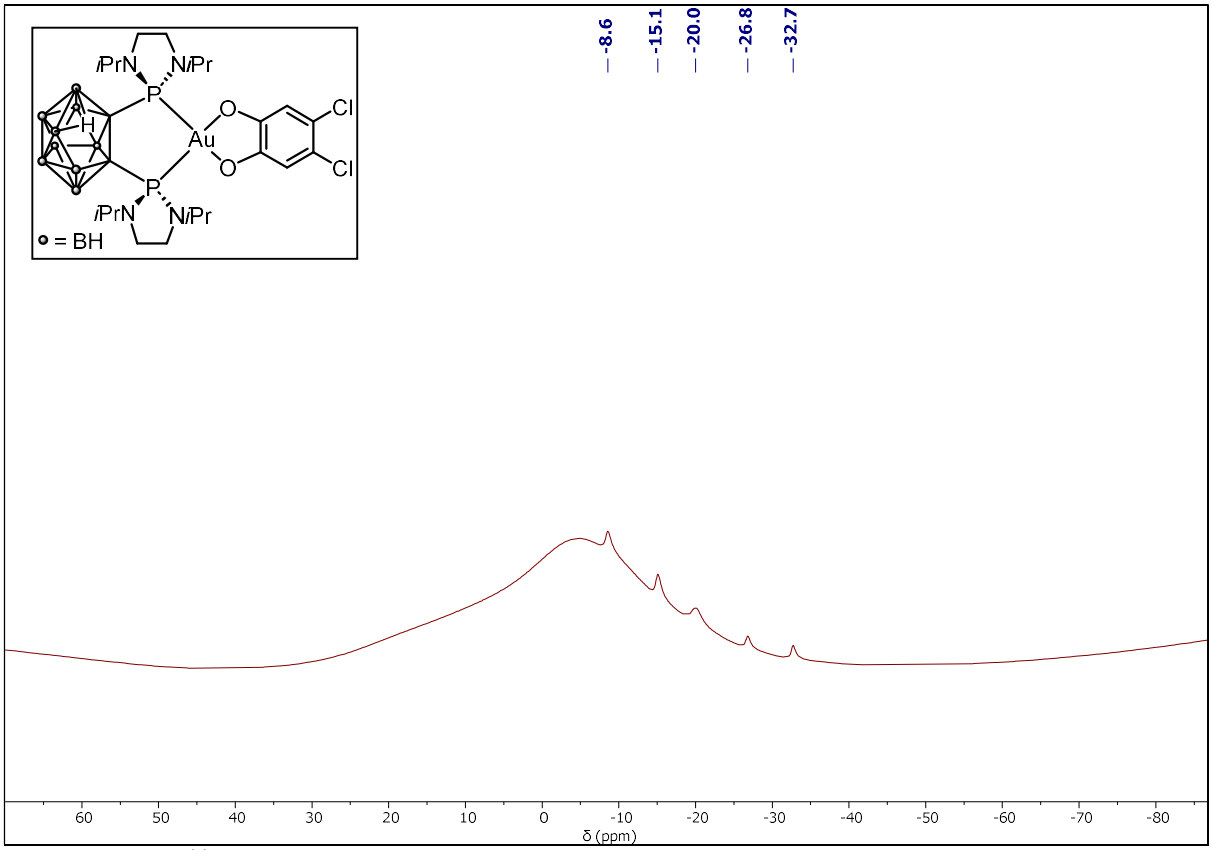


Figure S36. ^{11}B NMR spectrum of **7c** in CD_2Cl_2.

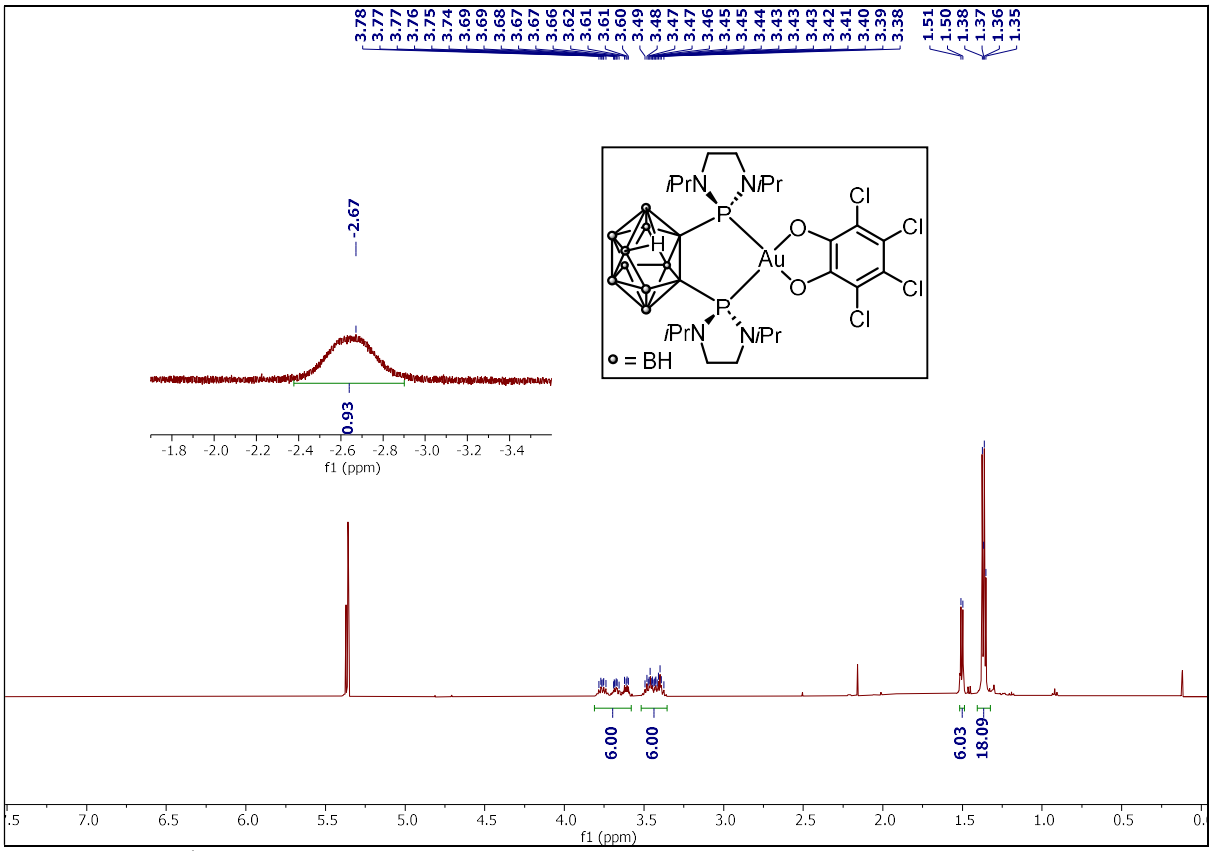


Figure S37. ^{1}H NMR spectrum of **7d** in CD_2Cl_2.

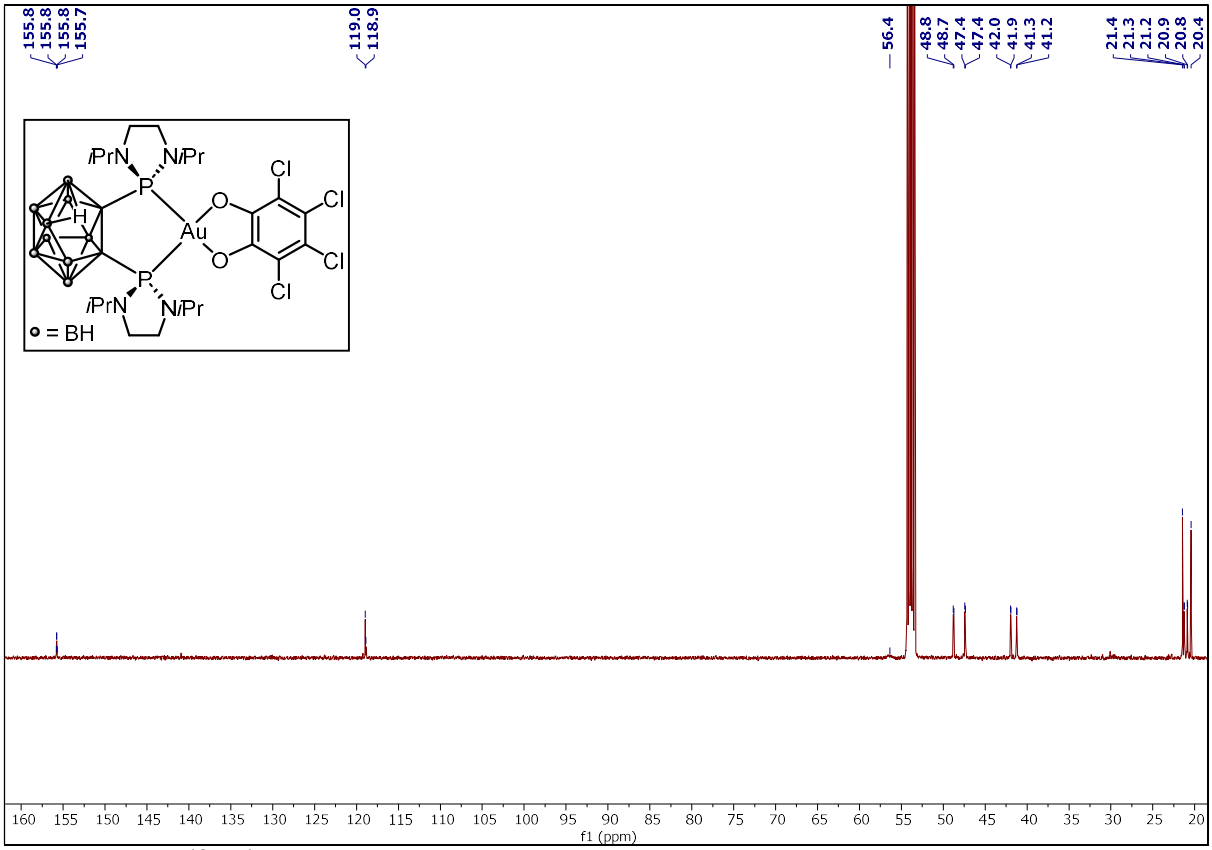


Figure S38. $^{13}C\{^{1}H\}$ NMR spectrum of **7d** in CD_2Cl_2.

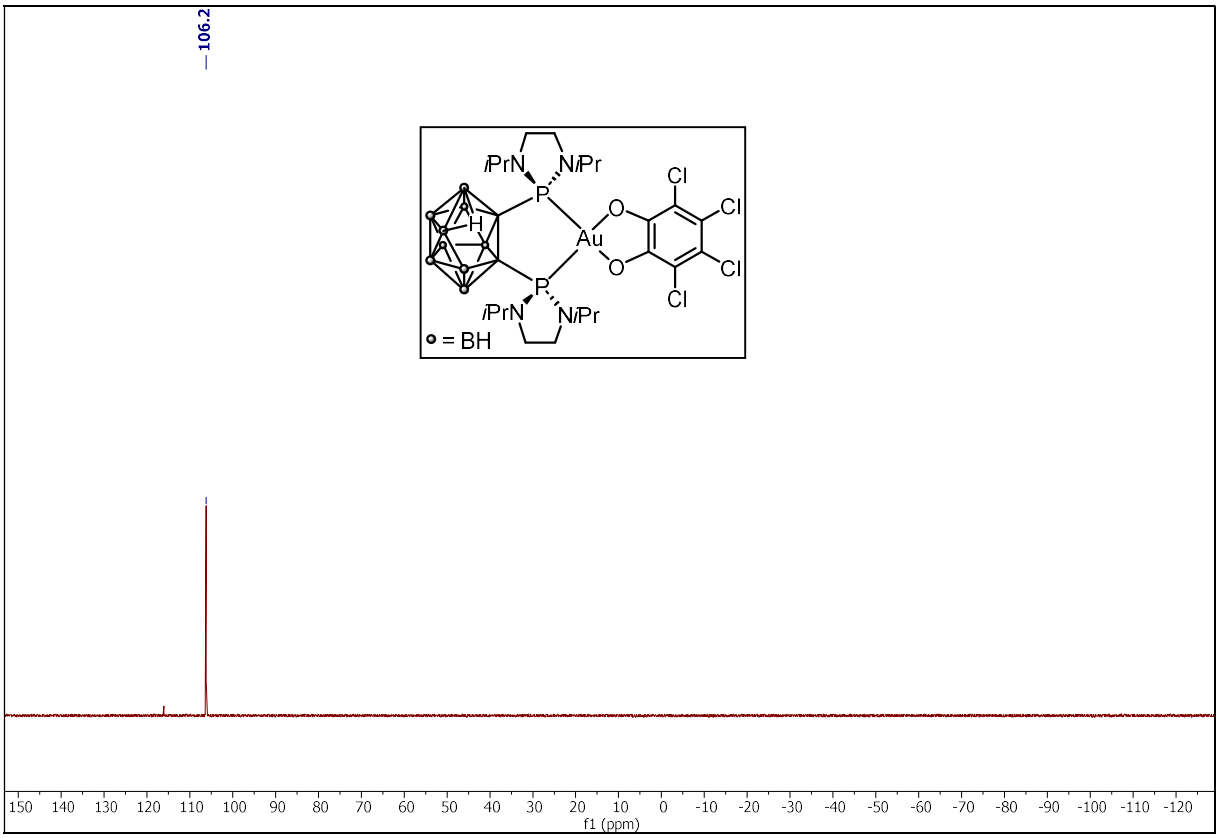


Figure S39. ^{31}P NMR spectrum of **7d** in CD_2Cl_2.

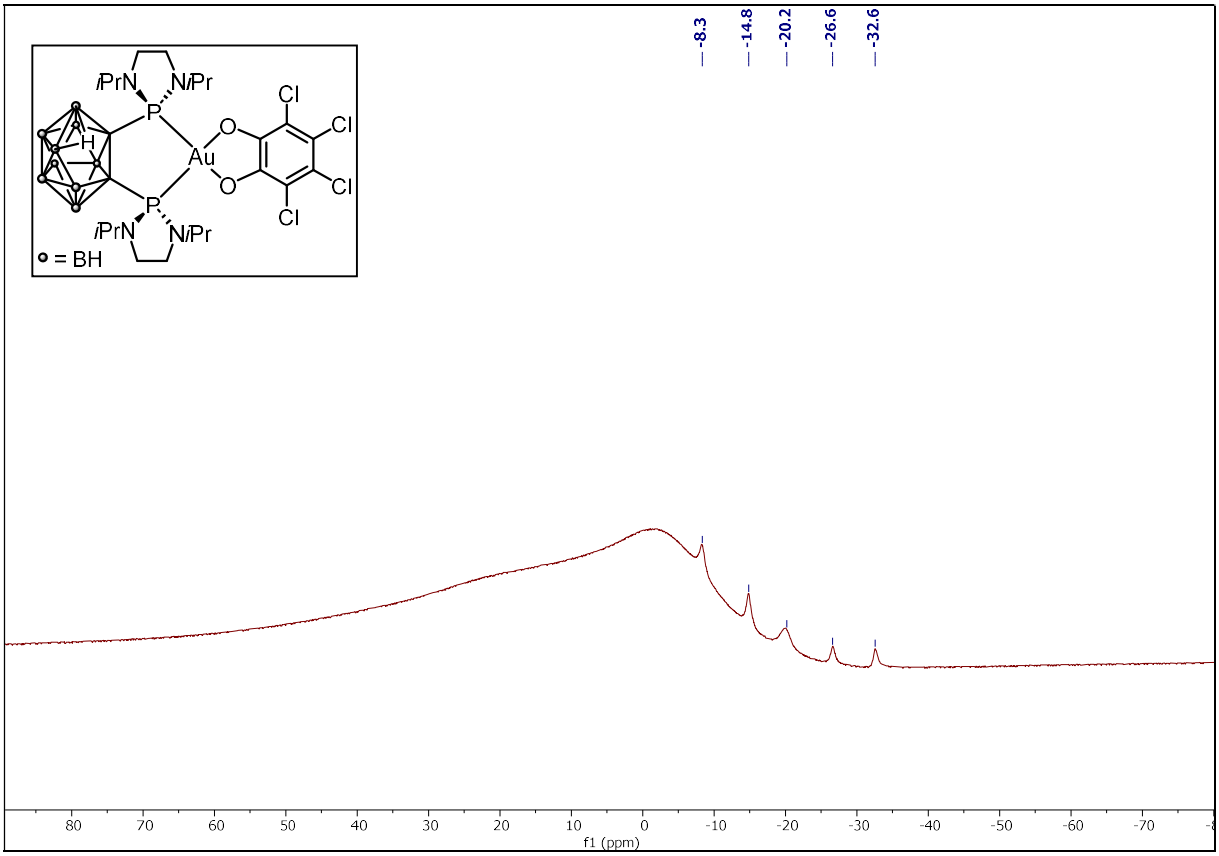
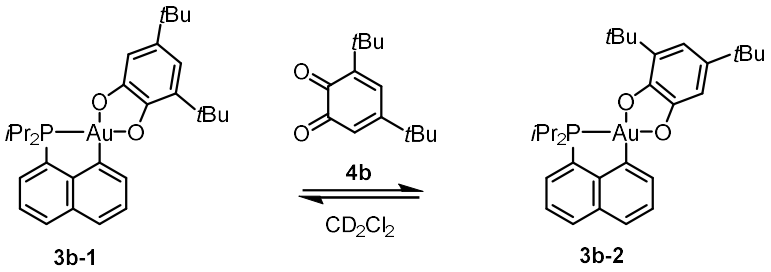


Figure S40. ^{11}B NMR spectrum of **7d** in CD_2Cl_2.

8. Isomerization experiment

To a solution of **3b-1** (0.01 mmol) in CD_2Cl_2 (0.3 ml) were added different amounts of **4b** (0, 0.5 and 1 equiv.) in CD_2Cl_2 (0.2 ml) and ^1H NMR of the mixtures were recorded immediately upon mixture and after 60 and 120 min.



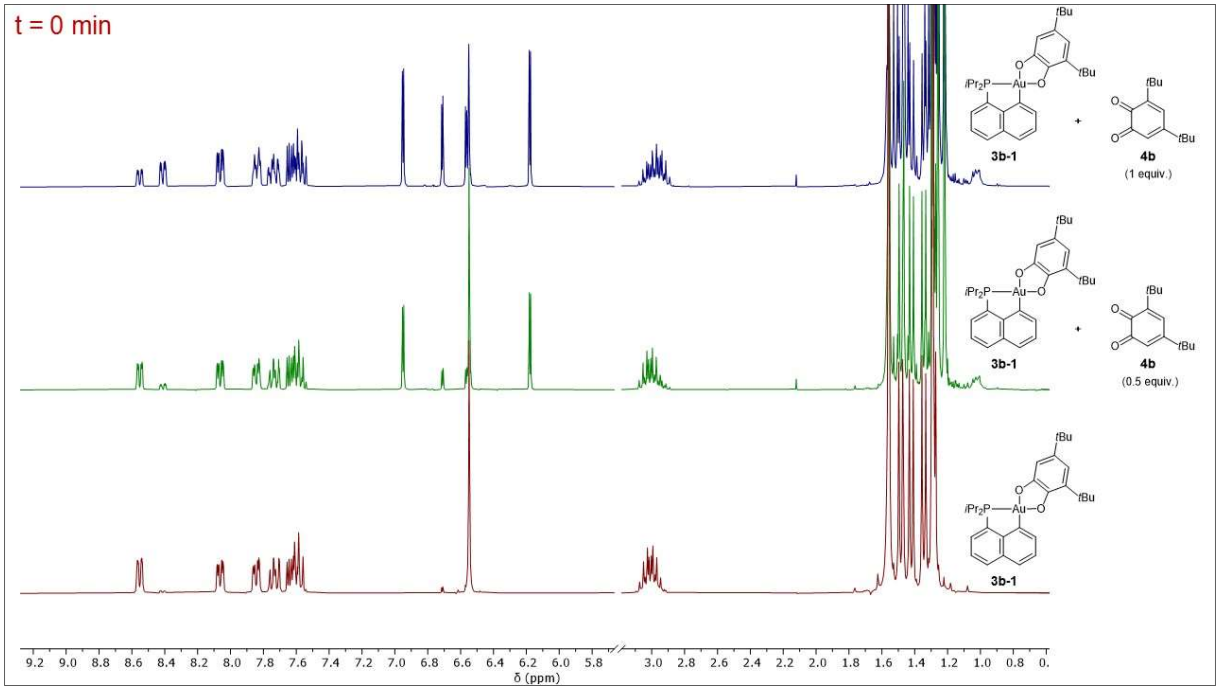


Figure S41. ^1H NMR spectra for the isomerization experiment in CD_2Cl_2 at **t = 0 min**.

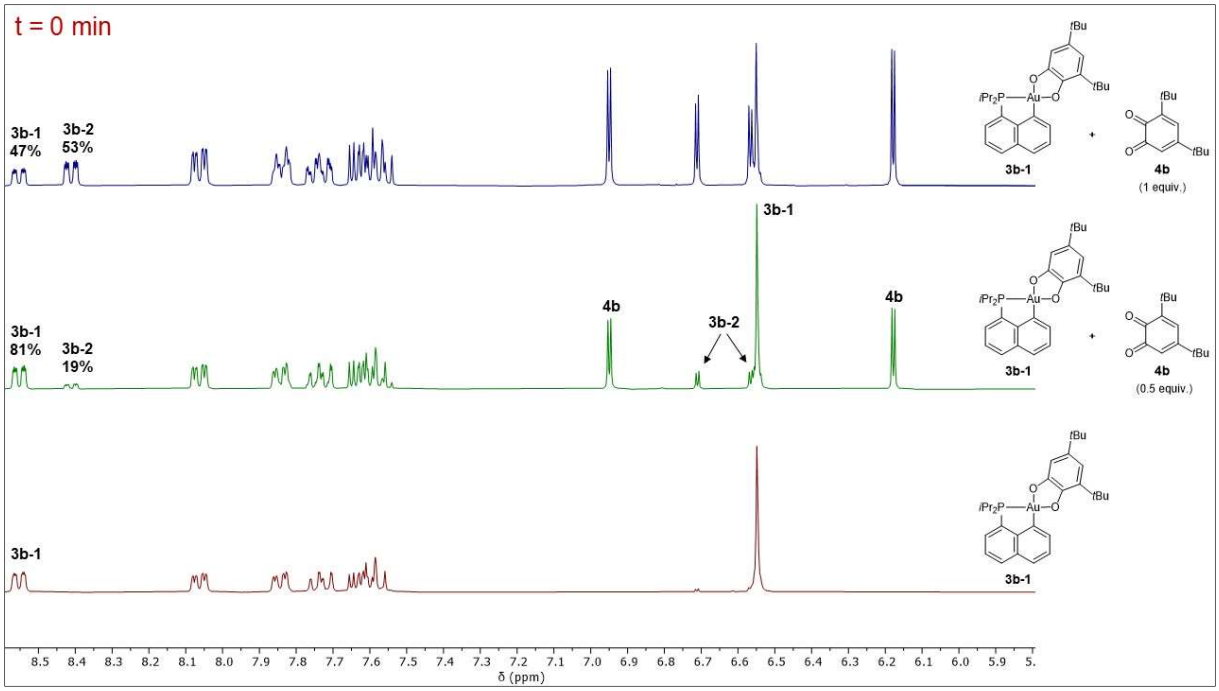


Figure S42. ^{1}H NMR spectra for the isomerization experiment in CD_2Cl_2 at **t = 0 min**. (5.8-8.6 ppm zone)

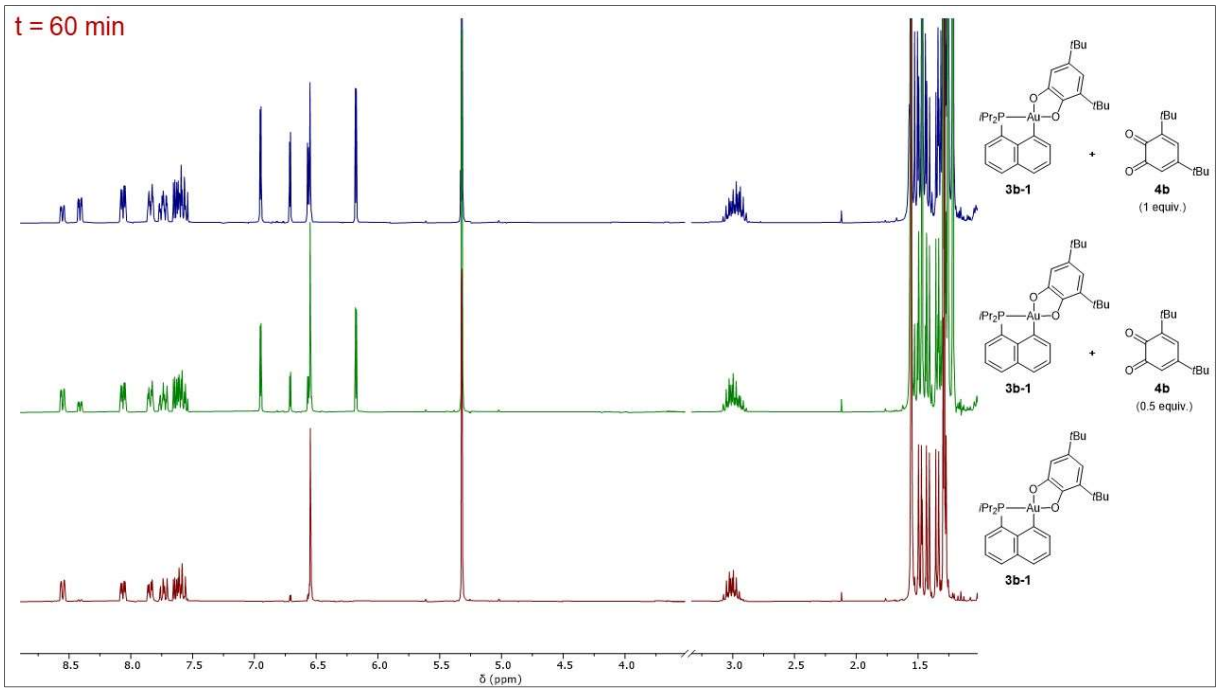


Figure S43. ^{1}H NMR spectra for the isomerization experiment in CD_2Cl_2 at **t = 60 min**.

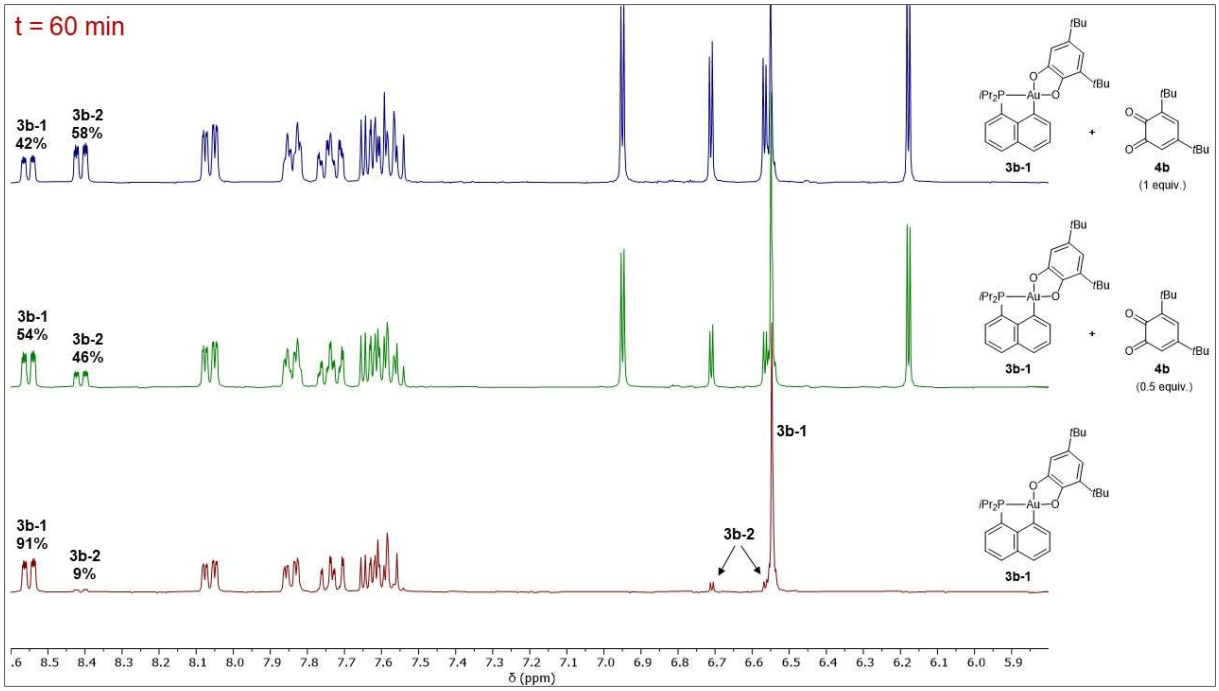


Figure S44. ^{1}H NMR spectra for the isomerization experiment in CD_2Cl_2 at **t = 60 min**. (5.8-8.6 ppm zone)

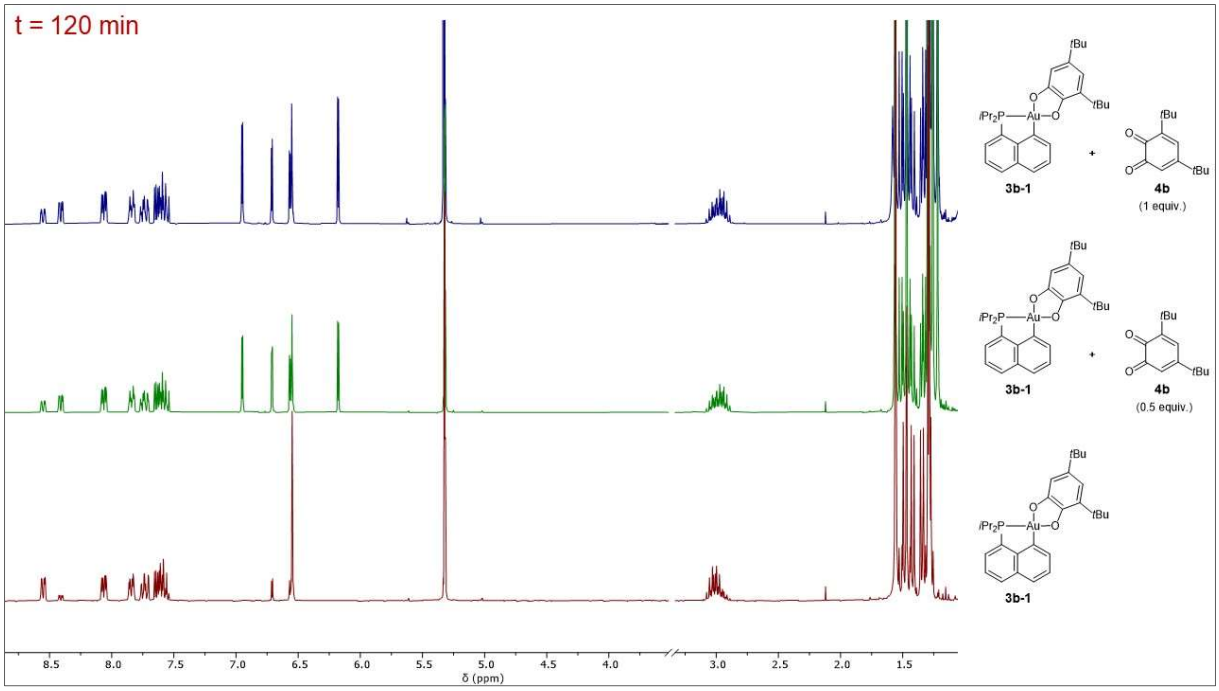


Figure S45. ^{1}H NMR spectra for the isomerization experiment in CD_2Cl_2 at **t = 120 min**.

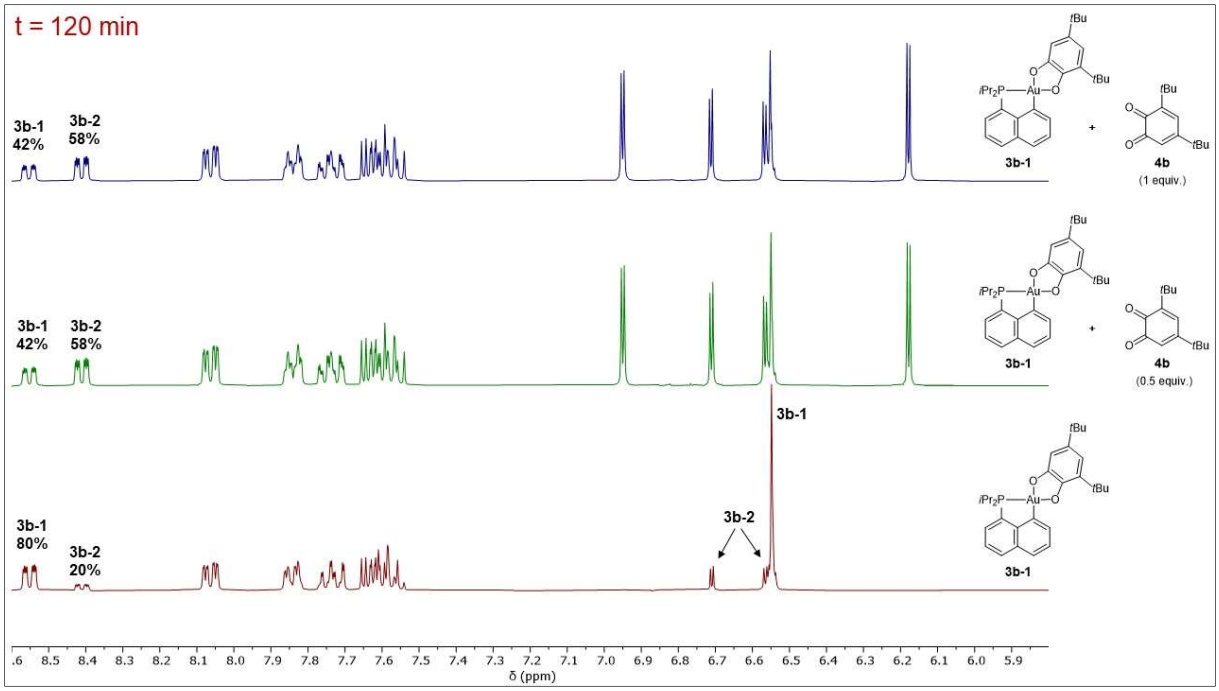


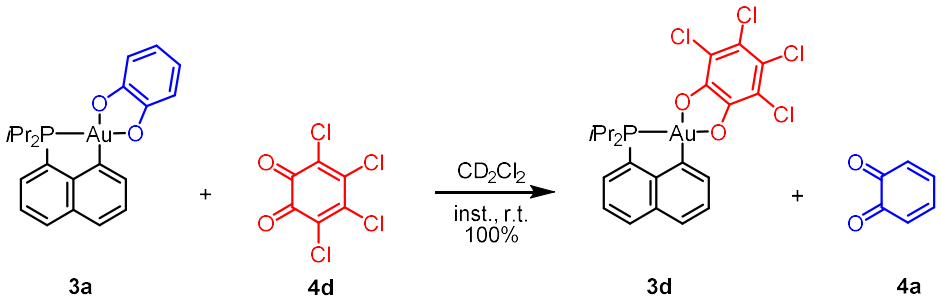
Figure S46. ^{1}H NMR spectra for the isomerization experiment in CD_2Cl_2 at **t = 120 min**. (5.8-8.6 ppm zone)

9. Catechol exchange experiments

P^C Systems

To a solution of the (P^C)Au catecholate complex (**3b-1** or **3a**) (0.01 mmol) in CD_2Cl_2 (250 µL) a solution of benzoquinone **4c** or **4d** (0.01 mmol, 1 equiv.) was added in CD_2Cl_2 (250 µL). The mixture was placed in an NMR tube and ^1H NMR spectrum was recorded immediately. The reaction of **3a** with **4d** was also monitored using $^{13}C\{^1H\}$ NMR.

9.1 (P^C)Au(pyrocatechol) to (P^C)Au(tetrachlorocatechol)



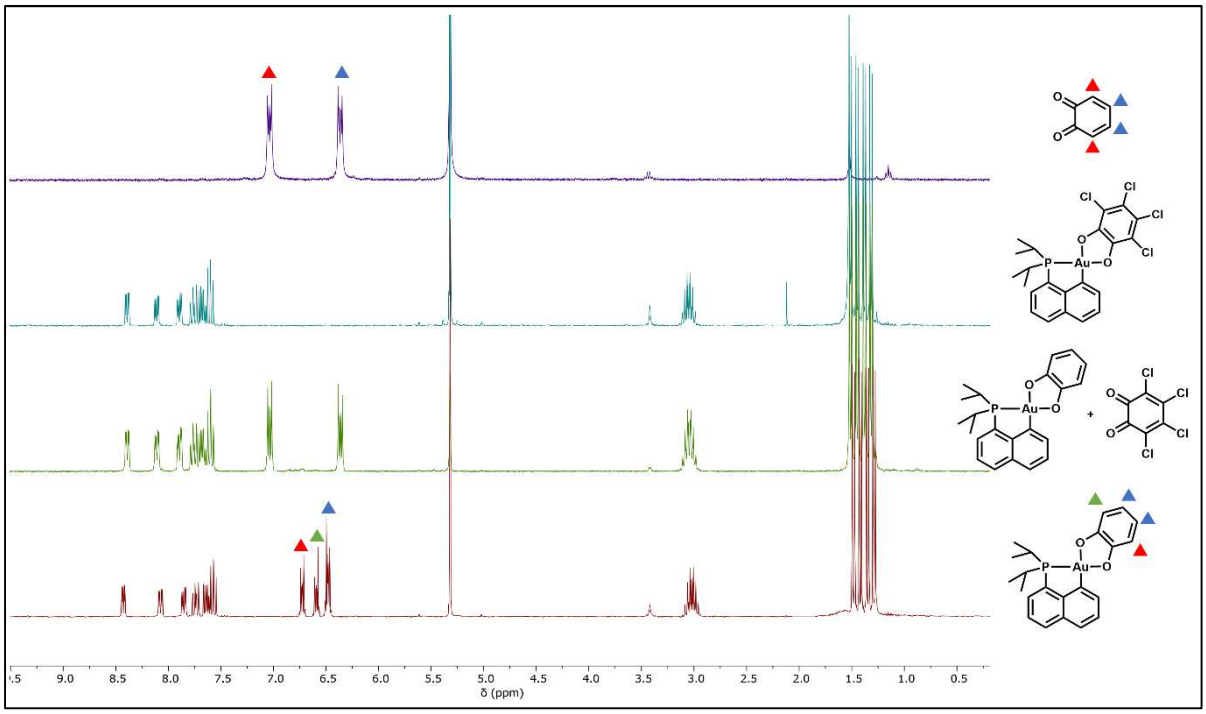


Figure S47. ^1H NMR spectra of the reaction of **3a** with **4d**.

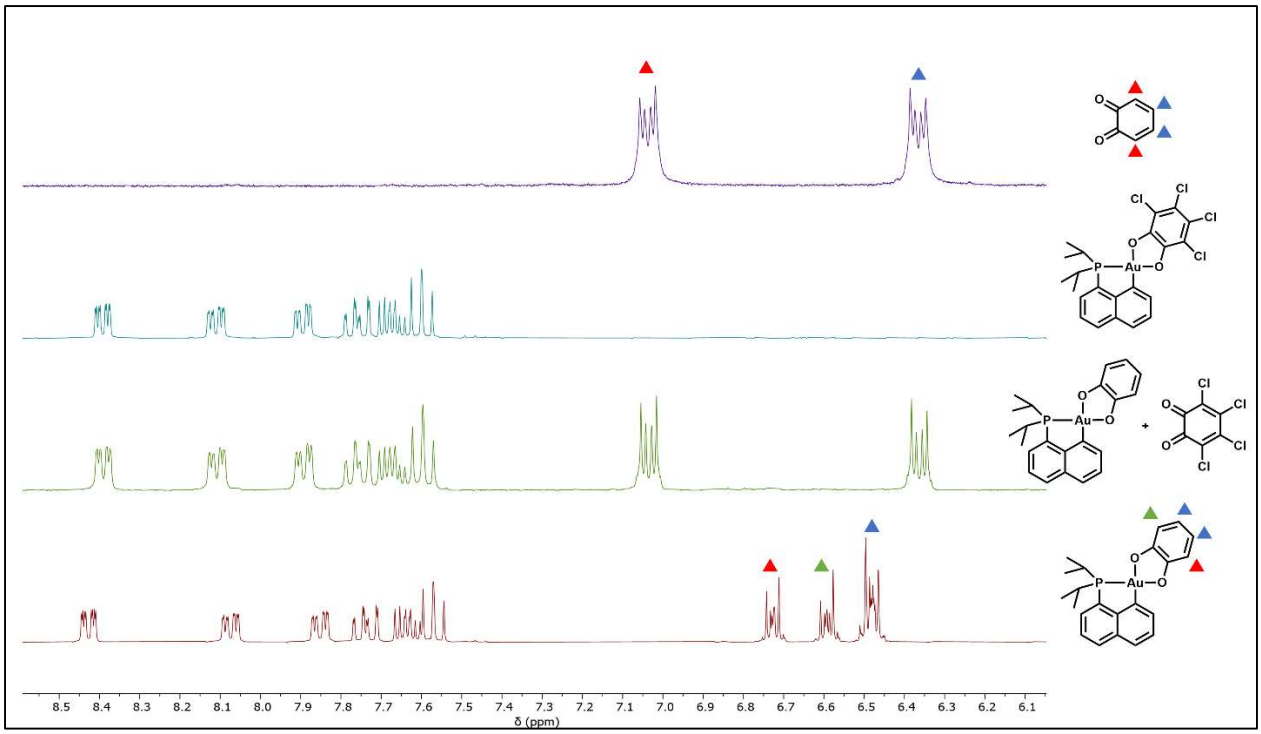


Figure S48. ^{1}H NMR spectra of the reaction of **3a** with **4d**.

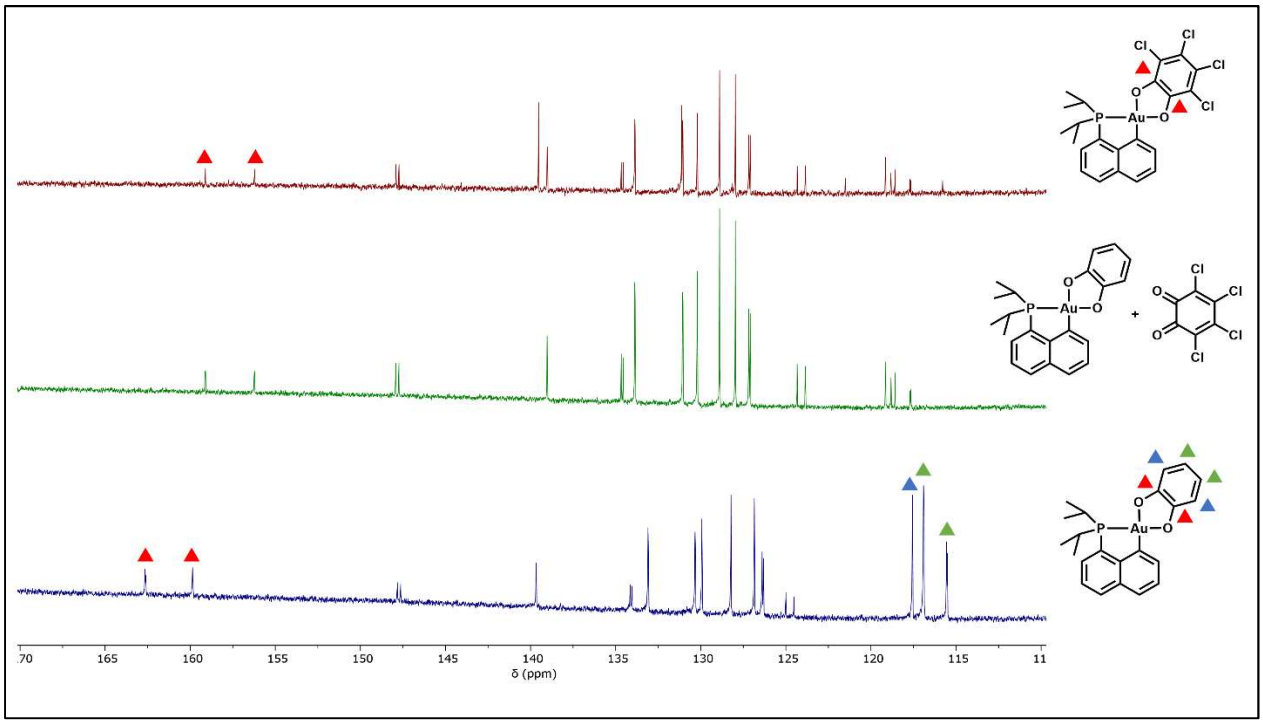


Figure S49. ^{13}C{^{1}H} NMR spectra of the reaction of **3a** with **4d**.

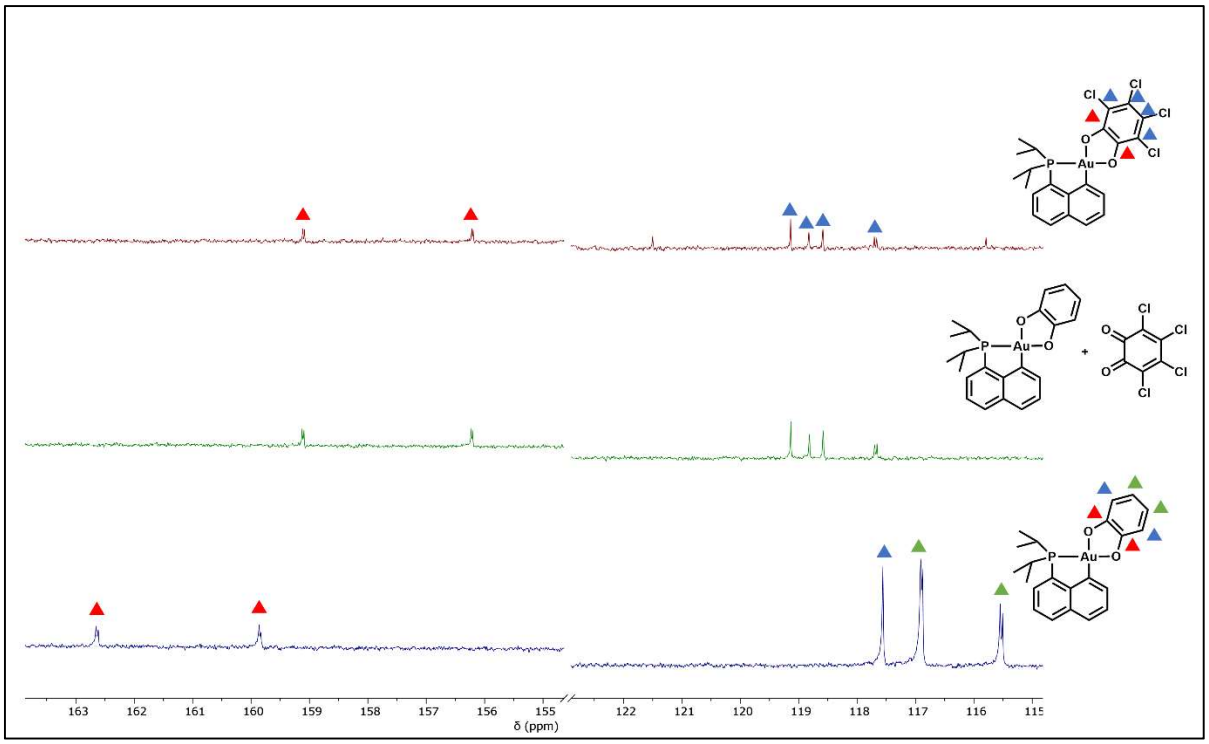
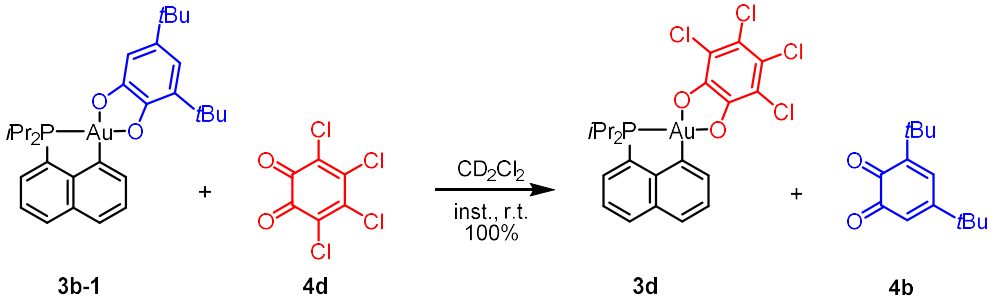


Figure S50. $^{13}C\{^{1}H\}$ NMR spectra of the reaction of **3a** with **4d**.

9.2 (P^C)Au(bis(*tert*-butyl)catechol) to (P^C)Au(tetrachlorocatechol)



3b-1 **4d** **3d** **4b**

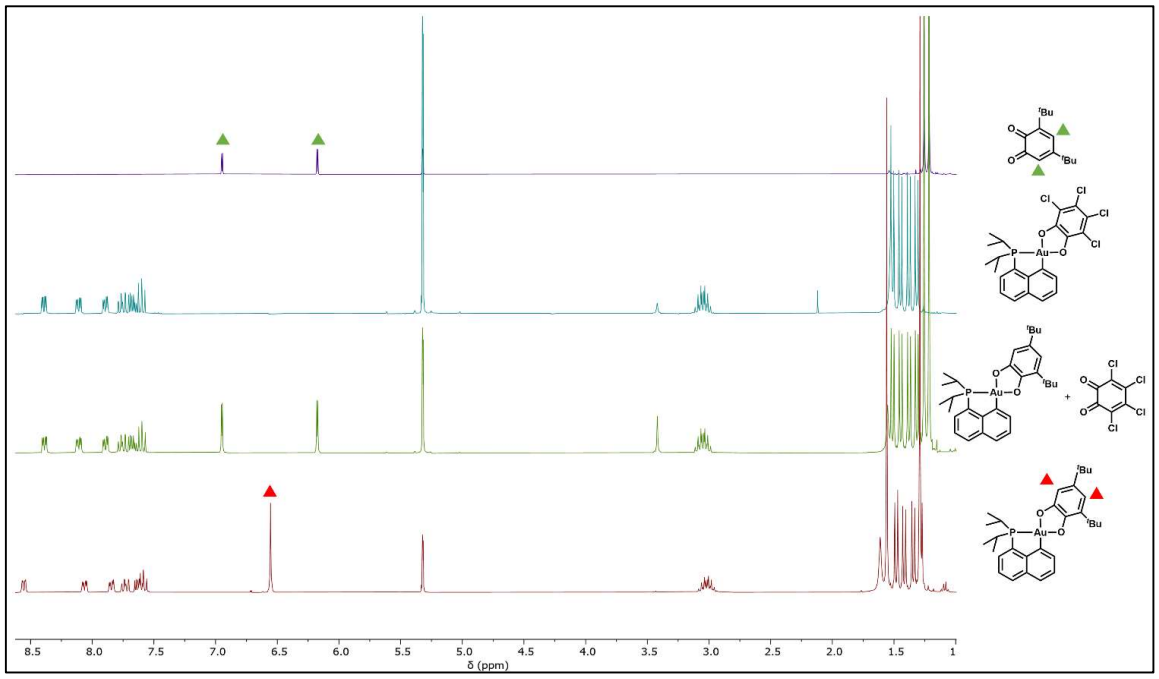


Figure S51. ^{1}H NMR spectra of the reaction of **3b-1** with **4d**.

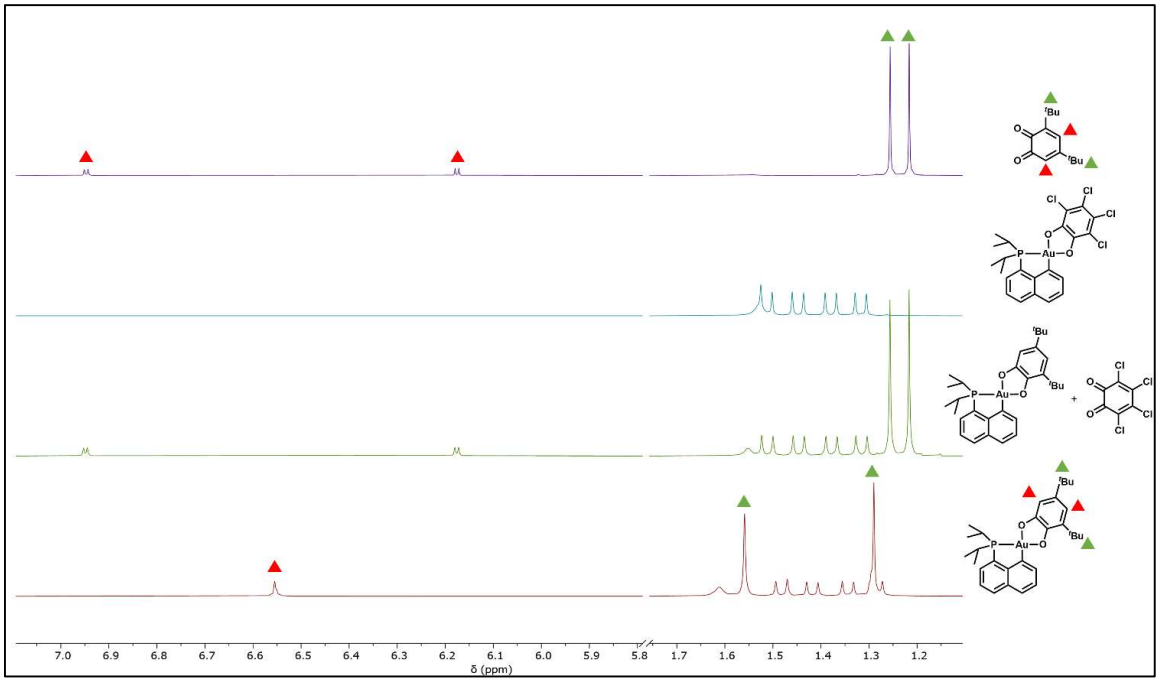
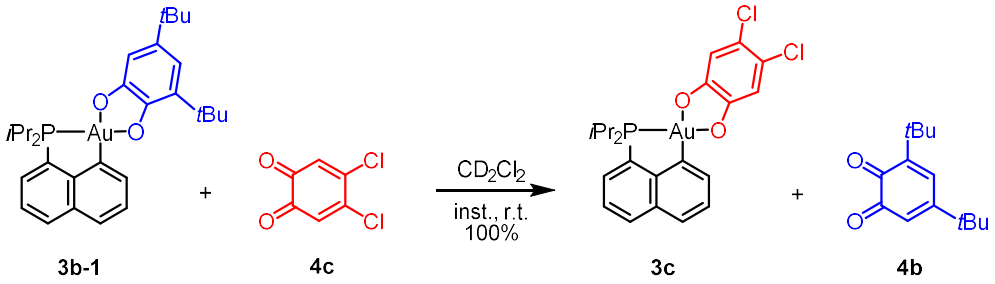


Figure S52. ^{1}H NMR spectra of the reaction of **3b-1** with **4d**.

9.3 (P^C)Au(bis(*tert*-butyl)catechol) to (P^C)Au(4,5-dichlorocatechol)



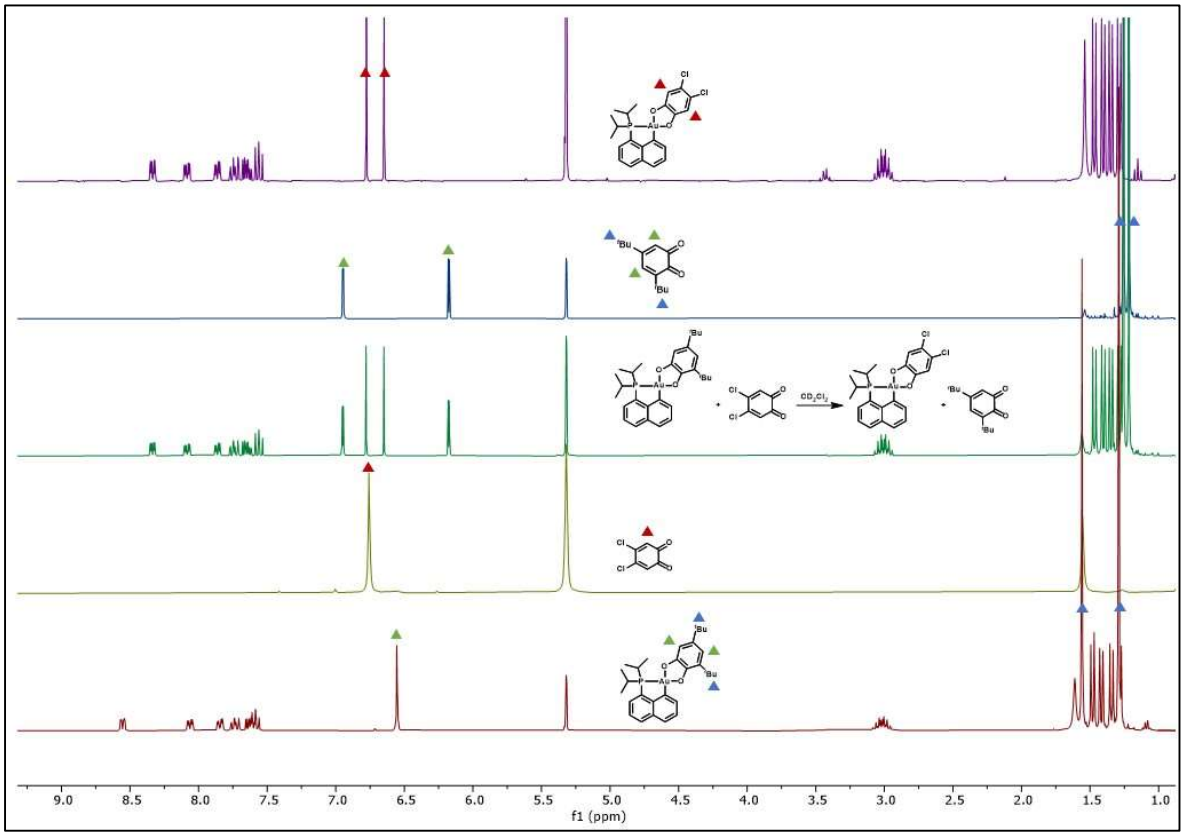


Figure S53. ^{1}H NMR spectra of the reaction of **3b-1** with **4c**.

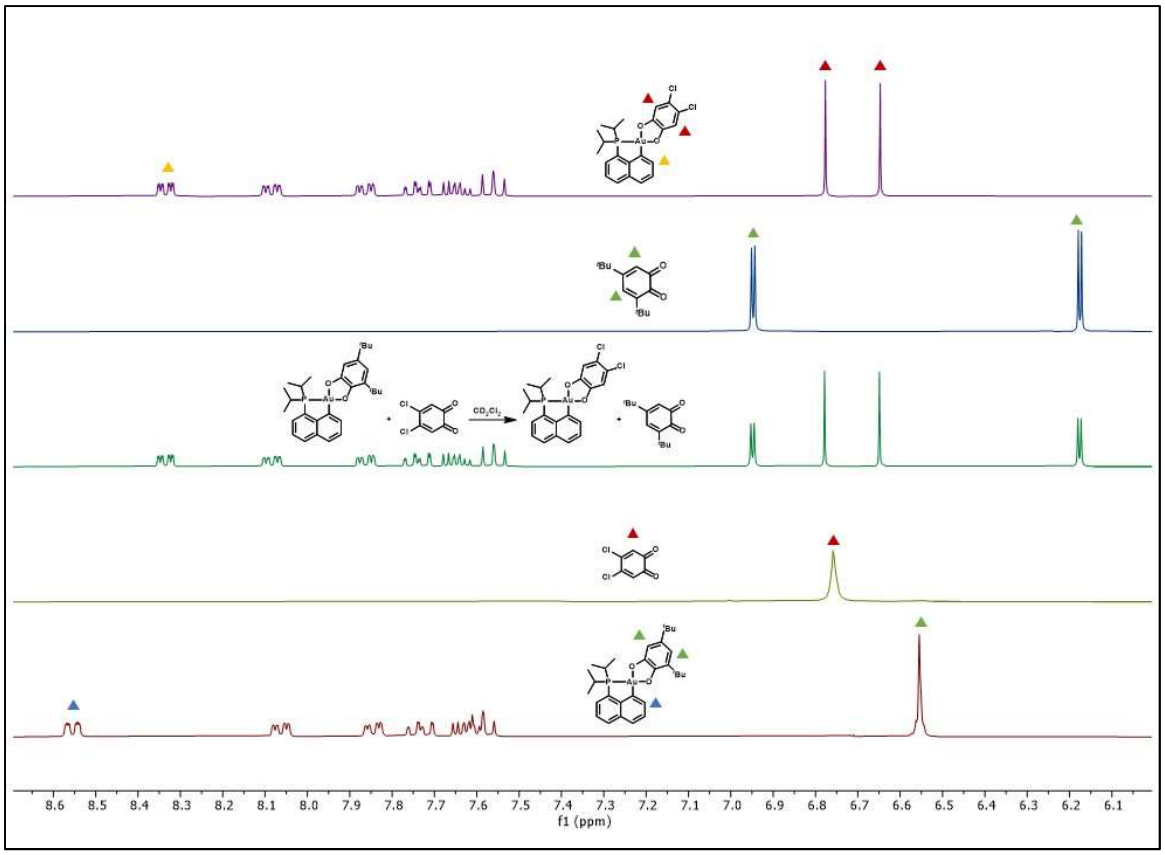


Figure S54. [1]H NMR spectra of the reaction of **3b-1** with **4c**.

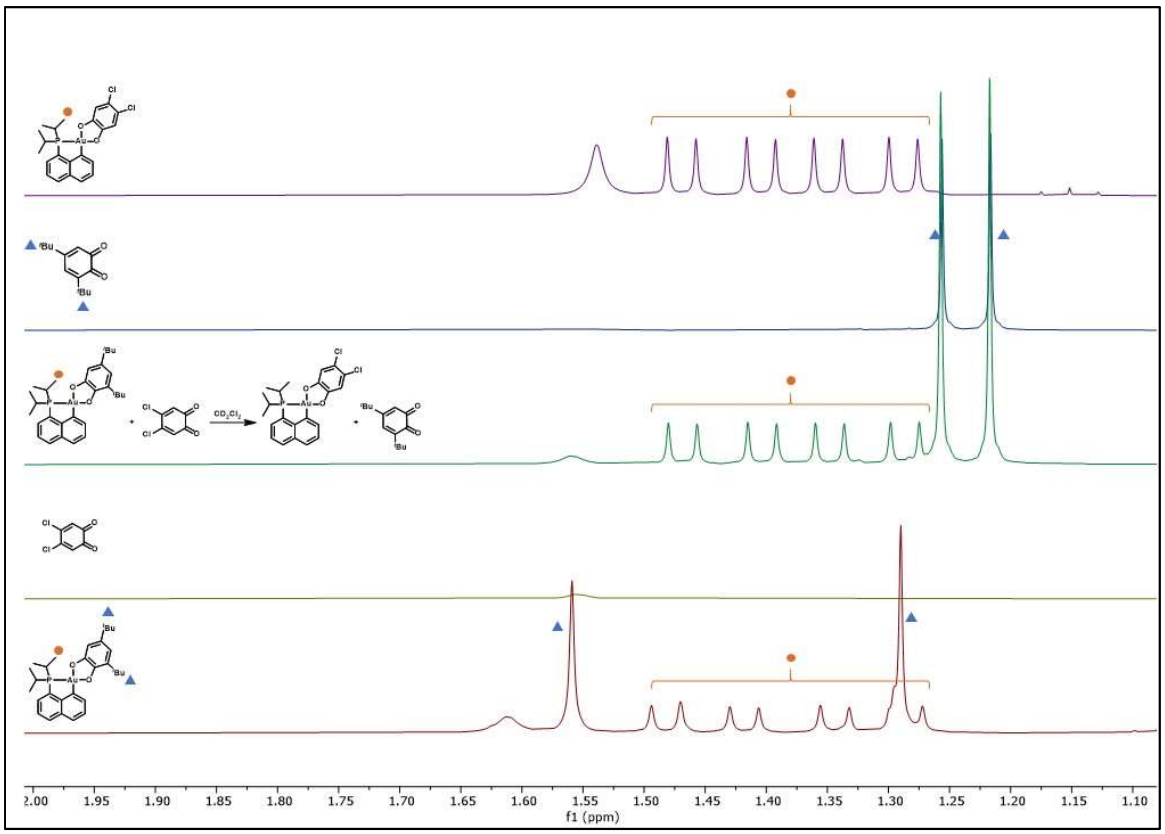
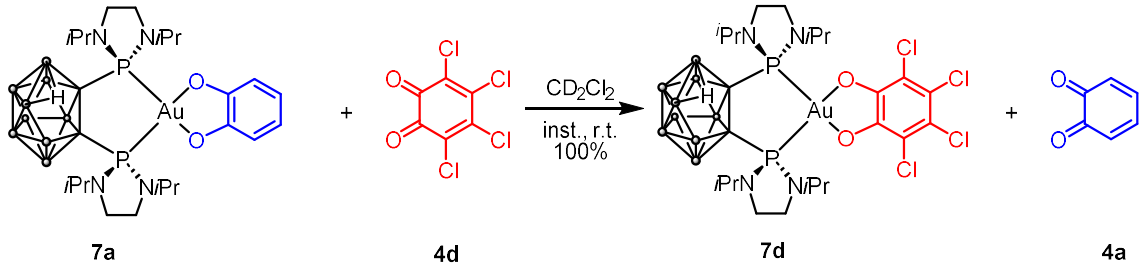


Figure S55. [1]H NMR spectra of the reaction of **3b-1** with **4c**.

P^P Systems

9.4 (P^P)Au(pyrocatechol) to (P^P)Au(tetrachlorocatechol)

To a solution of P^CAu catecholate **7a** or **7b** (0.01 mmol) in CD_2Cl_2 (250 µL) a solution of benzoquinone **4c** or **4d** (0.01 mmol, 1 equiv.) was added in CD_2Cl_2 (250 µL). The mixture was placed in an NMR tube and ^1H NMR spectrum was recorded immediately. As representative example, the exchange between **7a** and **4d**, was also monitored using $^{13}C\{^1H\}$ NMR.



7a **4d** **7d** **4a**

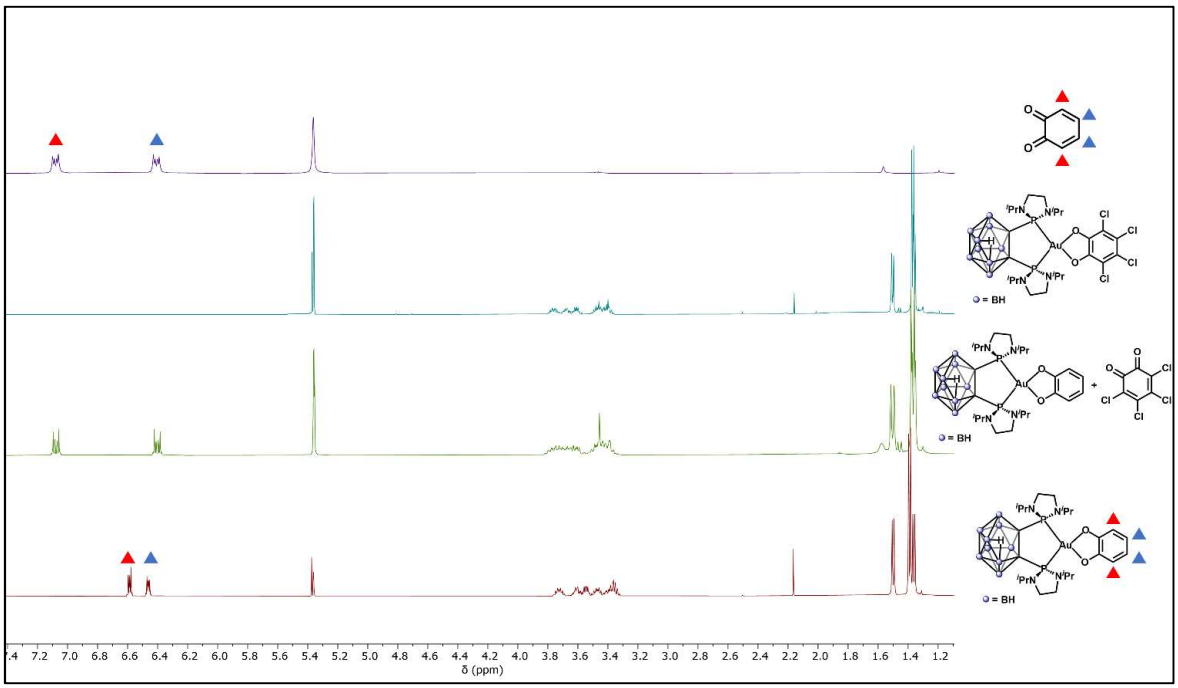


Figure S56. ^1H NMR spectra of the reaction of **7a** with **4d**.

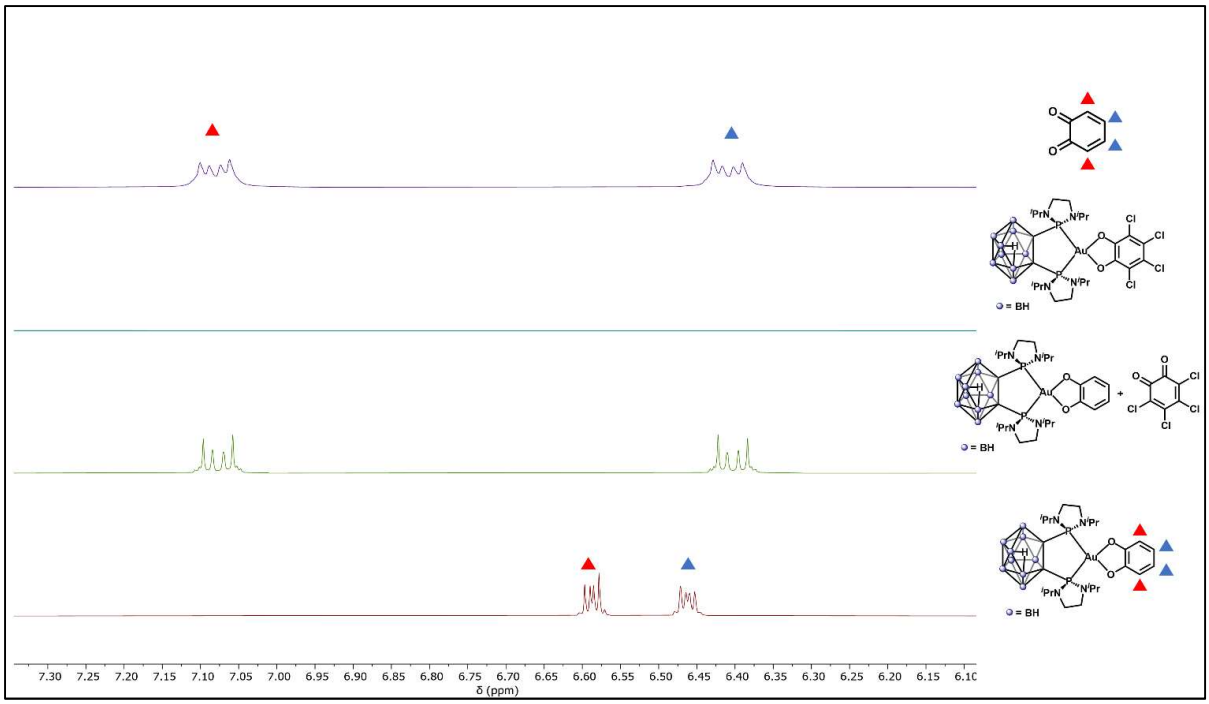


Figure S57. ^{1}H NMR spectra of the reaction of **7a** with **4d**.

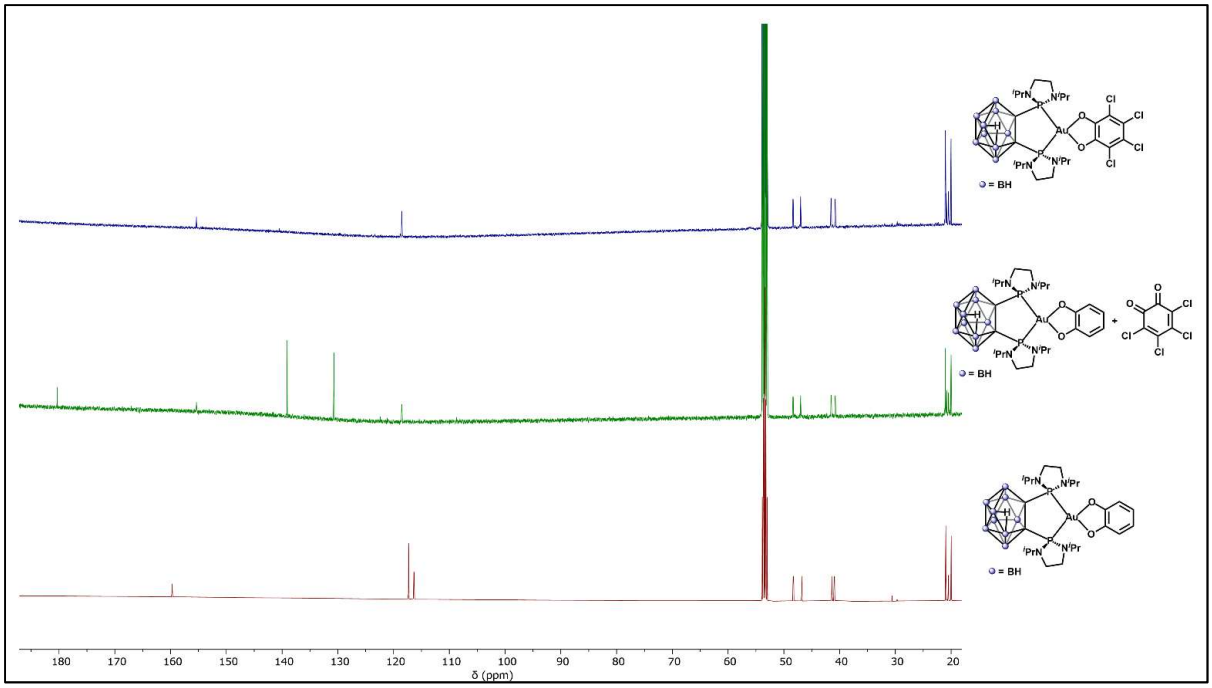


Figure S58. ^{13}C{^{1}H} NMR spectra of the reaction of **7a** with **4d**.

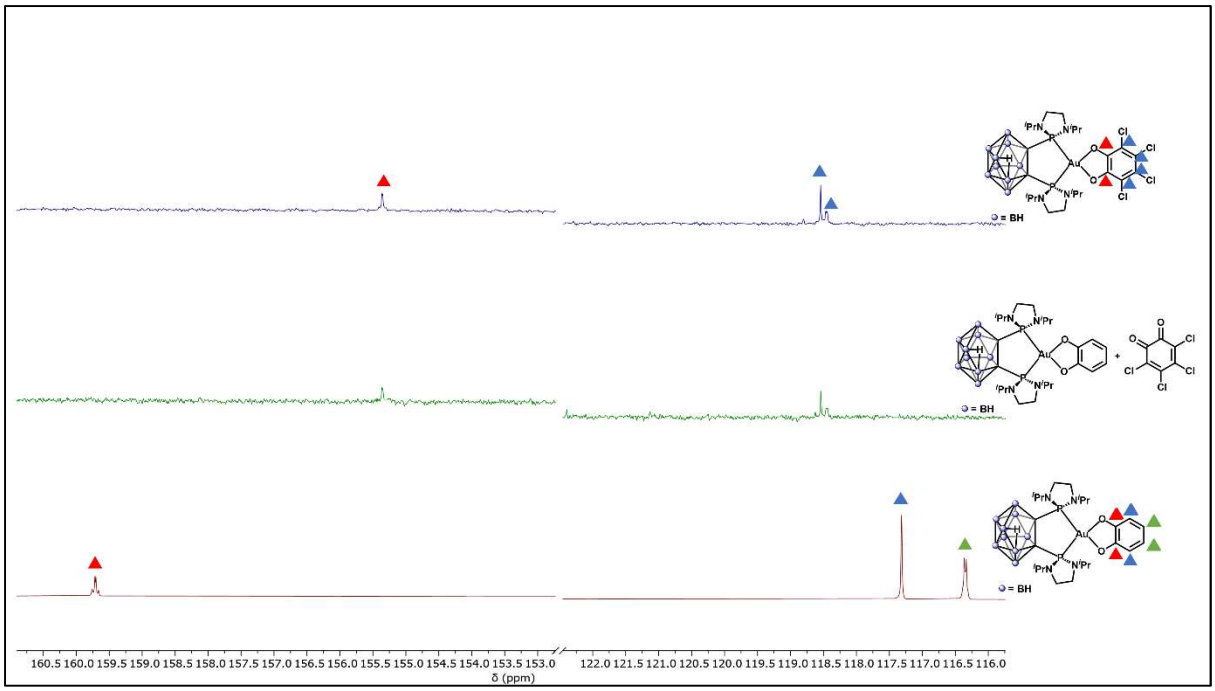
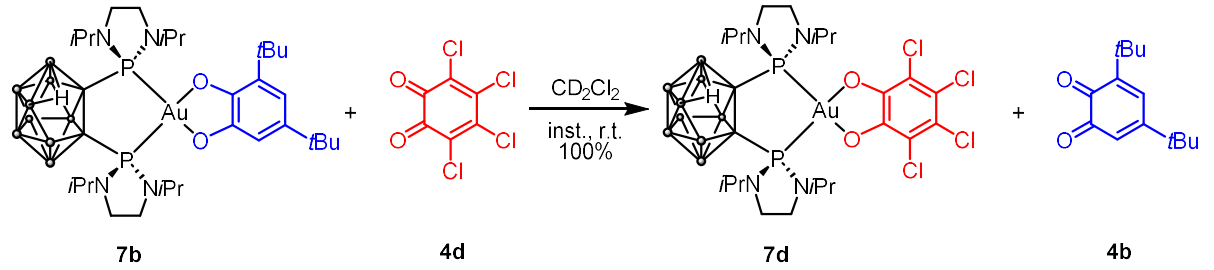


Figure S59. $^{13}C\{^{1}H\}$ NMR spectra of the reaction of **7a** with **4d**.

9.5 (P^P)Au(bis(*tert*-butyl)catechol) to (P^P)Au(tetrachlorocatechol)



7b **4d** **7d** **4b**

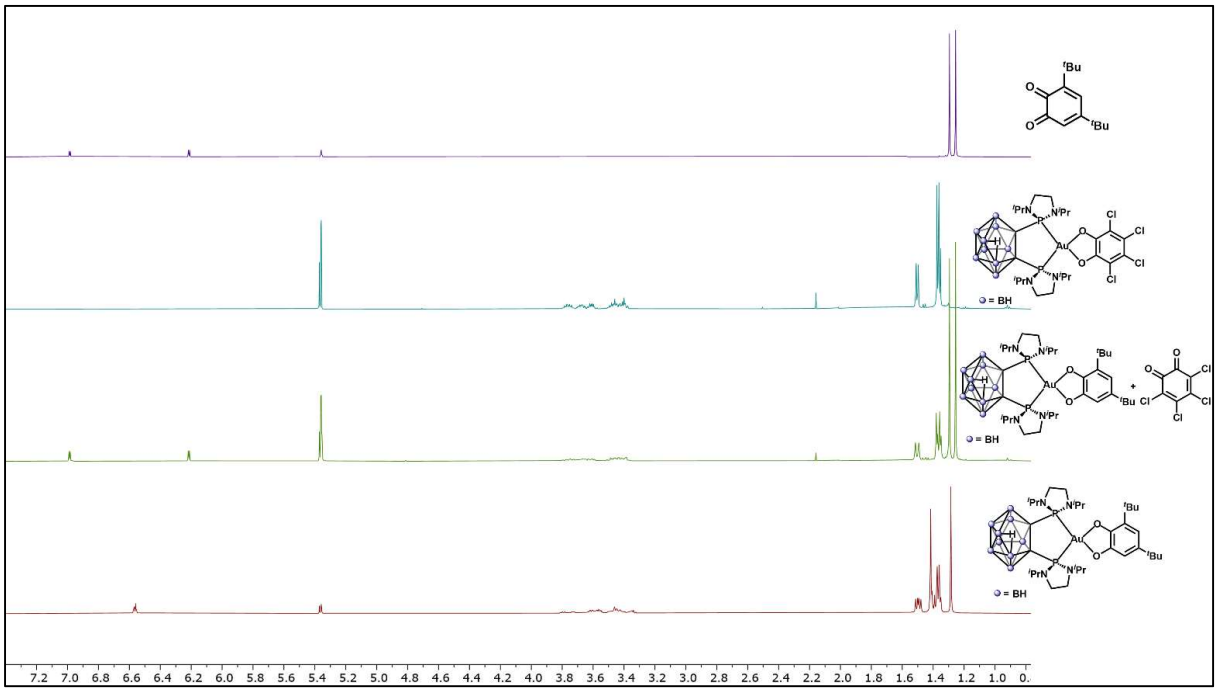


Figure S60. ^{1}H NMR spectra of the reaction of **7b** with **4d**.

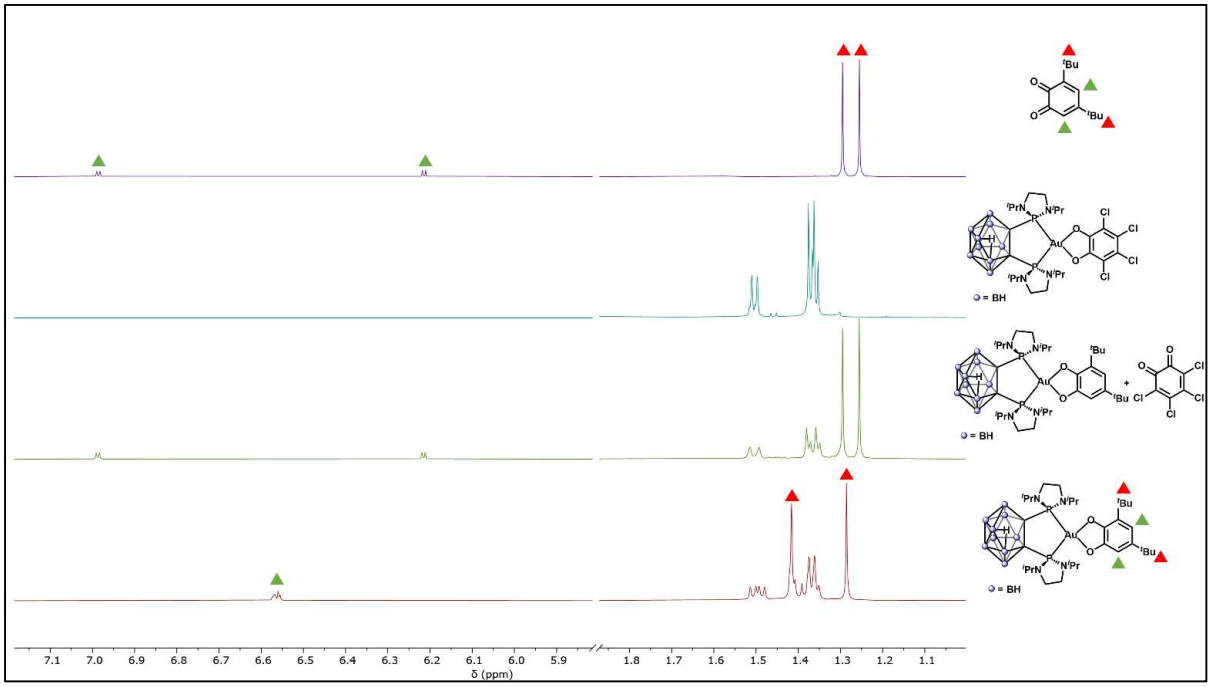
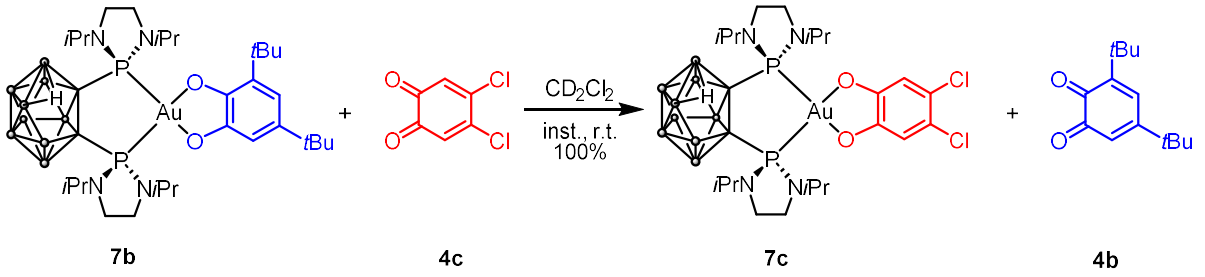


Figure S61. ^{1}H NMR spectra of the reaction of **7b** with **4d**.

9.6 (P^P)Au(bis(*tert*-butyl)catechol) to (P^P)Au(4,5-dichlorocatechol)



7b **4c** **7c** **4b**

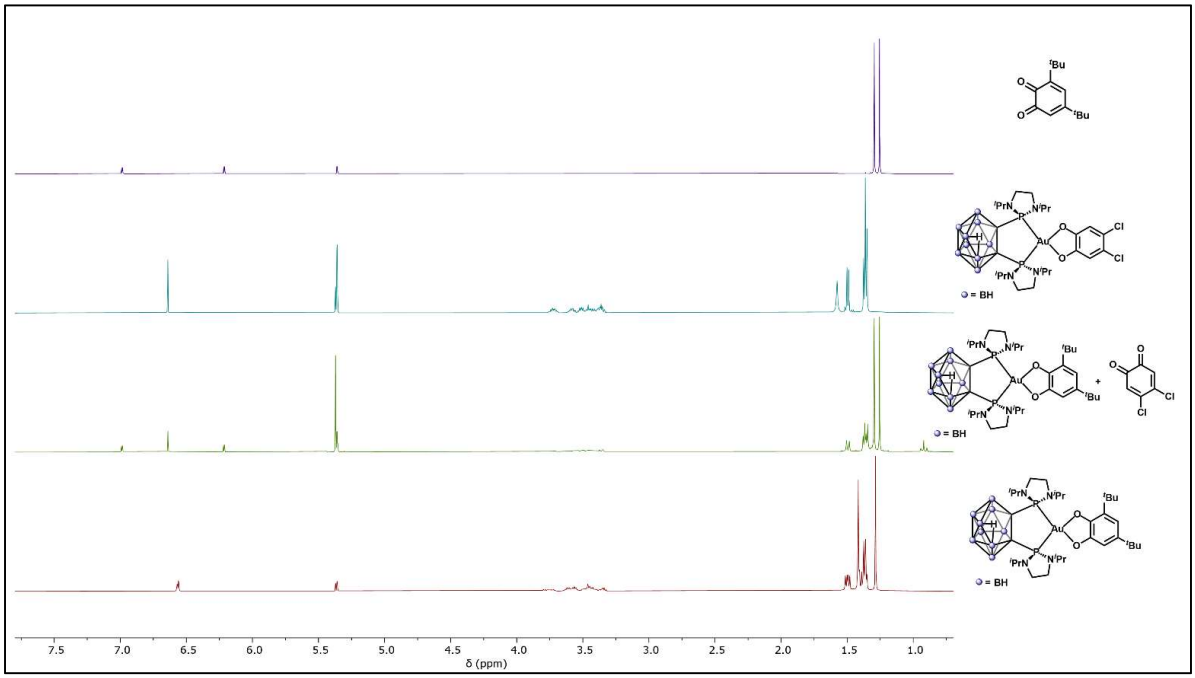


Figure S62. ^{1}H NMR spectra of the reaction of **7b** with **4c**.

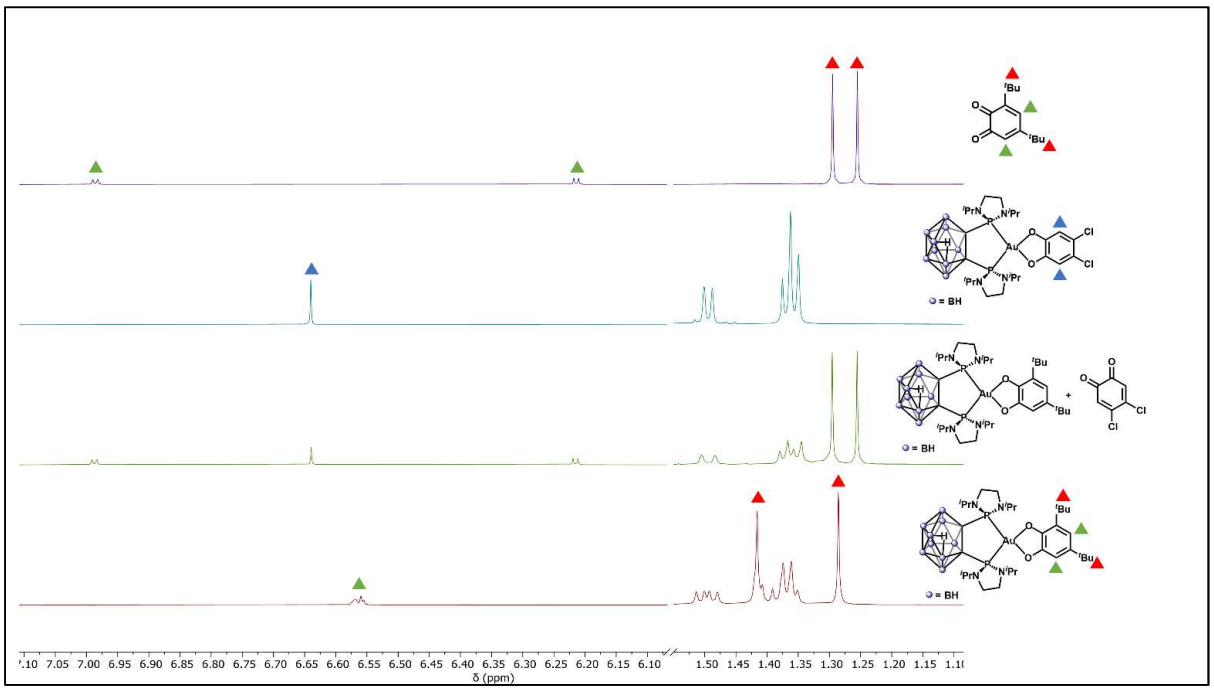
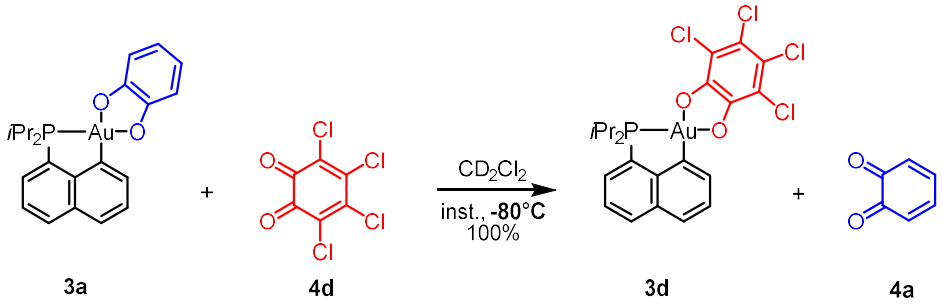


Figure S63. ^{1}H NMR spectra of the reaction of **7b** with **4c**.

9.7 Variable temperature catechol exchange experiment (VT-NMR)

A solution of (P^C)Au catecholate (**3a**) (0.01 mmol, 1 equiv.) in CD_2Cl_2 (250 µL) was placed in an NMR tube and frozen in liquid N_2. A solution of **4d** (0.01 mmol, 1 equiv.) in CD_2Cl_2 (250 µL) was then cooled down to -80 °C and added over the previous solution. The mixture was quickly placed in the NMR machine previously cooled down to -80 °C. The tube was left inside the machine at -80 °C for one minute before ^{1}H NMR was recorded (Figure S64).



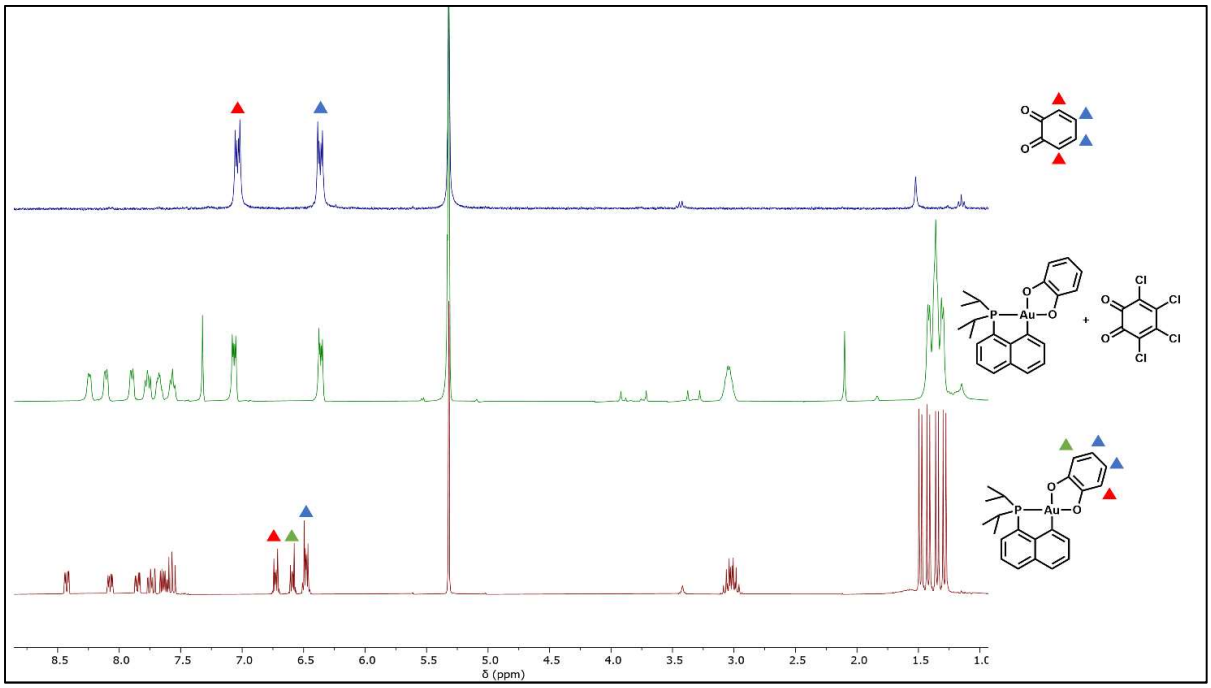
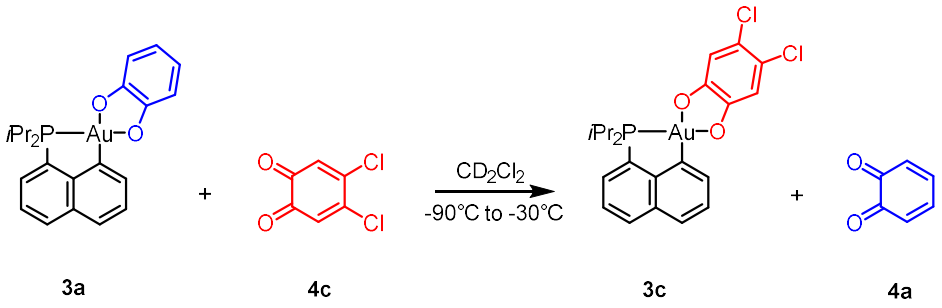
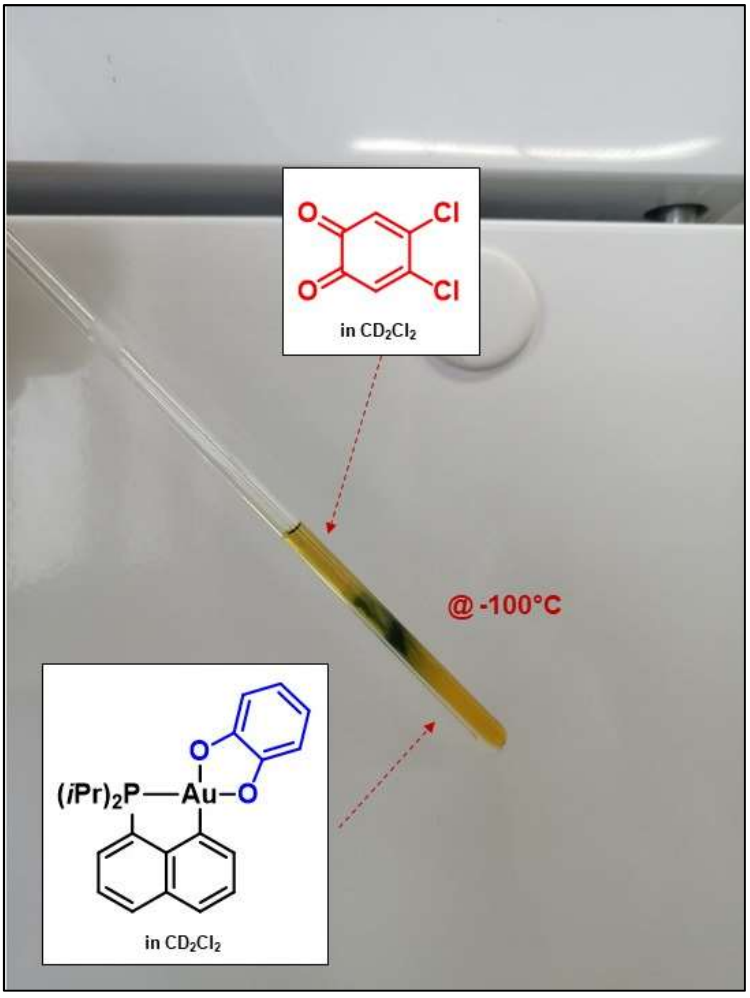


Figure S64. ^{1}H NMR spectra of the reaction of **3a** with **4d** at -80°C.

A solution of (P^C)Au catecholate (**3a**) (0.01 mmol) in CD_2Cl_2 (250 µL) was placed in an NMR tube and cooled to -100°C. A solution of **4c** (0.01 mmol, 1 equiv.) in CD_2Cl_2 (250 µL) was then added very slowly over the previous solution. At the interface of the two solutions a dark green colour appeared (see image below). The mixture was quickly placed in the NMR machine (with a previously precooled probe: -100 °C). The temperature of the sample was let to raise to -90°C and after a proton NMR was recorded. Then the temperature was raised by 10 °C and a new proton NMR was recorded. This was repeated until -30°C. This VT-NMR experiment shows, that the products (**3c** and **4a**) start to form even at -80°C, they become the major species in the mixture at -60°C and the reaction is complete at -40°C (Figure S65).





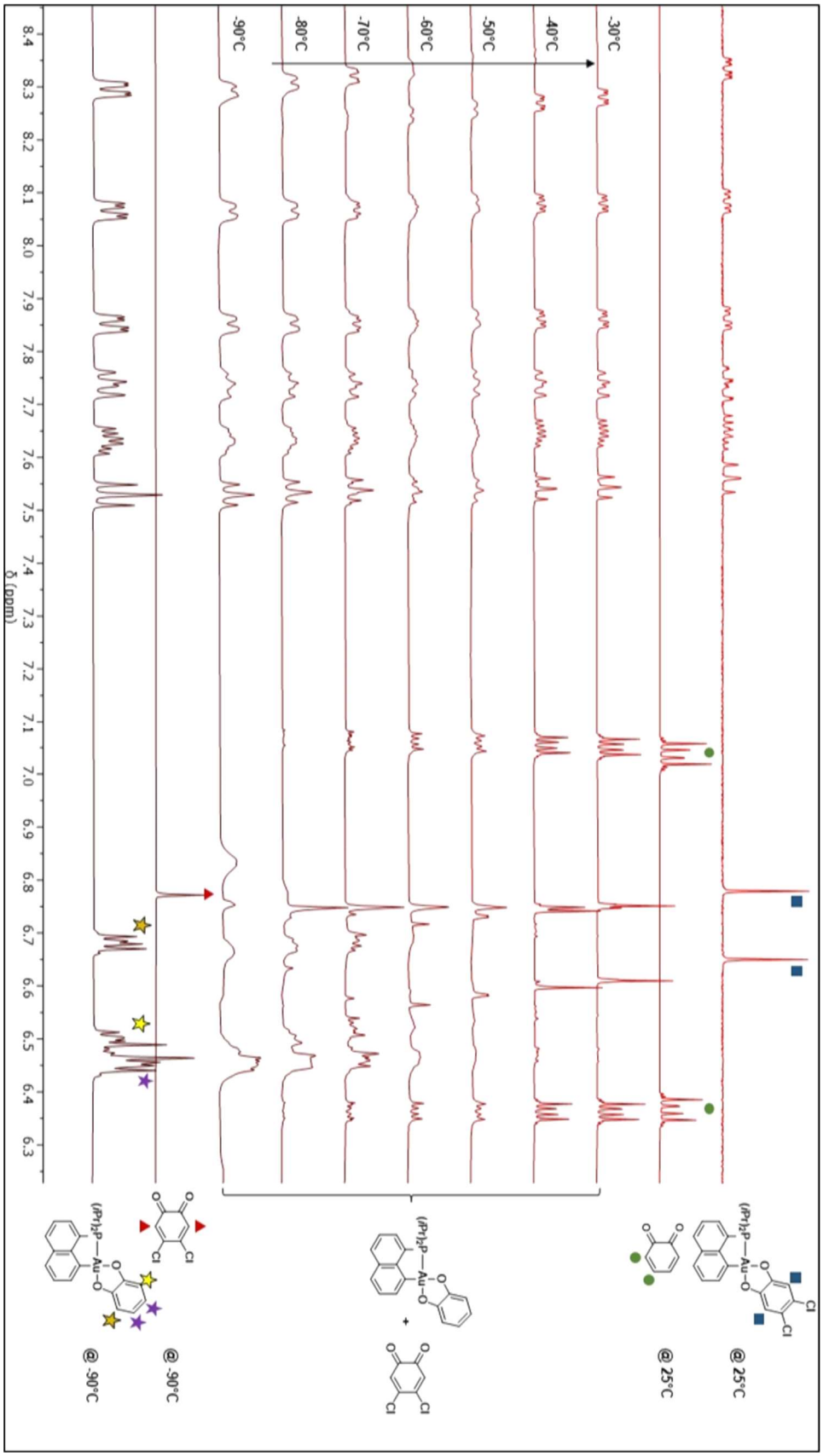


Figure S65. ^{1}H VT-NMR spectra of the reaction of **3a** with **4c** (-90°C to -30°C).

9.8 Low temperature catechol exchange experiment (VT UV-vis)

A solution of (P^C)Au catecholate (**3a**) (0.015 mmol, 10^{-2}M) in CH_2Cl_2 (1.5 mL) was placed in an cuvette and cooled to -100°C. Then a solution of **4c** (1 equiv., 10^{-2}M) in CH_2Cl_2 (1.5 mL) was added very slowly over the previous solution. Then the cuvette was quickly placed in a precooled (190K) optical cryostat. After 20 minutes the UV spectrum was recorded, that revealed a broad absorption band with a maximum at 745 nm, that could be attributed to a charge-transfer complex. The UV spectra was then consecutively recorded at 200K, 210K and 220K (Figure S66), that revealed the decrease of the absorption maximum.

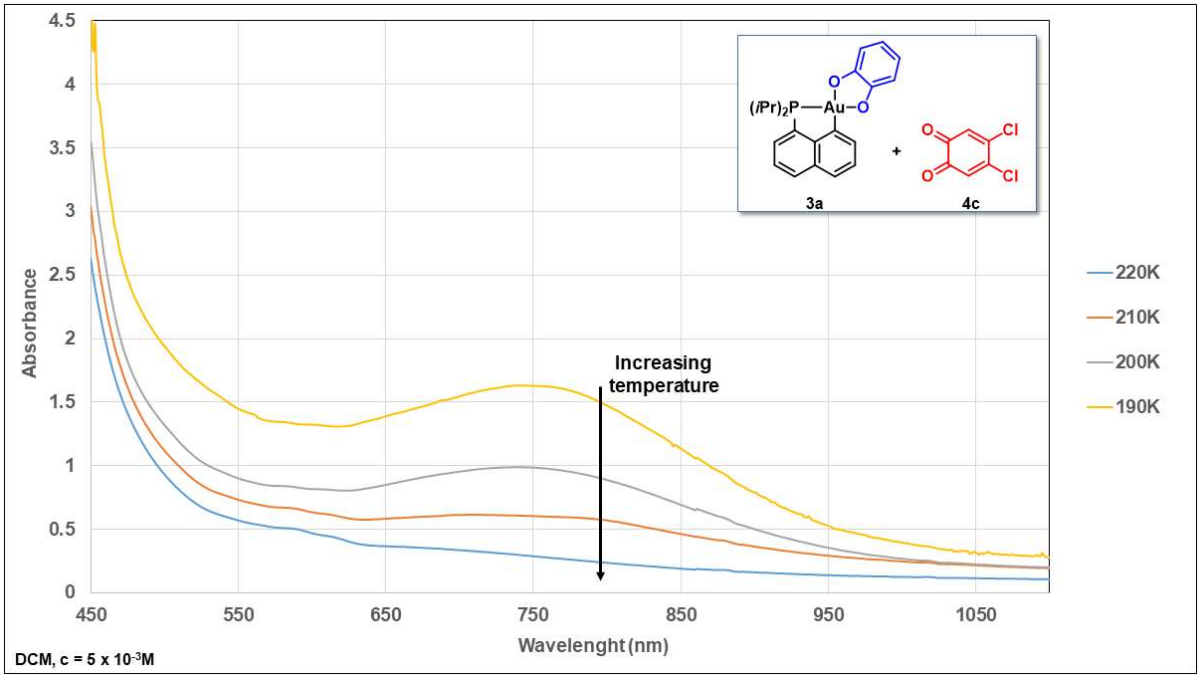


Figure S66. VT UV-vis spectra of the reaction of **3a** with **4c** (190K to 220K).

10. EPR analyses

10.1 Room Temperature EPR experiments

A mixture of catecholate (**3a** or **3b** or **3d**) (0.005 mmol) and (**4a** or **4b** or **4d**) (0.005 mmol) were dissolved in dry CH_2Cl_2 (0.3 ml) inside the glovebox and placed in an EPR tube. The EPR spectra of the mixture was recorded immediately at room temperature.

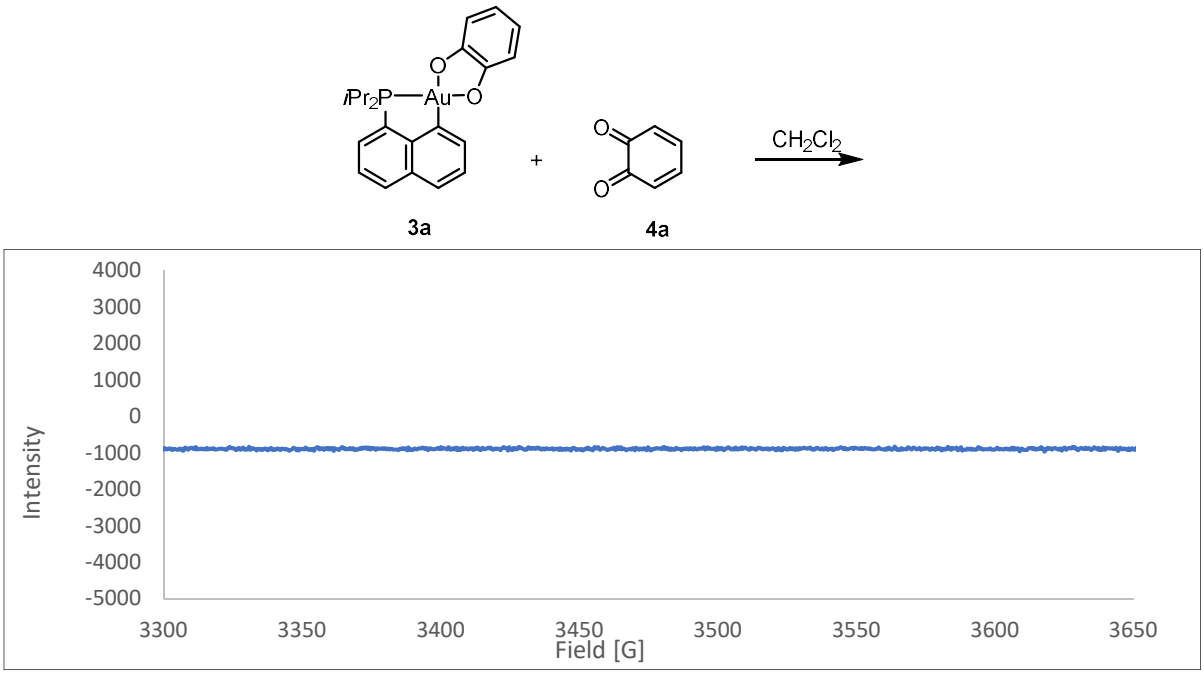


Figure S67. EPR spectrum of **3a** in the presence of **4a**.

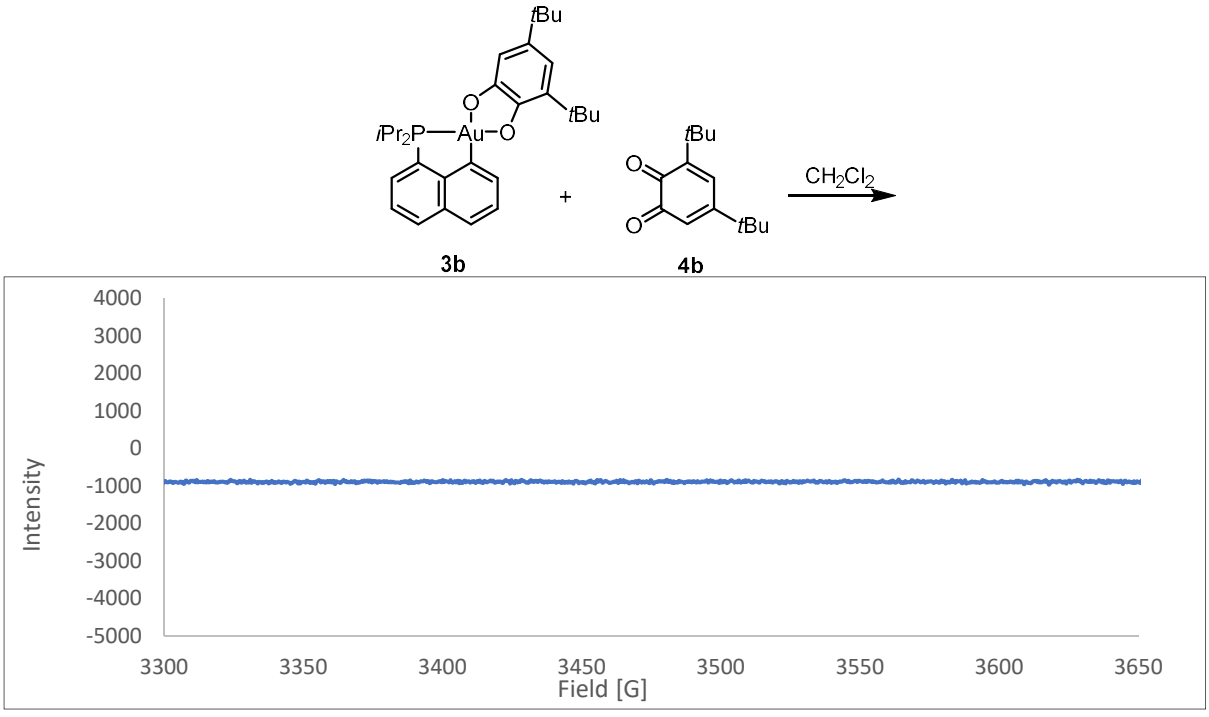


Figure S68. EPR spectrum of **3b** in the presence of **4b**.

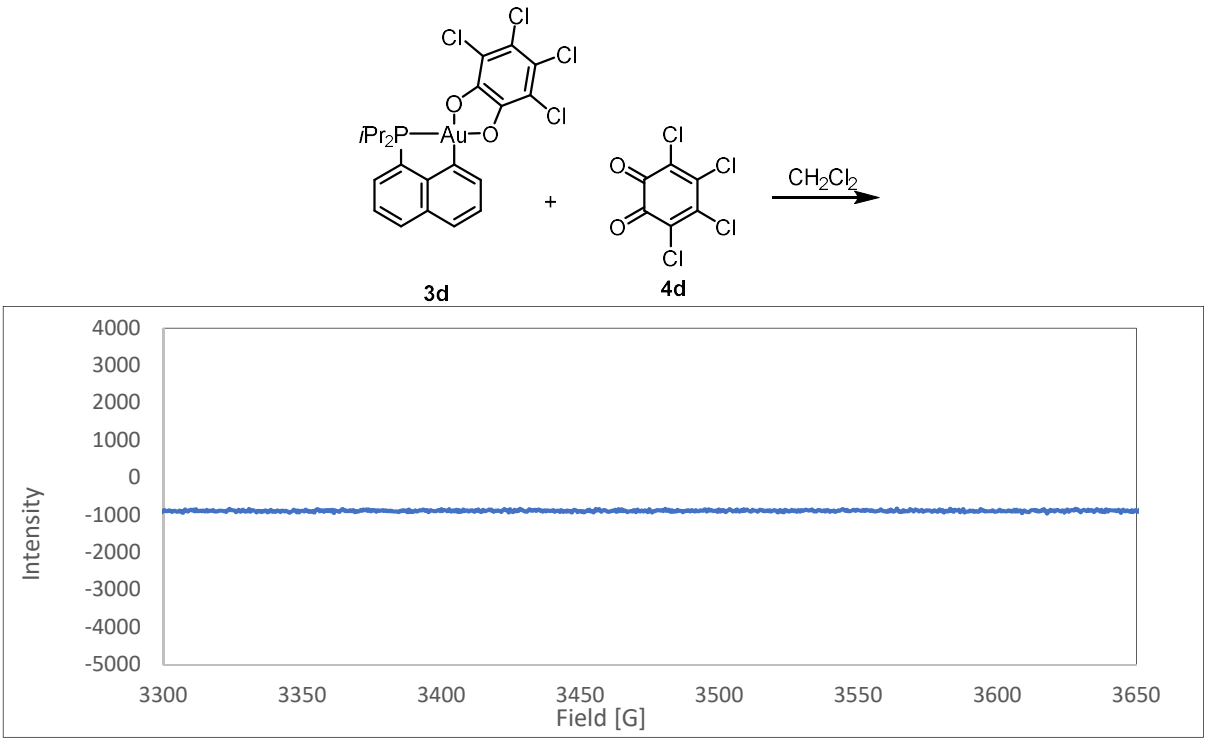
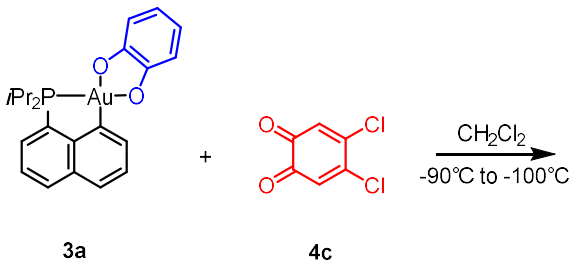
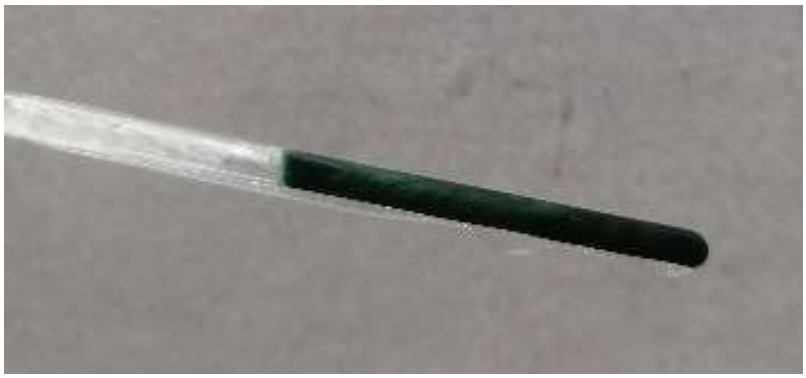


Figure S69. EPR spectrum of **3d** in the presence of **4d**.

10.2 Low Temperature EPR experiment

A solution of (P^C)Au catecholate (**3a**) (0.01 mmol) in CH_2Cl_2 (250 µL) was placed in an EPR tube and cooled to -100°C. A solution of **4c** (0.01 mmol, 1 equiv.) in CH_2Cl_2 (250 µL) was then added very slowly over the previous solution. Then the tube was shaken outside of the cooling bath to give a homogeneous deep green solution (see image below), that was immediately replaced into the bath. Then EPR spectra was recorded at 150K. (Figure S69).





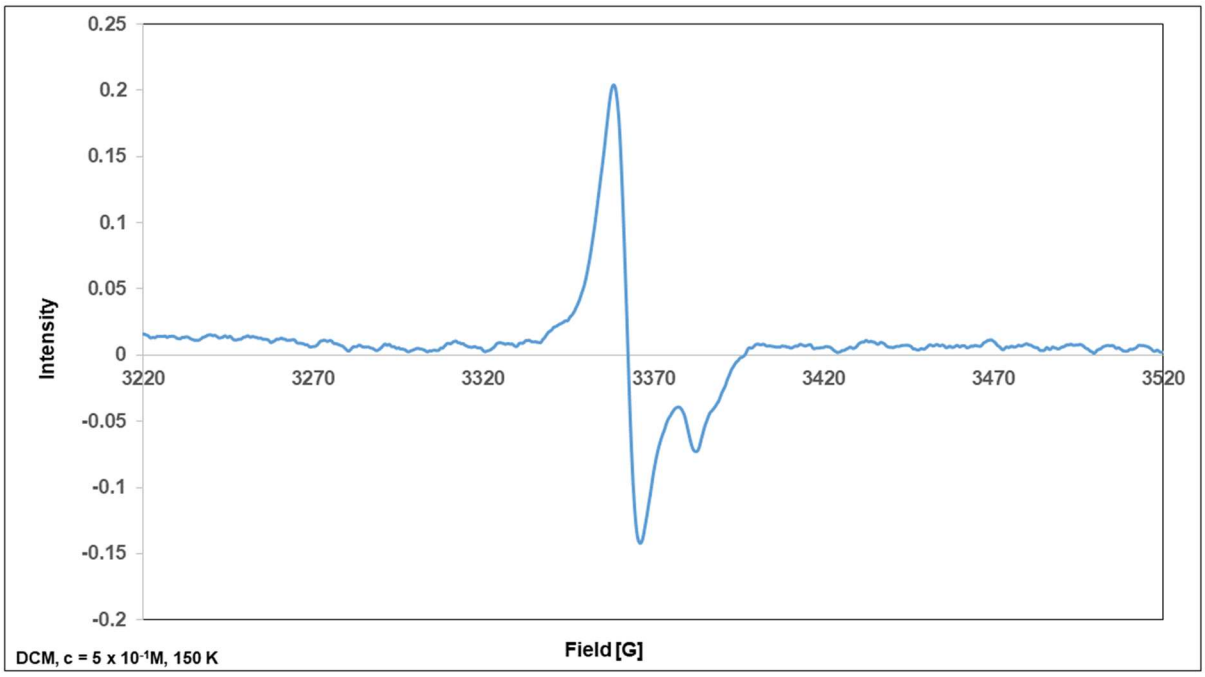


Figure S70. EPR spectrum of **3a** in the presence of **4c** at 150K.

11. Metrical parameters for the P^C gold(III) complexes

The ^{31}P NMR signals (85.6 - 95.6 ppm) are found in the typical region of gold(III) coordinated naphthalenyl diisopropylphosphine complexes.[6] XRD analyses confirmed the square planar geometry of the gold center (τ_4 = 0.02 – 0.04).[7] In addition, the C-O / C=C distances and MOS[8] values are clearly indicative for the catecholate moiety in the -2 oxidation state, which supports the gold(III) assignment.

	3a	**3b**	**3c**	**3d**
^{31}P (ppm)	88.7	85.6	92.0	95.6
τ_4	0.04	0.03	0.02	0.04
C=O (Å)	1.357(4)	1.358(4)	1.341(11)	1.330(3)
	1.355(4)	1.363(5)	1.347(12)	1.341(3)
C-C (Å)	1.410(5)	1.406(5)	1.414(13)	1.417(4)
MOS	-2.03(4)	-1.96(8)	-1.90(4)	-1.82(7)

Table S1. ^{31}P NMR values and key geometric parameters (Å) of complexes **3a**-**d**.

12. Crystallographic data

Crystallographic data were collected at low temperature (193(2) K) on a Bruker APEX II Quazar diffractometer equipped with a 30 W air-cooled microfocus source using MoK_α radiation (λ = 0.71073 Å) for **3a** and **7a**, and on a Bruker D8 VENTURE diffractometer equipped with a PHOTON III detector, using MoK_α radiation (λ = 0.71073 Å) or a microfocus source with CuK_α radiation (λ = 1.54184 Å) for **3d**, **3c**, **3b-2**, **7b** and **6**. Phi and Omega scans were performed for data collection. An empirical absorption correction was applied[9] and the structures were solved by intrinsic phasing method (ShelXT).[10] All non-hydrogen atoms were refined anisotropically by means of least-squares procedures on F^2 with ShelXL.[11] All the hydrogen atoms were refined isotropically at calculated positions using a riding model. For **3b-2**, the SQUEEZE[12] function of PLATON was used to remove the electron density contribution of the highly disordered solvent molecules from the model.

CCDC 2332329 (**3a**), 2332332 (**3b-2**), 2332331 (**3c**), 2332330 (**3d**), 2332335 (**6**), 2332334 (**7a**) and 2332333 (**7b**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre.

Crystal Data, Data Collection, and Structure Refinement for **3a**, **3b-2**, **3c**, **3d**, **6**, **7a**, and **7b**.

ID	**3a**	**3d**	**3c**	**3b-2**	**7b**	**7a**	**6**
formula	$C_{22}H_{24}AuO_2P$, $0.5(C_4H_8O)$	$C_{22}H_{20}AuCl_4O_2P$	$C_{22}H_{22}AuCl_2O_2P$	$C_{30}H_{40}AuO_2P$, $0.33(C_4H_{10}O)$	$C_{32}H_{64}AuB_9N_4O_2P_2$, $0.5(CH_2Cl_2)$	$C_{24}H_{49}AuB_9N_4O_2P_2$	$C_{18}H_{45}AuB_9Cl_2N_4P_2$, $CHCl_3$
M_r	584.40	686.12	617.24	685.02	935.53	781.87	864.05
crystal system	orthorhombic	orthorhombic	monoclinic	trigonal	monoclinic	monoclinic	monoclinic
space group	*Pbcn*	*Pbca*	$P2_1/c$	$R\bar{3}$	$P2_1/n$	$P2_1$	*C2/m*
a (Å)	15.7586(7)	15.3901(11)	10.7611(7)	28.7347(9)	11.279(4)	9.5342(8)	19.4759(13)
b (Å)	19.2635(7)	15.6458(9)	14.4997(9)	28.7347(9)	13.765(3)	17.6708(15)	17.3049(11)
c (Å)	14.1296(5)	19.2140(11)	13.7734(8)	20.9068(10)	29.733(9)	10.3038(9)	10.6632(6)
α (°)	90	90	90	90	90	90	90
β (°)	90	90	98.291(2)	90	94.479(14)	95.660(2)	102.725(2)
γ (°)	90	90	90	120	90	90	90
V (Å^3)	4289.3(3)	4626.6(5)	2126.6(2)	14949.7(12)	4602(2)	1727.5(3)	3505.5(4)
Z	8	8	4	18	4	2	4
ρ_{calc} (g cm^{-3})	1.810	1.970	1.928	1.370	1.350	1.503	1.637
μ (mm^{-1})	6.954	17.004	7.260	4.500	3.356	4.38	4.689
F(000)	2288	2640	1192	6189	1900	782	1708
crystal size (mm^3)	0.08 x 0.06 x 0.04	0.20 x 0.20 x 0.04	0.18 x 0.10 x 0.04	0.16 x 0.12 x 0.08	0.10 x 0.08 x 0.06	0.18 x 0.10 x 0.08	0.10 x 0.08 x 0.06
T/K	193(2)	193(2)	193(2)	193(2)	193(2)	192(2)	193(2)
measd reflns	45422	79862	145612	127299	51568	68579	115453
Unique reflns (Rint)	5542 (0.0658)	4573 (0.0512)	14871 (0.0355)	7640 (0.0562)	8416 (0.0478)	14523 (0.0507)	7561
Data/restraints/ parameters	5542 / 44 / 285	4573 / 0 / 276	14871 / 0 / 257	7640 / 76 / 388	8416 / 557 / 645	14523 / 1 / 387	7561 / 60 / 194
GOF on F^2	1.016	1.120	1.042	1.068	1.199	1.024	1.087
R_1[a] [I>2σ(I)]	0.0245	0.0219	0.0153	0.0294	0.0710	0.0331	0.0386
wR_2[b] [all data]	0.0508	0.0534	0.0373	0.0766	0.1619	0.0732	0.1107

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

13. Computational details

All calculations were performed on the real systems using the Gaussian 16 package[13] and the B3PW91 hybrid functional[14] with D3 dispersion correction of Grimme with Becke–Johnson damping (DFT-*D3*(*BJ*)).[15] All stationary points involved were fully optimized in the gas phase and by taking into account dichloromethane as solvent (DCM: CH_2Cl_2, optimization or single point calculations on the gas phase's geometry) by means of SMD model.[16] The gold atom was described with the relativistic electron core potential SDD and associated basis set,[17] augmented by a set of f-orbital polarization functions.[18] The 6-31G** basis set was employed for all other atoms. Frequency calculations were undertaken to confirm the nature of the stationary points, yielding one imaginary frequency for transition states (TS), corresponding to the expected process, and all of them positive for *minima*. The connectivity of the transition states and their adjacent *minima* was confirmed by intrinsic reaction coordinate (IRC) calculations.[19]

In order to have better insight on the bonding situation in the intermediate **RC1**, Energy Decomposition Analysis (EDA)[20] was performed with Amsterdam Density Functional 2019.102 program package[21] at ZORA-BP86-D3/TZ2P level of theory on the geometries optimized from Gaussian 16 at B3PW91-D3(BJ)/SDD+f(Au) 6-31G** (other atoms) level. This analysis is based on the EDA method of Morokuma and the ETS partitioning scheme of Ziegler and Rauk. The term ΔE_{int} can be mainly decomposed into different contributions: (i) electrostatic interaction energy between the fragments (ΔV_{elstat}), (ii) destabilizing Pauli repulsion from interactions between electrons on either fragment with the same spin (ΔE_{Pauli}), (iii) stabilizing orbital interaction (ΔE_{orb}):

$$\Delta E_{int} = \Delta V_{elstat} + \Delta E_{Pauli} + \Delta E_{orb}$$

Hirshfield charges were also computed. To further characterize the interaction between the substrates and metal fragments in the transition states, the Natural Orbital Chemical Valence (NOCV) approach was used.[22] *ETS-NOCV* scheme combines *charge* rearrangement (NOCV) and bond energy *analysis*. *It* is a powerful tool to quantitatively *analyze* chemical bonds, combining the extended transition state (*ETS*) method for energy decomposition *analysis* combined with the natural orbitals for chemical valence (*NOCV*) theory. In this approach, the ΔE_{orb} term is decomposed into the contributions from different natural orbitals of chemical valence (NOCV) eigenvalues (λ_i) as follows:

$$\Delta E_{orb} = \sum_{k} \Delta E_{orb}^{k} = \sum_{k=1}^{M/2} v_k [-F_{-k,-k}^{TS} + F_{k,k}^{TS}]$$

where $F^{TS}_{k,k}$ are diagonal Kohn-Sham matrix elements defined over NOCV with respect to the transition state (TS) density. The components ΔE^{k}_{orb} provide energetic estimation of $\Delta\rho^{k}$ and allow to characterize the importance of a particular electron flow channel for the bonding between considered molecular fragments.

Electrostatic Potential map (ESP) has also been computed at B3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms) level of theory. 3D DFT ESP maps were generated for the **RC1** complex and the two fragments, the (P,C)Au(O,O) complex and the 3,4,5,6-tetrachloro 1,2-benzoquinone in their ground state, using Gaussian16 software with 803 points, an isosurface of 0.02 and ±0.1 kT/e. The ESP has been ploted using PyMOL (1.8.6.2) molecular graphic software.[23]

In the intermediate **INT**, the π-π interaction was studied using Atoms-In Molecules analysis, QTAIM,[24] thanks to the AIMALL[25] software. The density ρ(r) was determined for the Bond Critical Points (BCP) associated to the π-π interaction interactions between the 2 rings. Laplacian of the density $\nabla^2\rho(r)$ indicates the regions where the density ρ(r) is depleted or concentrated. Delocalization bond indexes (δ) between the two main atoms involved in the π-π interaction were also calculated.

For the energy profile of the catechol exchange reaction at gold(III) with tetra-chloro quinone, a benchmark of functionals was also realized, such as PBE0[26]-D3(BJ), TPSS[27]-D3(BJ), B97D[28], M06[29], CAM-B3LYP[30]-D3(BJ) and WB97XD[31].

For the singlet state (S^0) of the intermediate **INT**, optimizations have been carried out with restricted DFT (B3PW91-D3(BJ)) and unrestricted-DFT (UB3PW91-D3(BJ)) by means of the broken-symmetry formalism[32] using B3PW91-D3(BJ) functional.

The absorption spectrum of (P,C)Au(O,O)H_4 (**3a**) and (P,C)Au(O,O)Cl_4 (**3d**) were calculated at SMD(DCM)-CAM-B3LYP/SDD+f(Au), 6-31G**(other atoms) level including the solvent on the geometry optimized at B3PW91-D3(BJ)/SDD+f(Au), 6-31G**(other atoms) by using time-dependent density functional theory (TD-DFT)[33] method. Solvents effects (DCM: dichloromethane) were included by means of the universal Solvation Model based on Density (SMD).[34]

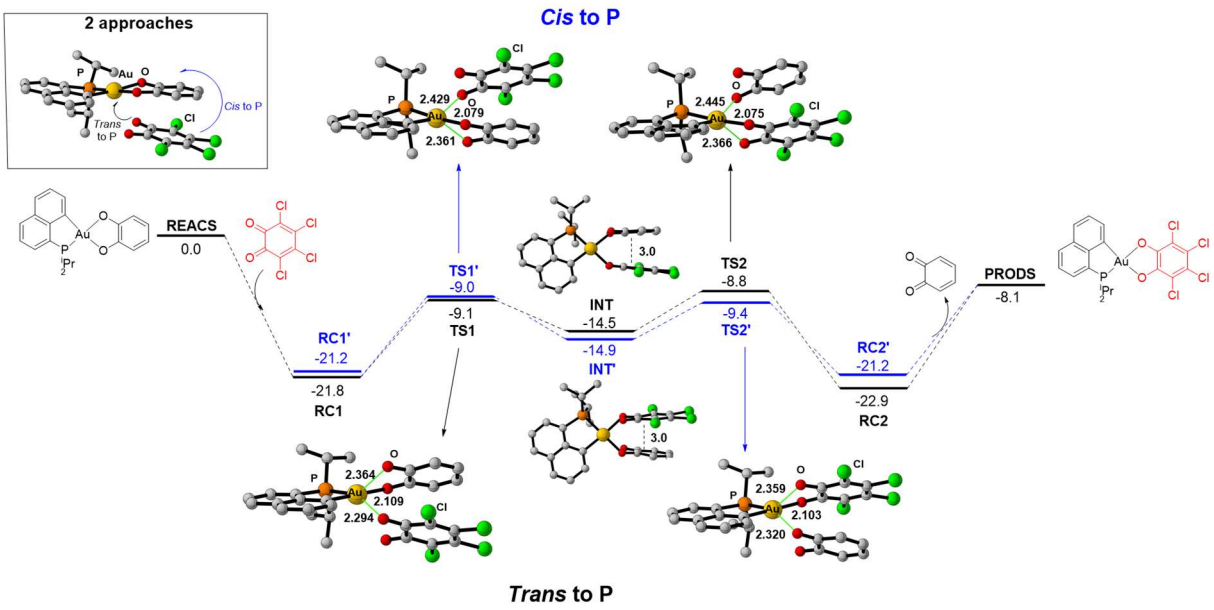


Figure S71. Energy profiles (ΔG in kcal/mol) of the catechol exchange reaction at gold(III) computed at B3PW91-D3(BJ)/SDD+f(Au), 6-31G** (other atoms) level of theory with the approach of 3,4,5,6-tetrachloro-1,2-benzoquinone in *trans* (black path) or *cis* (blue path) to P. Hydrogens omitted for clarity

Two approaches were considered for the reaction of the 3,4,5,6-tetrachloro-1,2-benzoquinone with the (P,C)Au(O,O) complex: *cis* or *trans* to P. The energy profiles were found to be very similar. The activation barriers are very close, with $\Delta G1^{\neq}$ 12.7 kcal/mol (*trans*) and 12.2 kcal/mol (*cis*) for the first Au–O bond exchange and $\Delta G2^{\neq}$ 13.0 kcal/mol (*trans*) and 11.8 kcal/mol (*cis*) for the second Au–O bond exchange.

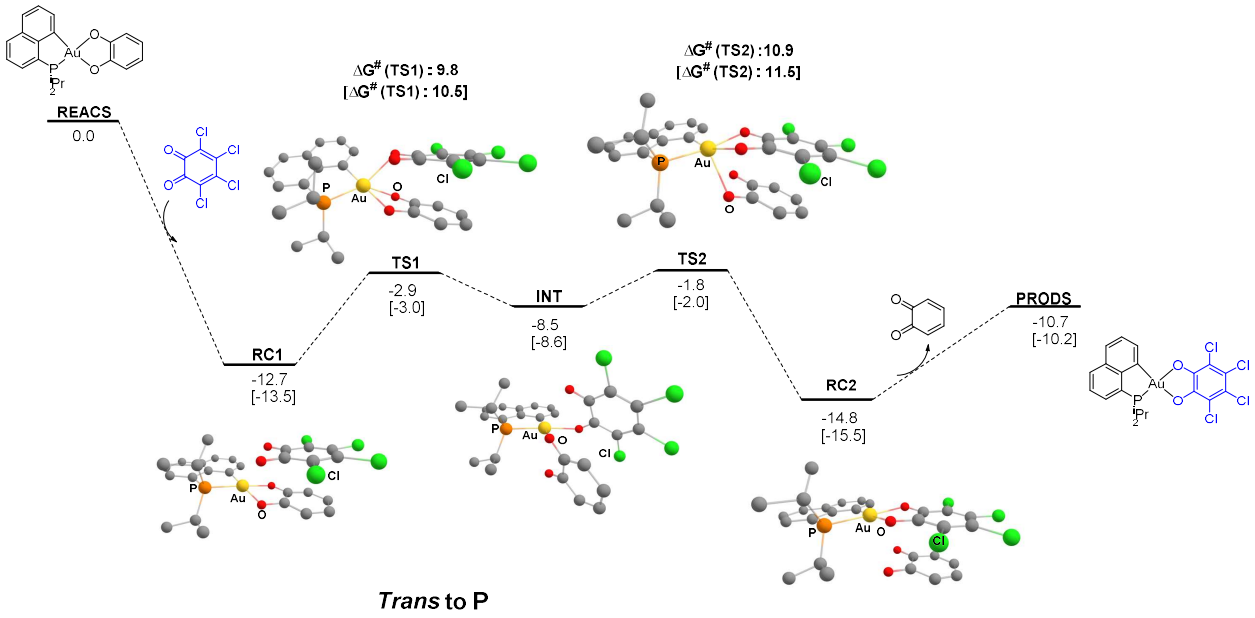


Figure S72. Energy profiles (ΔG in kcal/mol) of the catechol exchange reaction at Gold(III) computed at SMD(DCM)-B3PW91-D3(BJ)/SDD+f(Au), 6-31G** (other atoms)//B3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms) level of theory. Displacement of Au–O bond *trans* to P. For comparison, into brackets are reported the values computed at SMD(DCM)-B3PW91-D3(BJ)/SDD+f(Au), 6-31G** (other atoms). Hydrogens omitted for clarity.

In order to analyze the influence of the solvent (DCM: Dichloromethane), we computed the energy profile for the reaction of the 3,4,5,6-tetrachloro-1,2-benzoquinone with the (P,C)Au(O,O) complex (« *trans* to P » path) by including solvent upon optimization using SMD model or by single point calculations on the geometry optimized in gas phase. The two methodologies give very similar results. Comparison with the gas phase results has shown that in solvent all *minima* and transition states are shifted upwards. However, the activation barriers associated to the two Au–O bond exchanges are found very accessible and quite similar at ~ 10 kcal/mol for **TS1** (12.7 kcal/mol in gas phase) and ~11.2 kcal/mol for **TS2** (13.0 kcal/mol in gas phase).

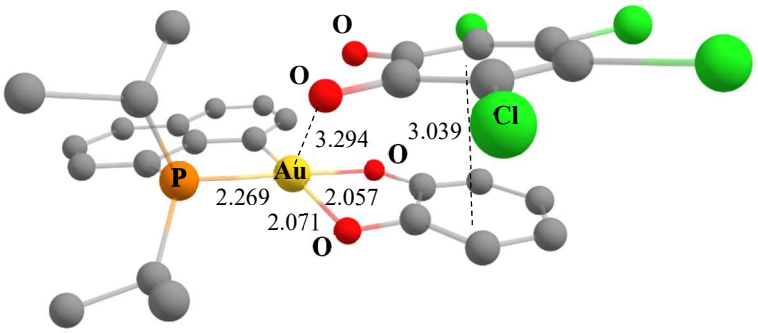


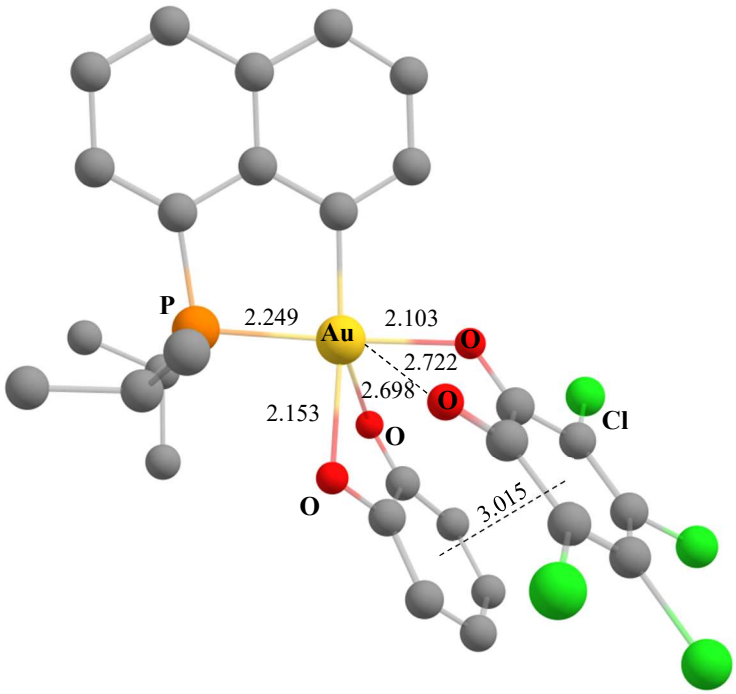
Figure S73. Main geometrical features for the charge transfer complex **RC1** computed at B3PW91-D3(BJ)/SDD+f(Au), 6-31G** (other atoms). Distances in Å. Hydrogen omitted for clarity.

We can notice a π-π stacking between the 2 rings with a distance between the centroids of each ring of 3.04 Å.

Table S2. Energy Decomposition Analysis (EDA) carried out at ZORA-BP86(D3)/TZ2VP for the complex **RC1**. Energies are in kcal/mol.

	RC1
ΔE_{Pauli}	59.88
ΔV_{elstat}	-34.89 (33.9%)[a]
ΔE_{orb}	-40.62 (39.5%)[a]
ΔE_{disp}	-27.32 (26.6 %)[a]
ΔE_{int}	-42.96
ΔE_{orb1} (ρ)	-27.32
Hirshfeld Charges[b]	0.42

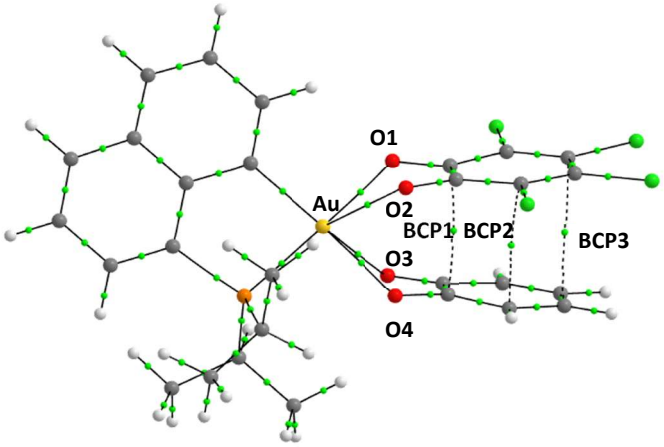
[a] Values into bracket (%) correspond to the percentage contribution to the total attractive interaction ($\Delta V_{elstat} + \Delta E_{orb} + \Delta E_{disp}$). [b] Hirshfeld charges for (P,C)Au(O,O) fragment.



It is noteworthy that optimization of **INT** has been performed with restricted DFT (B3PW91-D3(BJ)) and unrestricted-DFT (UB3PW91-D3(BJ)) by means of the broken-symmetry formalism[32] using B3PW91-D3(BJ) functional. For the U-BS formalism, the optimized structures of the restricted singlet state or that of the triplet state calculations have been taken as input structures. In all cases, the optimizations converge to the same structure, *i.e.* that of the restricted DFT calculation.

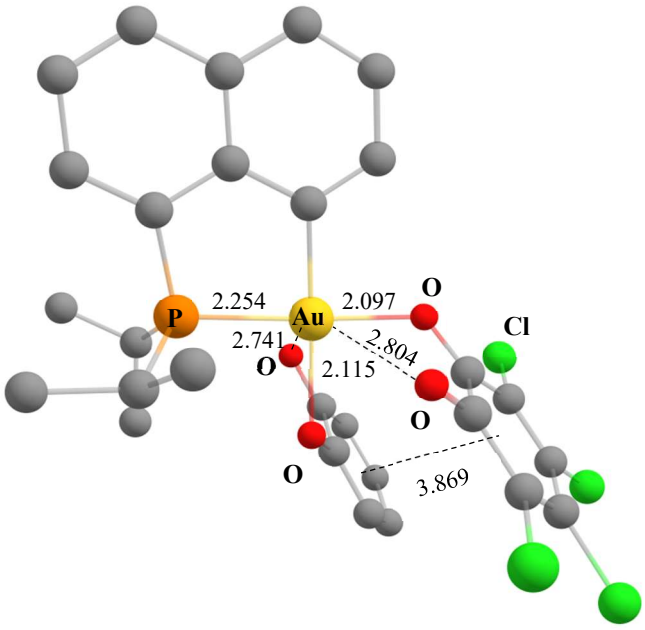
Figure S74. Main geometrical features of complex **INT** in singlet state, with 3,4,5,6-tetrachloro 1,2-catecholate moiety in *trans* to P. Main distances in Å. Calculations carried out at B3PW91-D3(BJ)/SDD+f(Au), 6-31G** (other atoms). Hydrogens omitted for clarity.

Table S3. AIM analysis for the complex **INT**. Calculations carried out at B3PW91-D3(BJ)/ SDD+f(Au),6-31G**(other atoms) level of theory.



BCP1		**BCP2**	
Distance C…C (Å)	2.706	**Distance C…C (Å)**	2.980
ρ(r)[a]	0.021	**ρ(r)[a]**	0.013
$\nabla^2\rho(r)$[b]	0.049	**$\nabla^2\rho(r)$[b]**	0.039
ε[c]	0.73	**ε[c]**	1.054
Bond index δ[d]	0.085	**Bond index δ[d]**	0.038
BCP3			
Distance C…C (Å)	3.121		
ρ(r)[a]	0.011		
$\nabla^2\rho(r)$[b]	0.028		
ε[c]	3.48		
Bond index δ[d]	0.049		
BCP (Au-O1)		**BCP (Au-O2)**	
Distance Au-O1 (Å)	2.103	**Distance Au-O2 (Å)**	2.722
ρ(r)[a]	0.095	**ρ(r)[a]**	0.027
$\nabla^2\rho(r)$[b]	0.40	**$\nabla^2\rho(r)$[b]**	0.096
ε[c]	0.06	**ε[c]**	0.039
Bond index δ[d]	0.561	**Bond index δ[d]**	0.156
BCP (Au-O3)		**BCP (Au-O4)**	
Distance Au-O3 (Å)	2.698	**Distance Au-O4 (Å)**	2.125
ρ(r)[a]	0.029	**ρ(r)[a]**	0.084
$\nabla^2\rho(r)$[b]	0.10	**$\nabla^2\rho(r)$[b]**	0.36
ε[c]	0.05	**ε[c]**	0.07
Bond index δ[d]	0.177	**Bond index δ[d]**	0.519

[a] Density at the main BCP in e.bohr^{-3}. [b] Laplacian of density at the main BCP in e.bohr^{-5}.
[c] Ellipticity. [d] Delocalization index



ΔE(S/T) : 0.9 kcal/mol (Singlet state the more stable)

Figure S75. Main geometrical features of the intermediate **INT^T** at triplet state, with 3,4,5,6-tetrachloro 1,2-catecholate moiety in *trans* to P. Main distances in Å. Calculations carried out at UB3PW91-D3(BJ)/SDD+f(Au), 6-31G** (other atoms). Hydrogens omitted for clarity. Energy gap between singlet and triplet state (ΔE(S/T)) in kcal/mol.

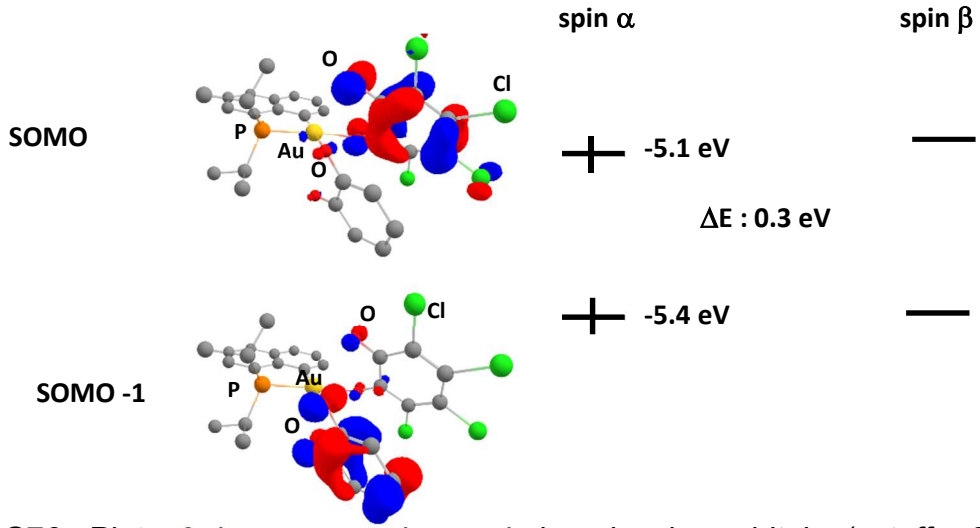


Figure S76. Plot of the two semi-occupied molecular orbitals (cutoff : 0.05) for intermediate **INT^T** at triplet state. Calculations carried out at UB3PW91-D3(BJ)/SDD+f(Au), 6-31G** (other atoms). Hydrogens omitted for clarity. Energy difference (ΔE) between the two mono-occupied MO in eV.

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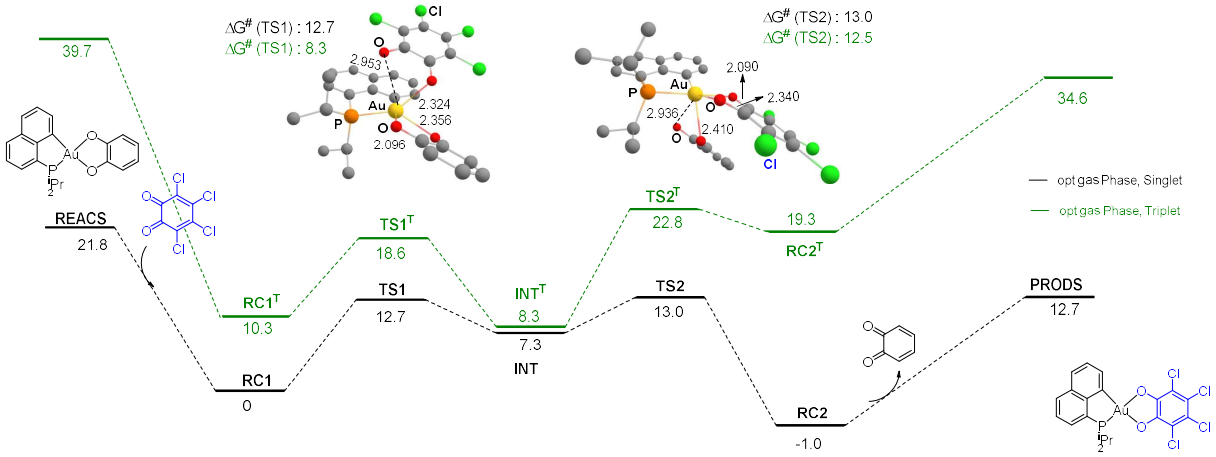
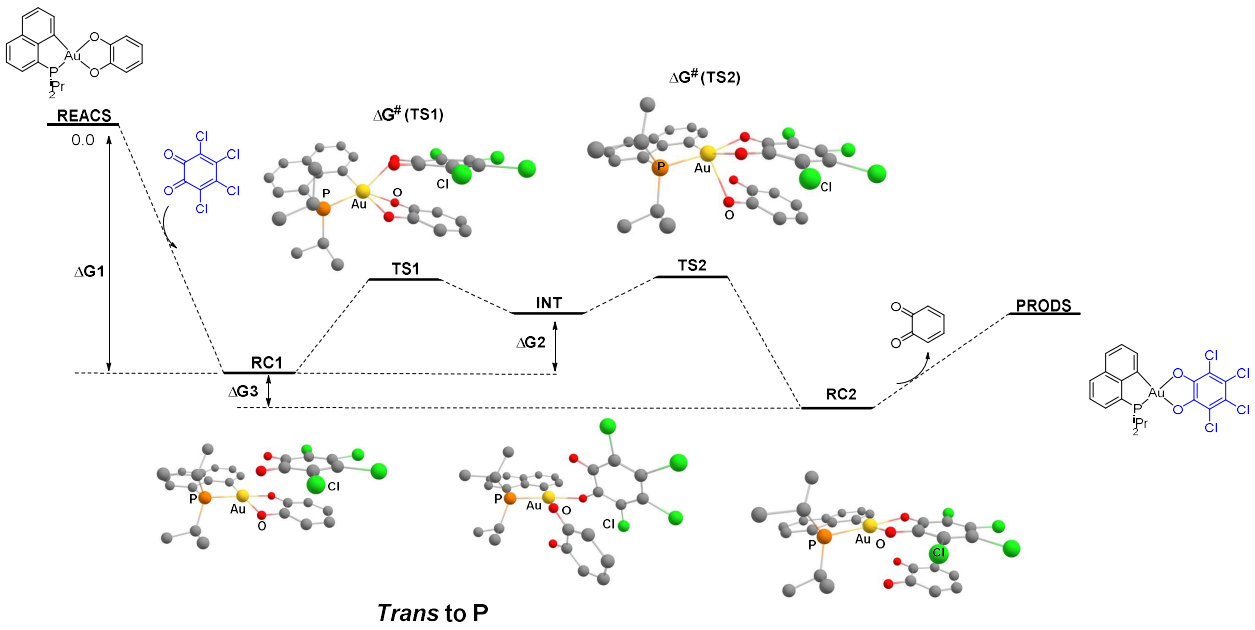


Figure S77. Energy profile (ΔG in kcal/mol) of the catechol exchange reaction at Gold(III) on the triplet PES (green path), computed at UB3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms) level of theory, with the approach of 3,4,5,6-tetrachloro-1,2-benzoquinone in *trans* to P. Energy profile for singlet state PES (black path) was plotted for comparison. Hydrogens omitted for clarity. Structures of the two transition states **TS1^{T}** and **TS2^{T}** at triplet state, with main distances in Å.



	Functional	ΔG1	ΔG# (TS1)	ΔG2	ΔG# (TS2)	ΔG3
Hybrid	**B3PW91-D3(BJ)**	-21.8	12.7	7.3	13.1	-1.0
Hybrid	**PBE0-D3(BJ)**	-16.9	13.7	8.4	13.9	-2.0
GGA	**B97D**	-22.2	12.1	6.9	13.8	1.6
Meta-GGA	**TPSS-D3(BJ)**	-22.0	10.8	5.8	11.7	2.1
Meta-GGA	**M06**	-16.0	12.3	8.0	11.7	-3.4
Long range GGA	**CAM-B3LYP-D3(BJ)**	-14.5	16.6	11.2	15.0	4.8
Long range GGA	**WB97XD**	-13.3	17.3	12.0	15.3	3.3

Figure S78. Energy profiles (ΔG in kcal/mol) of the catechol exchange reaction at Gold(III) computed at Functional/SDD+f(Au), 6-31G** (other atoms). Displacement of Au–O bond *trans* to P. Hydrogens omitted for clarity.

With all the functionals tested, the energy profile looks like very similar.

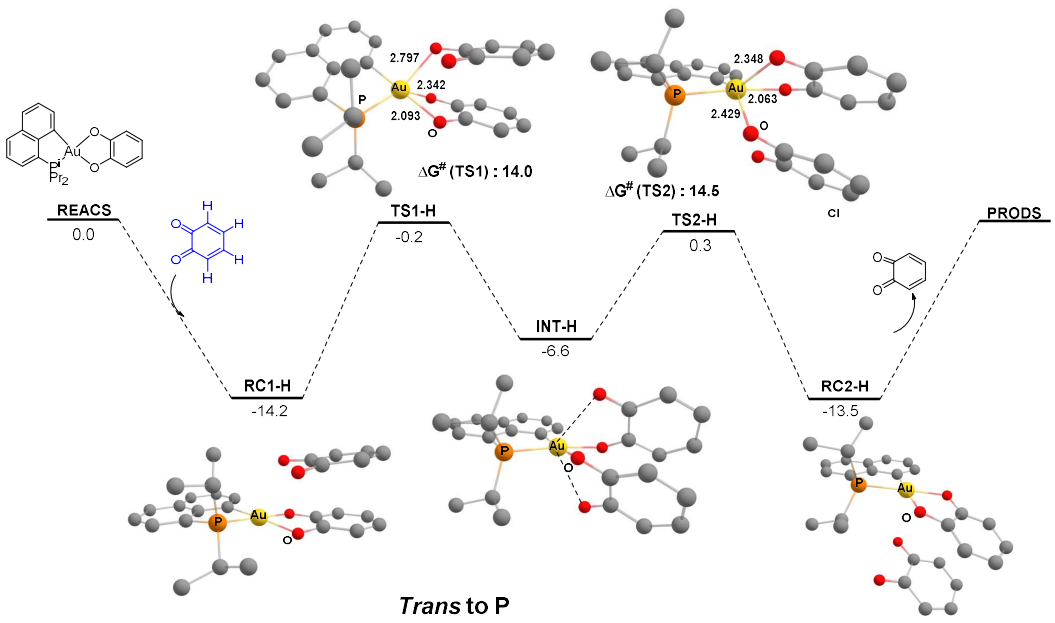


Figure S79. Energy profile (ΔG in kcal/mol) of the catechol exchange reaction with *o*-quinone at Gold(III) computed at B3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms) level of theory. Displacement of Au–O bond *trans* to P. Hydrogens omitted for clarity.

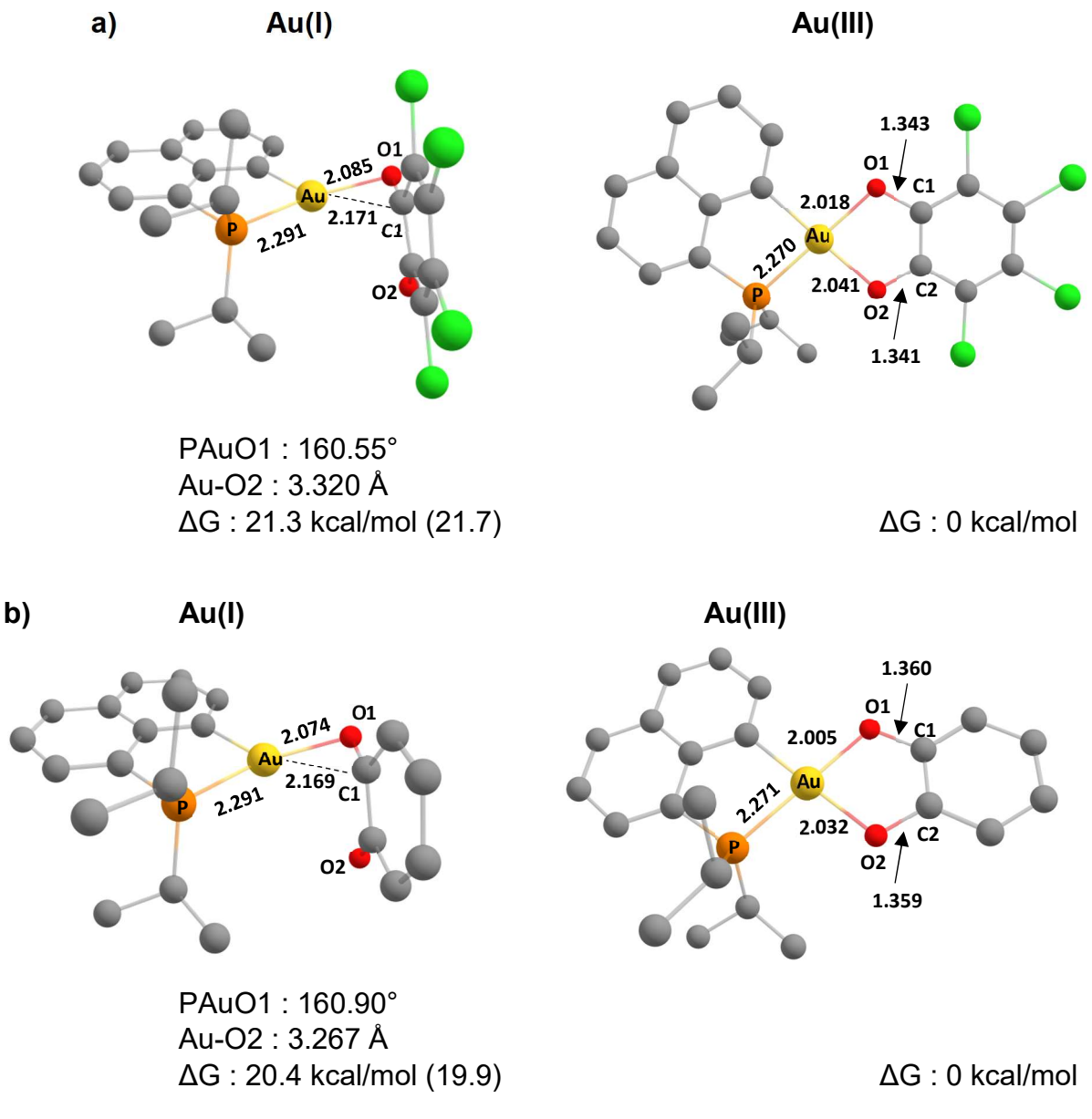


Figure S80. Relative stability (ΔG in kcal/mol) of Au(I) and Au(III) forms for (P,C)Au(O,O)Cl_4 (**a**) and (P,C)Au(O,O)H_4 (**b**) computed at B3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms) level of theory.
Into brackets values computed at SMD(DCM)-B3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms)//B3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms) level of theory.

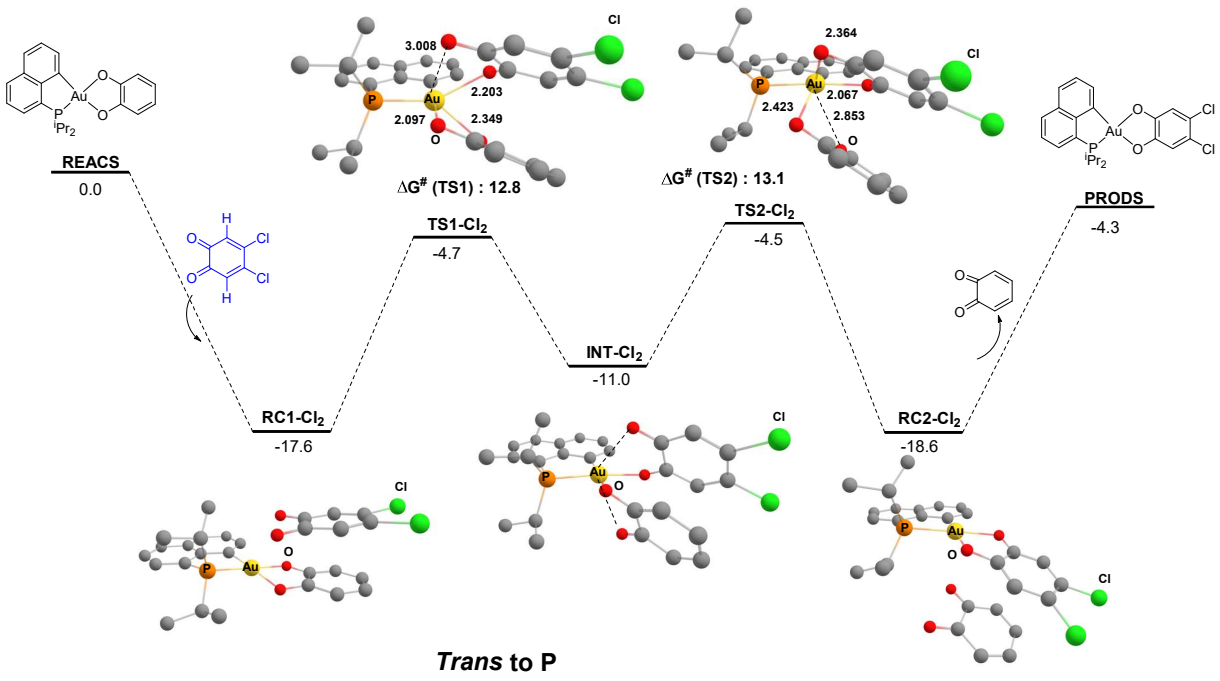
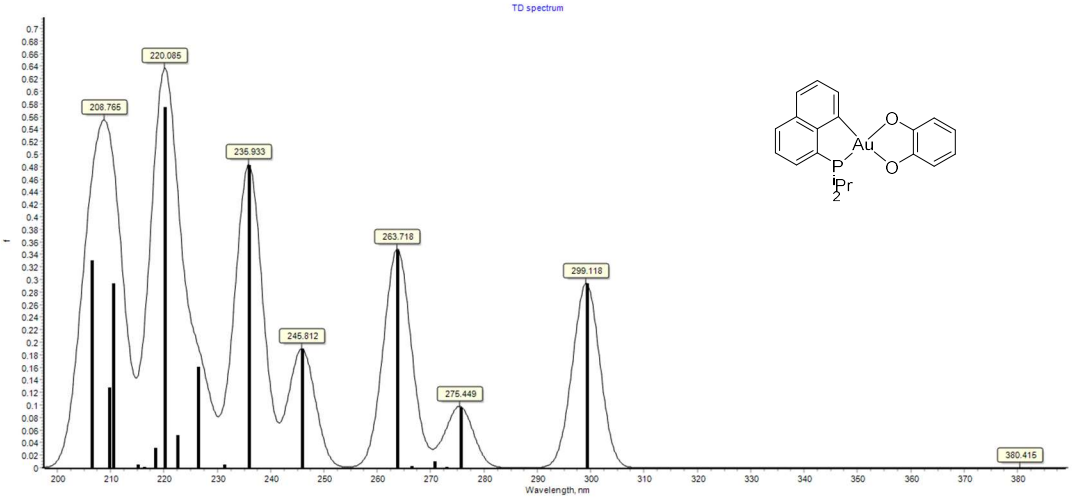


Figure S81. Energy profile (ΔG in kcal/mol) of the catechol exchange reaction at Gold(III) with 4,5-dichloro *o*-quinone computed at B3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms) level of theory. Displacement of Au–O bond *trans* to P. Hydrogens omitted for clarity.

(3a)



(3d)

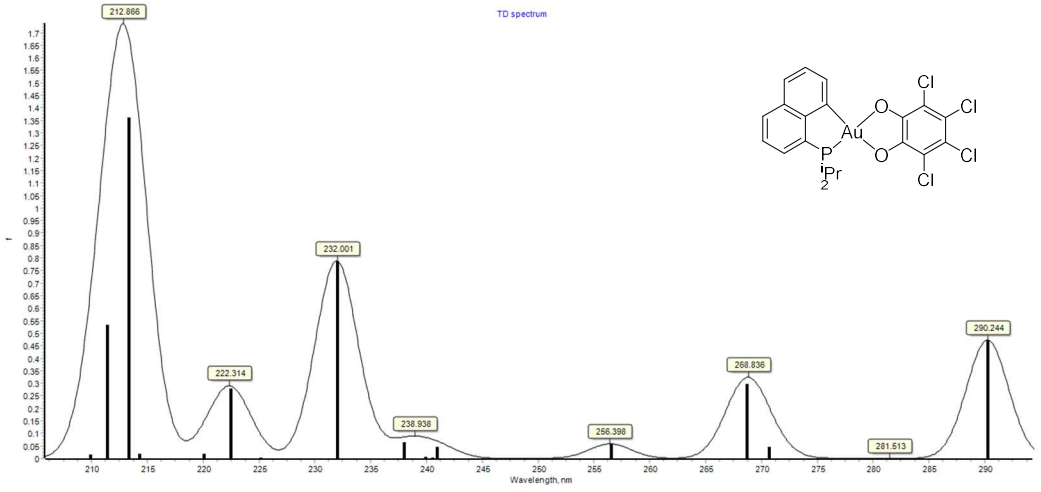


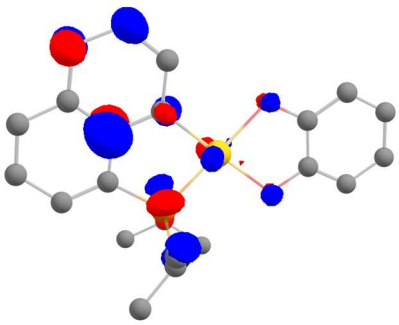
Figure S82. Simulation of the UV-Visible spectra for (P,C)Au(O,O)H_4 (**3a**) and (P,C)Au(O,O)Cl_4 (**3d**) computed by TD-DFT at SMD(DCM)-CAM-B3LYP//B3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms) level of theory.

	λ (nm)	Transition energy (eV)	f	Electronic transition
(P,C)Au(O,O)H$_4$ (3a)				
excited state 1	380.4	3.26	0.0001	HOMO → LUMO+1 LMCT
excited state 2	299.2	4.14	0.2936	mainly HOMO → LUMO (51.1 %) HOMO-2 → LUMO (34.5 %) LLCT & ILCT
excited state 3	275.5	4.50	0.0962	mainly HOMO-2 → LUMO (31.4 %) HOMO → LUMO (23.6 %) ILCT
excited state 4	273.0	4.54	0.0007	mainly HOMO-1→ LUMO+1 (41.6 %) HOMO-2→ LUMO+1 (28.1 %) LMCT
excited state 5	270.7	4.58	0.010	mainly HOMO-3 → LUMO (35.8 %) ILCT
(P,C)Au(O,O)Cl$_4$ (3d)				
excited state 1	354.8	3.49	0.0001	mainly HOMO → LUMO+1 (85.7 %) LMCT
excited state 2	290.2	4.27	0.4722	mainly HOMO → LUMO (44.6 %) HOMO-1 → LUMO (32.8 %) LLCT & ILCT
excited state 3	281.4	4.41	0.0004	mainly HOMO-1 → LUMO+1 (69.1 %) LMCT
excited state 4	275.1	4.51	0.0007	HOMO → LUMO+2 (47.7 %) mainly HOMO→ LUMO+5 (52.3 %) ILCT
excited state 5	270.6	4.58	0.045	mainly HOMO-3 → LUMO (40.2 %) HOMO-1 → LUMO+3 (26.1 %) LMCT

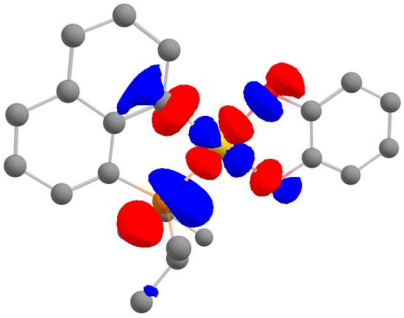
Table S4. TD-DFT calculations for (P,C)Au(O,O)H$_4$ (**3a**) and (P,C)Au(O,O)Cl$_4$ (**3d**) : absorption wavelength λ (in nm) associated to the 5 first excited states and transition energies (in eV), oscillator strength f, associated electronic transitions. Calculations carried out at SMD(DCM)-CAM-B3LYP//B3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms) level of theory. For Molecular Orbitals see Figure S81.

(P,C)Au(O,O)H_4 (**3a**)

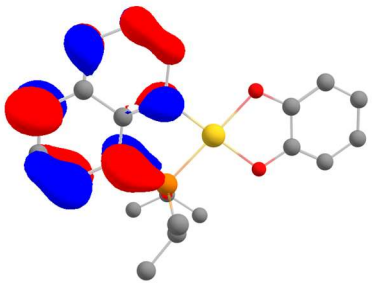
LUMO+4



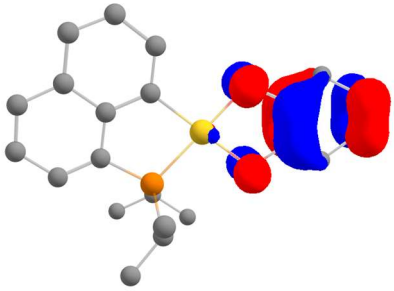
LUMO+1



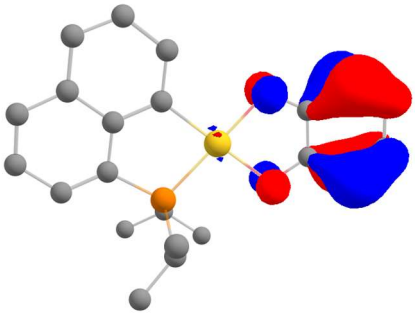
LUMO



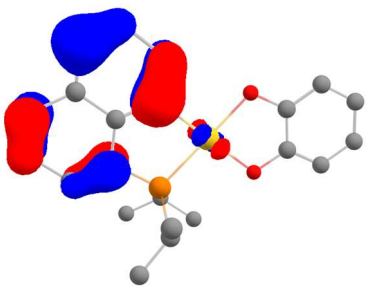
HOMO



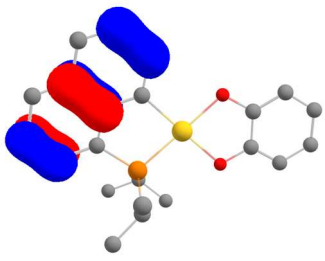
HOMO-1



HOMO-2



HOMO-3



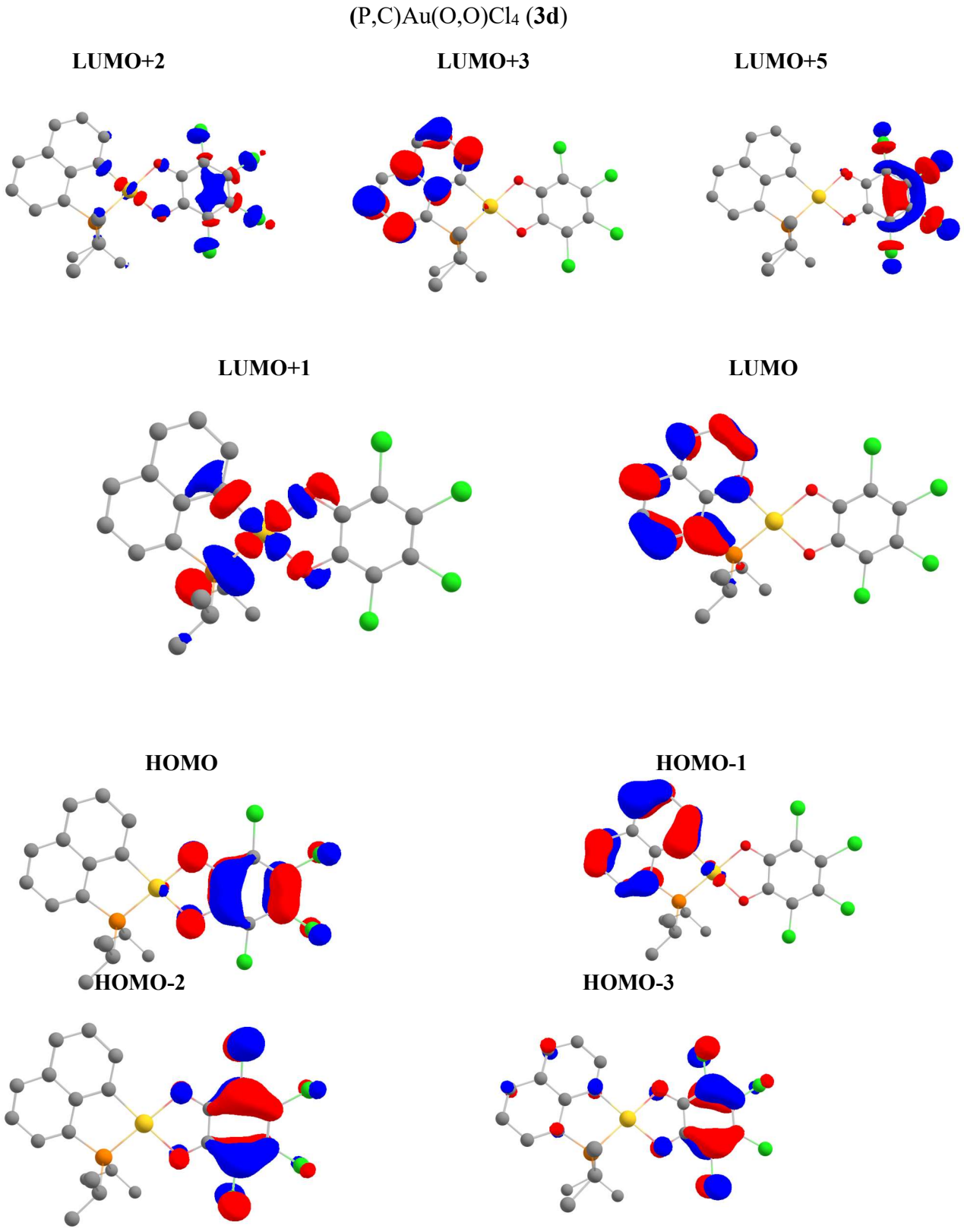


Figure S83. Main molecular orbitals (cutoff : 0.05) involved in the main transitions for UV-Visible spectra of (P,C)Au(O,O)H_4 (**3a**) and (P,C)Au(O,O)Cl_4 (**3d**), computed at SMD(DCM)-CAM-B3LYP//B3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms) level of theory.

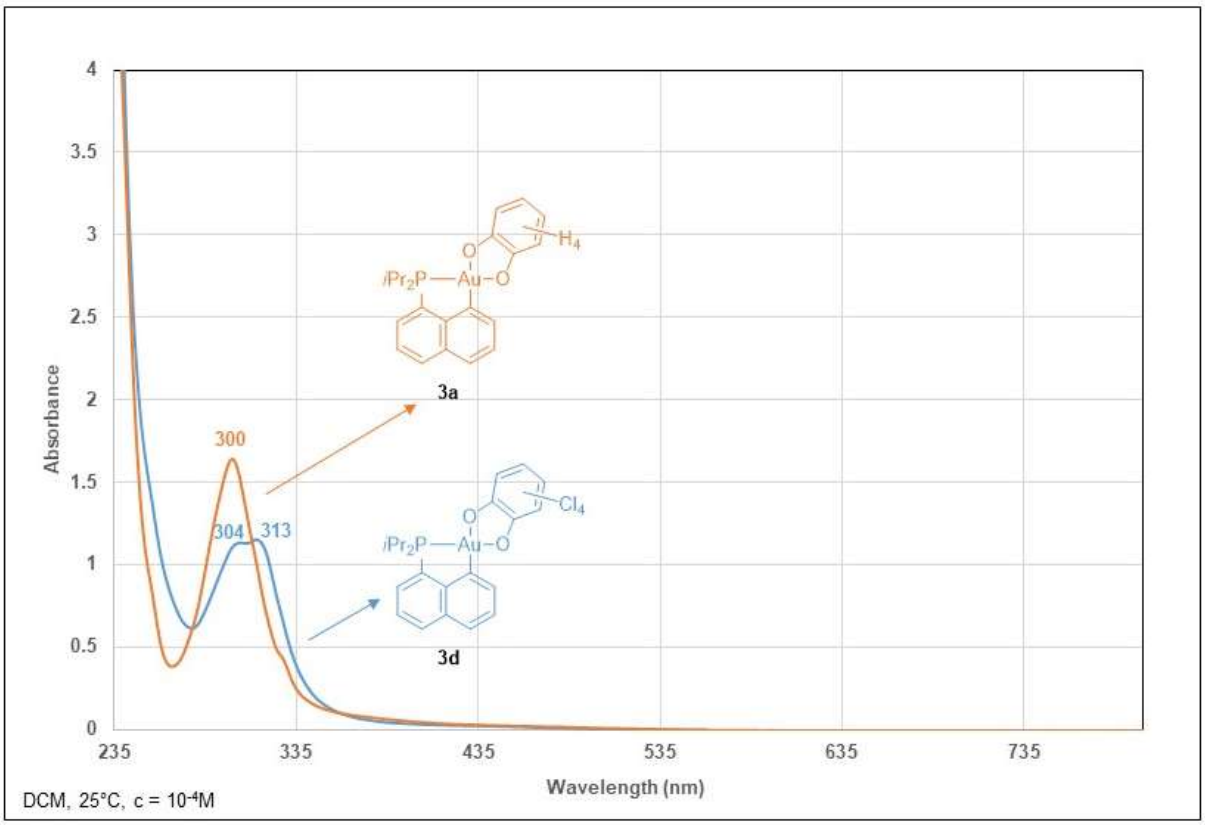
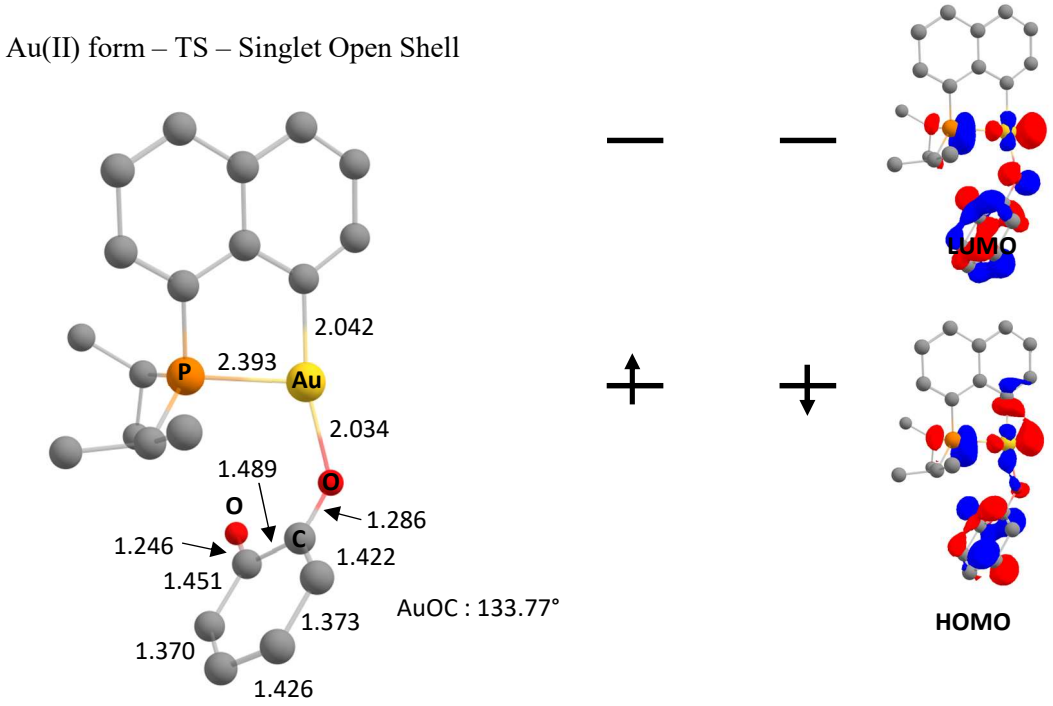


Figure S84. UV absorption spectra for complexes **3a** and **3d**.

For (P,C)Au(O,O)H$_4$ (**3a**), the Au(II) semi-quinone form has only been located as a transition state on the Singlet Open Shell Potential Energy Surface (PES), connecting the two forms Au(III) and Au(I). As *minimum*, this form converges to the Au(III) form.



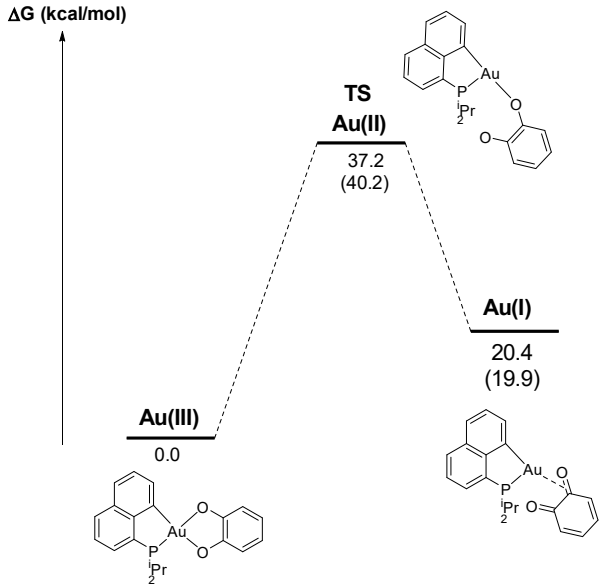


Figure S85. Au(II) semi-quinone form for (P,C)Au(O,O)H$_4$ (**3a**) localized as transition state (TS) on the singlet surface. Frontier Molecular Orbitals (cutoff :0.05). Energy profile (ΔG in kcal/mol) computed at UB3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms) level of theory. Into brackets, values at SMD(DCM)-UB3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms)//UB3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms).

For (P,C)Au(O,O)H$_4$ (**3a**), the Au(II) semi-quinone form has also been located as a *minimum* on the triplet state Potential Energy Surface (PES).

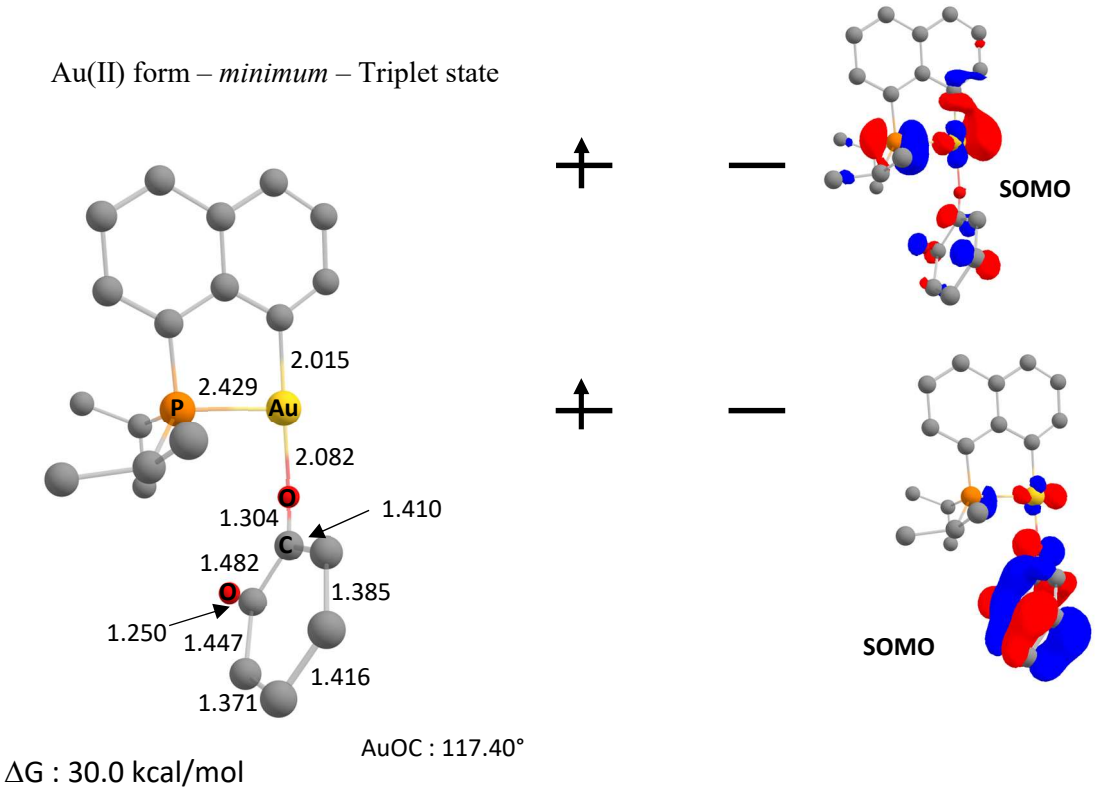


Figure S86. Au(II) semi-quinone form for (P,C)Au(O,O)H$_4$ (**3a**) localized on the triplet state Potential Energy Surface, computed at UB3PW91-D3(BJ)/SDD+f (Au), 6-31G** (other atoms) level of theory. Frontier Molecular Orbitals (cutoff :0.05). Relative energy (ΔG in kcal/mol) from closed shell singlet Au(III) form.

13. Z-matrices and energies in au

Optimization GAS PHASE, Singlet state

- Approach *trans* to P

RC1

Au	-1.054276000	-0.286323000	0.696341000
P	-2.558509000	1.268458000	0.011105000
O	0.384045000	0.977220000	1.486457000
O	0.286136000	-1.709239000	1.335534000
C	-2.467144000	-1.588989000	0.118289000
C	-4.062254000	0.277191000	-0.162875000
C	-3.779845000	-1.116885000	-0.161708000
C	-4.817999000	-2.043277000	-0.475447000
C	-6.115132000	-1.533377000	-0.730758000
H	-6.915364000	-2.233647000	-0.954988000
C	-6.369435000	-0.180635000	-0.704663000
H	-7.370185000	0.188682000	-0.905296000
C	-5.334097000	0.740784000	-0.436370000
H	-5.548883000	1.803153000	-0.454775000
C	1.492796000	0.299337000	1.697927000
C	2.706405000	0.928224000	2.033231000
C	3.828839000	0.162284000	2.286507000
C	3.759142000	-1.246264000	2.261436000
C	2.576216000	-1.897059000	1.965805000
C	1.432220000	-1.143817000	1.646786000
C	-4.502302000	-3.423456000	-0.521609000
C	-2.187663000	-2.933038000	0.042361000
H	-1.179590000	-3.284837000	0.235891000
C	-3.217603000	-3.849844000	-0.279378000
H	-5.287263000	-4.135918000	-0.758900000
H	-2.980266000	-4.908469000	-0.328982000
H	2.510116000	-2.978210000	1.929112000
H	4.652248000	-1.827999000	2.465541000
H	4.772467000	0.648814000	2.510324000
H	2.734796000	2.012189000	2.056090000
C	-2.659020000	2.609174000	1.277725000
H	-2.477452000	2.064084000	2.211995000
C	-4.017198000	3.300514000	1.380205000
C	-1.495409000	3.581401000	1.057039000
H	-0.540942000	3.056464000	0.965251000
H	-1.651769000	4.191244000	0.162494000
H	-1.431723000	4.258446000	1.914251000
H	-4.283757000	3.826377000	0.459428000
H	-3.973825000	4.045271000	2.181215000
H	-4.814785000	2.594636000	1.622880000
C	-2.142788000	1.938846000	-1.651481000
H	-1.178308000	2.432449000	-1.499194000
C	-3.188115000	2.932149000	-2.156355000
C	-1.932536000	0.774308000	-2.619364000
H	-1.109924000	0.134291000	-2.291944000
H	-2.840866000	0.172955000	-2.728183000
H	-1.676643000	1.179575000	-3.603330000
H	-4.162260000	2.452104000	-2.289419000
H	-2.871449000	3.307754000	-3.134331000
H	-3.308227000	3.795377000	-1.497055000
O	0.879591000	1.673138000	-1.112966000
O	0.646480000	-1.021960000	-1.388938000
C	1.887039000	0.975614000	-1.047310000
C	3.227928000	1.520848000	-0.874273000
C	4.324180000	0.708404000	-0.796351000
C	4.194141000	-0.733684000	-0.878153000
C	2.969968000	-1.321730000	-1.054438000
C	1.754962000	-0.529617000	-1.167806000
Cl	2.785850000	-3.023917000	-1.208813000
Cl	5.620337000	-1.700275000	-0.801108000
Cl	5.892608000	1.384776000	-0.568914000
Cl	3.338705000	3.233543000	-0.732938000

Σ of electronic & zero-point Energies -3699.299449

Σ of electronic & thermal Free Energies -3699.369066

INT

Au	-0.928909000	0.182283000	-0.142309000
P	-2.764125000	-1.115517000	-0.221464000
O	0.304641000	-1.580164000	-0.219731000
O	0.336584000	-0.123984000	-2.505470000
C	-2.212716000	1.681056000	0.228430000
C	-4.072817000	0.044215000	0.227130000
C	-3.594679000	1.373346000	0.389162000
C	-4.519846000	2.410253000	0.714526000
C	-5.882905000	2.064214000	0.885672000
H	-6.589994000	2.849220000	1.140111000
C	-6.318246000	0.766516000	0.736218000
H	-7.367336000	0.524533000	0.873172000
C	-5.409988000	-0.258063000	0.397051000
H	-5.773163000	-1.271299000	0.264761000
C	1.412054000	-1.440394000	-0.862555000
C	2.595314000	-2.119173000	-0.470898000
C	3.755470000	-1.932619000	-1.179927000
C	3.776563000	-1.141343000	-2.370158000
C	2.653947000	-0.525390000	-2.839225000
C	1.407074000	-0.637121000	-2.127595000
C	-4.035802000	3.734120000	0.853811000
C	-1.776821000	2.977863000	0.363110000
H	-0.725182000	3.207894000	0.233044000
C	-2.700398000	4.004728000	0.676073000
H	-4.735059000	4.527746000	1.100959000
H	-2.334568000	5.021923000	0.780255000
H	2.660104000	0.081915000	-3.737054000
H	4.717197000	-1.026692000	-2.900127000
H	4.673310000	-2.403600000	-0.843597000
H	2.562840000	-2.722056000	0.430222000
C	-3.001441000	-1.763789000	-1.935435000
H	-2.684513000	-0.908622000	-2.545092000
C	-4.450061000	-2.105477000	-2.280111000
C	-2.031366000	-2.917447000	-2.193964000
H	-1.009383000	-2.645036000	-1.924032000
H	-2.316635000	-3.813871000	-1.634615000
H	-2.050176000	-3.168028000	-3.258414000
H	-4.833020000	-2.934419000	-1.678182000
H	-4.498686000	-2.413094000	-3.329306000
H	-5.112923000	-1.247163000	-2.151053000
C	-2.576782000	-2.454628000	1.023247000
H	-1.689906000	-2.993693000	0.667539000
C	-3.776475000	-3.398423000	1.091709000
C	-2.250968000	-1.824304000	2.380193000
H	-1.318333000	-1.255148000	2.350637000
H	-3.059235000	-1.165609000	2.714216000
H	-2.136565000	-2.620235000	3.122432000
H	-4.670632000	-2.875877000	1.443600000
H	-3.561368000	-4.195603000	1.809907000
H	-4.000133000	-3.870309000	0.131958000
O	0.780496000	-0.090942000	1.958798000

O	0.709047000	1.498388000	-0.234993000
C	1.853989000	0.178742000	1.393757000
C	3.140818000	-0.307541000	1.832531000
C	4.301757000	0.034848000	1.177090000
C	4.268662000	0.895828000	0.035284000
C	3.062763000	1.414510000	-0.416209000
C	1.836666000	1.022494000	0.175373000
Cl	2.997929000	2.557475000	-1.707605000
Cl	5.748926000	1.374894000	-0.713224000
Cl	5.818804000	-0.599984000	1.706014000
Cl	3.136122000	-1.369972000	3.190609000

Σ of electronic & zero-point Energies -3699.287541

Σ of electronic & thermal Free Energies -3699.357405

RC2

Au	0.913419000	0.368754000	-0.522423000
P	2.570582000	-1.162975000	-0.299973000
O	-0.926324000	-2.708243000	2.042236000
O	-0.012678000	-0.130022000	2.062567000
C	2.333915000	1.693097000	-0.019216000
C	3.921148000	-0.163170000	0.365787000
C	3.617823000	1.225825000	0.379906000
C	4.614446000	2.154956000	0.802280000
C	5.875730000	1.649297000	1.203450000
H	6.637563000	2.351281000	1.531800000
C	6.143203000	0.298951000	1.186831000
H	7.114890000	-0.067397000	1.502516000
C	5.162575000	-0.622074000	0.760507000
H	5.392575000	-1.681545000	0.754360000
C	-1.734004000	-1.793430000	2.129573000
C	-3.170419000	-2.000757000	2.266667000
C	-4.005127000	-0.942489000	2.378577000
C	-3.527190000	0.425798000	2.365551000
C	-2.211964000	0.725008000	2.237444000
C	-1.224851000	-0.336614000	2.128801000
C	4.296703000	3.535553000	0.805856000
C	2.057271000	3.040411000	-0.000915000
H	1.071588000	3.393192000	-0.287948000
C	3.050199000	3.961337000	0.412611000
H	5.050648000	4.248843000	1.126513000
H	2.811715000	5.020835000	0.421384000
H	-1.848605000	1.746992000	2.209382000
H	-4.259090000	1.223341000	2.446471000
H	-5.075767000	-1.103763000	2.460420000
H	-3.527757000	-3.024337000	2.248962000
C	1.999302000	-2.524508000	0.797614000
H	1.300714000	-2.010487000	1.471724000
C	3.104017000	-3.174886000	1.626777000
C	1.182056000	-3.525677000	-0.022228000
H	0.386504000	-3.026552000	-0.581369000
H	1.809263000	-4.106318000	-0.706700000
H	0.695943000	-4.215588000	0.670586000
H	3.840385000	-3.700407000	1.010398000
H	2.642145000	-3.913572000	2.288736000
H	3.625888000	-2.447477000	2.252903000
C	3.083274000	-1.789613000	-1.957063000
H	2.187934000	-2.302165000	-2.329510000
C	4.245981000	-2.778418000	-1.875626000
C	3.405948000	-0.608596000	-2.872993000
H	2.550519000	0.062505000	-2.985449000
H	4.246130000	-0.026046000	-2.482402000
H	3.682219000	-0.980207000	-3.864403000
H	5.150468000	-2.287276000	-1.505323000
H	4.465664000	-3.161333000	-2.877085000
H	4.024407000	-3.634239000	-1.234140000
O	-0.607858000	-0.943979000	-0.993428000
O	-0.610621000	1.728147000	-0.659073000
C	-1.767209000	-0.329204000	-0.848525000
C	-2.985308000	-1.024563000	-0.862764000
C	-4.195674000	-0.340627000	-0.707102000
C	-4.197086000	1.059068000	-0.563580000
C	-2.990791000	1.769468000	-0.586707000
C	-1.771128000	1.093760000	-0.698132000
Cl	-2.946932000	3.482699000	-0.353705000
Cl	-5.689942000	1.904991000	-0.348419000
Cl	-5.684986000	-1.219279000	-0.704175000
Cl	-2.931786000	-2.737813000	-1.087202000

Σ of electronic & zero-point Energies -3699.300346

Σ of electronic & thermal Free Energies -3699.370703

TS1

Au	0.965078000	0.216340000	0.344523000
P	2.758917000	-1.146900000	0.253179000
O	-0.353675000	-1.319985000	0.934074000
O	-0.413579000	1.172110000	2.009479000
C	2.254476000	1.632907000	-0.240192000
C	4.083808000	-0.025540000	-0.245138000
C	3.622726000	1.302537000	-0.443530000
C	4.543847000	2.309785000	-0.858202000
C	5.892621000	1.933296000	-1.072228000
H	6.601029000	2.693841000	-1.389522000
C	6.312442000	0.634348000	-0.889203000
H	7.349930000	0.368064000	-1.064325000
C	5.404720000	-0.361369000	-0.470240000
H	5.755529000	-1.377495000	-0.327689000
C	-1.462541000	-0.869597000	1.441496000
C	-2.629069000	-1.668263000	1.497482000
C	-3.789080000	-1.148876000	2.023817000
C	-3.817557000	0.153920000	2.593116000
C	-2.701904000	0.948039000	2.606101000
C	-1.480805000	0.485507000	2.026948000
C	4.066059000	3.631232000	-1.037596000
C	1.818522000	2.922853000	-0.426079000
H	0.770590000	3.165262000	-0.285329000
C	2.740243000	3.923378000	-0.821840000
H	4.760965000	4.405697000	-1.349350000
H	2.379252000	4.937949000	-0.962101000
H	-2.710735000	1.948431000	3.022847000
H	-4.748963000	0.524878000	3.009314000
H	-4.697802000	-1.741796000	2.008852000
H	-2.591613000	-2.659883000	1.059468000
C	3.089273000	-1.911319000	1.904495000
H	2.874724000	-1.078054000	2.585392000
C	4.538577000	-2.347136000	2.118315000
C	2.077460000	-3.027855000	2.173536000
H	1.052566000	-2.695911000	1.988154000
H	2.276549000	-3.905388000	1.551473000
H	2.159007000	-3.338606000	3.219373000
H	4.837624000	-3.141280000	1.428995000
H	4.639872000	-2.740139000	3.134871000
H	5.233854000	-1.511846000	2.011769000
C	2.453732000	-2.398228000	-1.061969000
H	1.494977000	-2.846044000	-0.770841000
C	3.541058000	-3.469814000	-1.142762000

C	2.268085000	-1.668001000	-2.393770000
H	1.436549000	-0.962329000	-2.346365000
H	3.182445000	-1.141620000	-2.684653000
H	2.034375000	-2.403559000	-3.168901000
H	4.509030000	-3.032664000	-1.406050000
H	3.278698000	-4.179059000	-1.933767000
H	3.652050000	-4.035646000	-0.215410000
O	-0.793082000	-1.043868000	-1.667781000
O	-0.712811000	1.456646000	-0.609854000
C	-1.852099000	-0.511138000	-1.320426000
C	-3.147091000	-1.154968000	-1.429629000
C	-4.302406000	-0.516750000	-1.053538000
C	-4.267471000	0.821871000	-0.531872000
C	-3.067264000	1.489719000	-0.397227000
C	-1.823285000	0.856911000	-0.720415000
Cl	-2.996289000	3.126949000	0.138389000
Cl	-5.749815000	1.614306000	-0.138896000
Cl	-5.822950000	-1.325679000	-1.174407000
Cl	-3.146990000	-2.772285000	-2.027159000

Σ of electronic & zero-point Energies -3699.280691

Σ of electronic & thermal Free Energies -3699.348825

TS2

Au	0.886419000	0.181130000	-0.169819000
P	2.666108000	-1.137116000	0.258501000
O	-0.368128000	-1.542560000	1.027113000
O	-0.181810000	0.828270000	2.347152000
C	2.262630000	1.620557000	-0.433730000
C	4.050960000	-0.070833000	-0.210739000
C	3.637429000	1.262639000	-0.470061000
C	4.615584000	2.263660000	-0.748462000
C	5.975249000	1.869651000	-0.799606000
H	6.726817000	2.621700000	-1.024079000
C	6.351850000	0.566018000	-0.565435000
H	7.399932000	0.287037000	-0.606223000
C	5.387668000	-0.415243000	-0.252388000
H	5.710194000	-1.425323000	-0.028131000
C	-1.406224000	-1.036939000	1.534076000
C	-2.683845000	-1.688289000	1.492252000
C	-3.782111000	-1.085820000	2.033799000
C	-3.686950000	0.183152000	2.700849000
C	-2.505429000	0.845784000	2.817589000
C	-1.292748000	0.287845000	2.260044000
C	4.183932000	3.596997000	-0.954372000
C	1.869524000	2.923338000	-0.615892000
H	0.818166000	3.185496000	-0.566328000
C	2.848580000	3.913411000	-0.877080000
H	4.923515000	4.363449000	-1.167178000
H	2.524187000	4.939111000	-1.025126000
H	-2.428713000	1.810906000	3.305516000
H	-4.594685000	0.622202000	3.104009000
H	-4.752394000	-1.567133000	1.964057000
H	-2.744025000	-2.641947000	0.978745000
C	2.745552000	-1.533428000	2.072983000
H	2.138869000	-0.727317000	2.503489000
C	4.162816000	-1.456738000	2.638426000
C	2.065223000	-2.865868000	2.392555000
H	1.051423000	-2.902714000	1.991913000
H	2.639200000	-3.716628000	2.013306000
H	2.002836000	-2.970944000	3.480115000
H	4.814772000	-2.226564000	2.212879000
H	4.117423000	-1.626819000	3.718604000
H	4.625706000	-0.482873000	2.467842000
C	2.596326000	-2.658454000	-0.770305000
H	1.739411000	-3.200543000	-0.351976000
C	3.861683000	-3.511143000	-0.658761000
C	2.282288000	-2.282045000	-2.219900000
H	1.301234000	-1.810033000	-2.306475000
H	3.042724000	-1.606283000	-2.625215000
H	2.278728000	-3.189460000	-2.831859000
H	4.696911000	-3.031373000	-1.175970000
H	3.687044000	-4.476272000	-1.143811000
H	4.158176000	-3.708696000	0.374822000
O	-0.743148000	-0.983576000	-1.429361000
O	-0.699501000	1.500039000	-0.392830000
C	-1.855193000	-0.432004000	-1.155263000
C	-3.119380000	-1.055891000	-1.378056000
C	-4.301120000	-0.428477000	-1.021627000
C	-4.275514000	0.862906000	-0.431875000
C	-3.064841000	1.530814000	-0.255365000
C	-1.845609000	0.899104000	-0.563142000
Cl	-3.002857000	3.136778000	0.376428000
Cl	-5.757101000	1.637343000	0.003655000
Cl	-5.812895000	-1.237166000	-1.238009000
Cl	-3.099232000	-2.643845000	-2.054099000

Σ of electronic & zero-point Energies -3699.278583

Σ of electronic & thermal Free Energies -3699.348275

Quinone-H4

O	-1.726213000	-1.382062000	0.000028000
O	-1.726228000	1.382050000	0.000109000
C	-0.671058000	-0.777455000	-0.000106000
C	0.635929000	-1.450332000	-0.000187000
C	1.775150000	-0.729354000	-0.000106000
C	1.775145000	0.729366000	0.000093000
C	0.635919000	1.450336000	0.000168000
C	-0.671067000	0.777452000	-0.000066000
H	0.631822000	2.535745000	0.000348000
H	2.737881000	1.233428000	0.000206000
H	2.737890000	-1.233410000	-0.000148000
H	0.631836000	-2.535741000	-0.000285000

Σ of electronic & zero-point Energies -381.231414

Σ of electronic & thermal Free Energies -381.262127

Quinone-Cl4

O	-1.363906000	2.780192000	0.000061000
O	1.363899000	2.780194000	-0.000052000
C	-0.773888000	1.724969000	0.000330000
C	-1.455057000	0.415156000	0.000117000
C	-0.738189000	-0.740041000	0.000004000
C	0.738191000	-0.740040000	-0.000007000
C	1.455056000	0.415159000	-0.000111000
C	0.773885000	1.724970000	-0.000321000
Cl	3.165463000	0.452346000	-0.000146000
Cl	1.540903000	-2.254817000	0.000048000
Cl	-1.540898000	-2.254819000	-0.000065000
Cl	-3.165464000	0.452341000	0.000154000

Σ of electronic & zero-point Energies -2219.434972

Σ of electronic & thermal Free Energies -2219.473994

(P,C)Au(O,O)-H$_4$

Au	0.600926000	0.258823000	-0.051937000
P	-1.112069000	-1.231745000	-0.041248000
O	2.089770000	-1.121392000	0.036671000
O	2.101601000	1.587674000	-0.066670000
C	-0.861160000	1.645826000	-0.101443000
C	-2.563846000	-0.156184000	-0.045851000
C	-2.225108000	1.226912000	-0.077295000
C	-3.273645000	2.196098000	-0.079941000
C	-4.614368000	1.739927000	-0.040658000
H	-5.414095000	2.475969000	-0.040455000
C	-4.914180000	0.396700000	-0.001969000
H	-5.948719000	0.069667000	0.029281000
C	-3.882918000	-0.565891000	-0.006174000
H	-4.137710000	-1.619930000	0.015661000
C	3.286498000	-0.478018000	0.036139000
C	4.491910000	-1.173959000	0.087509000
C	5.700469000	-0.474310000	0.089771000
C	5.703970000	0.917962000	0.041265000
C	4.499988000	1.623516000	-0.010807000
C	3.291311000	0.931499000	-0.014203000
C	-2.929333000	3.569681000	-0.117158000
C	-0.568952000	2.991318000	-0.136136000
H	0.470004000	3.306919000	-0.151881000
C	-1.608705000	3.951179000	-0.146126000
H	-3.722763000	4.311801000	-0.120726000
H	-1.351086000	5.006087000	-0.174286000
H	4.480209000	2.708550000	-0.049781000
H	6.643657000	1.462763000	0.042945000
H	6.637304000	-1.022553000	0.130246000
H	4.466181000	-2.259307000	0.126119000
C	-1.044624000	-2.295694000	-1.549847000
H	-0.761790000	-1.568048000	-2.321656000
C	-2.371447000	-2.931937000	-1.958210000
C	0.098861000	-3.302619000	-1.396883000
H	1.027200000	-2.812555000	-1.083974000
H	-0.152280000	-4.078346000	-0.666386000
H	0.273177000	-3.798317000	-2.356643000
H	-2.733568000	-3.647614000	-1.215508000
H	-2.228351000	-3.478155000	-2.896005000
H	-3.146964000	-2.180536000	-2.123337000
C	-1.047841000	-2.231037000	1.505856000
H	-0.056758000	-2.699656000	1.452841000
C	-2.126629000	-3.306730000	1.613969000
C	-1.075838000	-1.274878000	2.700679000
H	-0.257649000	-0.551160000	2.657409000
H	-2.020414000	-0.723598000	2.741873000
H	-0.974217000	-1.847525000	3.627421000
H	-3.127048000	-2.864680000	1.631954000
H	-1.995304000	-3.854776000	2.552373000
H	-2.078595000	-4.032279000	0.799323000

Σ of electronic & zero-point Energies -1479.805497

Σ of electronic & thermal Free Energies -1479.860282

(P,C)Au(O,O)-Cl$_4$

Au	-0.534808000	0.234662000	-0.055334000
P	-2.281823000	-1.214519000	-0.051447000
O	0.935903000	-1.179724000	0.005529000
O	1.021584000	1.518457000	-0.058471000
C	-1.959405000	1.654073000	-0.081530000
C	-3.705599000	-0.104454000	-0.051106000
C	-3.331763000	1.269026000	-0.064002000
C	-4.352349000	2.266519000	-0.054341000
C	-5.704632000	1.845209000	-0.023722000
H	-6.484859000	2.601615000	-0.014905000
C	-6.039643000	0.509709000	-0.004052000
H	-7.082424000	0.209914000	0.020706000
C	-5.034899000	-0.480395000	-0.018909000
H	-5.317875000	-1.527377000	-0.010834000
C	2.132624000	-0.575446000	0.002637000
C	3.323015000	-1.303605000	0.028893000
C	4.563238000	-0.647157000	0.031453000
C	4.607002000	0.751990000	0.006656000
C	3.411519000	1.487852000	-0.022620000
C	2.177202000	0.835743000	-0.026398000
C	-3.969022000	3.630360000	-0.071625000
C	-1.624517000	2.989208000	-0.096328000
H	-0.577955000	3.279080000	-0.107175000
C	-2.638805000	3.976811000	-0.093444000
H	-4.741193000	4.394367000	-0.065759000
H	-2.351767000	5.024084000	-0.106177000
C	-2.221930000	-2.276810000	-1.560859000
H	-1.910204000	-1.558597000	-2.330323000
C	-3.566311000	-2.869694000	-1.978963000
C	-1.114708000	-3.322509000	-1.397639000
H	-0.168186000	-2.871543000	-1.082770000
H	-1.397176000	-4.088364000	-0.668575000
H	-0.953742000	-3.824893000	-2.355988000
H	-3.957712000	-3.571314000	-1.237743000
H	-3.431607000	-3.422991000	-2.913559000
H	-4.315206000	-2.093997000	-2.153938000
C	-2.226406000	-2.211697000	1.496054000
H	-1.249631000	-2.708661000	1.435812000
C	-3.335617000	-3.256561000	1.605096000
C	-2.223278000	-1.257015000	2.692359000
H	-1.383603000	-0.558174000	2.651369000
H	-3.150625000	-0.677657000	2.737427000
H	-2.136947000	-1.835055000	3.617044000
H	-4.322566000	-2.785645000	1.631199000
H	-3.213696000	-3.811668000	2.540313000
H	-3.312648000	-3.980020000	0.787570000
Cl	3.415852000	3.218871000	-0.056267000
Cl	6.126826000	1.579141000	0.010254000
Cl	6.026808000	-1.569957000	0.065220000
Cl	3.211844000	-3.033372000	0.056513000

Σ of electronic & zero-point Energies -3318.022345

Σ of electronic & thermal Free Energies -3318.084978

- Approach *cis* to P

RC1'

Au	-1.086789000	0.231231000	0.838869000
P	-2.553006000	-1.294866000	0.018262000
O	1.500356000	-2.327896000	-1.197359000
O	0.422320000	0.149217000	-1.425800000
C	-2.419492000	1.577881000	0.175272000
C	-3.747038000	-0.243919000	-0.840729000
C	-3.531769000	1.140254000	-0.597562000
C	-4.441075000	2.095251000	-1.142265000
C	-5.528237000	1.620666000	-1.916975000
H	-6.221048000	2.343507000	-2.339504000
C	-5.712264000	0.275203000	-2.142641000
H	-6.549068000	-0.066634000	-2.743468000
C	-4.819250000	-0.672467000	-1.598637000

H	-4.980587000	-1.727589000	-1.788382000
C	2.233531000	-1.353518000	-1.108932000
C	3.682148000	-1.441656000	-0.961483000
C	4.458722000	-0.320369000	-0.879354000
C	3.876666000	1.008667000	-0.943940000
C	2.524828000	1.181139000	-1.079337000
C	1.628525000	0.040180000	-1.202486000
C	-4.212338000	3.470390000	-0.890685000
C	-2.223855000	2.921296000	0.395428000
H	-1.360830000	3.253452000	0.963255000
C	-3.130805000	3.867001000	-0.140670000
H	-4.900099000	4.203080000	-1.303228000
H	-2.957177000	4.923243000	0.043179000
Cl	1.802573000	2.733412000	-1.215574000
Cl	4.921665000	2.377743000	-0.895859000
Cl	6.166076000	-0.459002000	-0.694115000
Cl	4.338122000	-3.027502000	-0.832888000
C	-1.660376000	-2.491885000	-1.057591000
H	-0.828846000	-1.885511000	-1.441038000
C	-2.479249000	-3.025566000	-2.230030000
C	-1.048456000	-3.592561000	-0.188785000
H	-0.446215000	-3.166939000	0.617488000
H	-1.809354000	-4.262126000	0.225549000
H	-0.370842000	-4.182076000	-0.809966000
H	-3.331413000	-3.632391000	-1.907389000
H	-1.831553000	-3.665993000	-2.836450000
H	-2.845533000	-2.220351000	-2.870949000
C	-3.439540000	-2.145538000	1.394924000
H	-2.646999000	-2.695864000	1.916238000
C	-4.500688000	-3.123798000	0.891691000
C	-4.034666000	-1.102255000	2.341160000
H	-3.265931000	-0.442721000	2.752059000
H	-4.774461000	-0.481534000	1.826153000
H	-4.535136000	-1.606697000	3.173357000
H	-5.303611000	-2.592989000	0.372151000
H	-4.947495000	-3.644034000	1.744694000
H	-4.089455000	-3.880331000	0.219493000
O	0.375039000	-1.086962000	1.478694000
O	0.252416000	1.605434000	1.542128000
C	1.493001000	-0.416223000	1.679901000
C	2.726783000	-1.060881000	1.891143000
C	3.860693000	-0.306964000	2.142014000
C	3.786823000	1.095299000	2.200742000
C	2.579810000	1.759501000	2.027936000
C	1.425125000	1.025579000	1.741828000
H	2.513752000	2.841061000	2.062035000
H	4.689595000	1.670067000	2.381396000
H	4.816642000	-0.802661000	2.274235000
H	2.757319000	-2.143859000	1.837032000

Σ of electronic & zero-point Energies -3699.298217

Σ of electronic & thermal Free Energies -3699.368091

TS1'

Au	0.972943000	-0.255752000	0.446472000
P	2.475232000	1.204677000	-0.392148000
O	-0.634725000	1.335740000	-0.437620000
O	-0.709222000	-1.084736000	-1.633311000
C	2.488729000	-1.571285000	0.355658000
C	4.014336000	0.255759000	-0.311627000
C	3.793074000	-1.102203000	0.039782000
C	4.890391000	-2.014547000	0.053821000
C	6.179754000	-1.510876000	-0.246815000
H	7.023338000	-2.195579000	-0.227251000
C	6.373753000	-0.185596000	-0.565994000
H	7.369891000	0.178148000	-0.797023000
C	5.283442000	0.708328000	-0.614641000
H	5.452304000	1.737556000	-0.909045000
C	-1.749727000	0.773760000	-0.623639000
C	-2.997219000	1.408018000	-0.314437000
C	-4.198358000	0.757315000	-0.503915000
C	-4.230178000	-0.565441000	-1.066289000
C	-3.071005000	-1.203121000	-1.434110000
C	-1.776667000	-0.570005000	-1.277017000
C	4.640072000	-3.374806000	0.359517000
C	2.268835000	-2.898987000	0.628619000
H	1.265878000	-3.248974000	0.846643000
C	3.361106000	-3.800881000	0.627119000
H	5.471190000	-4.073947000	0.371678000
H	3.172793000	-4.847019000	0.849383000
Cl	-3.069161000	-2.797485000	-2.085896000
Cl	-5.753647000	-1.355681000	-1.252613000
Cl	-5.683964000	1.549837000	-0.123435000
Cl	-2.922798000	3.024489000	0.284764000
C	2.053712000	1.619213000	-2.155297000
H	1.401192000	0.782030000	-2.431147000
C	3.276345000	1.628404000	-3.071456000
C	1.241495000	2.911953000	-2.259269000
H	0.363943000	2.886747000	-1.612129000
H	1.846507000	3.792553000	-2.024045000
H	0.895117000	3.019120000	-3.291889000
H	3.971277000	2.435198000	-2.816702000
H	2.940338000	1.798209000	-4.099036000
H	3.822884000	0.683698000	-3.045136000
C	2.556923000	2.709589000	0.659881000
H	1.583112000	3.184560000	0.488988000
C	3.684683000	3.659553000	0.251143000
C	2.658373000	2.301515000	2.131048000
H	1.773813000	1.748176000	2.453386000
H	3.548805000	1.689517000	2.309443000
H	2.741252000	3.202463000	2.747068000
H	4.657442000	3.244732000	0.528670000
H	3.566982000	4.606338000	0.786876000
H	3.693387000	3.883699000	-0.818795000
O	-0.379828000	0.815047000	2.058882000
O	-0.413228000	-1.689747000	1.034431000
C	-1.480444000	0.176279000	2.077580000
C	-2.682023000	0.696197000	2.644263000
C	-3.839496000	-0.036444000	2.601615000
C	-3.867591000	-1.330027000	2.014592000
C	-2.724889000	-1.907071000	1.507828000
C	-1.516180000	-1.176095000	1.497564000
H	-2.730421000	-2.894696000	1.059905000
H	-4.806148000	-1.873048000	1.971084000
H	-4.758163000	0.380341000	3.002128000
H	-2.646434000	1.693262000	3.067746000

Σ of electronic & zero-point Energies -3699.278603

Σ of electronic & thermal Free Energies -3699.348696

TS2'

Au	0.920961000	-0.283807000	-0.049910000
P	2.581023000	1.197717000	-0.413863000
O	-0.585955000	1.159661000	-0.309669000
O	-0.768738000	-1.342569000	-1.310923000
C	2.408930000	-1.600471000	0.194382000

C	4.061530000	0.172542000	-0.277765000
C	3.758218000	-1.178210000	0.037406000
C	4.821315000	-2.115194000	0.201002000
C	6.150901000	-1.648386000	0.055898000
H	6.966966000	-2.355204000	0.179874000
C	6.420188000	-0.329327000	-0.234699000
H	7.447109000	0.006567000	-0.337399000
C	5.369773000	0.597033000	-0.406118000
H	5.601896000	1.630052000	-0.640047000
C	-1.760262000	0.638138000	-0.520395000
C	-2.943485000	1.374613000	-0.305395000
C	-4.190934000	0.785679000	-0.487605000
C	-4.287507000	-0.537993000	-0.995701000
C	-3.144341000	-1.263553000	-1.283549000
C	-1.843929000	-0.714131000	-1.065079000
C	4.497154000	-3.461402000	0.499822000
C	2.125634000	-2.913201000	0.485968000
H	1.095710000	-3.228073000	0.614074000
C	3.183570000	-3.843909000	0.632787000
H	5.299953000	-4.182822000	0.621967000
H	2.940786000	-4.877583000	0.860653000
C	2.412319000	1.959101000	-2.091099000
H	2.064980000	1.108947000	-2.691434000
C	3.727906000	2.462649000	-2.684511000
C	1.310752000	3.022173000	-2.076010000
H	0.391143000	2.645429000	-1.620792000
H	1.626944000	3.917715000	-1.533356000
H	1.091637000	3.320416000	-3.105563000
H	4.159071000	3.279871000	-2.099949000
H	3.532745000	2.847269000	-3.690462000
H	4.468450000	1.664523000	-2.768937000
C	2.547071000	2.446390000	0.937568000
H	1.520235000	2.832331000	0.902479000
C	3.551351000	3.581341000	0.734506000
C	2.759220000	1.727137000	2.271157000
H	1.990934000	0.970351000	2.439857000
H	3.749401000	1.262950000	2.314078000
H	2.689088000	2.458883000	3.081290000
H	4.579305000	3.206412000	0.745093000
H	3.455041000	4.289170000	1.563530000
H	3.388715000	4.134754000	-0.192606000
O	-0.328303000	0.876052000	2.376424000
O	-0.428885000	-1.630138000	1.272347000
C	-1.418354000	0.296982000	2.308743000
C	-2.656698000	0.865219000	2.799851000
C	-3.826067000	0.181340000	2.691173000
C	-3.883119000	-1.126858000	2.101095000
C	-2.759612000	-1.746449000	1.636562000
C	-1.490321000	-1.079166000	1.681279000
H	-2.789162000	-2.733227000	1.187001000
H	-4.844073000	-1.626236000	2.028890000
H	-4.750676000	0.630358000	3.041526000
H	-2.606063000	1.859491000	3.229297000
Cl	-3.219694000	-2.883777000	-1.870726000
Cl	-5.846040000	-1.251159000	-1.214999000
Cl	-5.626208000	1.685017000	-0.148982000
Cl	-2.781796000	3.013219000	0.219922000

Σ of electronic & zero-point Energies -3699.280766

Σ of electronic & thermal Free Energies -3699.349206

INT'

Au	0.967757000	-0.368950000	0.054547000
P	2.456630000	1.258776000	-0.381321000
O	-0.548024000	1.138661000	0.222455000
O	-0.834360000	-0.384453000	-1.980493000
C	2.567648000	-1.576168000	0.152229000
C	4.030470000	0.393061000	-0.198248000
C	3.866215000	-0.998465000	0.044022000
C	5.024017000	-1.822077000	0.177258000
C	6.298146000	-1.209621000	0.083981000
H	7.182621000	-1.831793000	0.191453000
C	6.429697000	0.142925000	-0.137421000
H	7.416063000	0.590748000	-0.204070000
C	5.287894000	0.957588000	-0.287586000
H	5.409566000	2.017771000	-0.480637000
C	-1.731573000	0.775738000	-0.145561000
C	-2.895018000	1.275990000	0.486195000
C	-4.157079000	0.859274000	0.084635000
C	-4.303165000	0.000369000	-1.048795000
C	-3.200172000	-0.434629000	-1.750699000
C	-1.863785000	-0.051952000	-1.365266000
C	4.849215000	-3.210107000	0.399313000
C	2.434147000	-2.928541000	0.361613000
H	1.445095000	-3.366271000	0.436975000
C	3.585721000	-3.743602000	0.482985000
H	5.726628000	-3.842363000	0.500669000
H	3.456935000	-4.808949000	0.649912000
Cl	-3.337161000	-1.486494000	-3.109366000
Cl	-5.886484000	-0.509120000	-1.516012000
Cl	-5.561828000	1.460385000	0.889030000
Cl	-2.681443000	2.418408000	1.764837000
C	2.225424000	1.871370000	-2.109404000
H	1.971860000	0.948065000	-2.644828000
C	3.486170000	2.470950000	-2.730459000
C	1.016888000	2.806631000	-2.173727000
H	0.140422000	2.356325000	-1.704427000
H	1.224661000	3.763739000	-1.685487000
H	0.779679000	3.010345000	-3.221735000
H	3.808705000	3.379585000	-2.214113000
H	3.270719000	2.743257000	-3.768315000
H	4.315959000	1.760820000	-2.735001000
C	2.242828000	2.583302000	0.873719000
H	1.209021000	2.909646000	0.703989000
C	3.206155000	3.755734000	0.694871000
C	2.331751000	1.960579000	2.269396000
H	1.554484000	1.208790000	2.427739000
H	3.311295000	1.500712000	2.436341000
H	2.196676000	2.747775000	3.017428000
H	4.242196000	3.446218000	0.860520000
H	2.972753000	4.523847000	1.438553000
H	3.131185000	4.218591000	-0.291921000
O	-0.263958000	-0.410581000	2.461030000
O	-0.402893000	-1.963957000	0.221130000
C	-1.369847000	-0.880618000	2.138523000
C	-2.581420000	-0.680212000	2.892852000
C	-3.759424000	-1.220472000	2.471368000
C	-3.834781000	-2.020963000	1.288768000
C	-2.716320000	-2.299535000	0.545751000
C	-1.470160000	-1.713855000	0.894151000
H	-2.756024000	-2.913994000	-0.347038000
H	-4.795167000	-2.426075000	0.987173000
H	-4.670702000	-1.035512000	3.031817000
H	-2.513323000	-0.063391000	3.781577000

Σ of electronic & zero-point Energies -3699.288337

Σ of electronic & thermal Free Energies -3699.358090

RC2'

Au	1.086788000	-0.231036000	0.838537000
P	2.553520000	1.294731000	0.018196000
O	-1.500658000	2.327710000	-1.197987000
O	-0.422696000	-0.149378000	-1.425639000
C	2.419376000	-1.577908000	0.175151000
C	3.747612000	0.243565000	-0.840437000
C	3.531912000	-1.140563000	-0.597425000
C	4.441094000	-2.095775000	-1.141955000
C	5.528641000	-1.621417000	-1.916263000
H	6.221381000	-2.344413000	-2.338644000
C	5.713156000	-0.275981000	-2.141693000
H	6.550285000	0.065679000	-2.742167000
C	4.820227000	0.671892000	-1.597900000
H	4.981919000	1.726994000	-1.787468000
C	-2.233846000	1.353387000	-1.109145000
C	-3.682447000	1.441612000	-0.961614000
C	-4.459092000	0.320397000	-0.879234000
C	-3.877090000	-1.008671000	-0.943578000
C	-2.525262000	-1.181222000	-1.079099000
C	-1.628939000	-0.040341000	-1.202404000
C	4.211880000	-3.470860000	-0.890535000
C	2.223297000	-2.921275000	0.395238000
H	1.360096000	-3.253205000	0.962922000
C	3.130076000	-3.867198000	-0.140761000
H	4.899502000	-4.203733000	-1.302984000
H	2.956093000	-4.923405000	0.042955000
C	1.661486000	2.491750000	-1.058132000
H	0.830490000	1.885363000	-1.442581000
C	2.481389000	3.025987000	-2.229624000
C	1.048553000	3.591981000	-0.189509000
H	0.445470000	3.166027000	0.615969000
H	1.808928000	4.261486000	0.225865000
H	0.371514000	4.181718000	-0.811130000
H	3.333301000	3.632631000	-1.905994000
H	1.834230000	3.666704000	-2.836313000
H	2.848169000	2.221033000	-2.870590000
C	3.439683000	2.145353000	1.395052000
H	2.646863000	2.695106000	1.916566000
C	4.500475000	3.124267000	0.892353000
C	4.035196000	1.101932000	2.340933000
H	3.266793000	0.441586000	2.751161000
H	4.775637000	0.482047000	1.825858000
H	4.534951000	1.606266000	3.173619000
H	5.303331000	2.594134000	0.372012000
H	4.947510000	3.643709000	1.745720000
H	4.088832000	3.881375000	0.221068000
O	-0.375008000	1.087220000	1.478659000
O	-0.252591000	-1.605150000	1.541689000
C	-1.492976000	0.416571000	1.679777000
C	-2.726760000	1.061260000	1.891069000
C	-3.860644000	0.307398000	2.142122000
C	-3.786830000	-1.094879000	2.200940000
C	-2.579881000	-1.759122000	2.027949000
C	-1.425228000	-1.025241000	1.741620000
H	-2.757308000	2.144243000	1.836936000
H	-4.816560000	0.803140000	2.274433000
H	-4.689595000	-1.669587000	2.381816000
H	-2.513836000	-2.840685000	2.062106000
Cl	-1.803092000	-2.733522000	-1.215198000
Cl	-4.922095000	-2.377725000	-0.895222000
Cl	-6.166420000	0.459129000	-0.693840000
Cl	-4.338379000	3.027532000	-0.833365000

Σ of electronic & zero-point Energies -3699.298218
Σ of electronic & thermal Free Energies -3699.368099

Optimization SOLVENT DCM, Singlet state, approach *trans* to P

(P,C)Au(O,O)H$_4$

Au	0.594555000	0.253560000	-0.046680000
P	-1.130201000	-1.237404000	-0.043945000
O	2.114927000	-1.120516000	0.064147000
O	2.129865000	1.589070000	-0.078907000
C	-0.864658000	1.642063000	-0.101954000
C	-2.572576000	-0.149461000	-0.014777000
C	-2.230069000	1.230300000	-0.059339000
C	-3.272456000	2.205521000	-0.057086000
C	-4.616403000	1.757416000	0.003763000
H	-5.411932000	2.497931000	0.008893000
C	-4.918644000	0.415000000	0.057366000
H	-5.953567000	0.090842000	0.105837000
C	-3.891872000	-0.553890000	0.045139000
H	-4.149407000	-1.606602000	0.078249000
C	3.302441000	-0.480544000	0.051858000
C	4.512555000	-1.173751000	0.110861000
C	5.726525000	-0.477745000	0.101276000
C	5.733514000	0.913853000	0.031479000
C	4.526532000	1.619918000	-0.027585000
C	3.310881000	0.935070000	-0.018910000
C	-2.922046000	3.578329000	-0.111220000
C	-0.565611000	2.986291000	-0.154367000
H	0.471524000	3.306163000	-0.186569000
C	-1.600135000	3.953774000	-0.161154000
H	-3.712864000	4.323385000	-0.111276000
H	-1.335662000	5.006724000	-0.203317000
H	4.514253000	2.705683000	-0.082196000
H	6.673945000	1.458412000	0.022993000
H	6.661638000	-1.029565000	0.147929000
H	4.489019000	-2.259539000	0.164771000
C	-1.078009000	-2.245820000	-1.588403000
H	-0.795023000	-1.497294000	-2.339376000
C	-2.418087000	-2.852826000	-1.995688000
C	0.044689000	-3.278441000	-1.477845000
H	0.989226000	-2.817826000	-1.171596000
H	-0.209236000	-4.065077000	-0.760755000
H	0.191709000	-3.750531000	-2.454325000
H	-2.785986000	-3.573903000	-1.261466000
H	-2.284275000	-3.382619000	-2.944691000
H	-3.181616000	-2.086197000	-2.146079000
C	-1.032718000	-2.262127000	1.481516000
H	-0.039376000	-2.721991000	1.403981000
C	-2.092631000	-3.357226000	1.573494000
C	-1.056073000	-1.334320000	2.696593000
H	-0.262968000	-0.581844000	2.648104000
H	-2.017240000	-0.817392000	2.780794000
H	-0.908031000	-1.927025000	3.604621000
H	-3.100474000	-2.935846000	1.624068000
H	-1.926415000	-3.929062000	2.492401000
H	-2.043279000	-4.053752000	0.733901000

Σ of electronic & zero-point Energies -1479.846696
Σ of electronic & thermal Free Energies -1479.900729

(P,C)Au(O,O)-Cl4

Au	-0.549092000	0.228119000	-0.059498000
P	-2.310364000	-1.217226000	-0.067060000
O	0.961014000	-1.181942000	0.021843000
O	1.048568000	1.517032000	-0.078624000
C	-1.971469000	1.649156000	-0.078254000
C	-3.722964000	-0.096331000	0.003548000
C	-3.344767000	1.273241000	-0.022821000
C	-4.357628000	2.277393000	0.012399000
C	-5.712061000	1.864210000	0.086473000
H	-6.487102000	2.625356000	0.117192000
C	-6.049768000	0.529474000	0.121276000
H	-7.092342000	0.233026000	0.180241000
C	-5.051065000	-0.467499000	0.076245000
H	-5.336553000	-1.513399000	0.095104000
C	2.145892000	-0.581006000	0.012818000
C	3.343016000	-1.301356000	0.052733000
C	4.586058000	-0.646571000	0.049759000
C	4.631272000	0.748932000	0.005335000
C	3.432961000	1.482065000	-0.036341000
C	2.192838000	0.838686000	-0.034751000
C	-3.967020000	3.640005000	-0.022521000
C	-1.628470000	2.982499000	-0.111204000
H	-0.583690000	3.274947000	-0.151726000
C	-2.635779000	3.978552000	-0.085315000
H	-4.735024000	4.407961000	0.003052000
H	-2.340879000	5.023653000	-0.112007000
C	-2.290034000	-2.189395000	-1.634314000
H	-1.994420000	-1.431444000	-2.370702000
C	-3.652223000	-2.748286000	-2.039475000
C	-1.197512000	-3.256649000	-1.558186000
H	-0.234292000	-2.835027000	-1.255327000
H	-1.466888000	-4.050897000	-0.855604000
H	-1.076745000	-3.710615000	-2.546623000
H	-4.032053000	-3.475985000	-1.318042000
H	-3.542087000	-3.259197000	-3.001611000
H	-4.394867000	-1.957037000	-2.164260000
C	-2.200477000	-2.269338000	1.437145000
H	-1.221285000	-2.752869000	1.329367000
C	-3.287641000	-3.338115000	1.525794000
C	-2.177275000	-1.365305000	2.669829000
H	-1.362884000	-0.635712000	2.623316000
H	-3.121548000	-0.822997000	2.780395000
H	-2.031714000	-1.981207000	3.562539000
H	-4.281883000	-2.890856000	1.610876000
H	-3.114809000	-3.936684000	2.426058000
H	-3.276108000	-4.014015000	0.668151000
Cl	3.444340000	3.218293000	-0.092989000
Cl	6.155217000	1.578879000	-0.000201000
Cl	6.053065000	-1.572095000	0.101651000
Cl	3.239668000	-3.034892000	0.106778000

Sum of electronic and zero-point Energies= -3318.066897
Sum of electronic and thermal Free Energies= -3318.128680

Quinone-H4

O	1.729622000	1.372051000	-0.000219000
O	1.729615000	-1.372058000	0.000133000
C	0.664115000	0.777557000	-0.000034000
C	-0.634640000	1.453264000	-0.000148000
C	-1.773411000	0.729611000	-0.000071000
C	-1.773415000	-0.729605000	0.000081000
C	-0.634647000	-1.453262000	0.000159000
C	0.664111000	-0.777559000	0.000138000
H	-0.636432000	-2.539080000	0.000248000
H	-2.736863000	-1.231512000	0.000111000
H	-2.736857000	1.231523000	-0.000142000
H	-0.636421000	2.539082000	-0.000289000

Σ of electronic & zero-point Energies -381.246708
Σ of electronic & thermal Free Energies -381.277436

Quinone-Cl4

O	-1.359818000	2.779445000	0.000194000
O	1.359818000	2.779445000	-0.000178000
C	-0.772751000	1.720323000	0.000071000
C	-1.453307000	0.415139000	0.000070000
C	-0.738014000	-0.739371000	0.000021000
C	0.738014000	-0.739371000	-0.000026000
C	1.453307000	0.415139000	-0.000069000
C	0.772751000	1.720323000	-0.000065000
Cl	3.167079000	0.453412000	-0.000135000
Cl	1.540955000	-2.254124000	-0.000026000
Cl	-1.540955000	-2.254124000	0.000014000
Cl	-3.167079000	0.453412000	0.000138000

Σ of electronic & zero-point Energies -2219.449203
Σ of electronic & thermal Free Energies -2219.489118

RC1

Au	-1.089306000	-0.243120000	0.685295000
P	-2.672323000	1.260911000	0.030939000
O	0.371149000	1.082218000	1.357420000
O	0.309313000	-1.611872000	1.370544000
C	-2.461723000	-1.609110000	0.152636000
C	-4.090086000	0.191349000	-0.305702000
C	-3.765671000	-1.189675000	-0.234242000
C	-4.753159000	-2.160632000	-0.577022000
C	-6.040183000	-1.703763000	-0.958143000
H	-6.798936000	-2.438592000	-1.213410000
C	-6.331136000	-0.358905000	-1.012359000
H	-7.321160000	-0.027566000	-1.309944000
C	-5.349520000	0.604751000	-0.693273000
H	-5.594080000	1.658508000	-0.760100000
C	1.479801000	0.433612000	1.629278000
C	2.677470000	1.098130000	1.963724000
C	3.801890000	0.365934000	2.296557000
C	3.754355000	-1.043390000	2.345237000
C	2.589432000	-1.728078000	2.050159000
C	1.441921000	-1.013831000	1.658907000
C	-4.403157000	-3.533572000	-0.528511000
C	-2.149924000	-2.949646000	0.174675000
H	-1.152256000	-3.272621000	0.454184000
C	-3.131695000	-3.912543000	-0.166912000
H	-5.152067000	-4.276664000	-0.787519000
H	-2.865067000	-4.965217000	-0.138975000
H	2.541874000	-2.811228000	2.082988000
H	4.646347000	-1.598347000	2.618990000
H	4.728620000	0.879936000	2.530997000
H	2.690234000	2.182932000	1.938617000
C	-2.967067000	2.449604000	1.412822000
H	-2.846260000	1.813008000	2.298109000
C	-4.370476000	3.050186000	1.443249000

C	-1.862808000	3.508508000	1.413499000
H	-0.866630000	3.058710000	1.391185000
H	-1.961880000	4.187237000	0.561324000
H	-1.947433000	4.104073000	2.327953000
H	-4.579786000	3.658051000	0.559402000
H	-4.446119000	3.701419000	2.320300000
H	-5.140681000	2.280680000	1.531511000
C	-2.156491000	2.090595000	-1.525866000
H	-1.218200000	2.585828000	-1.254247000
C	-3.175511000	3.117442000	-2.015613000
C	-1.854978000	1.024440000	-2.577981000
H	-1.057448000	0.355091000	-2.246330000
H	-2.748207000	0.439144000	-2.820111000
H	-1.520683000	1.522293000	-3.494037000
H	-4.122637000	2.641586000	-2.286218000
H	-2.777809000	3.598356000	-2.915306000
H	-3.372735000	3.899485000	-1.279307000
O	1.019194000	1.690874000	-1.272739000
O	0.706106000	-1.010015000	-1.403750000
C	1.997864000	0.966322000	-1.129950000
C	3.353665000	1.475456000	-0.952600000
C	4.422909000	0.637688000	-0.806303000
C	4.249850000	-0.800241000	-0.819555000
C	3.011430000	-1.357234000	-0.994134000
C	1.821509000	-0.538694000	-1.173138000
Cl	2.783307000	-3.063024000	-1.085533000
Cl	5.645411000	-1.806477000	-0.669600000
Cl	6.011032000	1.278603000	-0.592107000
Cl	3.521773000	3.192007000	-0.919868000

Σ of electronic & zero-point Energies -3699.341066

Σ of electronic & thermal Free Energies -3699.411312

TS1

Au	0.995436000	0.172918000	0.296088000
P	2.833282000	-1.160262000	0.232246000
O	-0.360790000	-1.352813000	0.833639000
O	-0.419262000	1.135517000	1.934360000
C	2.273586000	1.618641000	-0.243494000
C	4.133724000	-0.001578000	-0.244750000
C	3.651349000	1.319657000	-0.428276000
C	4.558379000	2.353473000	-0.805750000
C	5.920608000	2.010325000	-0.997212000
H	6.618294000	2.791463000	-1.286733000
C	6.361438000	0.716875000	-0.823656000
H	7.407983000	0.473422000	-0.977861000
C	5.466617000	-0.306050000	-0.440868000
H	5.835182000	-1.316475000	-0.304909000
C	-1.454406000	-0.919169000	1.375644000
C	-2.608976000	-1.737155000	1.469797000
C	-3.753372000	-1.246311000	2.052029000
C	-3.783237000	0.052923000	2.631613000
C	-2.682438000	0.868191000	2.603617000
C	-1.477490000	0.433142000	1.972490000
C	4.057093000	3.669270000	-0.972108000
C	1.815121000	2.904077000	-0.413822000
H	0.761694000	3.130002000	-0.287565000
C	2.721680000	3.932081000	-0.776801000
H	4.743197000	4.461880000	-1.256798000
H	2.341157000	4.941298000	-0.905696000
H	-2.694324000	1.860785000	3.040630000
H	-4.699439000	0.398008000	3.101169000
H	-4.647421000	-1.860946000	2.082842000
H	-2.569896000	-2.731012000	1.036140000
C	3.125521000	-1.876369000	1.910162000
H	2.849750000	-1.042185000	2.566858000
C	4.583910000	-2.241849000	2.182182000
C	2.163598000	-3.038949000	2.155023000
H	1.127380000	-2.762531000	1.942251000
H	2.426461000	-3.907692000	1.544415000
H	2.230421000	-3.334971000	3.206458000
H	4.942215000	-3.037696000	1.524596000
H	4.657254000	-2.603855000	3.212969000
H	5.245627000	-1.378615000	2.083730000
C	2.576338000	-2.438731000	-1.063272000
H	1.674968000	-2.966718000	-0.728290000
C	3.740332000	-3.424444000	-1.165688000
C	2.288899000	-1.744272000	-2.393599000
H	1.411813000	-1.096595000	-2.324400000
H	3.149291000	-1.153477000	-2.723786000
H	2.089924000	-2.506599000	-3.153425000
H	4.658092000	-2.922381000	-1.484334000
H	3.491355000	-4.173086000	-1.924689000
H	3.930320000	-3.950124000	-0.227870000
O	-0.948644000	-1.065883000	-1.791558000
O	-0.751345000	1.419571000	-0.707003000
C	-1.970976000	-0.514871000	-1.370707000
C	-3.287222000	-1.120762000	-1.421171000
C	-4.409043000	-0.457828000	-0.988677000
C	-4.315682000	0.871696000	-0.458610000
C	-3.091526000	1.501518000	-0.368682000
C	-1.875735000	0.847219000	-0.761891000
Cl	-2.955248000	3.137674000	0.169728000
Cl	-5.759885000	1.703047000	0.004473000
Cl	-5.959266000	-1.220822000	-1.067739000
Cl	-3.363731000	-2.728377000	-2.051579000

Σ of electronic & zero-point Energies -3699.326429

Σ of electronic & thermal Free Energies -3699.394664

TS2

Au	0.912860000	0.149834000	-0.098505000
P	2.748924000	-1.158354000	0.219826000
O	-0.398755000	-1.366778000	1.238876000
O	-0.378919000	1.125900000	2.360893000
C	2.257981000	1.610638000	-0.429926000
C	4.101148000	0.009280000	-0.050264000
C	3.646127000	1.315459000	-0.363534000
C	4.594340000	2.353512000	-0.609186000
C	5.972444000	2.028565000	-0.543140000
H	6.700661000	2.813161000	-0.729484000
C	6.389549000	0.750427000	-0.245626000
H	7.449379000	0.520789000	-0.198100000
C	5.451873000	-0.273690000	0.008242000
H	5.803591000	-1.268403000	0.255440000
C	-1.472416000	-0.869543000	1.667051000
C	-2.714224000	-1.593816000	1.654804000
C	-3.852738000	-1.021251000	2.138994000
C	-3.843621000	0.296714000	2.715641000
C	-2.706031000	1.035828000	2.793958000
C	-1.451341000	0.514439000	2.290643000
C	4.120298000	3.657273000	-0.900025000
C	1.821479000	2.883512000	-0.707683000
H	0.760927000	3.105911000	-0.746580000
C	2.770129000	3.910802000	-0.941198000
H	4.840102000	4.449381000	-1.084962000

H	2.408862000	4.911773000	-1.158521000
H	-2.695349000	2.031040000	3.225971000
H	-4.779272000	0.700606000	3.091284000
H	-4.790477000	-1.567002000	2.105165000
H	-2.710848000	-2.590823000	1.226502000
C	2.768600000	-1.880806000	1.924764000
H	2.199750000	-1.141140000	2.499423000
C	4.171047000	-1.987841000	2.519677000
C	2.019100000	-3.213235000	1.958761000
H	1.021518000	-3.132299000	1.523724000
H	2.576201000	-4.000074000	1.442437000
H	1.905014000	-3.517163000	3.004189000
H	4.806683000	-2.674983000	1.954111000
H	4.080317000	-2.380160000	3.537880000
H	4.668280000	-1.017248000	2.577146000
C	2.779687000	-2.462106000	-1.079129000
H	1.925314000	-3.102003000	-0.828659000
C	4.068209000	-3.284074000	-1.037888000
C	2.550604000	-1.830496000	-2.451886000
H	1.580094000	-1.331457000	-2.510155000
H	3.334934000	-1.104380000	-2.689487000
H	2.577163000	-2.616578000	-3.213194000
H	4.924457000	-2.684204000	-1.357955000
H	3.969898000	-4.122570000	-1.734650000
H	4.278097000	-3.694545000	-0.047378000
O	-0.748122000	-1.109340000	-1.319241000
O	-0.715973000	1.432943000	-0.408650000
C	-1.859446000	-0.540288000	-1.087171000
C	-3.124775000	-1.165675000	-1.293066000
C	-4.313494000	-0.511171000	-1.010864000
C	-4.295757000	0.815096000	-0.514931000
C	-3.082609000	1.480002000	-0.345021000
C	-1.855600000	0.824880000	-0.572286000
Cl	-3.029345000	3.137583000	0.152274000
Cl	-5.785307000	1.634252000	-0.187272000
Cl	-5.827821000	-1.321475000	-1.232931000
Cl	-3.105430000	-2.793044000	-1.883421000

Σ of electronic & zero-point Energies -3699.324050

Σ of electronic & thermal Free Energies -3699.393015

INT

Au	-0.949654000	0.162475000	-0.123771000
P	-2.814879000	-1.123089000	-0.204952000
O	0.322972000	-1.568496000	-0.198616000
O	0.421672000	-0.103661000	-2.498650000
C	-2.225982000	1.676753000	0.219811000
C	-4.106667000	0.066718000	0.209723000
C	-3.614380000	1.390192000	0.360770000
C	-4.528982000	2.444369000	0.658301000
C	-5.900849000	2.120811000	0.811712000
H	-6.599992000	2.919854000	1.043081000
C	-6.348789000	0.825941000	0.673615000
H	-7.402837000	0.597817000	0.797010000
C	-5.449342000	-0.216865000	0.363851000
H	-5.820972000	-1.228254000	0.245172000
C	1.429955000	-1.455866000	-0.835087000
C	2.593316000	-2.171434000	-0.433400000
C	3.758381000	-2.038942000	-1.141807000
C	3.814958000	-1.258651000	-2.340952000
C	2.720022000	-0.600475000	-2.815147000
C	1.465757000	-0.654652000	-2.105422000
C	-4.028957000	3.764285000	0.790444000
C	-1.773215000	2.969408000	0.350135000
H	-0.717453000	3.191027000	0.239665000
C	-2.686579000	4.014900000	0.634909000
H	-4.722690000	4.569477000	1.015031000
H	-2.306364000	5.027573000	0.734067000
H	2.753396000	-0.010926000	-3.725103000
H	4.757505000	-1.199534000	-2.876979000
H	4.654655000	-2.550335000	-0.805620000
H	2.535841000	-2.774647000	0.466591000
C	-3.035354000	-1.785527000	-1.912961000
H	-2.731729000	-0.931894000	-2.531181000
C	-4.481892000	-2.139626000	-2.253747000
C	-2.065362000	-2.941252000	-2.154526000
H	-1.037716000	-2.666870000	-1.906480000
H	-2.343301000	-3.822367000	-1.568485000
H	-2.100137000	-3.215705000	-3.213197000
H	-4.866636000	-2.952985000	-1.633415000
H	-4.516060000	-2.471416000	-3.296589000
H	-5.146013000	-1.278132000	-2.155580000
C	-2.648896000	-2.432756000	1.073481000
H	-1.734536000	-2.958859000	0.771920000
C	-3.818415000	-3.415331000	1.098359000
C	-2.415558000	-1.769006000	2.431212000
H	-1.533402000	-1.122587000	2.420809000
H	-3.282991000	-1.174590000	2.735438000
H	-2.257732000	-2.548027000	3.183610000
H	-4.753967000	-2.918254000	1.369483000
H	-3.615386000	-4.176324000	1.858826000
H	-3.952851000	-3.926264000	0.142554000
O	0.844630000	-0.074031000	2.006807000
O	0.719326000	1.479004000	-0.213934000
C	1.903947000	0.188768000	1.407868000
C	3.202584000	-0.278113000	1.822950000
C	4.352188000	0.066010000	1.144246000
C	4.292066000	0.909896000	-0.003042000
C	3.069724000	1.401852000	-0.440977000
C	1.854808000	1.014483000	0.179943000
Cl	2.971894000	2.537804000	-1.742566000
Cl	5.755510000	1.399090000	-0.785523000
Cl	5.888276000	-0.532958000	1.671109000
Cl	3.240053000	-1.310102000	3.210575000

Σ of electronic & zero-point Energies -3699.333414

Σ of electronic & thermal Free Energies -3699.403563

RC2

Au	0.928668000	0.346755000	-0.506855000
P	2.616692000	-1.168216000	-0.306686000
O	-0.954391000	-2.660621000	2.087260000
O	-0.076674000	-0.069853000	2.144619000
C	2.341261000	1.685027000	-0.012307000
C	3.954375000	-0.149892000	0.358187000
C	3.632692000	1.233826000	0.380374000
C	4.619583000	2.177061000	0.794419000
C	5.892333000	1.689691000	1.185448000
H	6.646003000	2.402673000	1.508721000
C	6.176943000	0.342740000	1.160029000
H	7.156851000	-0.012564000	1.463273000
C	5.206583000	-0.592063000	0.737334000
H	5.457024000	-1.646414000	0.715221000
C	-1.776392000	-1.757633000	2.170807000
C	-3.210294000	-1.987181000	2.300014000
C	-4.059741000	-0.941946000	2.421876000

C	-3.599806000	0.434032000	2.420452000
C	-2.289491000	0.753861000	2.299782000
C	-1.286013000	-0.292813000	2.188509000
C	4.285616000	3.554909000	0.797140000
C	2.049950000	3.030258000	-0.000652000
H	1.063227000	3.378435000	-0.289466000
C	3.033081000	3.966037000	0.406217000
H	5.033880000	4.276384000	1.112911000
H	2.781272000	5.022700000	0.410046000
H	-1.943117000	1.782377000	2.298241000
H	-4.342921000	1.219137000	2.519821000
H	-5.126983000	-1.118139000	2.517739000
H	-3.555883000	-3.015646000	2.287539000
C	2.070667000	-2.531114000	0.805174000
H	1.387967000	-2.019649000	1.495762000
C	3.201000000	-3.177889000	1.601666000
C	1.249319000	-3.539899000	0.001435000
H	0.433976000	-3.051646000	-0.537600000
H	1.870640000	-4.099779000	-0.704054000
H	0.800748000	-4.251295000	0.699383000
H	3.929544000	-3.679618000	0.958965000
H	2.762464000	-3.934392000	2.260846000
H	3.724569000	-2.453409000	2.229852000
C	3.105052000	-1.775739000	-1.975321000
H	2.208391000	-2.292361000	-2.338331000
C	4.274352000	-2.758189000	-1.918900000
C	3.402188000	-0.585390000	-2.885976000
H	2.547083000	0.092702000	-2.960147000
H	4.263650000	-0.015085000	-2.524308000
H	3.636731000	-0.952151000	-3.890147000
H	5.183545000	-2.269145000	-1.557570000
H	4.474059000	-3.124988000	-2.930919000
H	4.064447000	-3.622538000	-1.285131000
O	-0.620713000	-0.967153000	-0.956612000
O	-0.621295000	1.707765000	-0.645224000
C	-1.775833000	-0.349676000	-0.825072000
C	-2.999601000	-1.035489000	-0.856065000
C	-4.212517000	-0.348410000	-0.726124000
C	-4.212627000	1.049034000	-0.593646000
C	-3.001148000	1.752169000	-0.598849000
C	-1.779029000	1.076330000	-0.683008000
Cl	-2.960112000	3.475020000	-0.407564000
Cl	-5.709310000	1.906628000	-0.430081000
Cl	-5.706972000	-1.224187000	-0.751204000
Cl	-2.955534000	-2.751405000	-1.092138000

Σ of electronic & zero-point Energies -3699.343443

Σ of electronic & thermal Free Energies -3699.414591

Optimisation GAS PHASE, Triplet state

RC1^{T}

Au	1.338966000	-0.188668000	-0.508125000
P	1.028866000	-2.360424000	0.124352000
O	3.278519000	0.220687000	0.246030000
O	1.637708000	1.743446000	-1.251976000
C	-0.499339000	-0.388690000	-1.296620000
C	-0.674216000	-2.677359000	-0.385412000
C	-1.229048000	-1.591713000	-1.110606000
C	-2.554920000	-1.692005000	-1.623227000
C	-3.263501000	-2.899946000	-1.414153000
H	-4.278530000	-2.979299000	-1.792428000
C	-2.696055000	-3.947689000	-0.726423000
H	-3.258254000	-4.862134000	-0.566890000
C	-1.392797000	-3.840547000	-0.198996000
H	-0.977619000	-4.669948000	0.360563000
C	3.540222000	1.482209000	0.131925000
C	4.671732000	2.077011000	0.740743000
C	4.906288000	3.417864000	0.561279000
C	4.038087000	4.221103000	-0.234284000
C	2.934973000	3.684073000	-0.848992000
C	2.649962000	2.307771000	-0.680096000
C	-3.116790000	-0.570014000	-2.279446000
C	-1.063141000	0.682577000	-1.948878000
H	-0.511571000	1.608548000	-2.065435000
C	-2.390311000	0.586263000	-2.430161000
H	-4.139714000	-0.629053000	-2.637897000
H	-2.836836000	1.453303000	-2.906165000
H	2.254506000	4.279202000	-1.446593000
H	4.254474000	5.279056000	-0.344697000
H	5.764182000	3.882983000	1.036796000
H	5.318229000	1.452670000	1.347573000
C	2.106468000	-3.351317000	-1.012772000
H	1.792251000	-3.024002000	-2.011695000
C	1.847716000	-4.851475000	-0.877745000
C	3.580249000	-2.994496000	-0.810329000
H	3.763984000	-1.922140000	-0.912765000
H	3.935449000	-3.299559000	0.179165000
H	4.187110000	-3.521484000	-1.553000000
H	2.071718000	-5.213031000	0.131485000
H	2.497474000	-5.396057000	-1.570113000
H	0.813566000	-5.107064000	-1.118199000
C	1.523700000	-2.843517000	1.846587000
H	2.324048000	-3.573733000	1.667626000
C	0.394417000	-3.530508000	2.614447000
C	2.115036000	-1.646227000	2.594982000
H	2.985814000	-1.235572000	2.079417000
H	1.367981000	-0.856127000	2.692425000
H	2.427246000	-1.981273000	3.589668000
H	-0.489607000	-2.893187000	2.655885000
H	0.741942000	-3.716481000	3.635680000
H	0.130057000	-4.497698000	2.178538000
O	-0.747776000	-0.848780000	1.954167000
O	0.664404000	1.447325000	1.560475000
C	-1.340700000	0.178725000	1.562039000
C	-2.749041000	0.194475000	1.269113000
C	-3.363360000	1.294284000	0.706014000
C	-2.615721000	2.485442000	0.449863000
C	-1.277823000	2.558993000	0.785987000
C	-0.568913000	1.434049000	1.336607000
Cl	-0.354834000	3.991593000	0.494291000
Cl	-3.400628000	3.824053000	-0.314193000
Cl	-5.038205000	1.237741000	0.282209000
Cl	-3.623455000	-1.255989000	1.611189000

Σ of electronic & zero-point Energies -3699.282060

Σ of electronic & thermal Free Energies -3699.352621

INT^{T}

Au	0.845503000	-0.097035000	-0.235235000
P	2.643372000	0.959961000	0.620292000
O	-0.503485000	1.249716000	0.678723000
O	0.201993000	2.000222000	-1.882363000
C	2.170096000	-1.463388000	-0.881962000
C	3.992826000	-0.148442000	0.158162000
C	3.549022000	-1.285046000	-0.572189000

C	4.505649000	-2.255675000	-0.996555000
C	5.866509000	-2.049465000	-0.661511000
H	6.597999000	-2.786836000	-0.981243000
C	6.269392000	-0.943302000	0.052398000
H	7.317524000	-0.805274000	0.298072000
C	5.328417000	0.022126000	0.467501000
H	5.665487000	0.892912000	1.018713000
C	-1.346827000	1.878918000	-0.090471000
C	-2.630277000	2.209038000	0.385710000
C	-3.539153000	2.836419000	-0.441842000
C	-3.196473000	3.188283000	-1.775038000
C	-1.949919000	2.915822000	-2.269803000
C	-0.958063000	2.256074000	-1.463881000
C	4.053817000	-3.379034000	-1.731569000
C	1.767037000	-2.565242000	-1.598544000
H	0.716700000	-2.697490000	-1.835041000
C	2.718958000	-3.522840000	-2.024521000
H	4.777078000	-4.120717000	-2.058330000
H	2.377703000	-4.385190000	-2.589673000
H	-1.666901000	3.167875000	-3.286714000
H	-3.939652000	3.670463000	-2.402911000
H	-4.538742000	3.049698000	-0.075414000
H	-2.890473000	1.914118000	1.397165000
C	2.820109000	2.636584000	-0.131410000
H	2.417089000	2.472675000	-1.138014000
C	4.261227000	3.131724000	-0.231482000
C	1.894366000	3.625218000	0.579574000
H	0.882849000	3.227365000	0.676338000
H	2.267673000	3.884453000	1.575139000
H	1.840941000	4.545926000	-0.008086000
H	4.715976000	3.286506000	0.751789000
H	4.264424000	4.096359000	-0.748614000
H	4.890356000	2.444238000	-0.800861000
C	2.461635000	1.031964000	2.449280000
H	1.567560000	1.652929000	2.586421000
C	3.660739000	1.677847000	3.142991000
C	2.174201000	-0.373814000	2.982126000
H	1.251902000	-0.789548000	2.568630000
H	2.998735000	-1.056973000	2.753809000
H	2.066781000	-0.327522000	4.070235000
H	4.556463000	1.060215000	3.030667000
H	3.452768000	1.760607000	4.214190000
H	3.878004000	2.681423000	2.769173000
O	-0.744691000	-1.613314000	1.501946000
O	-0.778451000	-1.033691000	-1.175176000
C	-1.829005000	-1.342760000	0.953838000
C	-3.079514000	-1.254805000	1.678945000
C	-4.266744000	-0.986685000	1.034787000
C	-4.290805000	-0.795362000	-0.382594000
C	-3.119321000	-0.855814000	-1.127760000
C	-1.874932000	-1.074484000	-0.497840000
Cl	-3.117036000	-0.574915000	-2.829252000
Cl	-5.781084000	-0.429618000	-1.158057000
Cl	-5.739216000	-0.865380000	1.927956000
Cl	-2.997621000	-1.487648000	3.381158000

Σ of electronic & zero-point Energies -3699.281848

Σ of electronic & thermal Free Energies -3699.356081

TS1^{T}

Au	1.233980000	0.260502000	-0.147587000
P	1.997700000	-1.865408000	-0.027839000
O	2.767117000	1.135878000	0.982090000
O	1.729859000	2.243899000	-1.316590000
C	-0.259408000	-0.613860000	-1.166623000
C	0.483871000	-2.802795000	-0.322297000
C	-0.489362000	-2.001215000	-0.974925000
C	-1.706050000	-2.588422000	-1.422106000
C	-1.924430000	-3.958001000	-1.131490000
H	-2.864430000	-4.410890000	-1.433765000
C	-0.978676000	-4.709271000	-0.469775000
H	-1.172375000	-5.754696000	-0.252050000
C	0.251387000	-4.138527000	-0.074058000
H	0.994939000	-4.754977000	0.419856000
C	3.070593000	2.353220000	0.642143000
C	3.958884000	3.121244000	1.426612000
C	4.280981000	4.405531000	1.048414000
C	3.736594000	4.984234000	-0.131357000
C	2.877200000	4.274456000	-0.926935000
C	2.506922000	2.935498000	-0.584944000
C	-2.639917000	-1.768440000	-2.103378000
C	-1.155178000	0.145609000	-1.880484000
H	-0.974103000	1.203990000	-2.039491000
C	-2.356057000	-0.445296000	-2.346900000
H	-3.584310000	-2.197780000	-2.423671000
H	-3.073915000	0.177527000	-2.871277000
H	2.444188000	4.694277000	-1.828735000
H	4.006438000	6.002470000	-0.394894000
H	4.956716000	4.992634000	1.663218000
H	4.360259000	2.673932000	2.330069000
C	3.144864000	-2.170632000	-1.445500000
H	2.586438000	-1.712794000	-2.272033000
C	3.361013000	-3.646295000	-1.777380000
C	4.441032000	-1.384473000	-1.244124000
H	4.242513000	-0.332872000	-1.018021000
H	5.043121000	-1.800355000	-0.430807000
H	5.041986000	-1.428451000	-2.157114000
H	3.933243000	-4.166058000	-1.006005000
H	3.923874000	-3.722153000	-2.713121000
H	2.411120000	-4.169110000	-1.914024000
C	2.800923000	-2.165703000	1.598302000
H	3.497874000	-1.319801000	1.669620000
C	3.582342000	-3.477934000	1.683058000
C	1.762918000	-2.035370000	2.713198000
H	1.225120000	-1.088143000	2.664659000
H	1.018248000	-2.833766000	2.656310000
H	2.273605000	-2.106480000	3.678411000
H	2.936770000	-4.347749000	1.533009000
H	4.011983000	-3.562258000	2.686185000
H	4.404580000	-3.528291000	0.966953000
O	-0.794255000	-0.551185000	1.838980000
O	-0.271865000	1.853867000	0.623815000
C	-1.727392000	0.098885000	1.335922000
C	-3.071430000	-0.423657000	1.233550000
C	-4.093976000	0.314386000	0.682020000
C	-3.847418000	1.639301000	0.200225000
C	-2.572547000	2.180852000	0.240970000
C	-1.463683000	1.432144000	0.734502000
Cl	-2.233078000	3.737562000	-0.427333000
Cl	-5.150179000	2.541139000	-0.482201000
Cl	-5.679372000	-0.357232000	0.537246000
Cl	-3.312938000	-2.033188000	1.802726000

Σ of electronic & zero-point Energies -3699.266488

Σ of electronic & thermal Free Energies -3699.339485

TS2^T

Au	-0.693545000	0.082246000	-0.442940000
P	-2.452312000	1.248271000	0.355288000
O	0.698159000	0.400965000	1.498312000
O	-1.389833000	-1.344802000	2.026663000
C	-2.107560000	-1.191900000	-1.101186000
C	-3.846889000	0.155379000	0.015656000
C	-3.464668000	-0.981989000	-0.740223000
C	-4.453604000	-1.927747000	-1.139452000
C	-5.797281000	-1.685334000	-0.760961000
H	-6.558466000	-2.402703000	-1.055574000
C	-6.145355000	-0.571088000	-0.030969000
H	-7.180744000	-0.407012000	0.250173000
C	-5.165936000	0.365208000	0.364116000
H	-5.459090000	1.232934000	0.944212000
C	0.918425000	-0.740967000	2.043159000
C	2.235345000	-1.141972000	2.395097000
C	2.480002000	-2.388091000	2.924230000
C	1.418401000	-3.307402000	3.146322000
C	0.125305000	-2.968090000	2.846662000
C	-0.203816000	-1.681682000	2.296531000
C	-4.046834000	-3.062251000	-1.884358000
C	-1.736551000	-2.299971000	-1.821492000
H	-0.695835000	-2.466995000	-2.078066000
C	-2.723844000	-3.239186000	-2.211053000
H	-4.794107000	-3.789593000	-2.188032000
H	-2.416051000	-4.113605000	-2.776702000
H	-0.699559000	-3.655192000	3.010814000
H	1.643386000	-4.287268000	3.558238000
H	3.497676000	-2.681890000	3.165141000
H	3.038469000	-0.434552000	2.210826000
C	-2.187002000	1.635935000	2.129998000
H	-1.684588000	0.712437000	2.447017000
C	-3.472669000	1.803874000	2.936104000
C	-1.214502000	2.808378000	2.258468000
H	-0.923648000	2.904509000	3.308626000
H	-0.300611000	2.632598000	1.686087000
H	-1.665695000	3.757350000	1.950619000
H	-4.070482000	2.662429000	2.614864000
H	-3.201418000	1.968442000	3.983662000
H	-4.091173000	0.904925000	2.893279000
C	-2.637854000	2.776540000	-0.660149000
H	-1.700417000	3.319530000	-0.487557000
C	-3.822276000	3.632301000	-0.210407000
C	-2.733006000	2.404883000	-2.140137000
H	-3.614913000	1.786780000	-2.335290000
H	-2.817269000	3.316713000	-2.739097000
H	-1.848888000	1.856863000	-2.474671000
H	-4.766886000	3.098445000	-0.350747000
H	-3.863548000	4.539749000	-0.820854000
H	-3.745258000	3.939166000	0.834962000
O	0.953008000	1.692457000	-0.858145000
O	0.951514000	-1.017081000	-1.117483000
C	2.050453000	1.069093000	-0.780453000
C	3.301387000	1.735164000	-0.565944000
C	4.480808000	1.021406000	-0.501044000
C	4.476981000	-0.403425000	-0.650422000
C	3.291280000	-1.090631000	-0.865643000
C	2.063857000	-0.391278000	-0.932351000
Cl	3.243763000	-2.804853000	-1.013016000
Cl	5.957901000	-1.267088000	-0.528942000
Cl	5.973713000	1.835402000	-0.227132000
Cl	3.253770000	3.443669000	-0.374696000

Σ of electronic & zero-point Energies -3699.259886
Σ of electronic & thermal Free Energies -3699.332710

RC2^T

Au	0.845912000	0.398083000	-0.450094000
P	2.539179000	-1.117342000	-0.412152000
O	-0.480558000	-2.927966000	2.281336000
O	0.397753000	-0.301120000	2.049241000
C	2.281448000	1.712431000	0.024096000
C	3.908525000	-0.132174000	0.233103000
C	3.589007000	1.247566000	0.333014000
C	4.591644000	2.172390000	0.747930000
C	5.879035000	1.668066000	1.057777000
H	6.647111000	2.364838000	1.382364000
C	6.163327000	0.324764000	0.958500000
H	7.154949000	-0.041000000	1.205170000
C	5.174834000	-0.590590000	0.537452000
H	5.418117000	-1.644549000	0.465431000
C	-1.297848000	-1.979125000	2.298030000
C	-2.715561000	-2.203171000	2.424516000
C	-3.632863000	-1.160972000	2.461591000
C	-3.188794000	0.162957000	2.386794000
C	-1.827459000	0.454564000	2.232883000
C	-0.836274000	-0.564916000	2.196960000
C	4.253300000	3.545367000	0.835165000
C	1.983189000	3.051150000	0.117173000
H	0.981237000	3.404113000	-0.104627000
C	2.982680000	3.968008000	0.525436000
H	5.011126000	4.255838000	1.152609000
H	2.728459000	5.021278000	0.597765000
H	-1.485737000	1.483256000	2.169675000
H	-3.906407000	0.976973000	2.424312000
H	-4.694043000	-1.371964000	2.549923000
H	-3.036209000	-3.238194000	2.494592000
C	2.055470000	-2.558100000	0.611520000
H	1.406431000	-2.098408000	1.373876000
C	3.215787000	-3.253127000	1.319236000
C	1.187673000	-3.508091000	-0.215850000
H	0.366368000	-2.979431000	-0.706295000
H	1.768355000	-4.058476000	-0.964143000
H	0.731487000	-4.221589000	0.473326000
H	3.914988000	-3.734627000	0.627638000
H	2.791226000	-4.031771000	1.959582000
H	3.769778000	-2.565106000	1.961853000
C	2.956537000	-1.604197000	-2.141679000
H	2.046985000	-2.103073000	-2.498279000
C	4.130088000	-2.583121000	-2.191710000
C	3.218297000	-0.359489000	-2.988949000
H	2.355485000	0.311623000	-3.000888000
H	4.078317000	0.200581000	-2.608867000
H	3.435596000	-0.657346000	-4.019201000
H	5.048404000	-2.110151000	-1.831579000
H	4.301519000	-2.888946000	-3.228451000
H	3.946930000	-3.485352000	-1.604267000
O	-0.719387000	-0.900242000	-0.928605000
O	-0.734999000	1.755313000	-0.511601000
C	-1.864974000	-0.300306000	-0.788287000
C	-3.087798000	-0.994712000	-0.863659000
C	-4.293252000	-0.309692000	-0.746059000
C	-4.306127000	1.096265000	-0.546304000
C	-3.112727000	1.799831000	-0.445535000
C	-1.871753000	1.125640000	-0.564240000

Cl	-3.071863000	3.495513000	-0.144877000
Cl	-5.808139000	1.919670000	-0.356305000
Cl	-5.780082000	-1.174479000	-0.813643000
Cl	-3.022868000	-2.702359000	-1.068011000

Σ of electronic & zero-point Energies -3699.266285

Σ of electronic & thermal Free Energies -3699.338381

(P,C)Au(O,O)-H_4^T

Au	0.607755000	0.333962000	-0.033479000
P	-1.188893000	-1.285763000	-0.015251000
O	2.280775000	-1.066634000	-0.012064000
O	2.567917000	1.657738000	-0.002862000
C	-0.894035000	1.711458000	-0.082815000
C	-2.588064000	-0.129066000	-0.091466000
C	-2.250682000	1.262791000	-0.102423000
C	-3.314460000	2.220659000	-0.131777000
C	-4.655526000	1.764964000	-0.147840000
H	-5.454461000	2.502012000	-0.170205000
C	-4.951322000	0.422808000	-0.135817000
H	-5.984104000	0.088069000	-0.148951000
C	-3.912122000	-0.529870000	-0.107349000
H	-4.166008000	-1.583709000	-0.103829000
C	3.457393000	-0.547004000	-0.002776000
C	4.625977000	-1.352504000	0.002008000
C	5.871818000	-0.771811000	0.016540000
C	6.021914000	0.643074000	0.026801000
C	4.925774000	1.466298000	0.021897000
C	3.605105000	0.919791000	0.005585000
C	-2.997877000	3.601699000	-0.141895000
C	-0.636361000	3.067778000	-0.093583000
H	0.392491000	3.415986000	-0.079004000
C	-1.687737000	4.013624000	-0.123032000
H	-3.809063000	4.324571000	-0.164007000
H	-1.451154000	5.074251000	-0.130431000
H	5.019151000	2.547540000	0.028968000
H	7.020802000	1.069502000	0.038224000
H	6.759102000	-1.398364000	0.020802000
H	4.498384000	-2.430466000	-0.005032000
C	-1.181005000	-2.385055000	-1.507874000
H	-0.814476000	-1.696903000	-2.281691000
C	-2.519653000	-2.949394000	-1.976635000
C	-0.116666000	-3.465524000	-1.296049000
H	0.835680000	-3.032935000	-0.973466000
H	-0.438032000	-4.196614000	-0.546757000
H	0.051759000	-4.007585000	-2.231980000
H	-2.957715000	-3.632734000	-1.243930000
H	-2.370111000	-3.514291000	-2.903639000
H	-3.240346000	-2.154992000	-2.181782000
C	-1.334777000	-2.270775000	1.548793000
H	-0.408138000	-2.859059000	1.555881000
C	-2.528413000	-3.216715000	1.658115000
C	-1.290182000	-1.284536000	2.719145000
H	-0.398776000	-0.652137000	2.679610000
H	-2.168077000	-0.630831000	2.711148000
H	-1.282041000	-1.832007000	3.667089000
H	-3.470340000	-2.661812000	1.666468000
H	-2.468563000	-3.774201000	2.599790000
H	-2.559350000	-3.944852000	0.844386000

Σ of electronic & zero-point Energies -1479.771734

Σ of electronic & thermal Free Energies -1479.831714

(P,C)Au(O,O)-Cl_4^T

Au	-0.604241000	0.398926000	-0.035067000
P	-2.347125000	-1.274607000	-0.006818000
O	1.091048000	-0.983970000	-0.011674000
O	1.423317000	1.713144000	0.000690000
C	-2.136454000	1.733007000	-0.092037000
C	-3.775602000	-0.158341000	-0.098459000
C	-3.478128000	1.242275000	-0.115177000
C	-4.568145000	2.169136000	-0.153386000
C	-5.895444000	1.674790000	-0.173088000
H	-6.714953000	2.388412000	-0.202471000
C	-6.152893000	0.324778000	-0.155445000
H	-7.175490000	-0.039358000	-0.171110000
C	-5.087260000	-0.597682000	-0.117243000
H	-5.310441000	-1.658446000	-0.107781000
C	2.267462000	-0.492977000	-0.009009000
C	3.422572000	-1.322810000	-0.015427000
C	4.692704000	-0.773159000	-0.005778000
C	4.871535000	0.649417000	0.009923000
C	3.778880000	1.491698000	0.013730000
C	2.440490000	0.969243000	0.002143000
C	-4.291169000	3.558759000	-0.168073000
C	-1.915456000	3.095246000	-0.106706000
H	-0.897992000	3.475282000	-0.089179000
C	-2.994207000	4.009680000	-0.144787000
H	-5.122722000	4.257641000	-0.197096000
H	-2.788184000	5.076358000	-0.155595000
C	-2.285637000	-2.393630000	-1.481758000
H	-1.934150000	-1.707095000	-2.263848000
C	-3.605100000	-3.003490000	-1.949047000
C	-1.192641000	-3.439822000	-1.243072000
H	-0.253268000	-2.980501000	-0.920247000
H	-1.500549000	-4.168861000	-0.486452000
H	-1.002067000	-3.990067000	-2.169664000
H	-4.029065000	-3.685493000	-1.206933000
H	-3.431178000	-3.580969000	-2.863663000
H	-4.346286000	-2.234059000	-2.175471000
C	-2.447313000	-2.234352000	1.574117000
H	-1.499828000	-2.788185000	1.587634000
C	-3.606944000	-3.220772000	1.694719000
C	-2.439979000	-1.229681000	2.729327000
H	-1.572012000	-0.565970000	2.682469000
H	-3.341126000	-0.608726000	2.712389000
H	-2.412338000	-1.763413000	3.684472000
H	-4.568399000	-2.700265000	1.689761000
H	-3.530390000	-3.758573000	2.646259000
H	-3.607338000	-3.964127000	0.894331000
Cl	3.948073000	3.204264000	0.030628000
Cl	6.468513000	1.296196000	0.022978000
Cl	6.076576000	-1.795900000	-0.012288000
Cl	3.169022000	-3.030494000	-0.035448000

Σ of electronic & zero-point Energies -3317.982074

Σ of electronic & thermal Free Energies -3318.050150

Optimization GAS PHASE, Singlet state, Au(I) forms

(P,C)Au(O,O)Cl_4 – Au(I)

Au	0.484137000	-0.890643000	-0.404624000
P	0.968545000	1.302512000	0.046451000
O	-1.805343000	-1.318982000	-2.769843000
O	-0.599240000	-2.656618000	-0.641025000
C	2.535950000	-1.157595000	-0.409986000
C	2.764981000	1.224161000	0.272638000
C	3.341733000	-0.049340000	-0.018346000
C	4.758615000	-0.203209000	0.091635000
C	5.535872000	0.905708000	0.506806000
H	6.612212000	0.782964000	0.595194000
C	4.952651000	2.117924000	0.795122000
H	5.563593000	2.957007000	1.112662000
C	3.557721000	2.284061000	0.671271000
H	3.120807000	3.254242000	0.878744000
C	-2.138985000	-1.058779000	-1.621283000
C	-3.120317000	-0.014920000	-1.284287000
C	-3.532631000	0.220004000	0.002639000
C	-3.028229000	-0.551062000	1.111060000
C	-2.085236000	-1.519085000	0.885860000
C	-1.516166000	-1.733919000	-0.438994000
C	5.333630000	-1.461882000	-0.213688000
C	3.134354000	-2.363733000	-0.698340000
H	2.527957000	-3.214353000	-0.995150000
C	4.539650000	-2.513025000	-0.603636000
H	6.410584000	-1.580232000	-0.132568000
H	4.987463000	-3.474779000	-0.837096000
C	0.550384000	2.447999000	-1.349814000
H	0.723637000	1.813172000	-2.228100000
C	1.445375000	3.680277000	-1.465074000
C	-0.935743000	2.800162000	-1.296564000
H	-1.559209000	1.913451000	-1.167346000
H	-1.155998000	3.496530000	-0.482394000
H	-1.234994000	3.276497000	-2.233706000
H	1.340708000	4.346089000	-0.603562000
H	1.152900000	4.247281000	-2.354594000
H	2.498260000	3.410536000	-1.567417000
C	0.140312000	1.829511000	1.610092000
H	-0.926940000	1.735664000	1.368174000
C	0.435305000	3.262049000	2.050917000
C	0.481535000	0.820983000	2.708439000
H	0.212622000	-0.199628000	2.426033000
H	1.551210000	0.841540000	2.939061000
H	-0.071584000	1.071080000	3.618295000
H	1.483155000	3.374539000	2.342086000
H	-0.175211000	3.500599000	2.927559000
H	0.205800000	3.998952000	1.278348000
Cl	-1.471388000	-2.502385000	2.159535000
Cl	-3.593764000	-0.219149000	2.711102000
Cl	-4.671385000	1.477058000	0.330434000
Cl	-3.775810000	0.849124000	-2.622690000

Σ of electronic & zero-point Energies -3317.986930

Σ of electronic & thermal Free Energies -3317.051038

(P,C)Au(O,O)H_4 – Au(I)

Au	-0.496413000	-0.874325000	0.003198000
P	0.370028000	1.244330000	-0.092315000
O	-2.961742000	-1.211753000	-2.114443000
O	-1.856181000	-2.429110000	0.193494000
C	1.484142000	-1.494966000	-0.098865000
C	2.148300000	0.901620000	0.027175000
C	2.489389000	-0.485797000	-0.017665000
C	3.871515000	-0.851810000	0.019180000
C	4.848689000	0.167951000	0.125485000
H	5.897094000	-0.117390000	0.160071000
C	4.491159000	1.494976000	0.182960000
H	5.252889000	2.264198000	0.263869000
C	3.132333000	1.867715000	0.124878000
H	2.873399000	2.920185000	0.141109000
C	-3.186370000	-0.746730000	-0.995867000
C	-4.006071000	0.447093000	-0.780073000
C	-4.322174000	0.900763000	0.464804000
C	-3.837008000	0.263184000	1.652765000
C	-3.020291000	-0.821463000	1.551613000
C	-2.600518000	-1.335109000	0.260049000
C	4.215721000	-2.224661000	-0.048244000
C	1.866793000	-2.817310000	-0.166067000
H	1.111793000	-3.595541000	-0.230604000
C	3.234928000	-3.181870000	-0.144782000
H	5.265392000	-2.504463000	-0.022384000
H	3.505857000	-4.232708000	-0.199219000
H	-2.649610000	-1.349438000	2.426546000
H	-4.133686000	0.643340000	2.625294000
H	-4.974119000	1.765372000	0.568546000
H	-4.416402000	0.911047000	-1.672627000
C	0.012541000	2.105764000	-1.696267000
H	-0.009999000	1.265772000	-2.402374000
C	1.082600000	3.092418000	-2.159145000
C	-1.381541000	2.730924000	-1.652878000
H	-2.135312000	2.027546000	-1.289173000
H	-1.401250000	3.619103000	-1.013540000
H	-1.672535000	3.041741000	-2.660622000
H	1.171880000	3.947990000	-1.483138000
H	0.805513000	3.481071000	-3.144528000
H	2.062369000	2.618832000	-2.245797000
C	-0.185884000	2.263788000	1.343848000
H	-1.272330000	2.322509000	1.191711000
C	0.395340000	3.674134000	1.420343000
C	0.078938000	1.474219000	2.627242000
H	-0.424341000	0.503890000	2.610398000
H	1.150689000	1.302979000	2.768809000
H	-0.293251000	2.036523000	3.489345000
H	1.468598000	3.644863000	1.626322000
H	-0.080043000	4.218680000	2.242934000
H	0.231762000	4.248520000	0.505785000

Σ of electronic & zero-point Energies -1479.770986

Σ of electronic & thermal Free Energies -1479.827742

(P,C)Au(O,O)H_4 – Au(II) – TS – Singlet Open-Shell

Au	0.083314000	-1.335846000	-0.294280000
P	0.149494000	1.056286000	-0.296008000
O	-1.892667000	-1.779886000	-0.133533000
O	-3.280199000	-0.168669000	-1.830517000
C	2.116326000	-1.229944000	-0.176212000
C	1.818985000	1.186904000	0.401431000
C	2.645123000	0.023278000	0.277083000
C	4.025995000	0.138716000	0.632719000
C	4.504949000	1.361858000	1.163761000
H	5.552773000	1.430704000	1.444986000
C	3.671479000	2.442767000	1.330239000
H	4.051282000	3.369761000	1.748593000
C	2.322456000	2.361218000	0.928957000
H	1.689347000	3.238052000	1.016391000
C	-2.912519000	-1.135474000	0.305644000
C	-3.308980000	-1.191808000	1.668158000
C	-4.391295000	-0.471384000	2.111341000

C	-5.115483000	0.373588000	1.219368000
C	-4.765306000	0.483473000	-0.097566000
C	-3.654451000	-0.269178000	-0.648515000
C	4.875466000	-0.981413000	0.456334000
C	2.995123000	-2.285134000	-0.339436000
H	2.626420000	-3.245327000	-0.688749000
C	4.371524000	-2.159947000	-0.036486000
H	5.925929000	-0.890514000	0.719051000
H	5.027380000	-3.015113000	-0.175557000
C	0.218425000	1.866418000	-1.963710000
H	0.829919000	1.144994000	-2.522664000
C	0.944441000	3.213499000	-1.966973000
C	-1.159114000	1.945144000	-2.615242000
H	-1.696877000	0.994906000	-2.579564000
H	-1.788524000	2.695821000	-2.127938000
H	-1.043036000	2.246424000	-3.661146000
H	0.406633000	3.965351000	-1.382605000
H	1.004323000	3.579199000	-2.997564000
H	1.960615000	3.133849000	-1.576294000
C	-1.122777000	1.749227000	0.830966000
H	-2.049847000	1.271364000	0.469865000
C	-1.333996000	3.262419000	0.804071000
C	-0.853047000	1.224478000	2.243223000
H	-0.705748000	0.140587000	2.248606000
H	0.038190000	1.689608000	2.673619000
H	-1.711617000	1.445601000	2.882929000
H	-0.459670000	3.798269000	1.184752000
H	-2.183880000	3.515896000	1.446489000
H	-1.556442000	3.632578000	-0.198048000
H	-5.313962000	1.119703000	-0.785413000
H	-5.962605000	0.936384000	1.602997000
H	-4.702377000	-0.539598000	3.149530000
H	-2.739472000	-1.834756000	2.333478000

Σ of electronic & zero-point Energies -1479.745310

Σ of electronic & thermal Free Energies -1479.801071

P,C)Au(O,O)H$_4$ – Au(II) – *minimum* – Triplet

P	-0.164924000	1.104472000	0.260199000
O	1.997873000	-1.425073000	0.832842000
O	4.219528000	-0.026138000	1.605492000
C	-2.018566000	-1.266204000	0.048216000
C	-1.920220000	1.225841000	-0.170101000
C	-2.647115000	-0.004955000	-0.209144000
C	-4.043251000	0.045326000	-0.519223000
C	-4.646106000	1.297249000	-0.795462000
H	-5.706174000	1.320460000	-1.034518000
C	-3.917502000	2.462442000	-0.766816000
H	-4.393709000	3.413653000	-0.983079000
C	-2.545088000	2.427924000	-0.447098000
H	-1.986580000	3.356944000	-0.412349000
C	2.826259000	-0.985020000	-0.072622000
C	2.628954000	-1.163070000	-1.457656000
C	3.508301000	-0.631285000	-2.386240000
C	4.643513000	0.106928000	-1.971214000
C	4.893144000	0.291837000	-0.635711000
C	4.016952000	-0.233275000	0.389170000
C	-4.788019000	-1.159400000	-0.548453000
C	-2.792505000	-2.410423000	0.009570000
H	-2.337226000	-3.377043000	0.204676000
C	-4.174944000	-2.358928000	-0.285434000
H	-5.848026000	-1.115113000	-0.782773000
H	-4.748723000	-3.281081000	-0.307132000
C	0.129035000	1.823025000	1.936692000
H	-0.371137000	1.089232000	2.583365000
C	-0.514412000	3.187349000	2.180913000
C	1.627859000	1.787526000	2.239945000
H	2.060125000	0.789623000	2.123135000
H	2.187302000	2.473259000	1.596561000
H	1.794608000	2.103915000	3.274163000
H	-0.079394000	3.965681000	1.548932000
H	-0.344798000	3.477435000	3.223226000
H	-1.593223000	3.163830000	2.010010000
C	0.878148000	1.877033000	-1.056546000
H	1.874731000	1.464980000	-0.853540000
C	0.960082000	3.402716000	-1.044089000
C	0.404802000	1.341659000	-2.408392000
H	0.344416000	0.250643000	-2.410254000
H	-0.580347000	1.741481000	-2.665889000
H	1.116075000	1.637911000	-3.184792000
H	-0.014352000	3.863286000	-1.229534000
H	1.633500000	3.727361000	-1.844644000
H	1.356957000	3.789549000	-0.103706000
H	5.758448000	0.846977000	-0.285900000
H	5.317121000	0.517026000	-2.718511000
H	3.327228000	-0.787302000	-3.445998000
H	1.764211000	-1.740248000	-1.779559000

Σ of electronic & zero-point Energies -1479.754197

Σ of electronic & thermal Free Energies -1479.812446

Optimization GAS PHASE, Singlet state, (P,C)Au(O,O)H$_4$ + o-quinone

- Approach *trans* to P

RC1-H

Au	0.119526000	-0.414094000	-0.490386000
P	1.663698000	1.227397000	-0.223706000
O	-1.425716000	0.737892000	-1.211469000
O	-1.252204000	-1.912222000	-0.760324000
C	1.628453000	-1.628339000	0.042503000
C	3.197453000	0.277884000	-0.072360000
C	2.952527000	-1.109978000	0.120137000
C	4.044779000	-1.979051000	0.415743000
C	5.347545000	-1.424564000	0.469964000
H	6.185537000	-2.083174000	0.682647000
C	5.561293000	-0.080391000	0.264104000
H	6.567423000	0.324304000	0.311771000
C	4.478842000	0.787496000	0.004105000
H	4.666325000	1.846940000	-0.128448000
C	-2.543873000	0.024577000	-1.213663000
C	-3.797250000	0.596533000	-1.464376000
C	-4.927884000	-0.206539000	-1.513876000
C	-4.820678000	-1.599821000	-1.367723000
C	-3.591817000	-2.196464000	-1.131964000
C	-2.443512000	-1.397824000	-1.016691000
C	3.776626000	-3.351031000	0.644061000
C	1.402913000	-2.963395000	0.286289000
H	0.391148000	-3.352737000	0.236292000
C	2.486406000	-3.823087000	0.587721000
H	4.603022000	-4.019408000	0.869015000
H	2.286783000	-4.874799000	0.771967000
H	-3.490315000	-3.269555000	-1.006937000
H	-5.711691000	-2.217356000	-1.434245000
H	-5.898555000	0.243755000	-1.697106000
H	-3.854337000	1.671006000	-1.600537000
C	1.616173000	2.343120000	-1.696070000
H	1.359223000	1.649652000	-2.506097000
C	2.942226000	3.016554000	-2.043943000
C	0.456693000	3.330326000	-1.527213000
H	-0.472912000	2.816573000	-1.268006000
H	0.677124000	4.074563000	-0.756393000
H	0.303627000	3.863145000	-2.470836000

H	3.283256000	3.691840000	-1.254565000
H	2.806262000	3.615396000	-2.950248000
H	3.729359000	2.285258000	-2.241282000
C	1.420763000	2.161892000	1.341229000
H	0.417734000	2.587604000	1.232766000
C	2.465506000	3.257781000	1.542639000
C	1.382166000	1.174446000	2.507775000
H	0.543151000	0.482896000	2.402393000
H	2.317517000	0.611543000	2.592221000
H	1.241766000	1.737180000	3.436147000
H	3.471636000	2.837874000	1.636688000
H	2.243582000	3.786678000	2.474859000
H	2.466921000	3.997364000	0.738301000
O	-1.709984000	2.116940000	1.336227000
O	-1.337043000	-0.565478000	1.850708000
C	-2.685717000	1.379256000	1.458603000
C	-4.056653000	1.866667000	1.433915000
C	-5.099481000	1.005388000	1.531132000
C	-4.905807000	-0.418734000	1.651707000
C	-3.662623000	-0.961100000	1.723180000
C	-2.480497000	-0.124322000	1.680683000
H	-4.197258000	2.937082000	1.320687000
H	-6.118001000	1.383743000	1.502281000
H	-5.781657000	-1.057839000	1.701485000
H	-3.502569000	-2.027759000	1.834435000

Σ of electronic & zero-point Energies -1861.081844

Σ of electronic & thermal Free Energies -1861.145106

TS1-H

Au	-0.057459000	0.192529000	-0.246568000
P	-1.795358000	-1.225975000	-0.036273000
O	1.380500000	-1.327081000	-0.303264000
O	1.435304000	0.850703000	-1.927068000
C	-1.463138000	1.617083000	-0.166516000
C	-3.218477000	-0.112331000	-0.011727000
C	-2.835941000	1.254030000	-0.073347000
C	-3.841620000	2.265274000	-0.031983000
C	-5.193962000	1.858684000	0.080678000
H	-5.966137000	2.622822000	0.112575000
C	-5.538801000	0.527280000	0.152091000
H	-6.581401000	0.239237000	0.242692000
C	-4.546198000	-0.474710000	0.106535000
H	-4.837927000	-1.517573000	0.162596000
C	2.524179000	-0.914328000	-0.791616000
C	3.726184000	-1.600150000	-0.533516000
C	4.914861000	-1.140247000	-1.064958000
C	4.934546000	-0.032695000	-1.947225000
C	3.782093000	0.650783000	-2.249415000
C	2.535684000	0.253694000	-1.682660000
C	-3.440588000	3.621932000	-0.102511000
C	-1.106205000	2.943317000	-0.227249000
H	-0.057303000	3.214213000	-0.281293000
C	-2.107689000	3.944475000	-0.199908000
H	-4.199501000	4.398744000	-0.075918000
H	-1.805832000	4.986579000	-0.251727000
H	3.778520000	1.508324000	-2.914427000
H	5.879883000	0.283991000	-2.378973000
H	5.842121000	-1.653111000	-0.829318000
H	3.692219000	-2.457581000	0.129675000
C	-1.861093000	-2.396769000	-1.466956000
H	-1.573142000	-1.745591000	-2.301757000
C	-3.247171000	-2.969718000	-1.759393000
C	-0.783920000	-3.471880000	-1.303254000
H	0.190201000	-3.029798000	-1.075570000
H	-1.042836000	-4.178301000	-0.508819000
H	-0.700537000	-4.038846000	-2.235422000
H	-3.619996000	-3.590370000	-0.940161000
H	-3.183999000	-3.604791000	-2.648823000
H	-3.977247000	-2.183039000	-1.961223000
C	-1.655872000	-2.096397000	1.580520000
H	-0.656974000	-2.548947000	1.540616000
C	-2.721368000	-3.172572000	1.786642000
C	-1.672664000	-1.049345000	2.696124000
H	-0.848887000	-0.341693000	2.583222000
H	-2.624703000	-0.509619000	2.715005000
H	-1.547754000	-1.556028000	3.657766000
H	-3.725212000	-2.737282000	1.802200000
H	-2.559152000	-3.649822000	2.758173000
H	-2.689924000	-3.954622000	1.024947000
O	1.442412000	-0.455895000	2.264567000
O	1.458540000	1.709662000	0.576723000
C	2.529053000	0.033264000	1.925451000
C	3.804988000	-0.450860000	2.406718000
C	4.971123000	0.125472000	2.002914000
C	4.985623000	1.220030000	1.081114000
C	3.820661000	1.751582000	0.599019000
C	2.555020000	1.198219000	0.965957000
H	3.813910000	2.592673000	-0.085325000
H	5.938455000	1.648237000	0.786472000
H	5.919457000	-0.251309000	2.377312000
H	3.783396000	-1.284523000	3.101621000

Σ of electronic & zero-point Energies -1861.062003

Σ of electronic & thermal Free Energies -1861.122734

INT-H

Au	0.065432000	-0.249553000	-0.111878000
P	1.735163000	1.233561000	0.135461000
O	-1.331365000	1.244216000	0.504283000
O	-1.445150000	0.713415000	-2.153703000
C	1.528737000	-1.600026000	-0.370396000
C	3.200632000	0.180551000	0.049696000
C	2.883009000	-1.179605000	-0.219705000
C	3.942188000	-2.129125000	-0.339329000
C	5.273471000	-1.676893000	-0.165231000
H	6.082221000	-2.397940000	-0.250125000
C	5.553056000	-0.356459000	0.106561000
H	6.580777000	-0.032701000	0.237385000
C	4.510527000	0.588160000	0.211189000
H	4.749343000	1.627313000	0.409446000
C	-2.486447000	1.179563000	-0.082946000
C	-3.684659000	1.491094000	0.596932000
C	-4.891907000	1.428927000	-0.062915000
C	-4.947344000	1.155811000	-1.459533000
C	-3.814416000	0.904369000	-2.182843000
C	-2.522089000	0.906467000	-1.550597000
C	3.617034000	-3.478316000	-0.622299000
C	1.250741000	-2.917866000	-0.649314000
H	0.219710000	-3.232703000	-0.766371000
C	2.304386000	-3.854969000	-0.776185000
H	4.418669000	-4.205561000	-0.715135000
H	2.060205000	-4.890521000	-0.994836000
H	-3.844146000	0.700235000	-3.248350000
H	-5.916014000	1.147503000	-1.952328000
H	-5.811395000	1.634704000	0.475424000
H	-3.623095000	1.720424000	1.654860000

C	1.705119000	2.454140000	-1.251316000
H	1.405698000	1.823028000	-2.097169000
C	3.059427000	3.088822000	-1.561548000
C	0.596185000	3.479659000	-1.012384000
H	-0.349666000	2.988484000	-0.775877000
H	0.852957000	4.164847000	-0.198246000
H	0.458487000	4.074906000	-1.919621000
H	3.425303000	3.705432000	-0.735480000
H	2.951268000	3.741179000	-2.433796000
H	3.817300000	2.338005000	-1.795906000
C	1.566394000	2.031435000	1.782398000
H	0.591224000	2.528867000	1.708091000
C	2.660026000	3.053096000	2.088442000
C	1.473432000	0.937299000	2.849514000
H	0.612740000	0.283476000	2.685252000
H	2.382780000	0.327662000	2.869924000
H	1.360810000	1.407091000	3.831660000
H	3.640287000	2.572759000	2.159308000
H	2.454172000	3.517884000	3.057747000
H	2.713535000	3.851352000	1.344236000
O	-1.392294000	-0.991221000	2.069086000
O	-1.435349000	-1.627963000	-0.588639000
C	-2.498379000	-1.180969000	1.524678000
C	-3.757503000	-1.131196000	2.222490000
C	-4.934522000	-1.343299000	1.561954000
C	-4.960918000	-1.622528000	0.164844000
C	-3.793461000	-1.740401000	-0.554430000
C	-2.547553000	-1.485340000	0.061413000
H	-3.794432000	-1.980812000	-1.611501000
H	-5.914342000	-1.792374000	-0.324880000
H	-5.875522000	-1.295387000	2.103608000
H	-3.723185000	-0.917855000	3.286107000

Σ of electronic & zero-point Energies -1861.070483

Σ of electronic & thermal Free Energies -1861.132945

TS2-H

Au	0.045491000	0.306310000	-0.250628000
P	1.689817000	-1.222748000	-0.047305000
O	-1.406894000	-1.565793000	0.283091000
O	-1.244001000	0.288750000	2.269998000
C	1.511233000	1.640338000	0.079875000
C	3.174484000	-0.186415000	-0.006429000
C	2.862090000	1.195368000	0.097754000
C	3.916004000	2.146573000	0.245895000
C	5.250100000	1.670413000	0.240352000
H	6.059386000	2.388867000	0.340102000
C	5.529995000	0.327763000	0.119343000
H	6.559655000	-0.015769000	0.122099000
C	4.486908000	-0.615879000	0.009508000
H	4.727819000	-1.671355000	-0.040285000
C	-2.471491000	-1.127117000	0.811807000
C	-3.767623000	-1.610320000	0.449443000
C	-4.891536000	-1.123393000	1.058837000
C	-4.801019000	-0.149667000	2.104424000
C	-3.601879000	0.348968000	2.517064000
C	-2.367389000	-0.105313000	1.918065000
C	3.581323000	3.514575000	0.396324000
C	1.213985000	2.970929000	0.247999000
H	0.178903000	3.294737000	0.252226000
C	2.264135000	3.907512000	0.407447000
H	4.378969000	4.243297000	0.508846000
H	2.012468000	4.956503000	0.533757000
H	-3.524868000	1.089937000	3.306387000
H	-5.719590000	0.198970000	2.569316000
H	-5.869495000	-1.492607000	0.766930000
H	-3.819051000	-2.354623000	-0.337514000
C	1.506754000	-2.143054000	1.557932000
H	0.868246000	-1.459144000	2.130935000
C	2.832311000	-2.336880000	2.291605000
C	0.747855000	-3.458287000	1.373276000
H	-0.204998000	-3.296638000	0.867398000
H	1.338649000	-4.195977000	0.821562000
H	0.538208000	-3.878896000	2.361822000
H	3.513103000	-2.993548000	1.739775000
H	2.631289000	-2.810963000	3.257471000
H	3.345360000	-1.391470000	2.478378000
C	1.706524000	-2.364987000	-1.487949000
H	0.784673000	-2.944039000	-1.354053000
C	2.915253000	-3.302317000	-1.499111000
C	1.596239000	-1.553689000	-2.780636000
H	0.654173000	-1.002487000	-2.824915000
H	2.428188000	-0.847564000	-2.873680000
H	1.636744000	-2.234836000	-3.636737000
H	3.826738000	-2.752879000	-1.749408000
H	2.771310000	-4.066303000	-2.269339000
H	3.069004000	-3.816692000	-0.546617000
O	-1.453961000	-0.320206000	-1.947397000
O	-1.438371000	1.738251000	-0.187828000
C	-2.572965000	0.218073000	-1.644666000
C	-3.814457000	-0.174795000	-2.223734000
C	-4.987740000	0.420866000	-1.827337000
C	-4.988349000	1.428153000	-0.833317000
C	-3.803899000	1.890936000	-0.290794000
C	-2.583578000	1.301238000	-0.659313000
H	-3.792087000	-0.963454000	-2.969085000
H	-3.787671000	2.679005000	0.453845000
H	-5.930741000	0.104444000	-2.264020000
H	-5.929209000	1.870691000	-0.520924000

Σ of electronic & zero-point Energies -1861.059822

Σ of electronic & thermal Free Energies -1861.121956

RC2-H

Au	-0.153413000	-0.493740000	-0.597100000
P	-1.629012000	1.208815000	-0.332470000
O	2.221083000	2.665165000	1.426789000
O	1.085182000	0.196252000	1.773893000
C	-1.644043000	-1.635920000	0.117484000
C	-2.979590000	0.398820000	0.557385000
C	-2.820227000	-1.012940000	0.625602000
C	-3.853844000	-1.804251000	1.209941000
C	-5.000490000	-1.144206000	1.717068000
H	-5.787223000	-1.741587000	2.170274000
C	-5.126869000	0.224644000	1.647033000
H	-6.011826000	0.710935000	2.045341000
C	-4.113330000	1.009406000	1.056467000
H	-4.233230000	2.085655000	1.006046000
C	2.947491000	1.683797000	1.550194000
C	4.398707000	1.765481000	1.608980000
C	5.146598000	0.642650000	1.743536000
C	4.555072000	-0.670946000	1.833160000
C	3.208429000	-0.848041000	1.803979000
C	2.315236000	0.289668000	1.701823000
C	-3.686005000	-3.209916000	1.260734000
C	-1.516097000	-3.004423000	0.184720000
H	-0.612948000	-3.477095000	-0.188164000
C	-2.545657000	-3.789442000	0.757217000

H	-4.468853000	-3.818519000	1.704588000
H	-2.421831000	-4.867728000	0.801239000
H	2.750077000	-1.827494000	1.884515000
H	5.213273000	-1.527564000	1.932839000
H	6.230408000	0.716841000	1.779843000
H	4.842303000	2.752825000	1.529281000
C	-0.830231000	2.603596000	0.561586000
H	-0.087116000	2.089905000	1.187542000
C	-1.766621000	3.411847000	1.455451000
C	-0.053035000	3.460731000	-0.439573000
H	0.621857000	2.845272000	-1.039980000
H	-0.716057000	4.035735000	-1.094737000
H	0.570622000	4.158024000	0.123412000
H	-2.536384000	3.945617000	0.888470000
H	-1.169284000	4.160247000	1.985079000
H	-2.255006000	2.785387000	2.205506000
C	-2.292179000	1.745237000	-1.969912000
H	-1.413178000	2.147818000	-2.487660000
C	-3.358226000	2.833058000	-1.844323000
C	-2.813027000	0.528645000	-2.735576000
H	-2.031618000	-0.221242000	-2.883133000
H	-3.642020000	0.053764000	-2.201574000
H	-3.177990000	0.843315000	-3.718196000
H	-4.244703000	2.451520000	-1.329376000
H	-3.669747000	3.153115000	-2.843671000
H	-2.996658000	3.714873000	-1.310489000
O	1.427541000	0.631370000	-1.277538000
O	1.195328000	-2.013405000	-0.787412000
C	2.538477000	-0.090075000	-1.181890000
C	3.811184000	0.475982000	-1.321920000
C	4.938000000	-0.333745000	-1.255752000
C	4.808965000	-1.720587000	-1.092848000
C	3.555570000	-2.311323000	-0.973048000
C	2.412588000	-1.508513000	-0.970113000
H	3.440144000	-3.381404000	-0.834321000
H	3.885428000	1.547917000	-1.470294000
H	5.698244000	-2.343746000	-1.065287000
H	5.923992000	0.110353000	-1.349435000

Σ of electronic & zero-point Energies -1861.081608

Σ of electronic & thermal Free Energies -1861.143980

Optimization GAS PHASE, Singlet state, (P,C)Au(O,O)H_4 + o-quinone-Cl2

- Approach *trans* to P

RC1-Cl_2

Au	-0.769786000	-0.374437000	0.592119000
P	-2.287369000	1.243278000	0.112380000
O	0.702829000	0.814174000	1.412869000
O	0.579650000	-1.852000000	1.055106000
C	-2.214703000	-1.618900000	-0.037912000
C	-3.794427000	0.277821000	-0.153708000
C	-3.525991000	-1.114172000	-0.266471000
C	-4.579214000	-2.002883000	-0.635437000
C	-5.872247000	-1.461184000	-0.840785000
H	-6.682124000	-2.134018000	-1.110031000
C	-6.110975000	-0.111742000	-0.710102000
H	-7.108886000	0.282733000	-0.873735000
C	-5.063695000	0.774277000	-0.377596000
H	-5.267761000	1.836549000	-0.306194000
C	1.816073000	0.111518000	1.541659000
C	3.043703000	0.701387000	1.876008000
C	4.167190000	-0.091582000	2.051872000
C	4.078139000	-1.491300000	1.950527000
C	2.880467000	-2.106588000	1.629145000
C	1.739141000	-1.321306000	1.390361000
C	-4.283249000	-3.380293000	-0.782565000
C	-1.958535000	-2.959704000	-0.206604000
H	-0.954924000	-3.338720000	-0.043413000
C	-3.003042000	-3.839245000	-0.580383000
H	-5.079956000	-4.063718000	-1.062419000
H	-2.781042000	-4.895306000	-0.703392000
H	2.797646000	-3.183794000	1.530551000
H	4.966233000	-2.095932000	2.103205000
H	5.119806000	0.370890000	2.288750000
H	3.086041000	1.780716000	1.974458000
C	-2.387776000	2.415973000	1.536708000
H	-2.208655000	1.757432000	2.395388000
C	-3.745103000	3.090943000	1.724574000
C	-1.223274000	3.407071000	1.442323000
H	-0.269378000	2.893851000	1.294656000
H	-1.373156000	4.119342000	0.625671000
H	-1.165638000	3.976994000	2.374737000
H	-4.008440000	3.732330000	0.879169000
H	-3.702484000	3.725536000	2.615505000
H	-4.544686000	2.361379000	1.871516000
C	-1.887529000	2.113983000	-1.457111000
H	-0.909689000	2.565046000	-1.260684000
C	-2.920010000	3.180397000	-1.818866000
C	-1.708760000	1.078202000	-2.567388000
H	-0.878686000	0.404498000	-2.342162000
H	-2.622178000	0.496106000	-2.727290000
H	-1.475688000	1.602788000	-3.499331000
H	-3.903746000	2.737396000	-2.001246000
H	-2.605990000	3.672058000	-2.744901000
H	-3.019183000	3.954743000	-1.054219000
O	1.214603000	1.989543000	-1.134822000
O	0.904034000	-0.722486000	-1.578265000
C	2.195744000	1.248186000	-1.143121000
C	3.552885000	1.744669000	-1.002994000
C	4.616369000	0.902987000	-0.978757000
C	4.445413000	-0.533629000	-1.095136000
C	3.209549000	-1.075438000	-1.251579000
C	2.021305000	-0.252466000	-1.329123000
H	3.684976000	2.814383000	-0.893153000
H	3.079556000	-2.144684000	-1.361762000
Cl	5.838103000	-1.568100000	-1.100832000
Cl	6.210018000	1.553218000	-0.776646000

Σ of electronic & zero-point Energies -2780.193916

Σ of electronic & thermal Free Energies -2780.260370

TS1-Cl_2

Au	-0.677161000	0.175078000	-0.324436000
P	-2.455121000	-1.177123000	-0.017978000
O	0.678924000	-1.402940000	-0.589362000
O	0.712357000	0.861521000	-2.089161000
C	-2.001057000	1.652326000	-0.046737000
C	-3.813759000	-0.005994000	0.196236000
C	-3.374090000	1.343724000	0.161491000
C	-4.321456000	2.394215000	0.346546000
C	-5.674855000	2.041113000	0.571042000
H	-6.403129000	2.835139000	0.713053000

C	-6.074562000	0.723862000	0.614037000
H	-7.116348000	0.476863000	0.792128000
C	-5.140063000	-0.316512000	0.425741000
H	-5.474785000	-1.347241000	0.461116000
C	1.794817000	-1.019045000	-1.150400000
C	2.980035000	-1.772212000	-1.031993000
C	4.142845000	-1.330421000	-1.628786000
C	4.149507000	-0.169728000	-2.442703000
C	3.015440000	0.584073000	-2.608114000
C	1.795152000	0.203596000	-1.970932000
C	-3.864259000	3.734093000	0.299606000
C	-1.587340000	2.962607000	-0.081195000
H	-0.536765000	3.191414000	-0.223291000
C	-2.532922000	4.003592000	0.088224000
H	-4.579030000	4.540718000	0.435251000
H	-2.187650000	5.032783000	0.055001000
H	3.004937000	1.485041000	-3.212545000
H	5.076815000	0.136873000	-2.916314000
H	5.062911000	-1.888887000	-1.490190000
H	2.958487000	-2.666174000	-0.418355000
C	-2.707787000	-2.268477000	-1.489844000
H	-2.466395000	-1.589423000	-2.317159000
C	-4.142440000	-2.761621000	-1.675090000
C	-1.676487000	-3.399612000	-1.478659000
H	-0.663686000	-3.016881000	-1.325497000
H	-1.896145000	-4.132235000	-0.696303000
H	-1.709672000	-3.922097000	-2.439412000
H	-4.468907000	-3.404482000	-0.853204000
H	-4.193344000	-3.354029000	-2.594159000
H	-4.847489000	-1.933295000	-1.771741000
C	-2.200633000	-2.132750000	1.535167000
H	-1.232779000	-2.625102000	1.376989000
C	-3.291914000	-3.171625000	1.792596000
C	-2.062300000	-1.144434000	2.694955000
H	-1.221505000	-0.466235000	2.536223000
H	-2.982281000	-0.567810000	2.832682000
H	-1.869043000	-1.704670000	3.614545000
H	-4.267395000	-2.695102000	1.929262000
H	-3.059112000	-3.706681000	2.718479000
H	-3.371940000	-3.912254000	0.994066000
O	1.028006000	-0.685047000	1.999999000
O	0.977652000	1.583411000	0.438622000
C	2.092473000	-0.211250000	1.578894000
C	3.383452000	-0.780546000	1.885556000
C	4.535721000	-0.237489000	1.401627000
C	4.512636000	0.930151000	0.563905000
C	3.324257000	1.529227000	0.243008000
C	2.077729000	1.002832000	0.696362000
H	3.302709000	2.420823000	-0.370857000
H	3.405263000	-1.665660000	2.509832000
Cl	5.996001000	1.643082000	0.009285000
Cl	6.054261000	-0.987402000	1.786979000

Σ of electronic & zero-point Energies -2780.175221

Σ of electronic & thermal Free Energies -2780.239898

INT-Cl_2

Au	-0.648539000	0.174291000	-0.162119000
P	-2.454053000	-1.121653000	0.179901000
O	0.616190000	-1.461820000	0.392905000
O	0.672532000	-0.942106000	-2.269919000
C	-1.970937000	1.673277000	-0.352613000
C	-3.799432000	0.082742000	0.165385000
C	-3.351992000	1.400441000	-0.127821000
C	-4.307017000	2.459018000	-0.196285000
C	-5.668095000	2.153120000	0.050634000
H	-6.397670000	2.957289000	0.005109000
C	-6.073645000	0.870416000	0.343661000
H	-7.121804000	0.659497000	0.530407000
C	-5.135226000	-0.181390000	0.397841000
H	-5.474180000	-1.188719000	0.613417000
C	1.741296000	-1.523380000	-0.242555000
C	2.930653000	-1.959759000	0.385732000
C	4.107489000	-2.014125000	-0.325010000
C	4.135039000	-1.737461000	-1.723379000
C	3.008245000	-1.364057000	-2.398410000
C	1.745782000	-1.245891000	-1.713000000
C	-3.853482000	3.765256000	-0.503254000
C	-1.566300000	2.952761000	-0.652821000
H	-0.515281000	3.155365000	-0.825877000
C	-2.518121000	3.998280000	-0.728558000
H	-4.575579000	4.574972000	-0.557167000
H	-2.175390000	5.001325000	-0.965194000
H	3.017159000	-1.147624000	-3.461662000
H	5.082198000	-1.809964000	-2.249261000
H	5.026388000	-2.301559000	0.175298000
H	2.892553000	-2.186215000	1.445430000
C	-2.624775000	-2.336030000	-1.202111000
H	-2.301538000	-1.740408000	-2.064764000
C	-4.054804000	-2.817178000	-1.441291000
C	-1.625359000	-3.478267000	-1.014619000
H	-0.619314000	-3.096651000	-0.830452000
H	-1.913547000	-4.130699000	-0.184407000
H	-1.602139000	-4.085332000	-1.924113000
H	-4.444253000	-3.391364000	-0.595731000
H	-4.062945000	-3.475712000	-2.315464000
H	-4.735984000	-1.986945000	-1.640236000
C	-2.283695000	-1.934343000	1.819208000
H	-1.371313000	-2.531488000	1.697547000
C	-3.461565000	-2.836359000	2.183775000
C	-2.022634000	-0.857286000	2.875784000
H	-1.108110000	-0.296415000	2.665649000
H	-2.861194000	-0.156285000	2.940514000
H	-1.909054000	-1.337691000	3.852557000
H	-4.380766000	-2.255998000	2.305281000
H	-3.254976000	-3.323599000	3.141725000
H	-3.637456000	-3.621878000	1.444931000
O	0.995861000	0.755013000	1.938646000
O	0.966648000	1.386833000	-0.726524000
C	2.081636000	0.827841000	1.329179000
C	3.360295000	0.626348000	1.952535000
C	4.522212000	0.706825000	1.236081000
C	4.507711000	1.008725000	-0.161413000
C	3.315950000	1.253940000	-0.807457000
C	2.085939000	1.127843000	-0.128573000
H	3.301493000	1.514027000	-1.858187000
H	3.374779000	0.393954000	3.010460000
Cl	6.034208000	0.414310000	2.041408000
Cl	5.992407000	1.187619000	-1.044447000

Σ of electronic & zero-point Energies -2780.183564

Σ of electronic & thermal Free Energies -2780.249861

TS2-Cl_2

Au	0.613081000	0.236713000	-0.162424000
P	2.377431000	-1.166213000	-0.040544000
O	-0.686591000	-1.645547000	0.636285000
O	-0.540122000	0.386647000	2.443131000

C	2.002983000	1.684360000	-0.055191000
C	3.781231000	-0.029777000	-0.155317000
C	3.379000000	1.331499000	-0.114979000
C	4.369697000	2.359048000	-0.114467000
C	5.730441000	1.973645000	-0.192908000
H	6.491074000	2.749684000	-0.203407000
C	6.096561000	0.647506000	-0.248590000
H	7.145540000	0.374466000	-0.304607000
C	5.118757000	-0.368886000	-0.217223000
H	5.430561000	-1.406849000	-0.223655000
C	-1.743424000	-1.239393000	1.199601000
C	-3.021791000	-1.840277000	0.969245000
C	-4.138548000	-1.365148000	1.598083000
C	-4.058642000	-0.291864000	2.545768000
C	-2.877916000	0.318385000	2.837219000
C	-1.648232000	-0.111958000	2.204251000
C	3.949703000	3.709096000	-0.030574000
C	1.622954000	3.000502000	0.042689000
H	0.570844000	3.255721000	0.104712000
C	2.612318000	4.013864000	0.055657000
H	4.699102000	4.495336000	-0.029759000
H	2.295585000	5.050050000	0.129292000
H	-2.809011000	1.137606000	3.545606000
H	-4.975162000	0.046196000	3.020406000
H	-5.106459000	-1.811273000	1.393314000
H	-3.069643000	-2.655524000	0.255683000
C	2.389564000	-2.059986000	1.588227000
H	1.782410000	-1.392935000	2.212301000
C	3.785825000	-2.186861000	2.195077000
C	1.672808000	-3.408372000	1.493007000
H	0.672291000	-3.298046000	1.072468000
H	2.243682000	-4.130494000	0.901484000
H	1.570537000	-3.818937000	2.502361000
H	4.436825000	-2.828440000	1.592307000
H	3.696355000	-2.648754000	3.183271000
H	4.274994000	-1.218491000	2.316930000
C	2.359561000	-2.338503000	-1.457668000
H	1.483948000	-2.966197000	-1.251740000
C	3.617792000	-3.204989000	-1.533730000
C	2.117851000	-1.563331000	-2.754662000
H	1.145781000	-1.065380000	-2.745445000
H	2.901371000	-0.815991000	-2.918196000
H	2.137639000	-2.260744000	-3.598089000
H	4.480020000	-2.607059000	-1.840962000
H	3.472608000	-3.983023000	-2.289419000
H	3.855889000	-3.701042000	-0.589075000
O	-0.967391000	-0.611000000	-1.702519000
O	-0.956604000	1.580429000	-0.098219000
C	-2.089145000	-0.114169000	-1.348314000
C	-3.340679000	-0.635267000	-1.773850000
C	-4.522101000	-0.096144000	-1.319993000
C	-4.515628000	0.999584000	-0.419380000
C	-3.320703000	1.580070000	-0.031956000
C	-2.097679000	1.039206000	-0.452059000
H	-3.341425000	-1.487934000	-2.442069000
H	-3.314970000	2.431291000	0.636974000
Cl	-6.002821000	1.685092000	0.162486000
Cl	-6.023941000	-0.811308000	-1.825322000

Σ of electronic & zero-point Energies -2780.173272

Σ of electronic & thermal Free Energies -2780.239490

RC2-Cl_2

Au	-0.664448000	-0.447551000	-0.530744000
P	-2.289249000	1.130943000	-0.398446000
O	1.326532000	2.890990000	1.581479000
O	0.353145000	0.354079000	1.929057000
C	-2.103211000	-1.699567000	0.098752000
C	-3.631373000	0.221028000	0.401506000
C	-3.360805000	-1.170942000	0.507744000
C	-4.365189000	-2.039520000	1.029582000
C	-5.597646000	-1.472338000	1.438129000
H	-6.363562000	-2.128134000	1.843538000
C	-5.832333000	-0.120103000	1.332495000
H	-6.782206000	0.294570000	1.654850000
C	-4.846378000	0.740106000	0.803744000
H	-5.051691000	1.801593000	0.724337000
C	2.112681000	1.972779000	1.782308000
C	3.550561000	2.163918000	1.919629000
C	4.365161000	1.106252000	2.146585000
C	3.863547000	-0.246098000	2.240600000
C	2.539546000	-0.526537000	2.136447000
C	1.573070000	0.538151000	1.941619000
C	-4.084473000	-3.425107000	1.119375000
C	-1.865591000	-3.050909000	0.200049000
H	-0.901799000	-3.450996000	-0.098246000
C	-2.865741000	-3.912703000	0.711409000
H	-4.844405000	-4.092135000	1.516461000
H	-2.655762000	-4.975834000	0.784721000
H	2.152047000	-1.536695000	2.211258000
H	4.578344000	-1.047188000	2.399091000
H	5.436706000	1.257882000	2.234124000
H	3.928138000	3.176521000	1.822517000
C	-1.672513000	2.591927000	0.534671000
H	-0.939393000	2.143995000	1.219513000
C	-2.736401000	3.323661000	1.348456000
C	-0.897200000	3.505682000	-0.416623000
H	-0.132199000	2.946396000	-0.961094000
H	-1.555634000	4.020748000	-1.123891000
H	-0.376117000	4.255693000	0.181767000
H	-3.502240000	3.790166000	0.720385000
H	-2.244058000	4.120920000	1.913521000
H	-3.226653000	2.661726000	2.065970000
C	-2.864563000	1.597436000	-2.089114000
H	-1.984273000	2.066817000	-2.544679000
C	-4.022294000	2.594844000	-2.058694000
C	-3.225104000	0.335794000	-2.873993000
H	-2.376236000	-0.348192000	-2.953207000
H	-4.050463000	-0.201615000	-2.396730000
H	-3.539351000	0.611724000	-3.885241000
H	-4.912038000	2.144573000	-1.609133000
H	-4.279930000	2.882235000	-3.082888000
H	-3.776532000	3.506637000	-1.509643000
O	0.869230000	0.797759000	-1.121042000
O	0.816731000	-1.856244000	-0.602080000
C	2.020052000	0.165676000	-0.941743000
C	3.247957000	0.830322000	-1.004385000
C	4.434462000	0.123946000	-0.841629000
C	4.406488000	-1.264980000	-0.639891000
C	3.195311000	-1.951132000	-0.602580000
C	1.995073000	-1.251758000	-0.708405000
H	3.176317000	-3.021425000	-0.436597000
H	3.262881000	1.898805000	-1.180246000
Cl	5.877422000	-2.168878000	-0.430773000
Cl	5.938258000	0.994876000	-0.922202000

Σ of electronic & zero-point Energies -2780.195533

Σ of electronic & thermal Free Energies -2780.262010

o-quinone-Cl_2

O	2.933360000	1.387630000	0.000102000
O	2.933360000	-1.387630000	-0.000092000
C	1.885466000	0.772476000	0.000067000
C	0.580228000	1.442169000	0.000056000
C	-0.570045000	0.738760000	0.000029000
C	-0.570045000	-0.738760000	-0.000029000
C	0.580228000	-1.442169000	-0.000051000
C	1.885466000	-0.772476000	-0.000051000
Cl	-2.083443000	-1.565370000	-0.000048000
Cl	-2.083443000	1.565370000	0.000035000
H	0.577758000	-2.526008000	-0.000087000
H	0.577758000	2.526008000	0.000089000

Σ of electronic & zero-point Energies -1300.337048
Σ of electronic & thermal Free Energies -1300.372095

(P,C)Au(O,O)Cl_2

Au	-0.172855000	0.238446000	-0.062720000
P	-1.914244000	-1.219234000	-0.044286000
O	1.298853000	-1.171609000	0.012937000
O	1.361467000	1.540181000	-0.083064000
C	-1.607737000	1.651727000	-0.096913000
C	-3.344087000	-0.116459000	-0.032549000
C	-2.978547000	1.259194000	-0.062375000
C	-4.006619000	2.249513000	-0.052789000
C	-5.355767000	1.820012000	-0.003460000
H	-6.140608000	2.571700000	0.006050000
C	-5.681976000	0.482822000	0.033334000
H	-6.722462000	0.176465000	0.072367000
C	-4.670572000	-0.500386000	0.017049000
H	-4.946395000	-1.549115000	0.037430000
C	2.499072000	-0.550286000	0.006820000
C	3.690635000	-1.265367000	0.048943000
C	4.914321000	-0.592836000	0.045764000
C	4.944608000	0.801405000	0.000771000
C	3.751621000	1.526081000	-0.042055000
C	2.530642000	0.861392000	-0.039912000
C	-3.634310000	3.615878000	-0.088438000
C	-1.286379000	2.990145000	-0.129656000
H	-0.241990000	3.286122000	-0.153178000
C	-2.306795000	3.970960000	-0.127533000
H	-4.412189000	4.374131000	-0.082695000
H	-2.027666000	5.020246000	-0.154393000
C	-1.874693000	-2.276727000	-1.558158000
H	-1.581758000	-1.552346000	-2.329254000
C	-3.218700000	-2.881626000	-1.958710000
C	-0.753814000	-3.310429000	-1.417201000
H	0.188729000	-2.844662000	-1.111140000
H	-1.016780000	-4.082812000	-0.687521000
H	-0.599018000	-3.806368000	-2.380019000
H	-3.591546000	-3.591139000	-1.215473000
H	-3.093742000	-3.428183000	-2.898736000
H	-3.978081000	-2.112585000	-2.116996000
C	-1.849344000	-2.222460000	1.499536000
H	-0.868629000	-2.710904000	1.434630000
C	-2.948548000	-3.276971000	1.613874000
C	-1.847091000	-1.269832000	2.697571000
H	-1.014771000	-0.562611000	2.650635000
H	-2.779851000	-0.699805000	2.749596000
H	-1.748692000	-1.847998000	3.621074000
H	-3.939575000	-2.815089000	1.645046000
H	-2.817640000	-3.831622000	2.548278000
H	-2.923660000	-3.999681000	0.795716000
Cl	6.450041000	1.677791000	-0.004605000
Cl	6.380021000	-1.533446000	0.099767000
H	3.664379000	-2.348333000	0.085266000
H	3.772069000	2.608948000	-0.077738000

Σ of electronic & zero-point Energies -2398.918220
Σ of electronic & thermal Free Energies -2398.977166

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