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Electronic Supporting Information

for

Gold carbonyl cations and beyond: Synthesis of homoleptic gold(I) complexes with P_4 and P_4S_3 and the half-sandwich cation $[Au(C_6H_6)(CO)]^+$

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1. Compounds

1 $[Au(CO)_2][F\{Al(OC(CF_3)_3)_3\}_2]$

2 $[Au(P_4)_2)][F\{Al(OC(CF_3)_3)_3\}_2]$

3 $[Au(P_4S_3)_2][F\{Al(OC(CF_3)_3)_3\}_2]$

4 $[Au(C_6H_6)(CO)][F\{Al(OC(CF_3)_3)_3\}_2]$

2. Abbreviations

4FB = 1,2,3,4-tetrafluorobenzene

5FB = pentafluorobenzene

o-dfb = *ortho*-difluorobenzene

$OR^F = OC(CF_3)_3$

$[Al(OR^F)_4]^- = [Al\{OC(CF_3)_3\}_4]^-$

$[F\{Al(OR^F)_3\}_2]^- = [\{(CF_3)_3CO\}_3Al\text{-}F\text{-}Al\{OC(CF_3)_3\}_3]^-$

FWHM = full width half maximum

Mes = mesitylene, 1,3,5-Trimethylbenzene

NMR = nuclear magnetic resonance

RT = room temperature

XRD = X-ray diffraction

Fc = ferrocene, bis(η^5-cyclopentadienyl)iron

TMS = tetramethylsilane

DFT = density functional theory

3. Materials and Methods

General Procedures

All reactions were performed under exclusion of moisture and air through usage of a nitrogen filled glovebox (O_2/H_2O < 1 ppm) and standard Schlenk technique. Special double-Schlenk tubes were used for all reactions, consisting of two Schlenk tubes connected by a G3 or G4 frit and equipped with grease-free PTFE or glass valves. Benzene, 1,2,3,4-tetrafluorobenzene (4FB, Fluorochem) and *ortho*-difluorobenzene (*o*-dfb, Apollo Scientific) were dried over CaH_2 and distilled. 4FB is usually contaminated with traces of less fluorinated benzenes. To remove these impurities, 4FB was stirred over $Ag[Al(OR^F)_4]$ at room temperature and condensed into a storage vessel. This procedure leads to the contamination of 4FB with traces of $HOC(CF_3)_3$ (< 1%). However, we could not observe an influence on the reactions by this impurity. Pentane was dried with a Grubbs apparatus (MBraun). Oxygen was removed from all solvents by purging with nitrogen and all solvents were stored over activated 3 Å molecular sieves. I_2 and P_4 were sublimated prior to use. P_4S_3 was purified by extraction with CS_2. Gold powder (Alfa Aeser, 99.96% metals basis, 0.5-0.8 micron) was used without further purification. $Ag[Al(OR^F)_4]$[1] and $Ag[F\{Al(OR^F)_3\}_2]$[2] were synthesized according to literature.

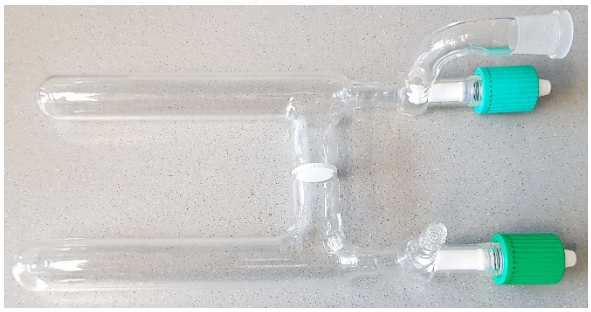


Figure S 1: Typical double-Schlenk tube which was used for all reactions.

NMR Spectroscopy

NMR spectroscopy was performed at RT either on a Bruker Avance II Widebore 400 MHz or a Bruker Avance III HD 300 MHz. The compounds were dissolved in a 5 mm thick-walled NMR tube with J. Young PTFE valve. The spectra were calibrated by using the ^1H signal of the solvent (4FB: δ = 6.97 ppm, rel. to TMS). The field corrections of other nuclei were adjusted accordingly. The Bruker Topspin software package (version 3.5 or 4.1.1) was used for measuring, processing, and creation of the graphical representations of the spectra. ^1H and $^{13}C\{^1H\}$ NMR spectra are referenced against TMS, ^{19}F NMR spectra

against $CFCl_3$, ^{27}Al NMR spectra against an aqueous solution of $Al(NO_3)_3$ (1.1 mM), and ^{31}P NMR spectra against an aqueous solution of H_3PO_4 (85%).

Vibrational Spectroscopy

FTIR spectra were measured with a Bruker ALPHA with a ZnSe or diamond ATR unit inside a glovebox. The spectra were recorded in the range of 4000 to 550 cm^{-1} (ZnSe) or 4000 to 375 (diamond) with 64 scans and a resolution of 2 cm^{-1} at RT. Data processing was performed with the Bruker OPUS 7.5 software package and, if not stated otherwise, a baseline correction with 3 iterations was carried out. Raman spectra were recorded on a VERTEX 70 equipped with a Bruker RAM II Modul (1064 nm exciting line of a Nd-YAG laser) and liquid nitrogen cooled Ge detector. The samples were flame-sealed in soda-lime glass Pasteur pipettes. The spectra were measured at RT in the range of 4000-80 cm^{-1} with a resolution of 4 cm^{-1}. The data were processed with the Bruker OPUS 7.5 software package and, if not stated otherwise, a baseline correction with 5 iterations was performed. All IR and Raman spectra were normalized to 1 and the intensities are reported as follows: ≥ 0.8 = very strong (vs), ≥ 0.6 = strong (s), ≥ 0.4 = medium (m), ≥ 0.2 = weak (w), < 0.2 = very weak (vw). The graphical representations were created with Origin 2021.

Single-Crystal X-ray Diffraction

Single-crystal X-ray diffraction was performed on a Bruker D8 VENTURE dual wavelength Mo/Cu three-circle diffractometer equipped with microfocus sealed X-ray tubes using mirror optics as monochromator and a Bruker PHOTON III detector. Single crystals were selected under perfluoropolyalkylether oil (AB128330, ABCR GmbH & Co. KG), mounted on CryoLoops with a diameter of 0.1 to 0.2 mm and shock-cooled using an Oxford Cryostream 800 low temperature device. The data were gathered with Mo K_α radiation (λ = 0.71073 Å) at 100(2) K. The data were integrated with SAINT[3] (version 8.40B) and a multi-scan absorption correction using SADABS[4] was applied. The structures were solved by direct methods using SHELXT[5] and refined by full-matrix least-squares methods against F^2 by SHELXL[6] using the GUI software ShelXle.[7] Disordered moieties were refined using bond lengths restraints and displacement parameter restraints and were modeled with the program DSR.[8,9] The data were finalized with the tool FinalCif.[10] The graphical representations of the crystal structures were generated with OLEX2.[11] Crystallographic data for the structures reported here have been deposited with the Cambridge Crystallographic Data Centre[12] Copies of the data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Powder X-ray Diffraction

Powder diffractograms were measured on a STOE STADI P powder diffractometer equipped with a Ge-(111) monochromator and Mythen 1K detector using Mo $K_{\alpha 1}$ radiation (λ = 0. 709300 Å). The samples were transferred into a 0.5 mm thick capillary (Hilgenberg GmbH, wall thickness 0.01 mm) and the capillary was sealed with silicon grease. The samples were cooled to 100(10) K with an Oxford Cryostream low temperature device. Data acquisition, processing, and the calculation of powder diffractograms from single-crystal data was performed using the STOE WinXPOW® package.

Computational Details

Geometry optimizations with the B3LYP functional,[13–15] were performed with the Turbomole software (v7.2, v7.5 or v7.5.1).[16,17] Here, the basis set def2-TZVPP,[18] the resolution-of-identity (RI) approximation,[19–21] dispersion correction (D3BJ),[22,23] a fine integration grid (m4 or m5) and the default SCF convergence criteria (10^{-7} H) were used. Thermal and entropic contributions to the Gibbs free energy were calculated without scaling factor at standard conditions (298.15 K, 0.1 MPa) with the *FREEH* module. The integrated *EGRAD*[24] module was used to calculate Raman scattering cross sections. IR and Raman spectra were simulated without scaling factor and a FWHM of 10 cm^{-1}.

Geometry optimizations and single point calculations at the r2scan-3c and DLPNO-CCSD(T) level of theory were performed with ORCA (v5.0.4).[25–27] For the DLPNO-CCSD(T) calculations, the def2-QZVPP basis set,[28] tight convergence criteria (tightscf) and normal DLPNO thresholds were used.

4. Experimental Details

4.1 Synthesis and NMR Spectra of $[Au(CO)_2][F\{Al(OR^F)_3\}_2]$ 1

$Ag[F\{Al(OR^F)_3\}_2]$ (399.6 mg, 0.2512 mmol), Au powder (69.5 mg, 0.353 mmol, 1.4 eq) and I_2 (31.5 mg, 0.124 mg, 0.5 eq.) were weighed in one side of a double-Schlenk tube and 4FB (4 mL) was added. The solution was frozen with liquid nitrogen, the system evacuated, and the tube was flooded with CO (3 bar). The mixture was stirred at RT for 18 h and a suspension of an off-white solid in a yellow solution was obtained. The solution was filtered through the frit to the other side of the double-Schlenk tube. The CO atmosphere was removed, and *n*-pentane (ca. 25 mL) was added to the off-white solid. Crystallization by vapor diffusion of *n*-pentane into the yellow solution at RT yielded colorless crystals of **1** (Yield: 303.8 mg, 0.1750 mmol, 70%).

FTIR (ZnSe, ATR): $\tilde{\nu}/cm^{-1}$ = 2219 (vw), 1354 (vw), 1301 (w), 1266 (s), 1247 (vs), 1215 (vs), 1178(w), 971 (vs), 862 (vw), 760 (vw), 727 (vs), 639 (w), 568 (w).

FT Raman: Could not be obtained due to a very intense fluorescence background, which may be caused by very small quantities of elemental gold.

^{1}H NMR (300.18 MHz, 4FB, RT): *only solvent signal at 6.97 ppm.*

^{13}C{^{1}H} NMR (75.48 MHz, 4FB, RT): δ = 173.8 (*minor unknown impurity*), 120.8 (q, ^1J(C,F) = 292 Hz, 18C, $[F\{Al(OC(\mathbf{C}F_3)_3)_3\}_2]^-$), 85.9 (*minor unknown impurity*),78.7 (m, 6C, $[F\{Al(O\mathbf{C}(CF_3)_3)_3\}_2]^-$) ppm.

No signal of the carbonyl ligands of **1** were observed in the ^{13}C NMR, which might be caused by dynamic exchange processes. The signal at 173.8 was also observed in the ^{13}C NMR of **4** with similar intensity compared to the solvent, which justifies the assignment as an impurity.

^{19}F NMR (282.45 MHz, 4FB, RT): δ = –76.2 (s, 54F, $[F\{Al(OC(C\mathbf{F}_3)_3)_3\}_2]^-$, –184.8 (br. s, 1F, $[\mathbf{F}\{Al(OC(CF_3)_3)_3\}_2]^-$) ppm.

^{27}Al NMR (78.22 MHz, 4FB, RT): *The signal of the anion is too broad to be visible.*

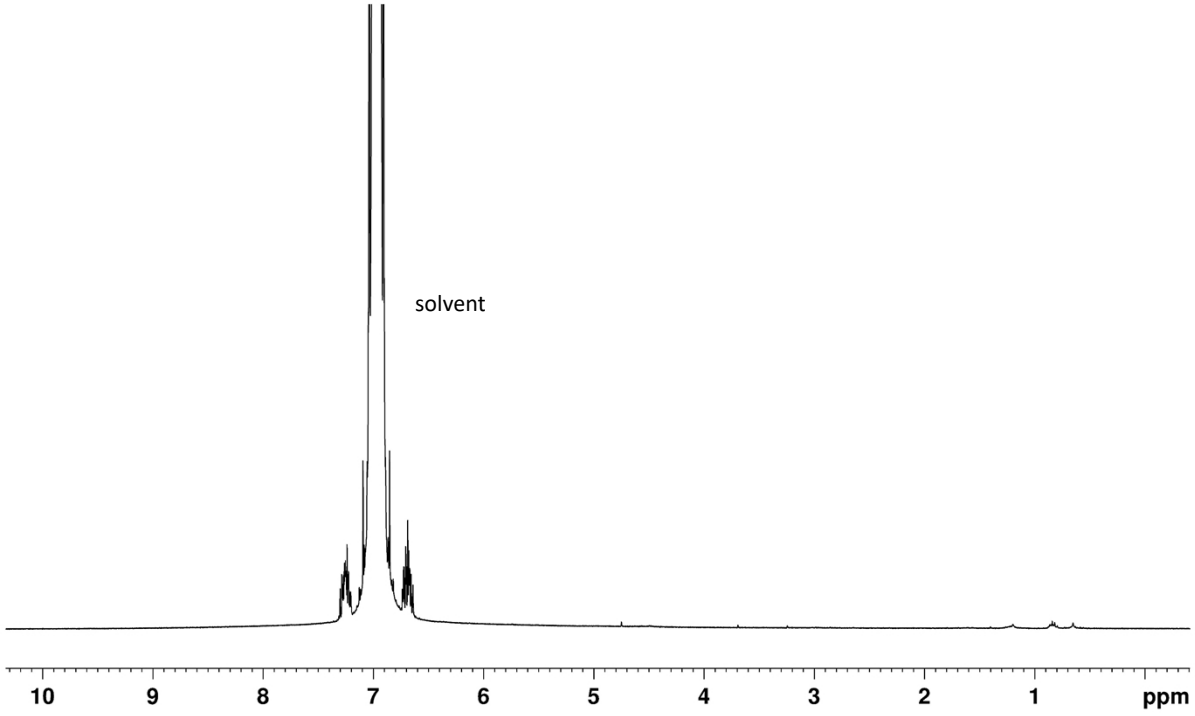


Figure S 2: ^{1}H NMR (300.18 MHz, 4FB, RT) spectrum of **1**.

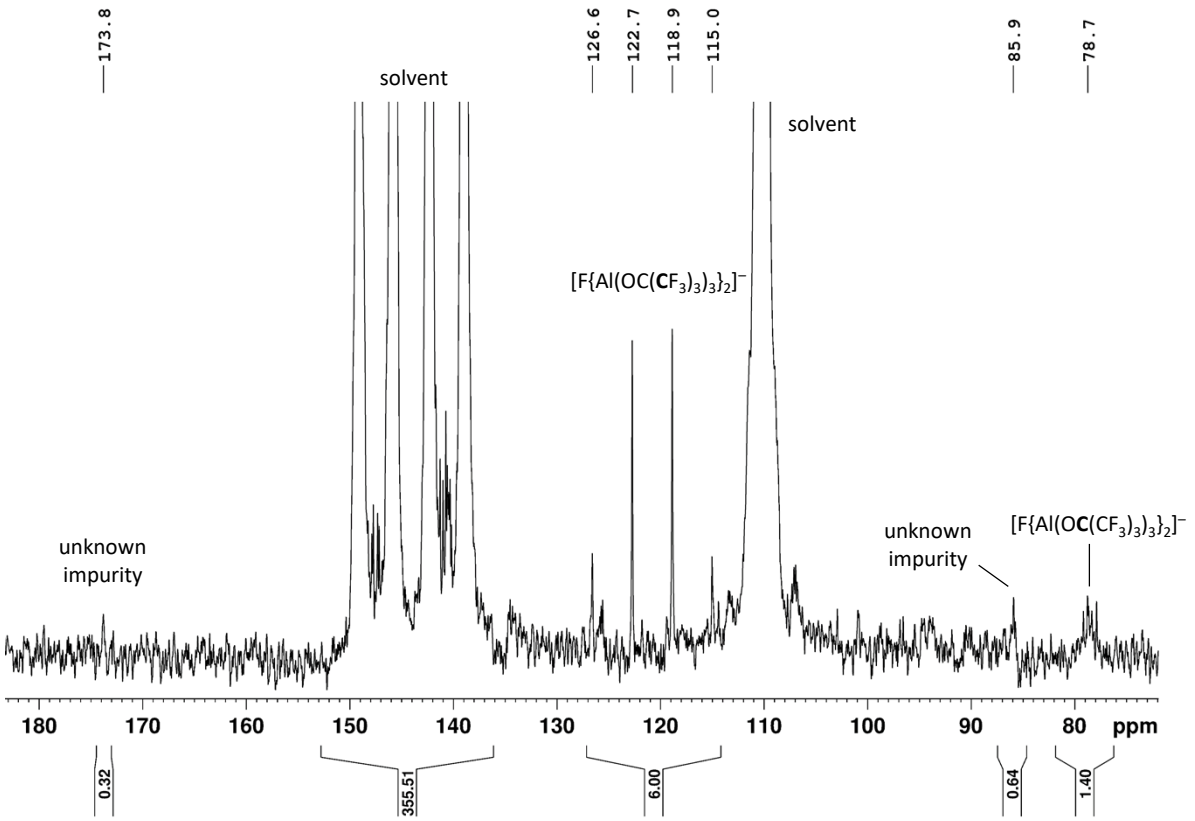


Figure S 3: ^{13}C{^{1}H} NMR (75.48 MHz, 4FB, RT) spectrum of **1**.

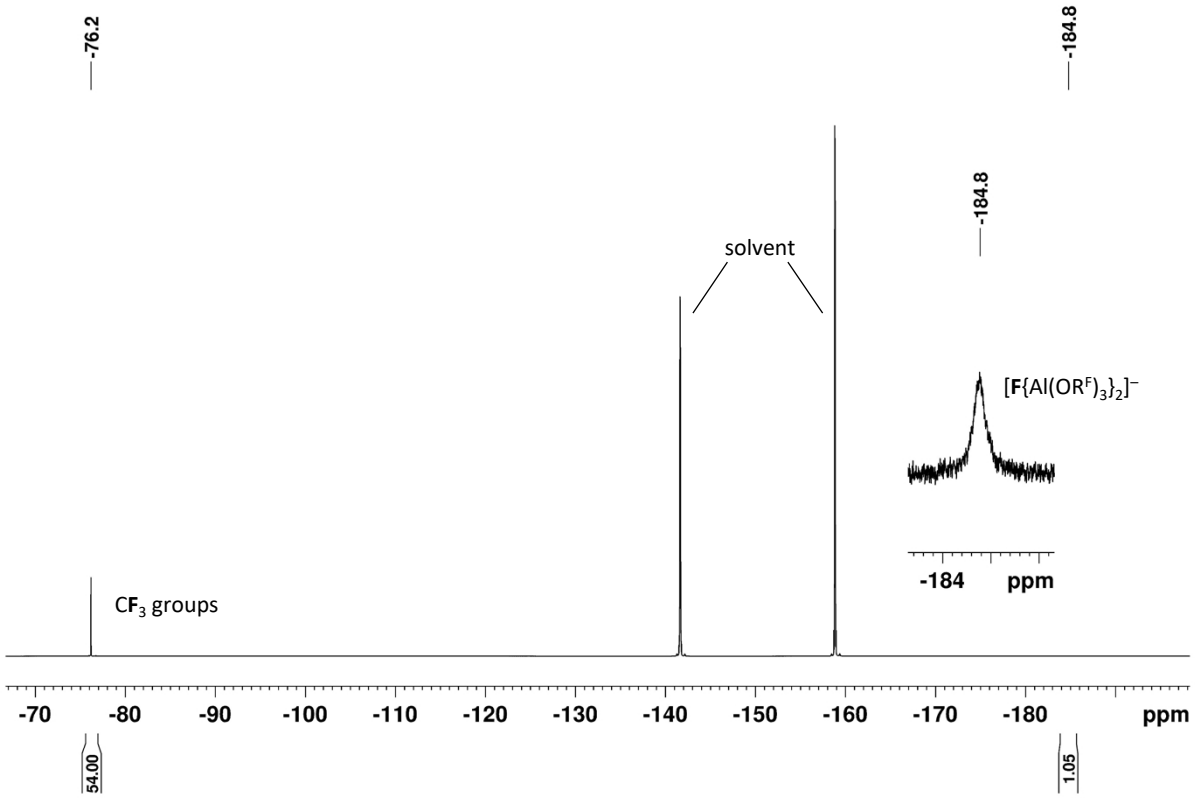


Figure S 4: ^{19}F NMR (282.45 MHz, 4FB, RT) spectrum of **1**.

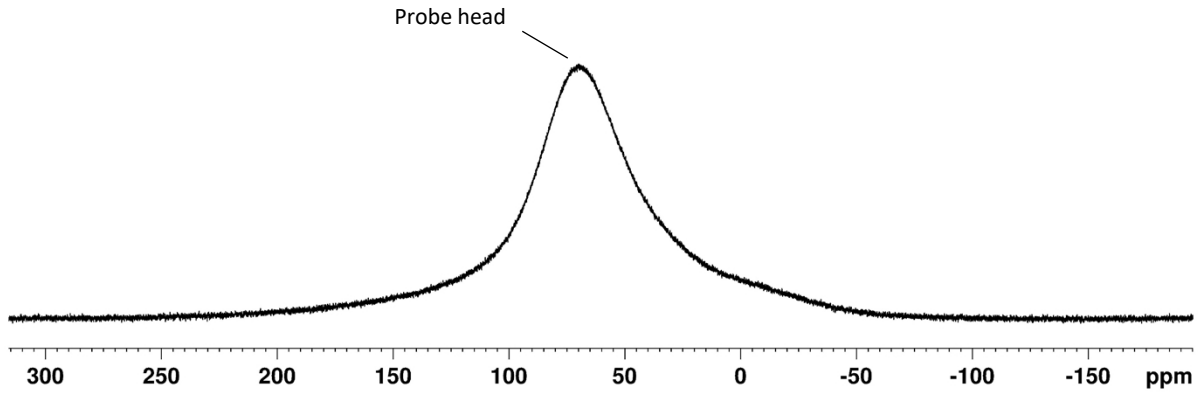


Figure S 5: ^{27}Al NMR (78.22 MHz, 4FB, RT) spectrum of **1**.

4.2 Synthesis and NMR Spectra of $[Au(P_4)_2][F\{Al(OR^F)_3\}_2]$ 2

Inside a glovebox, $[Au(CO)_2][F\{Al(OR^F)_3\}_2]$ (148.3mg, 0.08542 mmol) and P_4 (22.3 mg, 0.180 mmol, 2.1 eq.) were transferred into one side of a double-Schlenk tube and dissolved in 4FB (2.4 mL). The mixture was stirred for 2 h at RT and a brown solution and some dark precipitate was obtained. The solution was filtered, and *n*-pentane (ca. 25 mL) was added to the empty side of the double-Schlenk tube. Crystallization by vapor diffusion of *n*-pentane into the brown solution at RT yielded colorless crystals of **2** (Yield:112.3 mg, 0.05825 mmol, 68%).

FTIR (Diamond, ATR): $\tilde{\nu}/cm^{-1}$ = 1355 (vw), 1300 (w), 1274 (m), 1266 (m), 1238 (vs), 1211 (vs), 1179 (m), 970 (vs), 863 (w), 760 (vw), 726 (vs), 642 (w), 568 (vw), 537 (w), 449 (w).

FT Raman (3000 scans, 25 mW): $\tilde{\nu}/cm^{-1}$ = 817 (vw), 753 (w), 593 (vs), 570 (vw), 539 (vw), 467 (w), 392 (w), 382 (w), 325 (w), 91 (w).

^{1}H NMR (300.18 MHz,4FB, RT): *only solvent signal at 6.97 ppm and some very minor impurities.*

^{19}F NMR (282.45 MHz, 4FB, RT): δ = –76.1 (*minor unknown impurity*), –76.2 (s, 54F, $[F\{Al(OC(C\mathbf{F}_3)_3)_3\}_2]^-$, –184.8 (br. s, 1F, $[\mathbf{F}\{Al(OC(CF_3)_3)_3\}_2]^-$) ppm.

^{27}Al NMR (78.22 MHz, 4FB, RT): δ = 39.8 (br. s, 1Al, $[F\{\mathbf{Al}(OC(CF_3)_3)_3\}_2]^-$) ppm.

^{31}P NMR (121.52 MHz, 4FB, RT): δ = –458.1 (s, 8 P, $[Au(\mathbf{P}_4)_2]^+$) ppm.

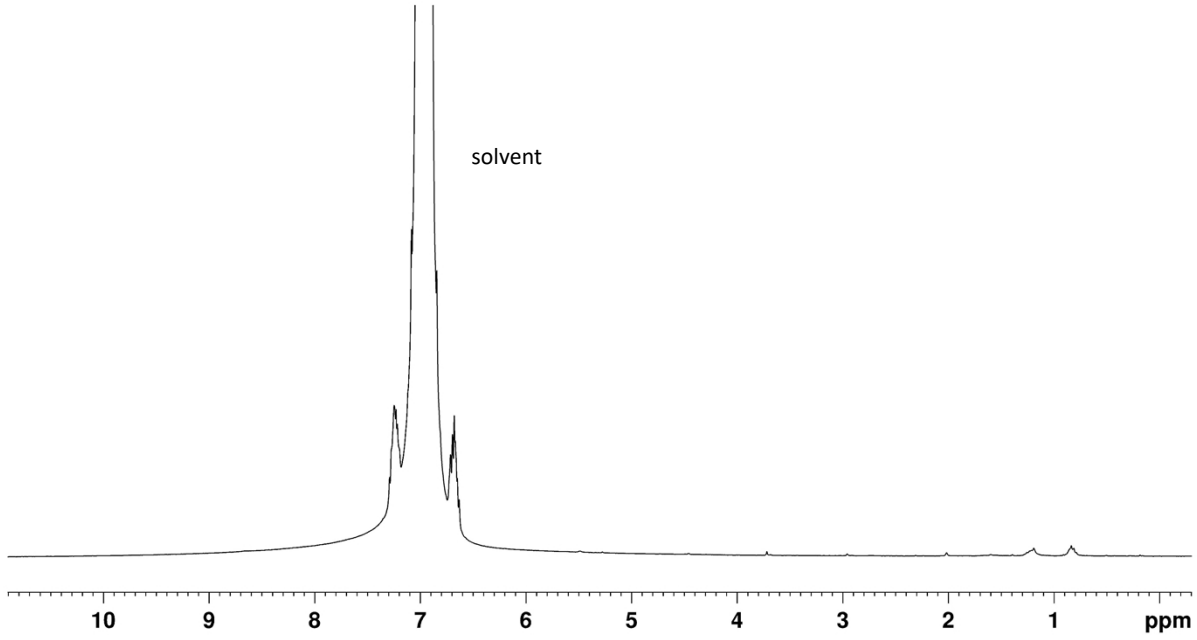


Figure S 6: ^{1}H NMR (300.18 MHz, 4FB, RT) spectrum of **2**.

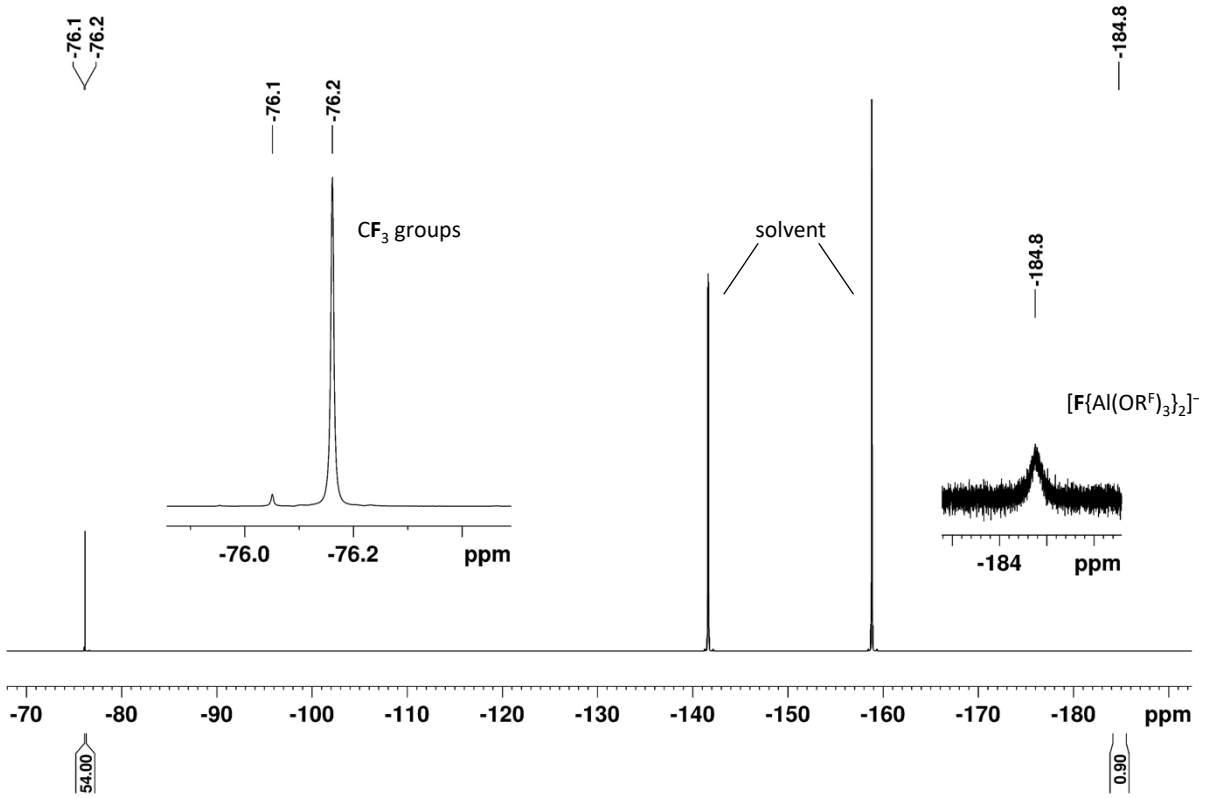


Figure S 7: ^{19}F NMR (282.45 MHz, 4FB, RT) spectrum of **2**.

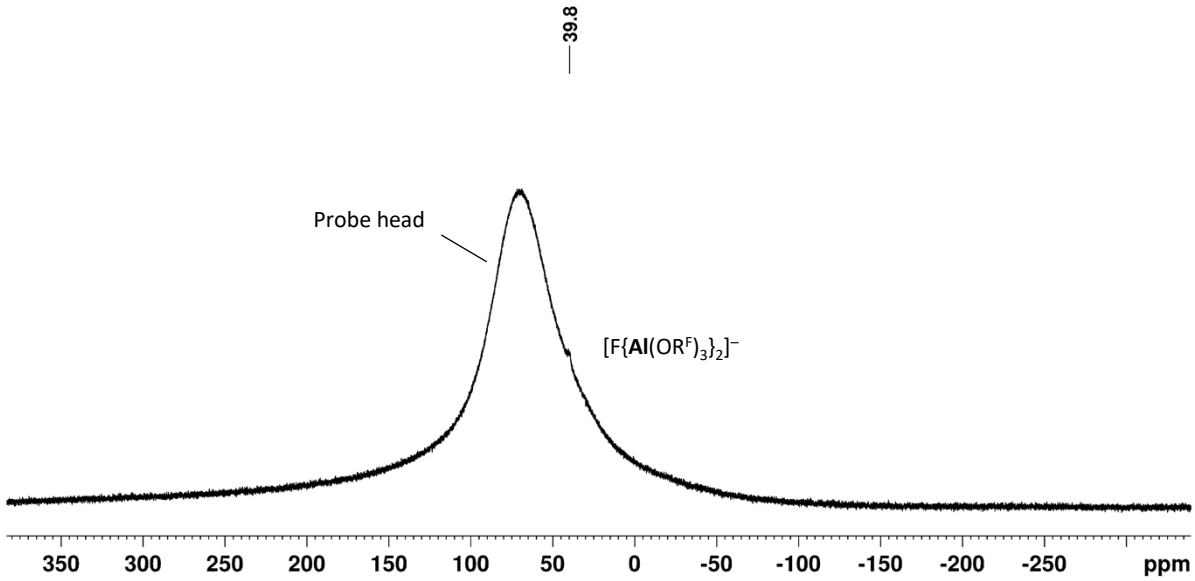


Figure S 8: ^{27}Al NMR (78.22 MHz, 4FB, RT) spectrum of **2**.

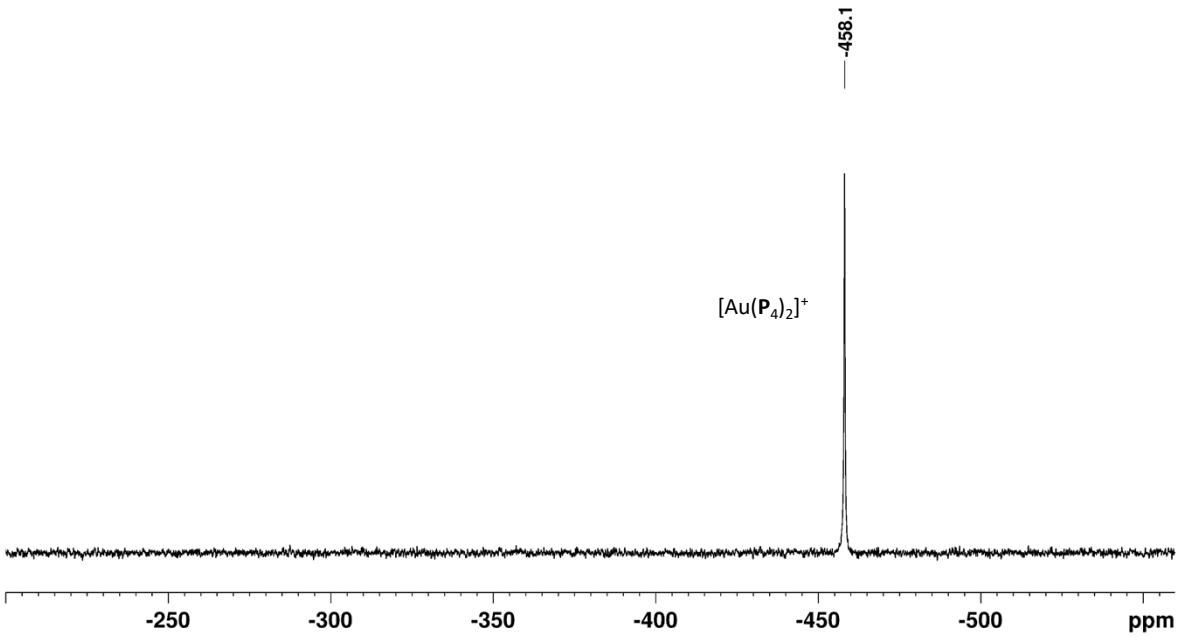


Figure S 9: ^{31}P NMR (121.52 MHz, 4FB, RT) spectrum of **2**.

4.3 Synthesis and NMR Spectra of $[Au(P_4S_3)_2][F\{Al(OR^F)_3\}_2]$ 3

Inside a glovebox, $[Au(CO)_2][F\{Al(OR^F)_3\}_2]$ (199.6mg, 0.1150 mmol) and P_4S_3 (56.2 mg, 0.255 mmol, 2.1 eq.) were transferred into one side of a double-Schlenk tube and dissolved in 4FB (2.4 mL). The mixture was stirred for 1 h at RT and a suspension of a dark precipitate in an orange solution was obtained. The solution was filtered and *n*-pentane (ca. 25 mL) was added to the empty side of the double-Schlenk tube. Crystallization by vapor diffusion of *n*-pentane into the orange solution at RT yielded colorless crystals of **3** (Yield:128.6 mg, 0.06065 mmol, 61%).

FTIR (Diamond, ATR): $\tilde{\nu}/cm^{-1}$ = 1354 (vw), 1299 (w), 1276 (m), 1238 (vs), 1213 (vs), 1171 (m), 1163 (m), 972 (vs), 864 (w), 759 (vw), 726 (vs), 635 (w), 568 (w), 536 (w), 527 (vw), 521 (vw), 500 (vw), 477 (vw), 471 (vw), 449 (m), 437 (m), 427 (vw), 383 (vw).

FT Raman (5,000 scans, 20 mW): $\tilde{\nu}/cm^{-1}$ = 1495 (vw), 1279 (vw), 816 (vw), 753 (m), 569 (vw), 538 (w), 523 (s), 485 (s), 439 (m), 427 (vw), 427 (vw), 394 (s), 370 (vw), 340 (s), 324 (w), 286 (vs), 223 (m), 171 (vw), 107 (vs).

^{1}H NMR (300.18 MHz, 4FB, RT): *only solvent signal at 6.97 and some very minor impurities.*

^{13}C{^{1}H} NMR (75.48 MHz, $F_4C_6H_2$, RT): δ = 120.8 (q, ^1J(C,F) = 292 Hz, 18C, $[F\{Al(OC(\mathbf{C}F_3)_3)_3\}_2]^-$), 78.6 (m, 6C, $[F\{Al(O\mathbf{C}(CF_3)_3)_3\}_2]^-$) ppm.

^{19}F NMR (282.45 MHz, 4FB, RT): δ = –76.1 (s, 54F, $[F\{Al(OC(C\mathbf{F}_3)_3)_3\}_2]^-$, –184.8 (br. s, 1F, $[\mathbf{F}\{Al(OC(CF_3)_3)_3\}_2]^-$) ppm.

^{27}Al NMR (78.22 MHz, $F_4C_6H_2$, RT): δ = 38.5 (br. s, 1Al, $[F\{\mathbf{Al}(OC(CF_3)_3)_3\}_2]^-$) ppm.

^{31}P NMR (121.52 MHz, 4FB, RT): δ = 80.7 (q, ^2J(P,P) = 61.3 Hz, 2P, $[Au(\mathbf{P}^aS_3P^b{}_3)_2]^+$), –122.8 (d, ^2J(P,P) = 61.3 Hz, 6P, $[Au(P^aS_3\mathbf{P}^b{}_3)_2]^+$) ppm.

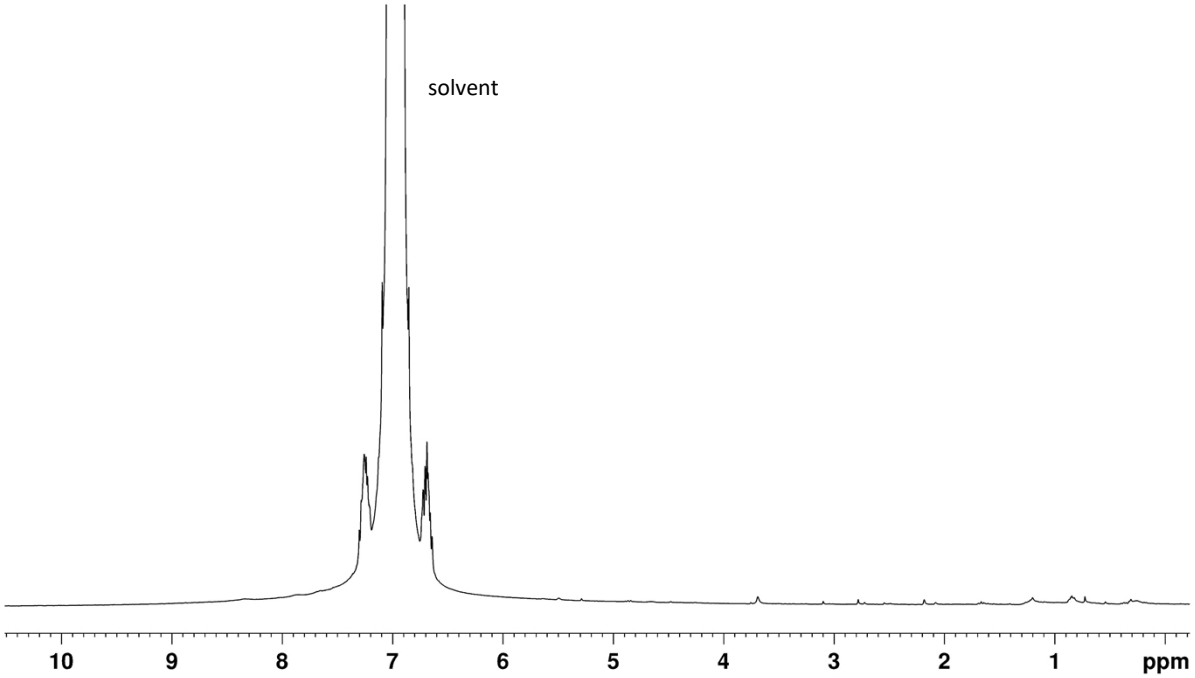


Figure S 10: ^{1}H NMR (300.18 MHz, $F_4C_6H_2$, RT) spectrum of **3**.

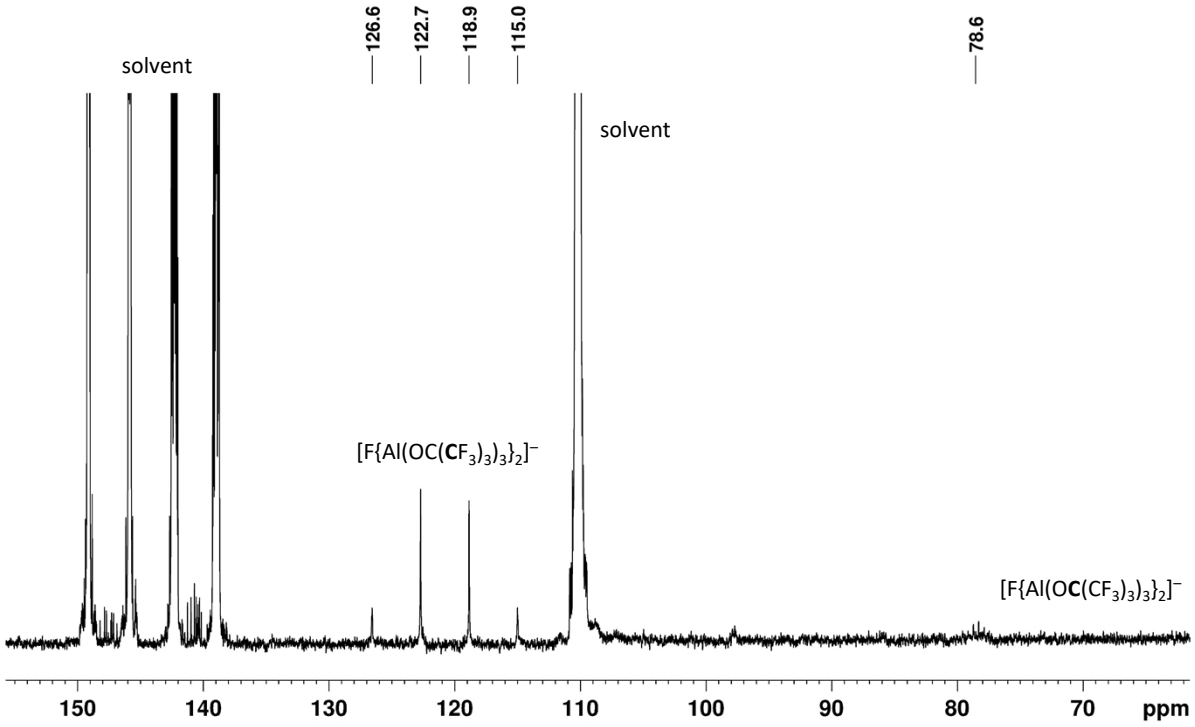


Figure S 11: $^{13}C\{^{1}H\}$ NMR (75.48 MHz, 4FB, RT) spectrum of **3**.

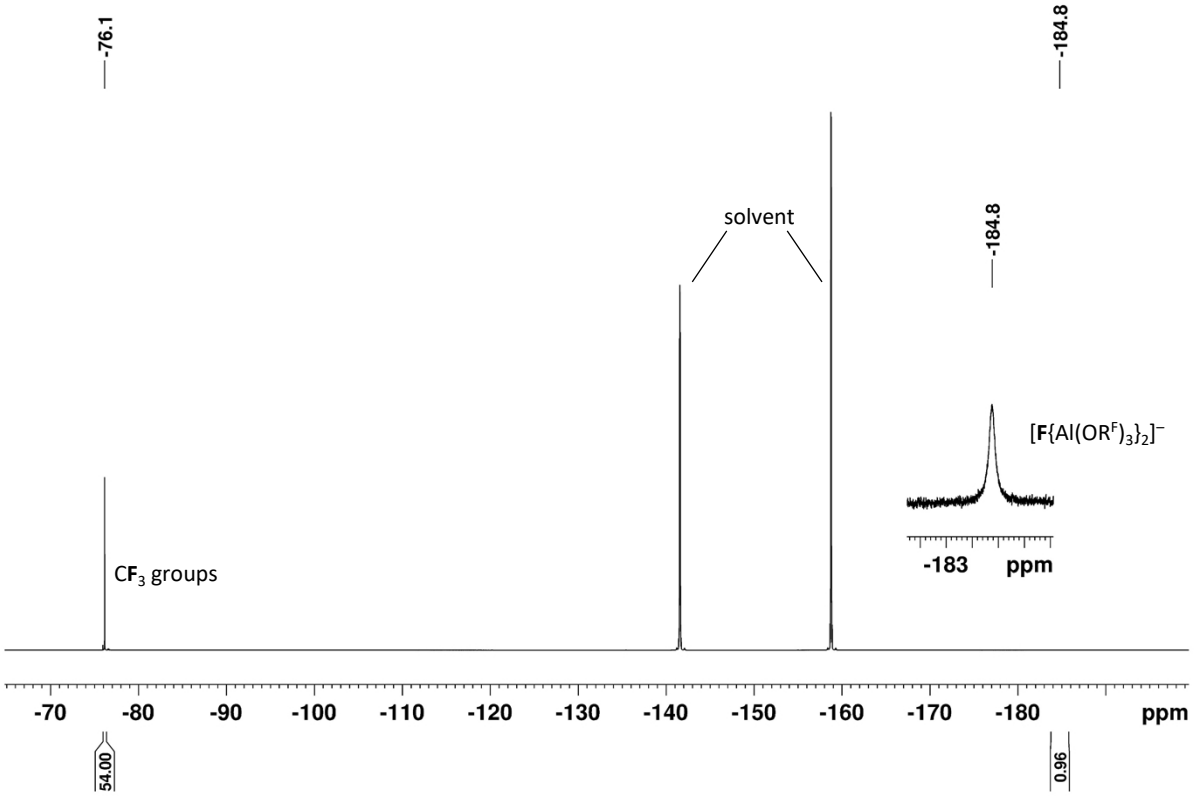


Figure S 12: ^{19}F NMR (282.45 MHz, 4FB, RT) spectrum of **3**.

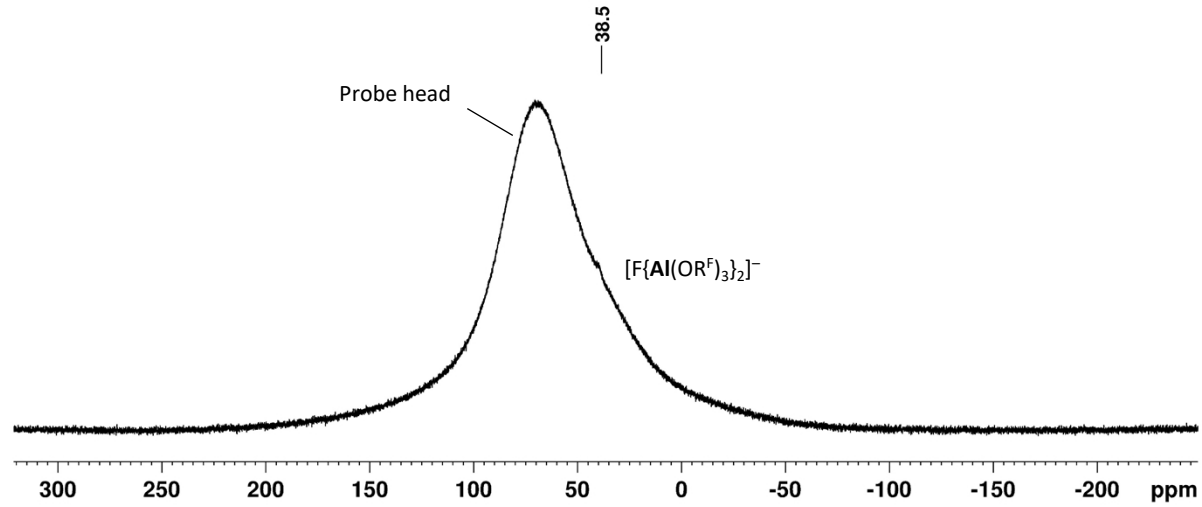


Figure S 13: ^{27}Al NMR (78.22 MHz, 4FB, RT) spectrum of **3**.

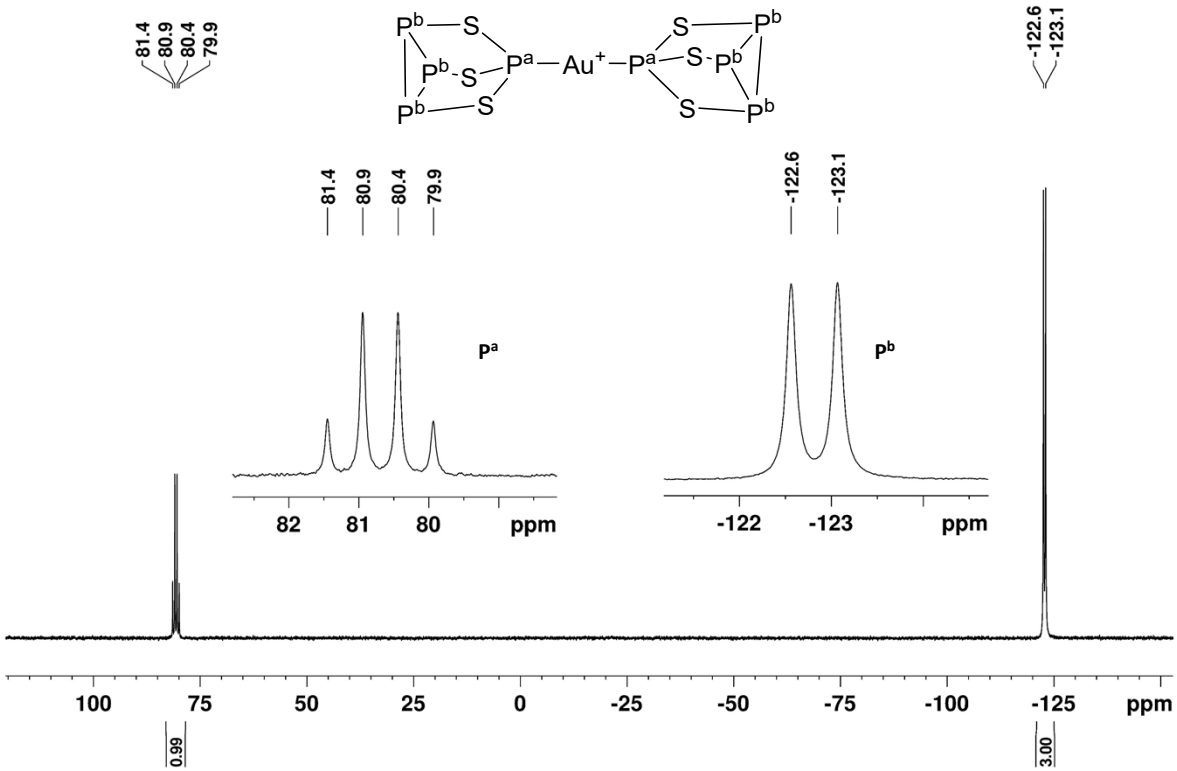


Figure S 14: ^{31}P NMR (121.52 MHz, 4FB, RT) spectrum of **3**.

4.4 Synthesis and NMR Spectra of $[Au(C_6H_6)(CO)][F\{Al(OR^F)_3\}_2]$ 4

A solution of $[Au(CO)_2][F\{Al(OR^F)_3\}_2]$ (73.9 mg, 0.0426 mmol) in 4FB (2 mL) was prepared and cooled to –35 °C. A solution of benzene (0.09 mL, 0.48 mol L^{-1}, 3 mg, 0.04 mmol, 1.0 eq.) in 4FB was added to the mixture. The reaction solution was stirred for 20 min at –35 °C and cold *n*-heptane (20 mL) was added to precipitate the product. The solvent was removed, and the product was shortly dried *in vacuo*. The product (18 mg, 0.010 mmol, 23%) was obtained as an off-white solid. Colorless crystals of **3** were obtained by layering of a 4FB solution with hexanes at –30 °C.

FTIR (ZnSe, ATR): $\tilde{\nu}/cm^{-1}$ = 2200 (vw), 1524(vw), 1516(vw), 1474(vw), 1468 (vw), 1355 (vw), 1301 (w), 1278 (m), 1267 (m), 1245 (vs), 1216 (vs), 1180 (w), 975 (vs), 864 (vw), 760 (vw), 728 (vs), 713 (w), 632 (vw), 569 (vw).
FT Raman: *Could not be obtained due to the temperature sensitivity of the compound.*

^{1}H NMR (400.17 MHz, 4FB, 233 K): 8.00 (s, 6H, $[Au(C_6\mathbf{H}_6)(CO)]^+$) ppm.

^{13}C{^{1}H} NMR (100.62 MHz, 4FB, 233 K): δ = 172.1 (*minor unknown impurity*), 127.6 (s, 6C, $[Au(\mathbf{C}_6H_6)(CO)]^+$), 120.7 (q, ^{1}J(C,F) = 292 Hz, 18C, $[F\{Al(OC(\mathbf{C}F_3)_3)_3\}_2]^-$), 78.1 (m, 6C, $[F\{Al(O\mathbf{C}(CF_3)_3)_3\}_2]^-$) ppm.

No signal of the carbonyl ligands of **4** were observed in the ^{13}C NMR, which might be caused by dynamic exchange processes. The signal at 172.1 was also observed in the ^{13}C NMR of **1** with similar intensity compared to the solvent, which justifies the assignment as a impurity.

^{19}F NMR (376.54 MHz, $F_4C_6H_2$, 233 K): δ = –76.6 (s, 54F, $[F\{Al(OC(C\mathbf{F}_3)_3)_3\}_2]^-$, –184.9 (br. s, 1F, $[\mathbf{F}\{Al(OC(CF_3)_3)_3\}_2]^-$) ppm.

^{27}Al NMR (104.27 MHz, 4FB, 233 K): *The signal of the anion was too broad to be visible.*

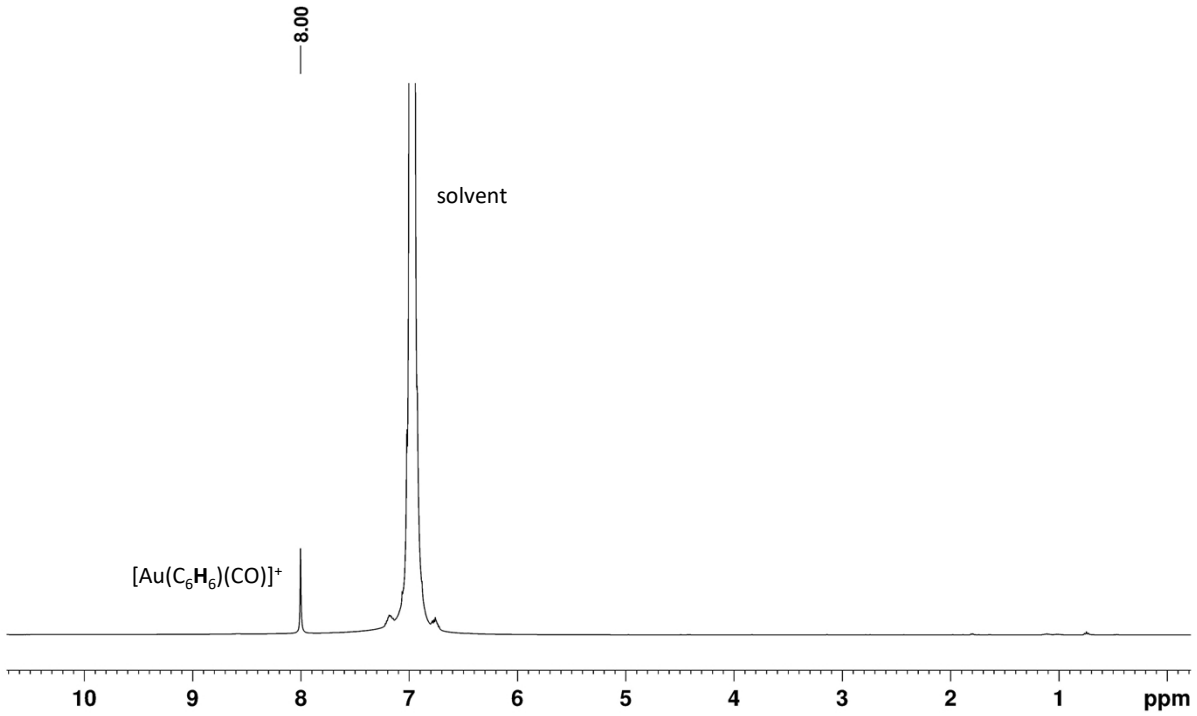


Figure S 15: ^{1}H NMR (400.17 MHz, $F_4C_6H_2$, 233 K) spectrum of **4**.

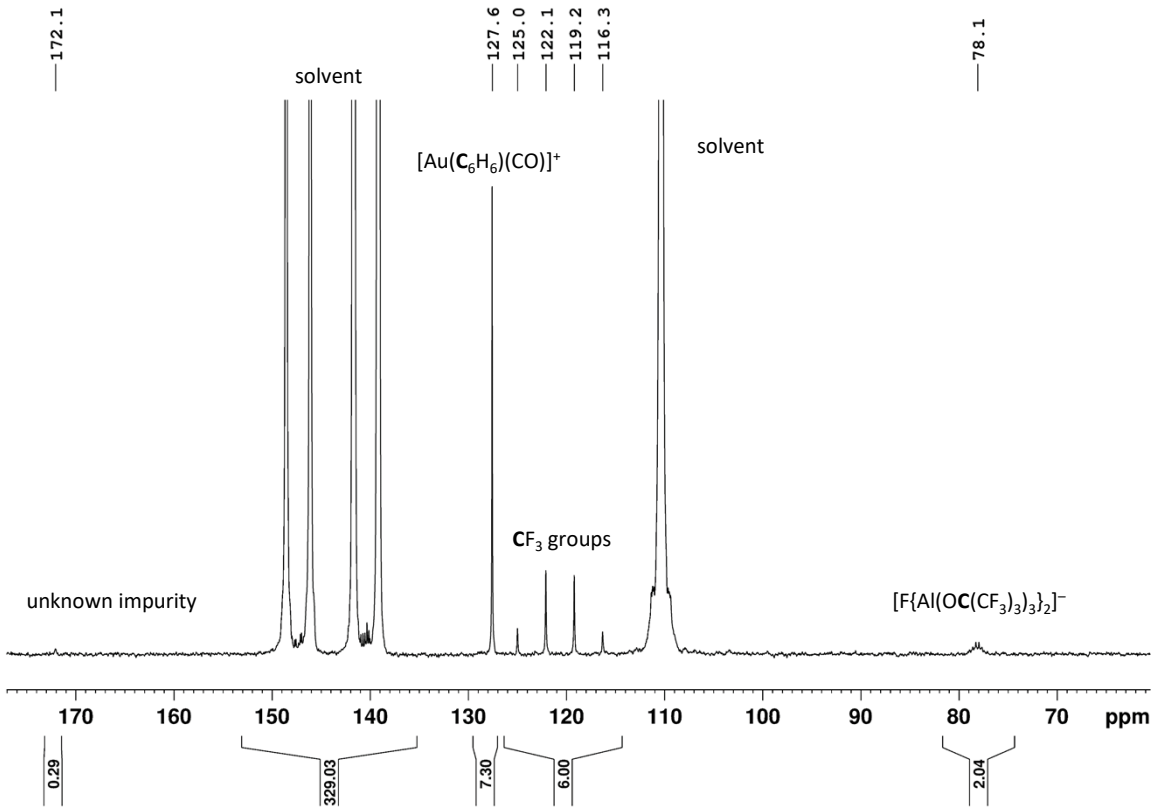


Figure S 16: $^{13}C\{^{1}H\}$ NMR (100.62 MHz, 4FB, 233 K) spectrum of **4**.

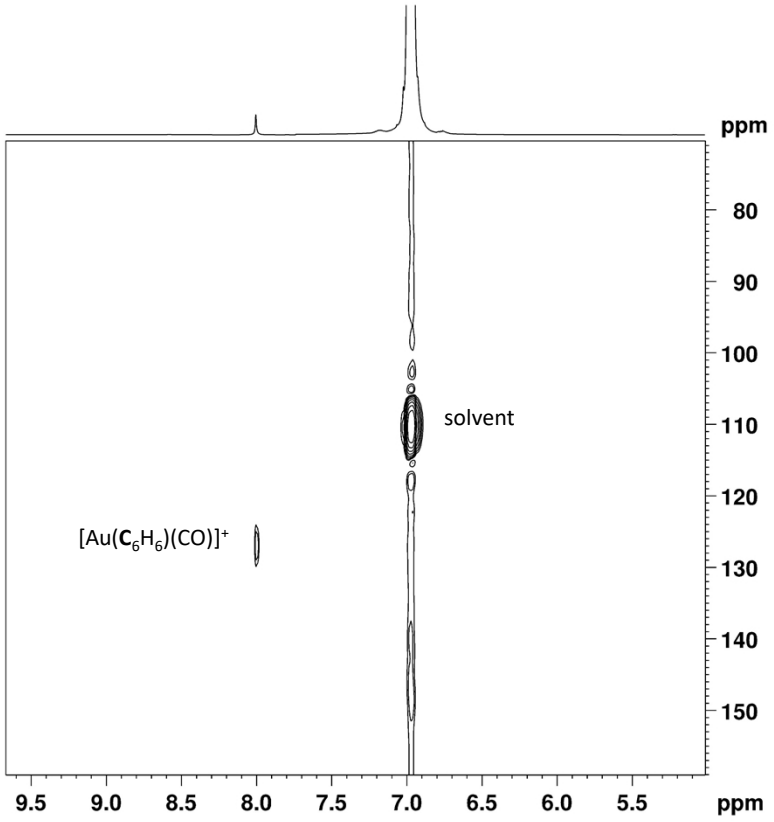


Figure S 17: $^{1}H,^{13}C$-HMBC NMR (400.17 MHz, 4FB, 233 K) spectrum of **4**.

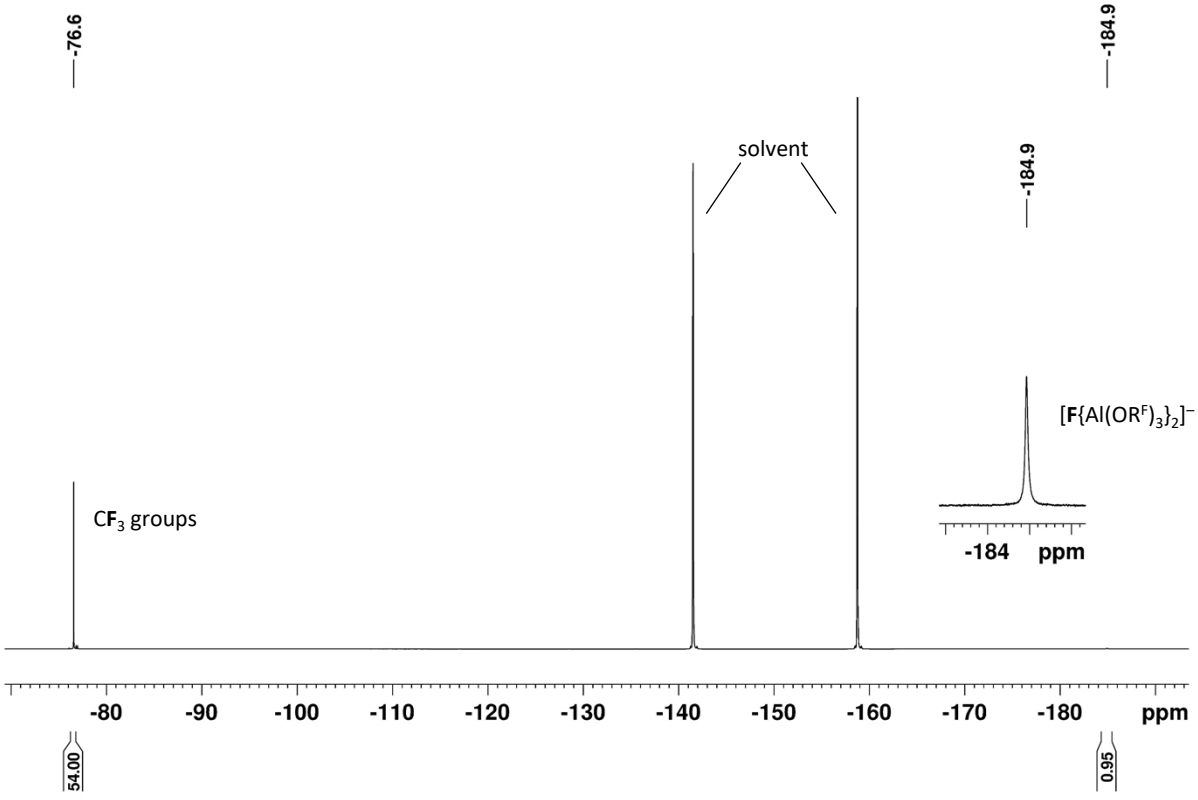


Figure S 18: ^{19}F NMR (376.53 MHz, 4FB, 233 K) spectrum of **4**.

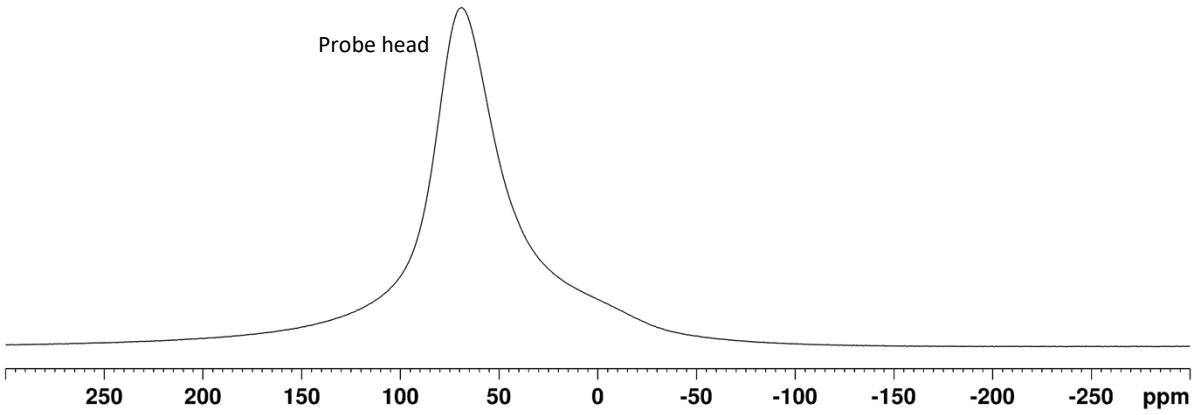


Figure S 19: ^{27}Al NMR (104.27 MHz, 4FB, 233 K) spectrum of **4**.

4.5 Reactions of $[Au(CO)_2]^+$ with acetylene

$[Au(CO)_2][F\{Al(OR^F)_3\}_2]$ (55.4 mg, 0.0319 mmol) was dissolved in 4FB (3 mL). The solution was frozen with liquid nitrogen, the system evacuated, and the tube was flooded with C_2H_2 (2 bar). The mixture was stirred for 10 min at RT. Meanwhile, a large amount of a black solid precipitated. The reaction was repeated at –35 °C with the same observation.

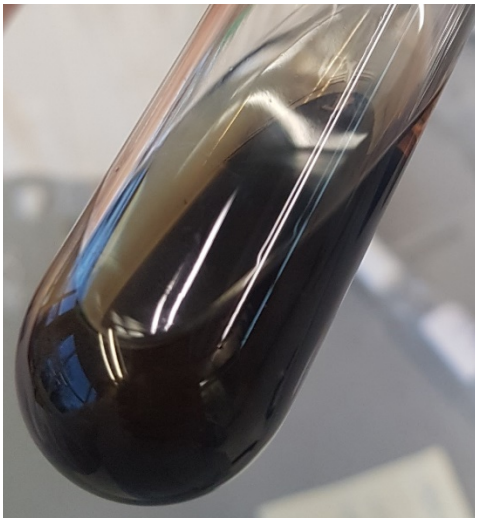


Figure S 20: Black solid after the reaction of **1** in 4FB with acetylene at RT.

5. Vibrational Spectra and Analysis

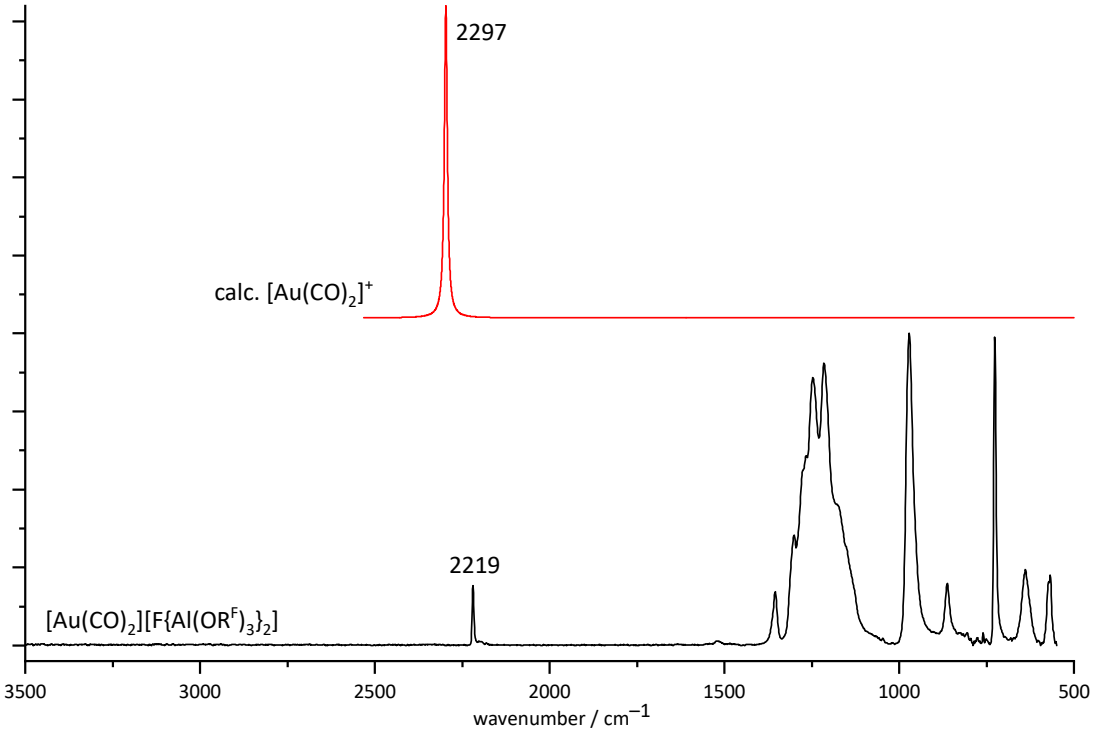


Figure S6-1: IR spectrum of **1** (black) and the calculated spectrum of $[Au(CO)_2]^+$ at the B3LYP(D3BJ)/def2-TZVPP level of theory (red).

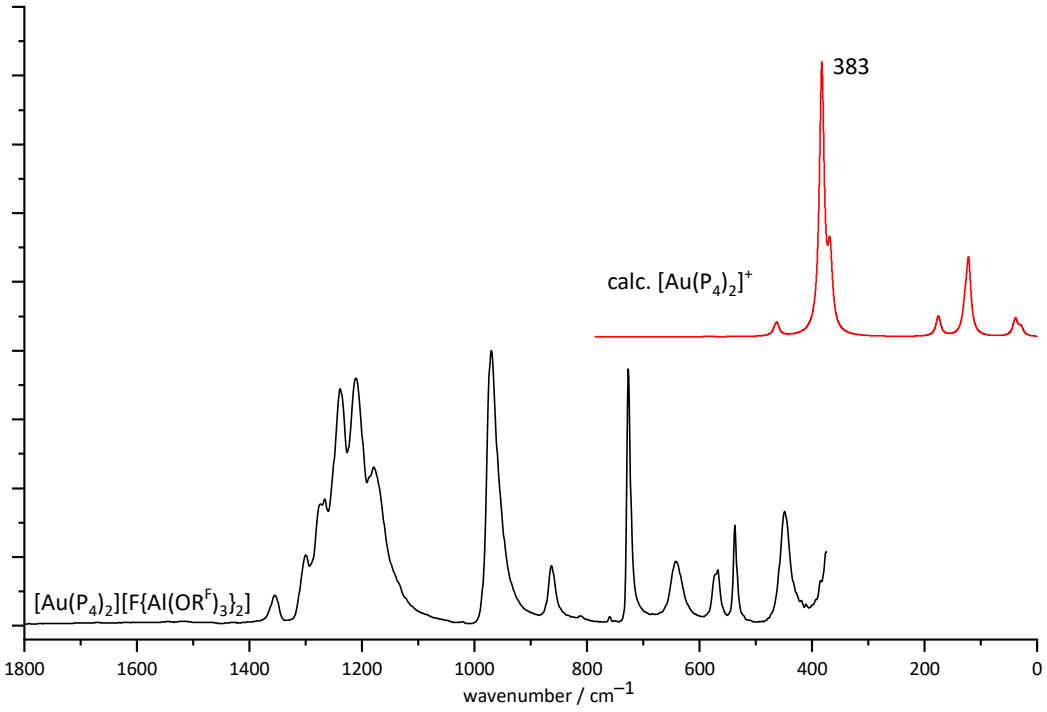


Figure S 21: IR spectrum of **2** (black) and the calculated spectrum of $[Au(P_4)_2]^+$ at the B3LYP(D3BJ)/def2-TZVPP level of theory (red). The vibrational bands of the $[Au(P_4)_2]^+$ cation are expected below 400 cm^{-1}, which is beyond the spectral range of the IR spectrometer. Therefore, only the vibrational bands of the anion are visible above 400 cm^{-1}.

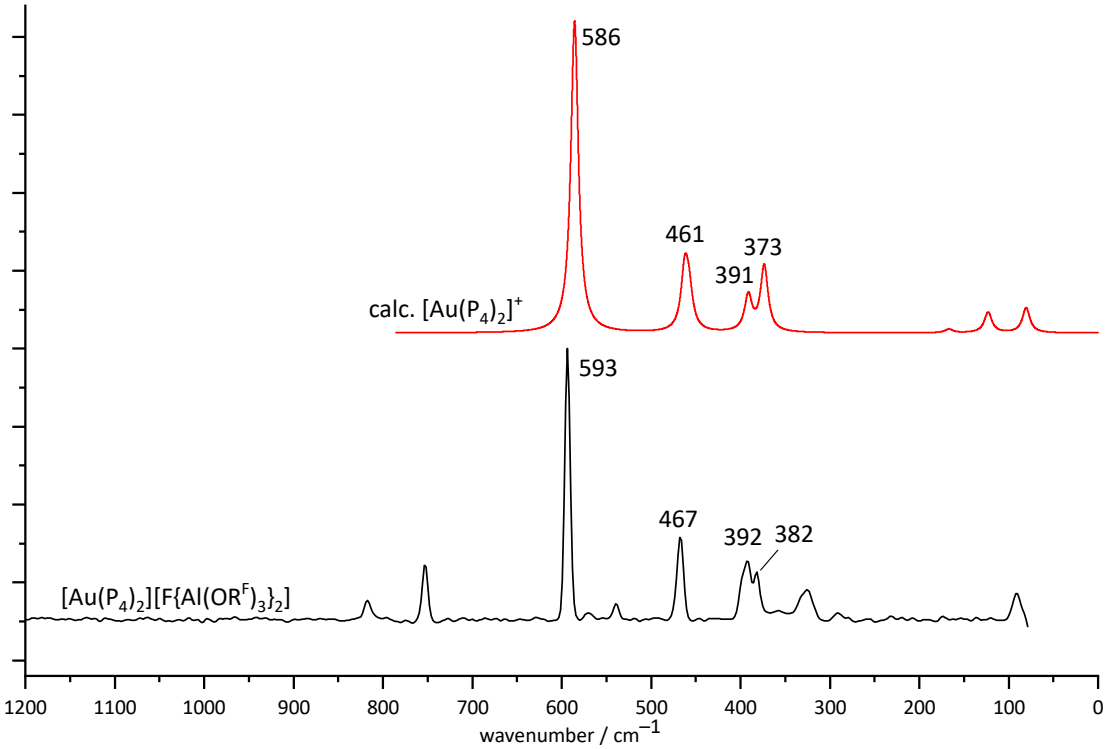


Figure S 22: Raman spectrum (3,000 scans, 25 mW, individual baseline correction) of **2** (black) and the calculated spectrum of $[Au(P_4)_2]^+$ at the B3LYP(D3BJ)/def2-TZVPP level of theory (red).

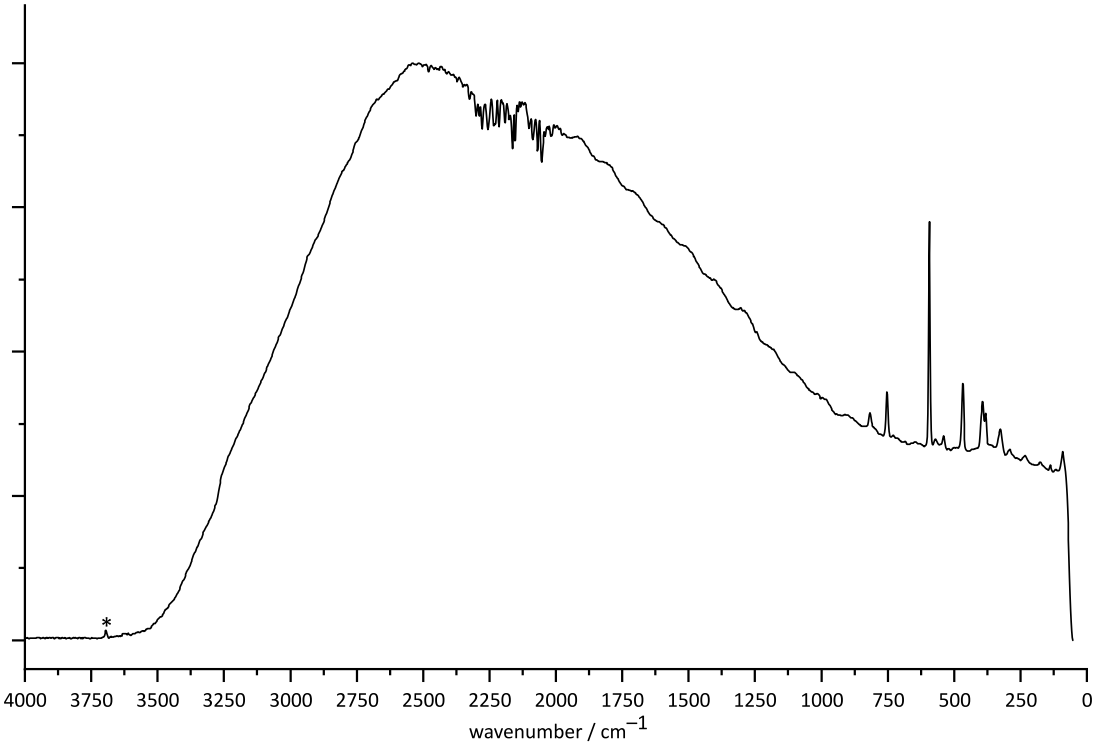


Figure S 23: Raman spectrum (3,000 scans,25 mW) of **2** (black) without baseline correction. The band marked with "*" is an artifact of the spectrometer.

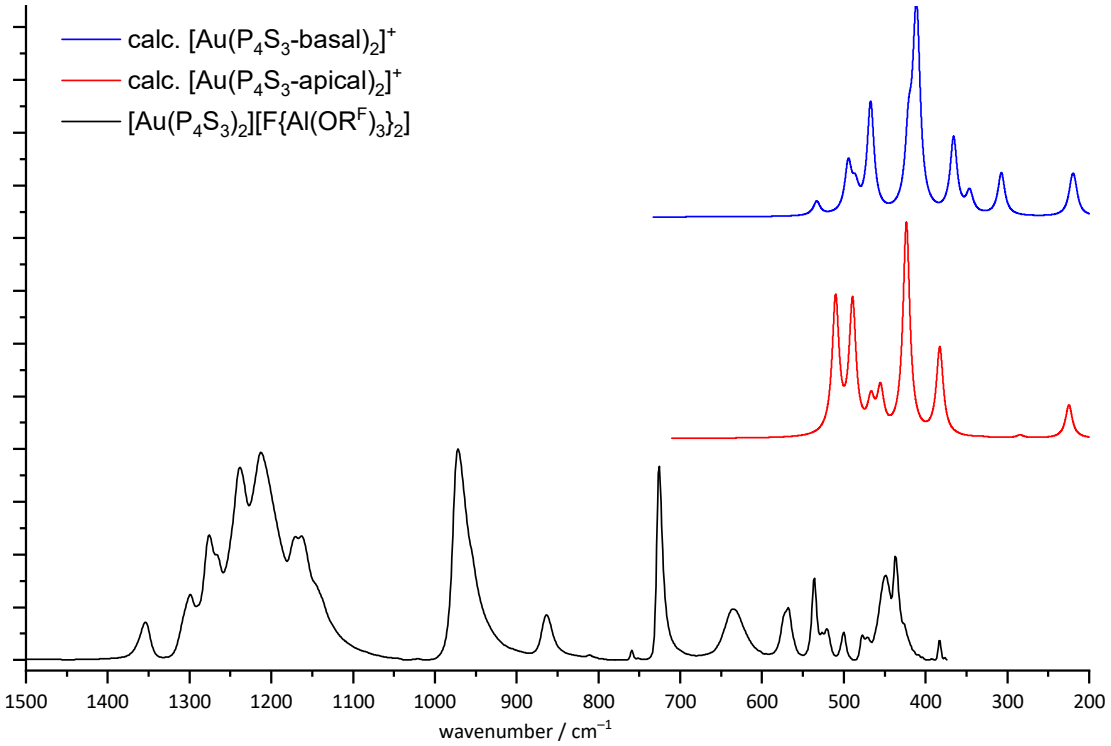


Figure S 24: IR spectrum of **3** (black) and the calculated spectrum of $[Au(P_4S_3)_2]^+$ with the coordination of the apical phosphor atom (red) or one of the basal phosphor atoms (blue) at the B3LYP(D3BJ)/def2-TZVPP level of theory. The calculated vibrational spectra were scaled by 1.02549.

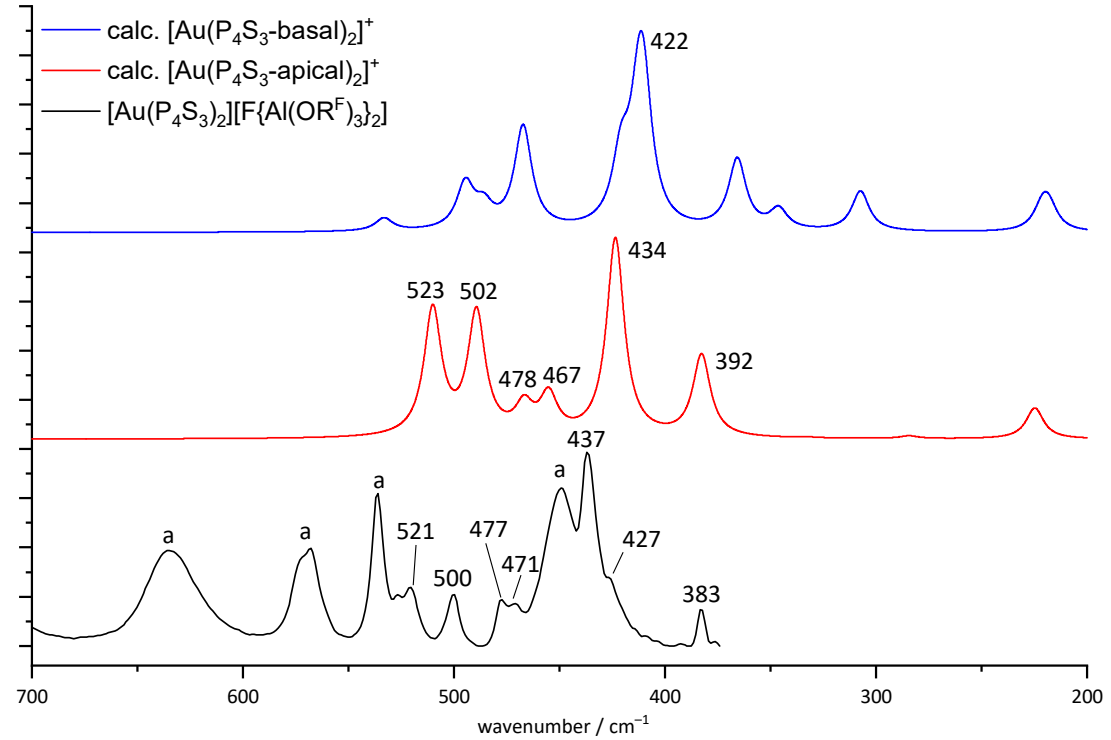


Figure S 25: IR spectrum between 700 cm^{-1} and 200 cm^{-1} of **3** (black) and the calculated spectrum of $[Au(P_4S_3)_2]^+$ with the coordination of the apical phosphor atom (red) or one of the basal phosphor atoms (blue) at the B3LYP(D3BJ)/def2-TZVPP level of theory. The bands marked with "a" are caused by the $[F\{Al(OR^F)_3\}_2]^-$ anion. The calculated vibrational spectra were scaled by 1.02549.

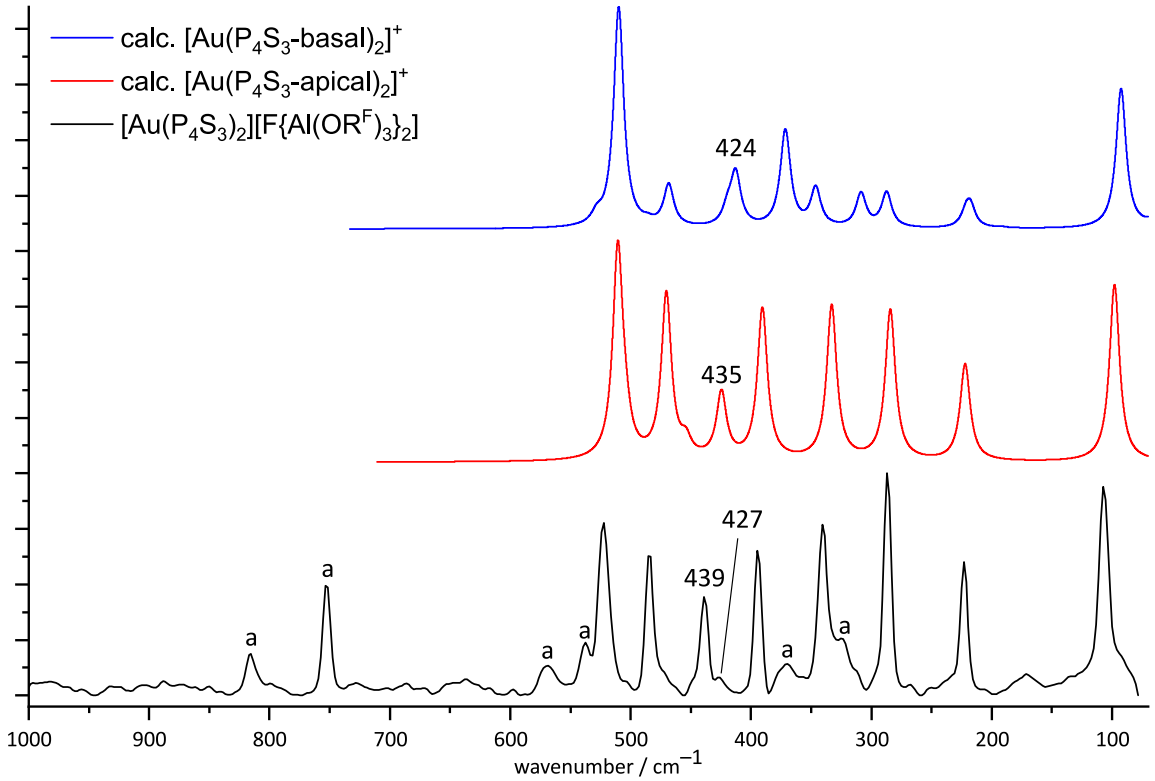


Figure S 26: Raman spectrum (5,000 scans, 20 mW, individual baseline correction) of **3** (black) and the calculated spectrum of $[Au(P_4S_3)_2]^+$ with the coordination of the apical phosphor atom (red) or one of the basal phosphor atoms (blue) at the B3LYP(D3BJ)/def2-TZVPP level of theory. The band marked with "a" are caused by the $[F\{Al(OR^F)_3\}_2]^-$ anion. The calculated vibrational spectra were scaled by 1.02549.

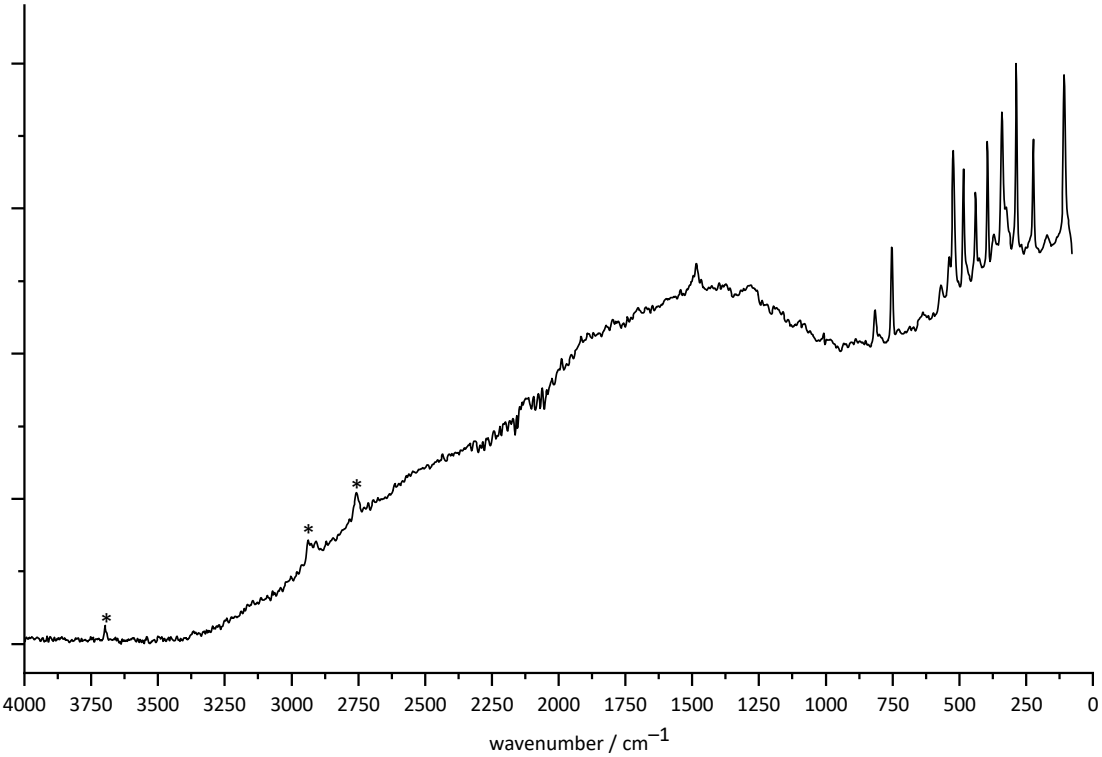


Figure S 27: Raman spectrum (5,000 scans, 20 mW) of **3** (black) without baseline correction. The bands marked with "*" are artifacts of the spectrometer.

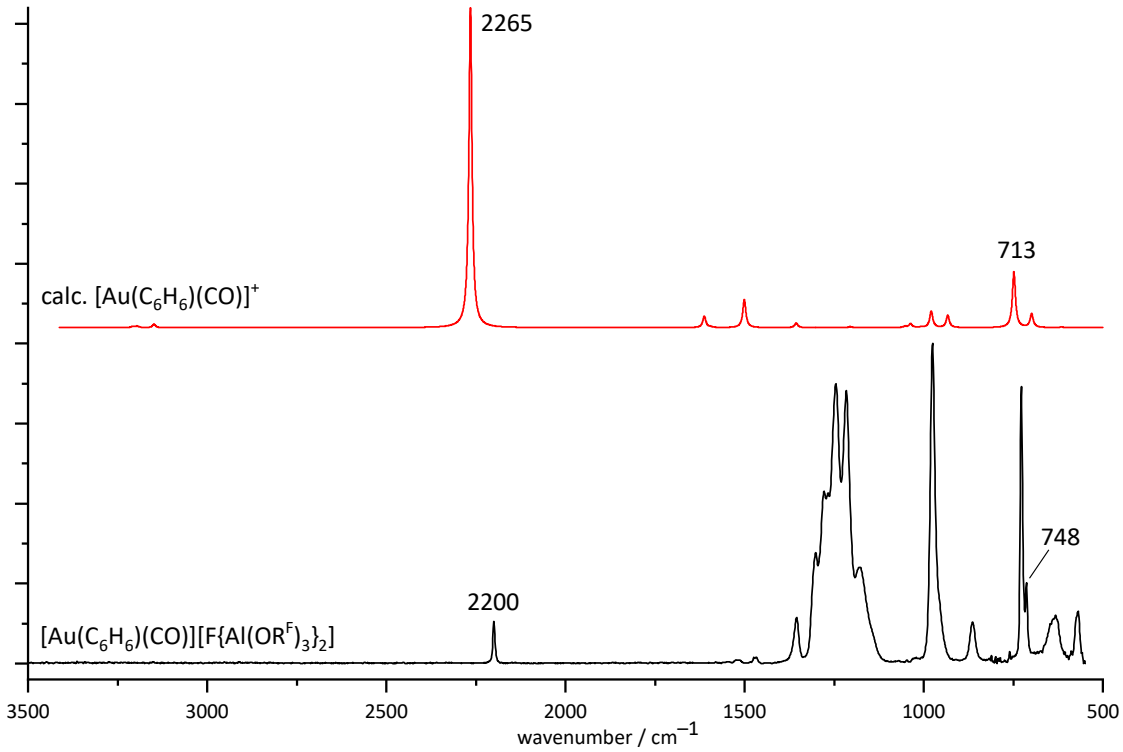


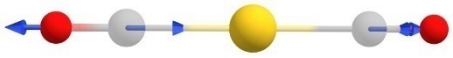
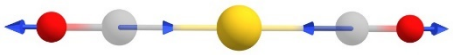
Figure S 28: IR spectrum of **4** (black) and the calculated spectrum of $[Au(C_6H_6)(CO)]^+$ at the B3LYP(D3BJ)/def2-TZVPP level of theory (red).

Table S 1: Assignment of IR and Raman vibrations of compound **1**, **2**, **3** and **4**.

1	**2**		**3**		**4**	$[F\{Al(OR^F)_3\}_2]^{-}$ [a]		**Assignment**[b]
IR	**IR**	**Raman**	**IR**	**Raman**	**IR**	**IR**	**Raman**	
		91 (w)						
				107 (vs)				$[Au(P_4S_3)_2]^+$
				171 (vw)				
				223 (m)				$[Au(P_4S_3)_2]^+$
							234 (vvw)	
				286 (vs)			291 (vw)	$[Au(P_4S_3)_2]^+$ + C–C
		325 (w)		324 (w)			328 (ms)	C–C, Al–O
				340 (s)				$[Au(P_4S_3)_2]^+$
				370 (vw)			370 (vw)	C–C, C–F, Al–O
		382 (w)						$[Au(P_4)_2]^+$
			383 (vw)					$[Au(P_4S_3)_2]^+$
		392 (w)						$[Au(P_4)_2]^+$
				394 (s)				$[Au(P_4S_3)_2]^+$
			427 (vw)	427 (vw)				$[Au(P_4S_3\text{-basal})_2]^+$
			437 (m),	439 (m)				$[Au(P_4S_3)_2]^+$
	449 (w)		449 (m)					Al–O
		467 (w)						$[Au(P_4)_2]^+$
			471 (vw)					$[Au(P_4S_3)_2]^+$
			477 (vw)					$[Au(P_4S_3)_2]^+$
				485 (s)				$[Au(P_4S_3)_2]^+$
			500 (vw)					$[Au(P_4S_3)_2]^+$
			521 (vw)	523 (s)				$[Au(P_4S_3)_2]^+$
			527 (vw)					
	537 (w)	539 (vw)	536 (w)	538 (w)			539 (vw)	C–C, C–O
568 (w)	568 (vw)	570 (vw)	568 (w)	569 (vw)	569 (vw)	568 (vw)	571 (vw)	Al–O, C–C
		593 (vs)						sym. $[Au(P_4)_2]^+$
639 (w)	642 (w)		635 (w)		632 (vw)	639 (w)		Al–F–Al
					713 (w)			C_6H_6, out-of-plane C–H bend
727 (vs)	726 (vs)		726 (vs)		728 (vs)	726 (vvs)		C–C, C–O
		753 (w)		753 (m)		751 (vvw)	753 (ms)	Al–O
760 (vw)	760 (vw)		759 (vw)		760 (vw)	760 (vvw)		C–C, C–O
		817 (vw)		816 (vw)			818 (vw)	Al–O
862 (vw)	863 (w)		864 (w)		864 (vw)	865 (w)		Al–O, Al–F–Al
971 (vs)	970 (vs)		972 (vs)		975 (vs)	972 (vvs)	980 (vvw)[b]	C–C, C–F
							1131 (vvw)[b]	C–C, C–F
			1163 (m)					C–C, C–F
1178(w)	1179 (m)		1171 (m)		1180 (w)	1184 (s)	1180 (vvw) [b]	C–C, C–F
1215 (vs)	1211 (vs)		1213 (vs)		1216 (vs)	1216 (vvs)		C–C, C–F
1247 (vs)	1238 (vs)		1238 (vs)		1245 (vs)	1247 (vvs)	1244 (vvw)[b]	C–C, C–F
1266 (s)	1266 (m)				1267 (m)			C–C, C–F
	1274 (m)		1276 (m)		1278 (m)			
				1279 (vw)			1281 (vvw)[b]	C–C, C–F
1301 (w)	1300 (w)		1299 (w)		1301 (w)	1300 (mw)	1304 (vvw)[b]	C–C, C–F
1354 (vw)	1355 (vw)		1354 (vw)		1355 (vw)	1355 (vw)		C–C, C–F
				1495 (vw)				
					1468 (vw)			C_6H_6, in-plane C–H bend
					1474(vw)			C_6H_6, in-plane C–H bend
					1516(vw)			C_6H_6, ring deformation
					1524(vw)			C_6H_6, ring deformation
2219 (vw)					2200 (vw)			ν_{asym}(CO)

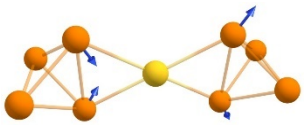
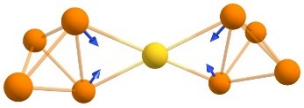
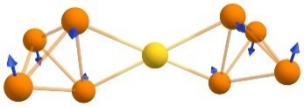
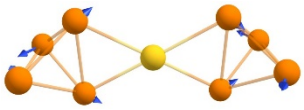
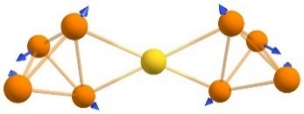
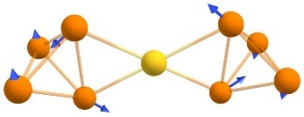
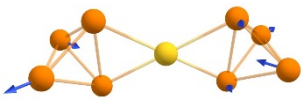
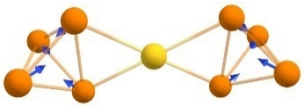
a) For comparison, the IR and Raman vibrations of the anion of $[Cr(CO)_6][F\{Al(OR^F)_3\}_2]$[29] are given. Here the intensities are given as: vvw = very very weak (< 0.1), vw = very weak (< 0.2), w = weak (< 0.3), mw = medium weak (< 0.4), m = medium (< 0.5), ms = medium strong (< 0.6), s = strong (< 0.7), vs = very strong (< 0.8), vvs = very very strong (≥ 0.9). b) Due to the low intensity, these bands were not observed in the Raman spectrum of **2** and **3**.

Table S 2: Observed and calculated (B3LYP(D3BJ)/def2-TZVPP) frequencies and intensities (in parentheses) of the most intense vibrational bands of the cation in **1**, together with the corresponding scaled displacement vectors.

1		**calc. $[Au(CO)_2]^+$**	
IR ν **/cm^{-1}**	**Raman** ν **/cm^{-1}**	**IR** ν **(CO)/cm^{-1}**	**Raman** ν **(CO)/cm^{-1}**
2219 (vw)		 2297 (100)	
	[a]		 2331 (100)

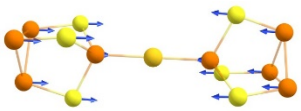
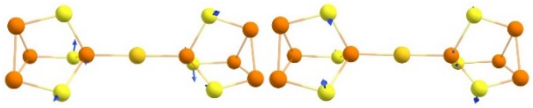
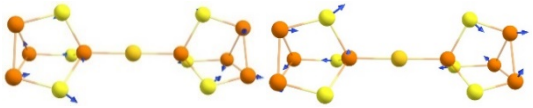
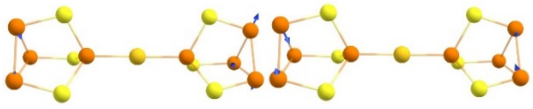
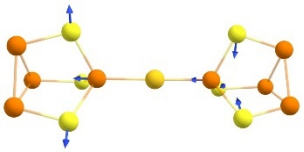
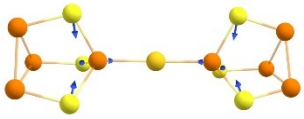
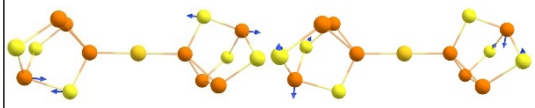
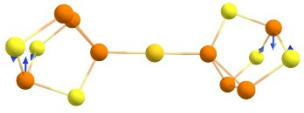
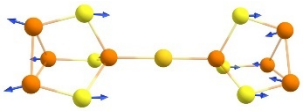
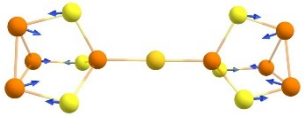
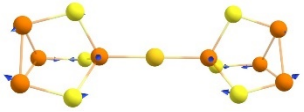
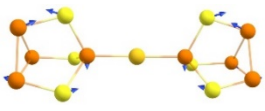
a) A Raman spectrum of **1** could not be obtained due to the decomposition of the compound during the measurement.

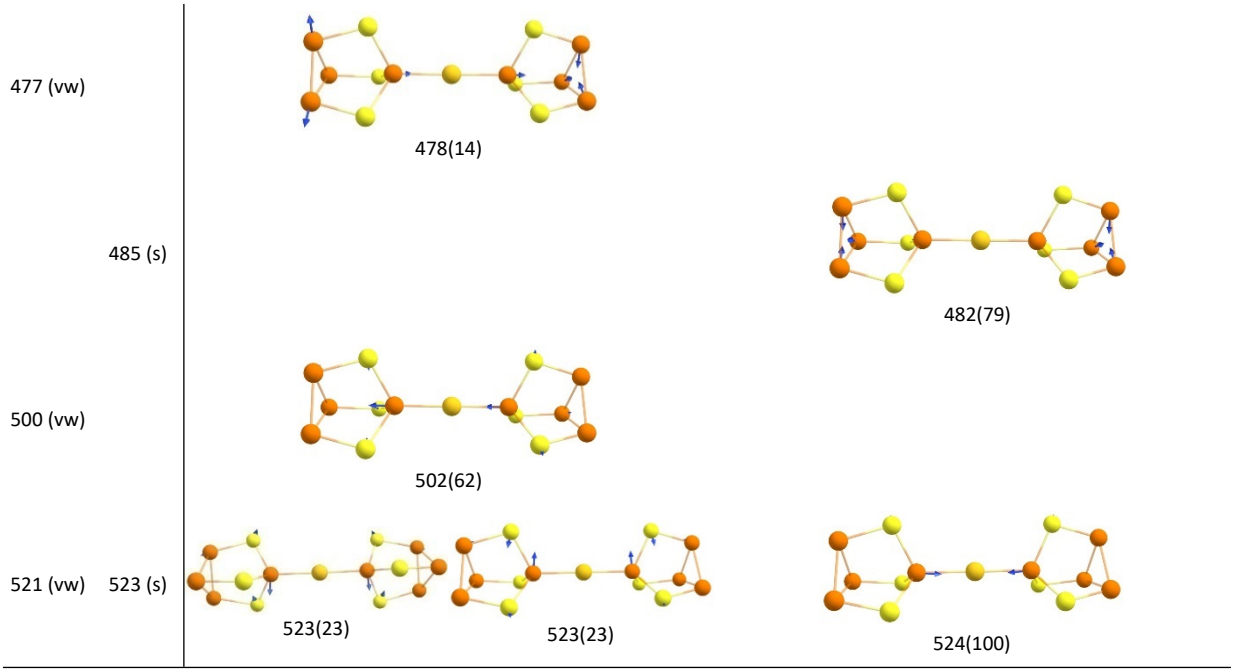
Table S 3: Observed and calculated (B3LYP(D3BJ)/def2-TZVPP) frequencies and intensities (in parentheses) of the most intense vibrational bands of the cation in **2**, together with the corresponding scaled displacement vectors.

2		**calc. $[Au(P_4)_2]^+$**	
IR ν **/cm^{-1}**	**Raman** ν **/cm^{-1}**	**IR** ν **(CO)/cm^{-1}**	**Raman** ν **(CO)/cm^{-1}**
[a]		 368 (27)	
	382 (w)		 373(13)  373 (8)
[a]		 383 (100)	
	392 (w)		 391 (11)
	467 (w)		 458(11)  462(19)
	593 (vs)		 586 (100)

a) Out of range of the experimental IR spectrum.

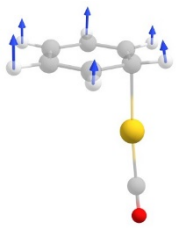
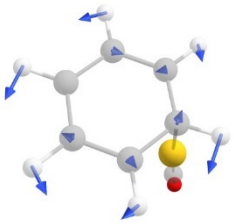
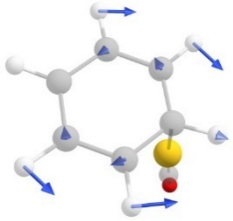
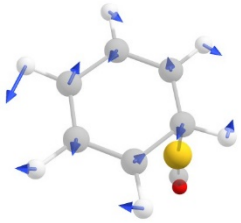
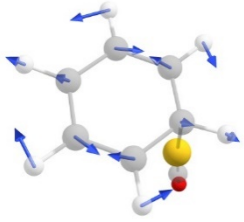
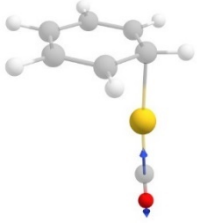
Table S 4: Observed and calculated (B3LYP(D3BJ)/def2-TZVPP) frequencies and intensities (in parentheses) of the most intense vibrational bands of the cation in **3**, together with the corresponding scaled displacement vectors. The calculated vibrational frequencies were scaled by 1.02549.

3		**calc. $[Au(P_4S_3)_2]^+$**	
IR ν /cm^{-1}	**Raman** ν /cm^{-1}	**IR** ν (CO)/cm^{-1}	**Raman** ν (CO)/cm^{-1}
	107 (vs)		 100(85)
	223 (m)		 228(23) 228(23)
	286 (vs)		 291(25) 291(36)
	340 (s)		 341(37) 341(37)
383 (vw)		 392(41)	
	394 (s)		 400(72)
427 (vw)[a]	427 (vw)[a]	 421(100)[a] 423(71)[a]	 423(22)[a]
437 (m),	439 (m)	 434(100)	 435(31)
471 (vw)		 467(10)	 467(10)



a) These vibrational bands are likely caused by the basal coordination of the P_4S_3 cage. The basal coordination of the P_4S_3 cage was also observed as a minority component in the crystal structure of **3** (Figure S 30).

Table S 5: Observed and calculated (B3LYP(D3BJ)/def2-TZVPP) frequencies and intensities (in parentheses) of the most intense vibrational bands of the cation in **4**, together with the corresponding scaled displacement vectors.

4	**calc. $[Au(C_6H_6)(CO)]^+$**
IR ν **/cm^{-1}**	**IR** ν **(CO)/cm^{-1}**
713 (w)	 748 (17)
1468 (vw)	 1500 (6)
1474(vw)	 1501 (3)
1516(vw)	 1594(0.2)
1524(vw)	 1612 (4)
2200 (vw)	 2265 (100)

6. Single-Crystal XRD Data

Table S 6: Crystallographic data for compounds **1**, **2**, **3** and **4**.

	1	**2**	**3**	**4**
CCDC number	2270712	2270713	2270715	2270714
Empirical formula	$C_{26}Al_2AuF_{55}O_8$	$C_{24}Al_2AuF_{55}O_6P_8$	$C_{24}Al_2AuF_{55}O_6P_8S_6$	$C_{37}H_8Al_2AuF_{59}O_7$
Formula weight	1736.19	1927.93	2120.29	1936.36
Temperature /K	100(2)	100(2)	100(2)	100(2)
Crystal system	triclinic	monoclinic	triclinic	monoclinic
Space group (number)	$P\bar{1}$ (2)	$C2/c$ (15)	$P\bar{1}$ (2)	$P2_1$ (4)
***a*/Å**	10.6511(15)	19.631(4)	10.475(2)	10.3633(17)
***b*/Å**	14.425(3)	12.986(2)	12.589(3)	21.779(5)
***c*/Å**	17.025(4)	20.436(5)	12.778(3)	12.483(3)
α/°	99.886(8)	90	116.446(8)	90
β/°	107.015(7)	90.606(11)	91.106(10)	98.548(8)
γ/°	107.198(6)	90	98.160(8)	90
Volume/Å³	2292.0(7)	5210(2)	1486.9(6)	2786.2(10)
Z	2	4	1	2
ρ_{calc}/g cm^{-3}	2.516	2.458	2.368	2.308
μ/mm^{-1}	3.521	3.343	3.143	2.918
***F*(000)**	1640	3648	1008	1844
Crystal size/mm³	0.30×0.18×0.08	0.14×0.12×0.09	0.172×0.042×0.04	0.483×0.318×0.126
Crystal color	colorless	colorless	colorless	colorless
Crystal shape	block	block	needle	block
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2Θ range/°	2.61 to 61.20 (0.70 Å)	3.76 to 61.18 (0.70 Å)	3.58 to 63.31 (0.68 Å)	3.30 to 72.81 (0.60 Å)
Index ranges	−15 ≤ h ≤ 15	−28 ≤ h ≤ 28	−15 ≤ h ≤ 15	−17 ≤ h ≤ 16
	−20 ≤ k ≤ 20	−18 ≤ k ≤ 18	−18 ≤ k ≤ 16	−36 ≤ k ≤ 34
	−24 ≤ l ≤ 24	−29 ≤ l ≤ 29	0 ≤ l ≤ 18	−19 ≤ l ≤ 19
Reflections collected	128923	297593	9917	317126
Independent reflections	14102	8007	9917	24148
	R_{int} = 0.0330	R_{int} = 0.0792	R_{int} = 0.0699	R_{int} = 0.0412
	R_{sigma} = 0.0175	R_{sigma} = 0.0181	R_{sigma} = 0.0358	R_{sigma} = 0.0235
Completeness to θ = 25.242°	100.0 %	100.0 %	99.9 %	100.0 %
Data/Restraints/Parameters	14102/13428/1213	8007/1731/435	9917/1922/527	24148/13737/1418
Goodness-of-fit on F^2	1.022	1.070	1.039	1.043
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0293	R_1 = 0.0185	R_1 = 0.0441	R_1 = 0.0325
	wR_2 = 0.0813	wR_2 = 0.0441	wR_2 = 0.1092	wR_2 = 0.0673
Final *R* indexes [all data]	R_1 = 0.0365	R_1 = 0.0215	R_1 = 0.0541	R_1 = 0.0471
	wR_2 = 0.0859	wR_2 = 0.0448	wR_2 = 0.1146	wR_2 = 0.0714
Largest peak/hole / e Å^{-3}	1.18/-0.91	0.52/-0.67	2.15/-1.18	1.36/-0.77

6.1 Crystal structure of $[Au(CO)_2][F\{Al(OR^F)_3\}_2]$ 1

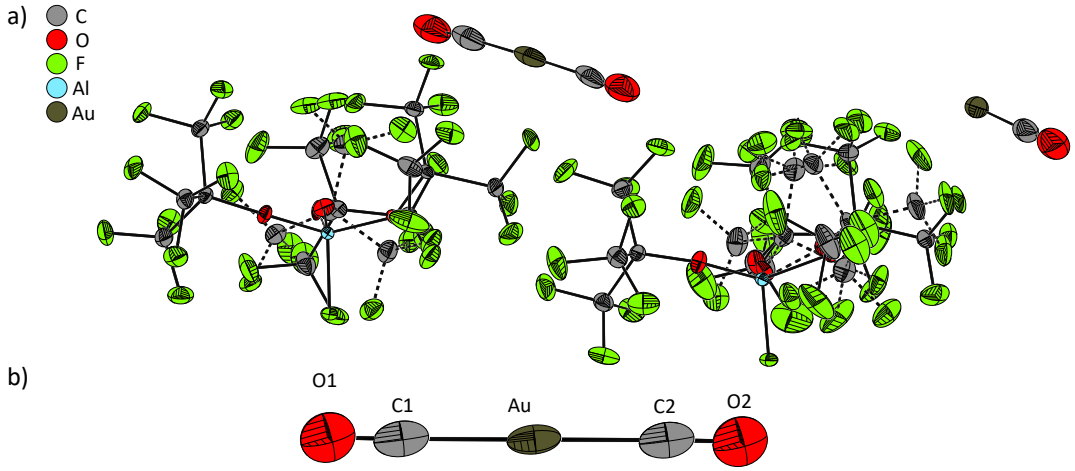


Figure S6-2: a) Asymmetric unit of **1** containing two half anion, one half cation and one disordered cation on a special position with an occupation of 50%. The minority part of disordered fragments is drawn with dashed bonds. **b)** Side view of one of the $[Au(CO)_2]^+$ cations in **1**. Thermal ellipsoids are shown at the 50% probability level.

Table S6-1: Experimental bond lengths [Å] and angles [°] of the $[Au(CO)_2]^+$ cations in **1** together with calculated values at the B3LYP(D3BJ)/def2-TZVPP level of theory.

	1	**calc. $[Au(CO)_2]^+$**
Au–C1	1.983(4)	2.001
Au_10–C1_10	1.981(9)	
Au_10–C2_10	1.977(10)	
Avg: Au–(CO)[a]	1.980(2)	
C1–O1	1.099(4)	1.114
C1_10–O1_10	1.088(10)	
C2_10–O2_10	1.118(11)	
Avg: C–O[a]	1.102(9)	
C1–Au–C1	180.0	180.0
C1_10–Au_10–C2_10	178.7(3)	

a) Standard deviation of the mean was calculated as $N^{-1/2}$ times the positive square root of the sample variance.[30]

6.2 Crystal structure of $[Au(P_4)_2][F\{Al(OR^F)_3\}_2]$ 2

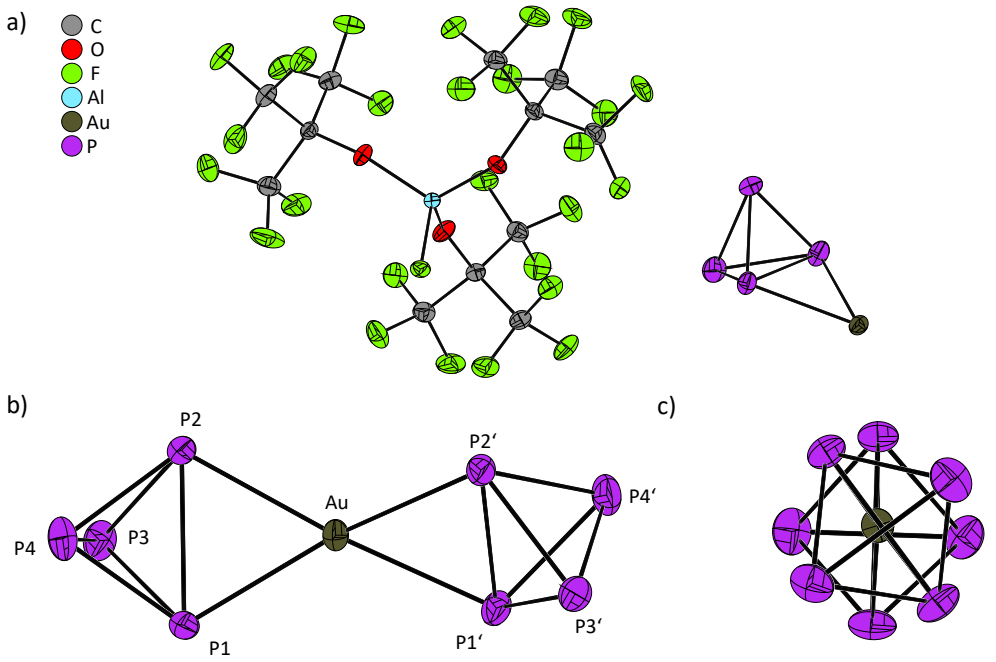


Figure S 29: a) Asymmetric unit of **2** containing one half cation and one half anion. **b), c)** Side view of the $[Au(P_4)_2]^+$ cations in **2**. Thermal ellipsoids are shown at the 50% probability level.

Table S 7: Experimental M–P bond lengths [Å] and torsion angle [°] of the $[Au(P_4)_2]^+$ cations in **2** together with calculated values at the B3LYP(D3BJ)/def2-TZVPP level of theory and literature-known compounds.

	2	**calc. $[Au(P_4)_2]^+$**	**$[Au(P_4)_2][GaCl_4]$[31]**	**$[Cu(P_4)_2][Al(OR^F)_4]$[32][a]**	**$[Ag(P_4)_2][Al(OR^F)_4]$[32][a]**	**$[Ag(P_4)_2][F\{Al(OR^F)_3\}_2]$[33]**
M–P1	2.4486(6)	2.508	2.4408(8)	2.3445(19)	2.548(2)	2.5403(10)
M–P2	2.4470(6)	2.508	2.4457(8)	2.3440(19)	2.564(2)	2.5382(9)
				2.3406(19)	2.550(2)	
				2.3452(19)	2.552(2)	
				2.3444(19)	2.562(2)	
				2.3430(18)	2.551(2)	
				2.3356(19)	2.552(2)	
				2.339(2)	2.554(2)	
P1–P2	2.3992(7)	2.4310	2.4094(12)	2.326(3)	2.329(3)	2.3298(11)
				2.350(3)	2.342(3)	
				2.349(3)	2.342(3)	
				2.343(3)	2.339(3)	
P3–P4	2.2095(8)	2.2379	2.2007(12)	2.183(3)	2.188(3)	2.1949(13)
				2.200(3)	2.195(3)	
				2.205(3)	2.199(3)	
				2.202(3)	2.210(3)	
P1-P2–P2’-P1’	37.36(3)	0.0	0.0	5.24(10)	8.49(13)	43.76(5)
				13.84(10)	4.16(11)	

a) $[Cu(P_4)_2][Al(OR^F)_4]$ and $[Ag(P_4)_2][Al(OR^F)_4]$ contain two crystallographically independent $[M(P_4)_2]^+$ cations with a total of 8 different M–P bonds.

It is noteworthy that the P1-P2–P2'-P1' torsion angle between the two P_4 molecules is highly sensitive towards the environment. In gas phase calculation (@B3LYP(D3BJ)/def2-TZVPP and r2scan-3c) and in the $[Au(P_4)_2][GaCl_4]$ salt, this torsion angle is close to 0°, resulting in an almost D_{2h} symmetric $[Au(P_4)_2]^+$ molecule. In the similar $[Ag(P_4)_2][Al(OR^F)_4]$ and $[Cu(P_4)_2][Al(OR^F)_4]$ salts, this torsion angle ranges between 4.16(11)° and 13.84(10)°.[32,34] In contrast, the torsion angle amounts to 43.76(5)° in $[Ag(P_4)_2][F\{Al(OR^F)_3\}_2]$[33] and 37.36(3)° in **2**, which reduces the symmetry of the $[Au(P_4)_2]^+$ cation to D_2. The differences in the torsion angles are likely caused by crystal-packing effects and the interactions with the different anions $[GaCl_4]^-$, $[Al(OR^F)_4]^-$, and $[F\{Al(OR^F)_3\}_2]^-$. In the gas phase, the energy difference ΔE between two conformers of the $[Au(P_4)_2]^+$ cation with a torsion angle of 0° and 90° amounts only to 0.8 kJ mol^{-1} at the CCSD(T)/def2-QZVPP//r2scan-3c level of theory (Figure S 37).

6.3 Crystal structure of $[Au(P_4S_3)_2][F\{Al(OR^F)_3\}_2]$ 3

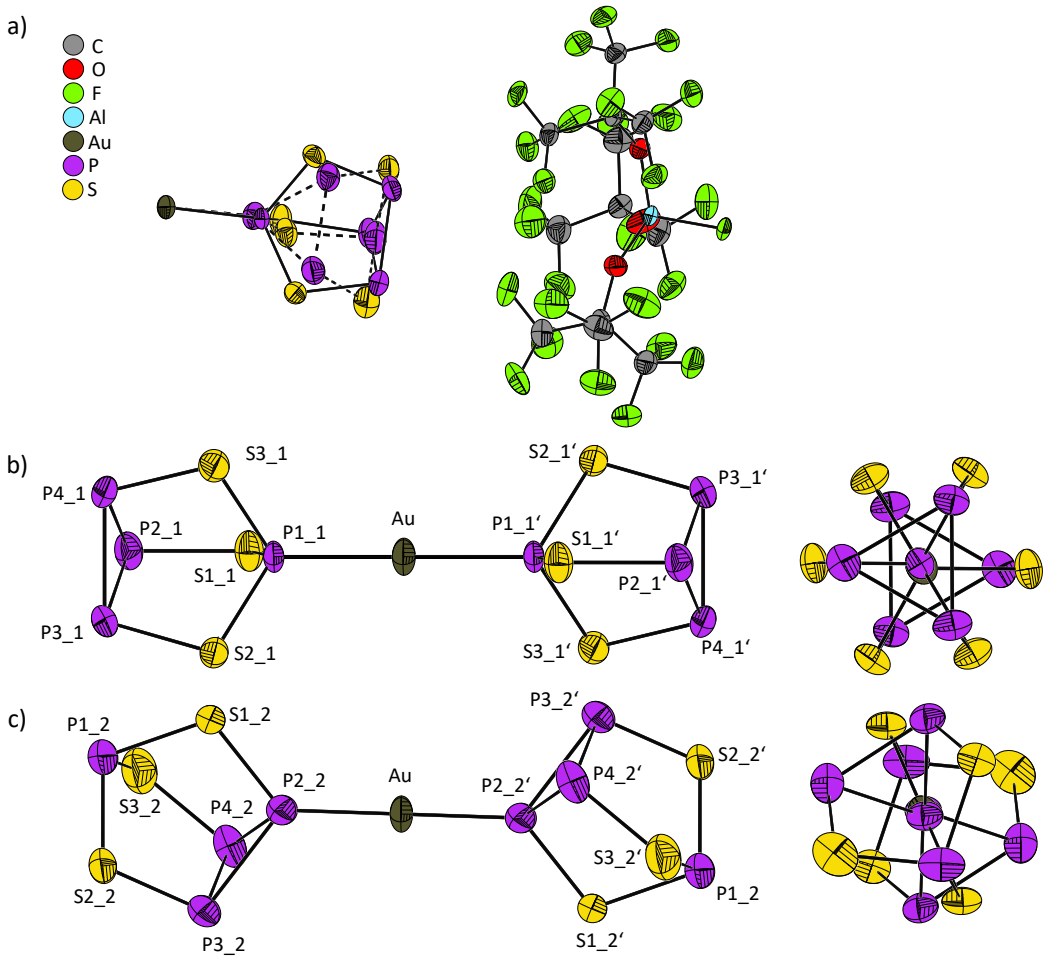


Figure S 30: Asymmetric unit of **3** containing a half anion and a half cation. The P_4S_3 cage of the cation is disordered and coordinates with the apical phosphor atom (86%) or one of the basal phosphor atoms (14%). The minority part of disordered fragments is drawn with dashed bonds. **b)** Top and side view of the majority part of the $[Au(P_4S_3)_2]^+$ cation in **3**. **c)** Top and side view of the minority part of the $[Au(P_4S_3)_2]^+$ cation in **3**. Thermal ellipsoids are shown at the 50% probability level.

Table S 8: Experimental bond lengths [Å] of the $[Au(P_4S_3)_2]^+$ cation in **3** together with calculated values at the B3LYP(D3BJ)/def2-TZVPP level of theory.

Apical coordination (majority part)			Basal coordination (minority part)		
	3	**calc. $[Au(P_4S_3)_2]^+$**		**3**	**calc. $[Au(P_4S_3)_2]^+$**
Au–P1_1	2.301(3)	2.327	Au–P2_2	2.14(2)	2.324
P1_1–S1_1	2.059(3)	2.088	P1_2–S1_2	2.12(3)	2.140
P1_1–S2_1	2.057(3)	2.088	P1_2–S2_2	2.05(2)	2.130
P1_1–S3_1	2.069(6)	2.088	P1_2–S3_2	2.01(2)	2.130
P2_1–S1_1	2.0897(18)	2.119	P2_2–S1_2	2.09(4)	2.077
P3_1–S2_1	2.0903(19)	2.119	P3_2–S2_2	2.068(12)	2.099
P4_1–S3_1	2.094(4)	2.119	P4_2–S3_2	2.089(14)	2.099
P2_1–P3_1	2.239(2)	2.269	P2_2–P3_2	2.26(2)	2.229
P3_1–P4_1	2.243(3)	2.269	P3_2–P4_2	2.216(18)	2.291
P4_1–P2_1	2.254(3)	2.269	P4_2–P2_2	2.25(2)	2.229

Table S 9: Comparison of the average bond lengths [Å] of the $[Au(P_4S_3)_2]^+$ cation in **3** with different literature-known complexes and free P_4S_3.

	3		**$[Ag(P_4S_3)_2]$ $[Al(OR^F)_4]$**[35]	**$[Ag(P_4S_3)]$ $[Al(OCH(CF_3)_2)_4]$**[35]	**$[Fe(Cp)(P_4S_3)]$ $[F\{Al(OR^F)_3\}_2]$**[36]	**γ-P_4S_3**[35]	**α-P_4S_3**[35]
	major	**minor**					
av. M–P_{basal}	–	2.14(2)[b]	2.529(9)	2.5471(8)	2.1978(7)[b]		
av. M–P_{apical}	2.301(3)[b]	–	–	2.459(2)	–		
av. M–S	–	–	2.6573(11)[b]	–	–		
av. P_{basal}–P_{basal}	2.245(8)	2.242(13)	2.237(5)	2.238(4)	2.226(16)	2.241(4)	2.2424(14)
av. P_{basal}–S	2.0913(13)	2.082(8)	2.083(4)	2.101(3)	2.074(4)	2.10553(3)	2.0992(16)
av. P_{apical}–S	2.062(4)	2.06(3)	2.112(4)	2.091(2)	2.107(5)	2.1082(12)	2.1104(17)

6.4 Crystal structure of $[Au(C_6H_6)(CO)][F\{Al(OR^F)_3\}_2]$ 4

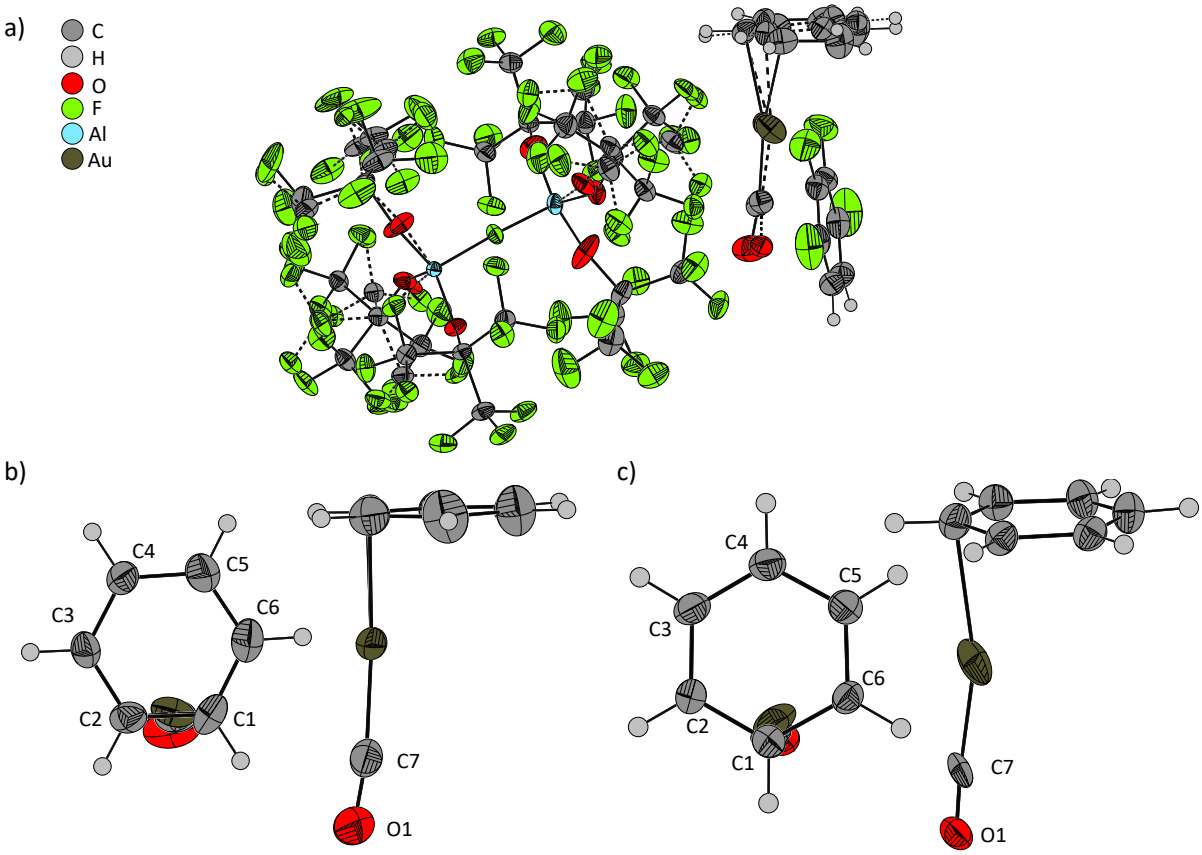


Figure S 31: a) Asymmetric unit of **4** containing one disordered cation (occupation 70%/30%) and one anion. The minority part of disordered fragments is drawn with dashed bonds. **b)** Top and side view of the majority part of the $[Au(C_6H_6)(CO)]^+$ cation in **4**. **c)** Top and side view of the minority part of the $[Au(C_6H_6)(CO)]^+$ cation in **4**. Thermal ellipsoids are shown at the 50% probability level.

Table S 10: Experimental bond lengths [Å] and angles [°] of the $[Au(C_6H_6)(CO)]^+$ cations in **4** together with calculated values at the B3LYP(D3BJ)/def2-TZVPP level of theory.

	4 majority part	**4** minority part	calc. $[Au(C_6H_6)(CO)]^+$
Au–C1	2.228(8)	2.394(16)	2.223
Au–C2	2.312(7)	2.554(18)	2.680
Au–C3	2.908(8)	3.083(18)	3.381
Au–C4	3.361(88)	3.454(17)	3.682
Au–C5	3.313(8)	3.352(13)	3.381
Au–C6	2.777(9)	2.851(11)	2.680
Au–C7	1.911(9)	1.884(17)	1.954
C7–O1	1.151(13)	1.02(2)	1.120
Au–C7–O1	171(2)	169(4)	179.0

7. Cyclic Voltammetry

Cyclic voltammetry was performed with a BioLogic VMP3 potentiostat inside a glovebox. The cyclic voltammograms of **1** and **2** were measured with a gold disc working electrode (d = 0.5 mm), a platinum wire as counter electrode and a platinum wire as quasi-reference electrode. All used solutions contained $[NBu_4][Al(OR^F)_4]$ (100 mM) as conducting salt. The measurements were performed with a solution of the sample (10 mM) in 4FB (**1**, Figure S 32) or 5FB (**2**, Figure S 33) and different scan rates. After the measurement of the pure sample, $[Fc][Al(OR^F)_4]$ (10mM) was added as an internal reference. In both cases, the oxidative and reductive process are coupled, as the oxidation is only observed if a reduction occurred first. However, due to the large separation of the anodic and cathodic peak potentials (0.39 V (**1**) or 0.80 V (**2**)) and the unusual shape of the cyclic voltammograms, we did not determine a half-wave potential and only report the peak potentials and currents (Table S 11). This large separation indicates that either the electron transfer reaction is quite slow, or more likely, that the electron transfer is coupled with a chemical reaction. In this case, the neutral $[Au(L)_2]^0$ (L = Co, P_4) complexes are likely not stable under these conditions at RT and (partial) ligand dissociation occurs. This conclusion is supported by the significantly smaller anodic peak current compared to the corresponding cathodic peak current in the CV of **2** and the considerably reduced bond dissociation Gibbs free energies of $[Au(L)_2]^0$ (L = Co: 20 kJ mol^{-1}, L = P_4: 108 kJ mol^{-1}) compared to $[Au(L)_2]^+$ (L = Co: 325 kJ mol^{-1}, L = P_4: 428 kJ mol^{-1}) (@DLPNO-CCSD(T)/def2-QZVPP//r2scan-3c, see Table S 14).

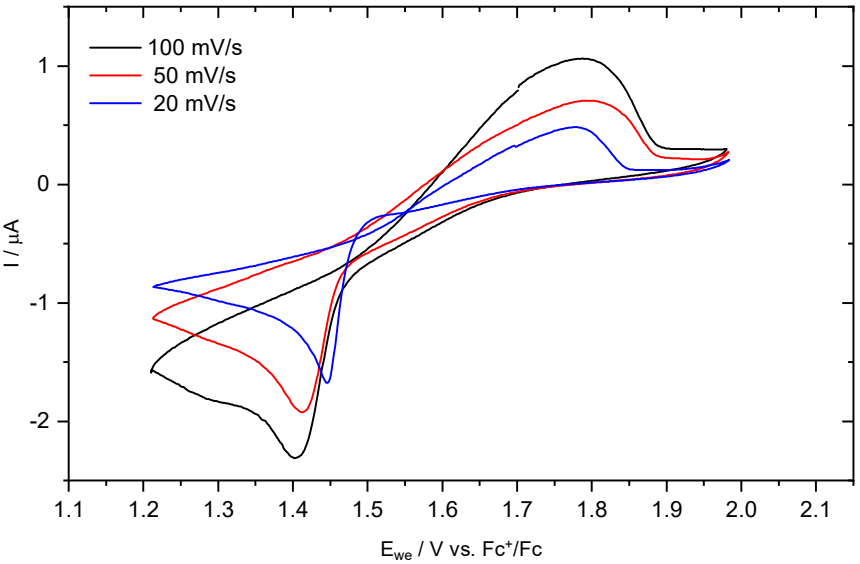


Figure S 32: Experimental cyclic voltammograms of **1** (10 mM) in 4FB at different scan rates.

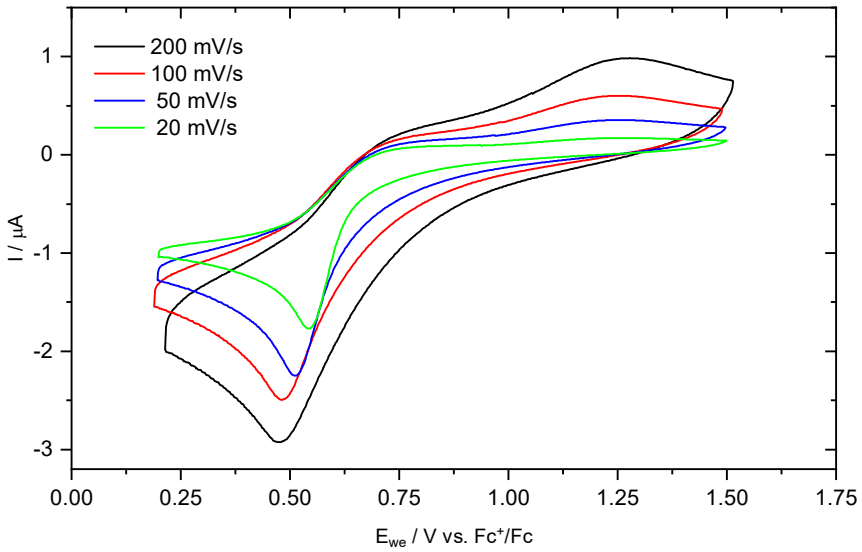


Figure S 33: Experimental cyclic voltammograms of **2** (10 mM) in 4FB at different scan rates.

Table S 11: Anodic and cathodic peak potentials vs. Fc^+/Fc and currents obtained by cyclic voltammetry of **1** and **2** at different scan rates.

	1				**2**			
***υ* / mV s^{-1}**	**E_{pc} / V**	**I_{pc} / µA**	**E_{pa} / V**	**I_{pa} / µA**	**E_{pc} / V**	**I_{pc} / µA**	**E_{pa} / V**	**I_{pa} / µA**
20	1.446	–1.678	1.779	0.4826	0.543	–1.769	1.256	0.1719
50	1.413	–1.922	1.794	0.7077	0.511	–2.247	1.255	0.3550
100	1.403	–2.311	1.787	1.062	0.484	–2.494	1.256	0.6027
200					0.477	–2.927	1.278	0.9852

8. Powder XRD Data

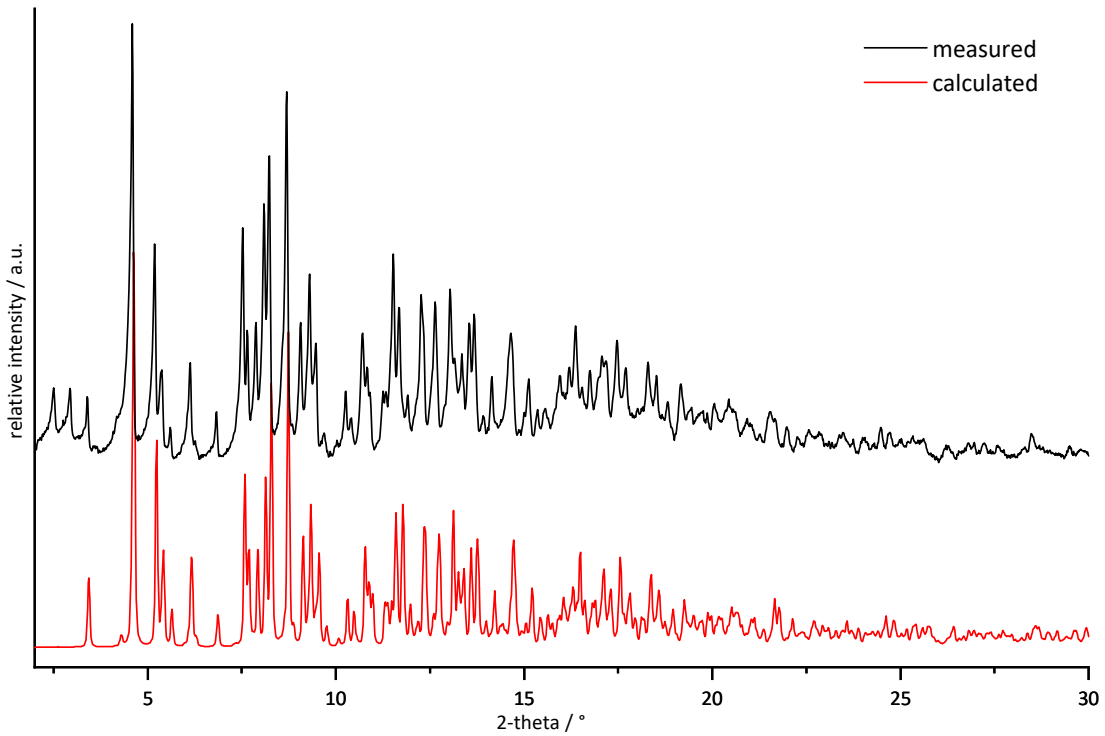


Figure S6-3: Measured powder XRD data of bulk material of **1** at 100 K (black) and calculated powder diffraction pattern, simulated with single-crystal data of **1** (red).

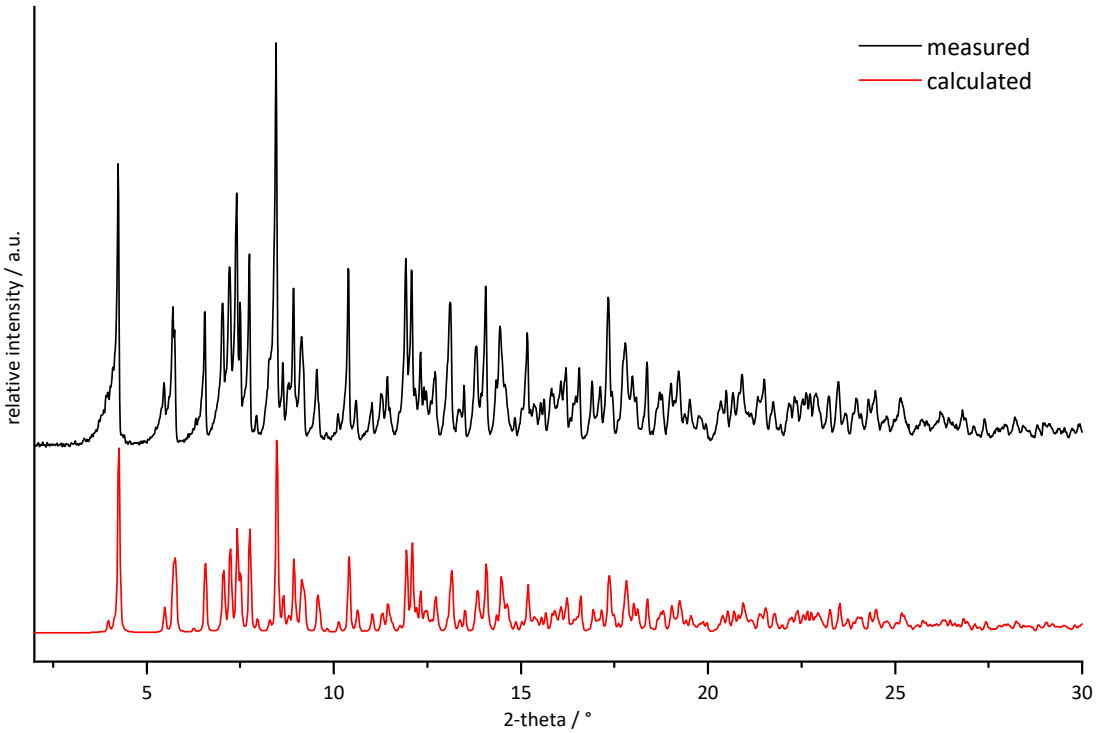


Figure S 34: Measured powder XRD data of bulk material of **2** at 100 K (black) and calculated powder diffraction pattern, simulated with single-crystal data of **2** (red).

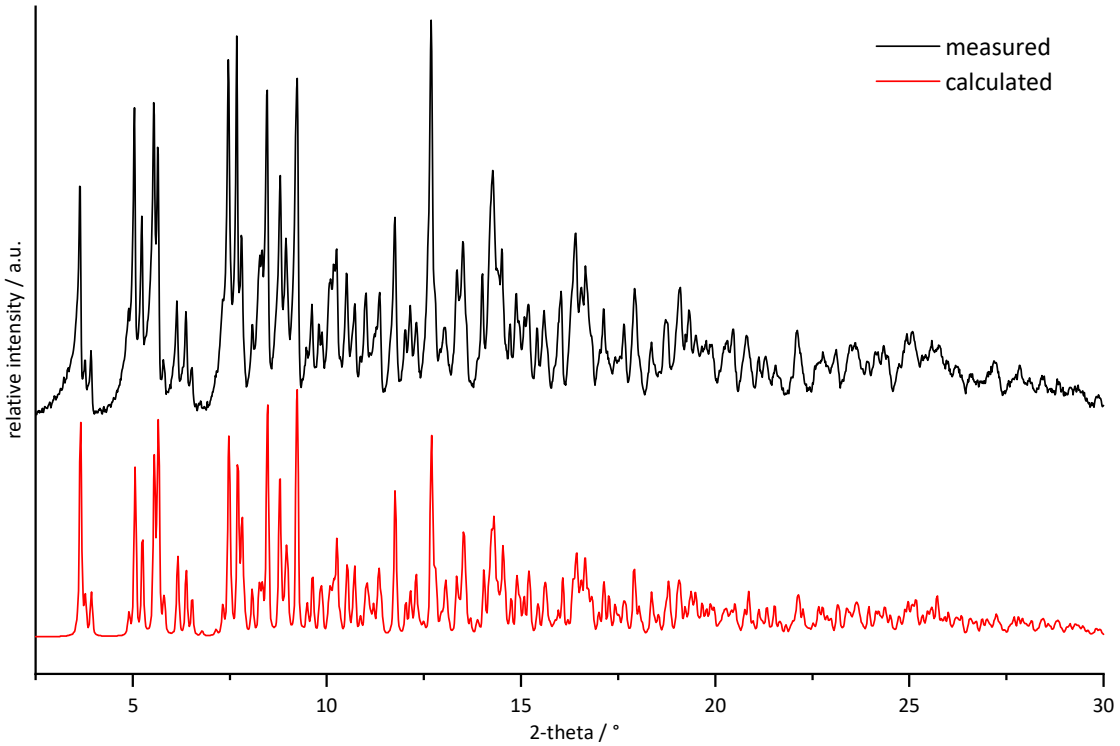


Figure S 35: Measured powder XRD data of bulk material of **3** at 100 K (black) and calculated powder diffraction pattern, simulated with single-crystal data of **3** (red).

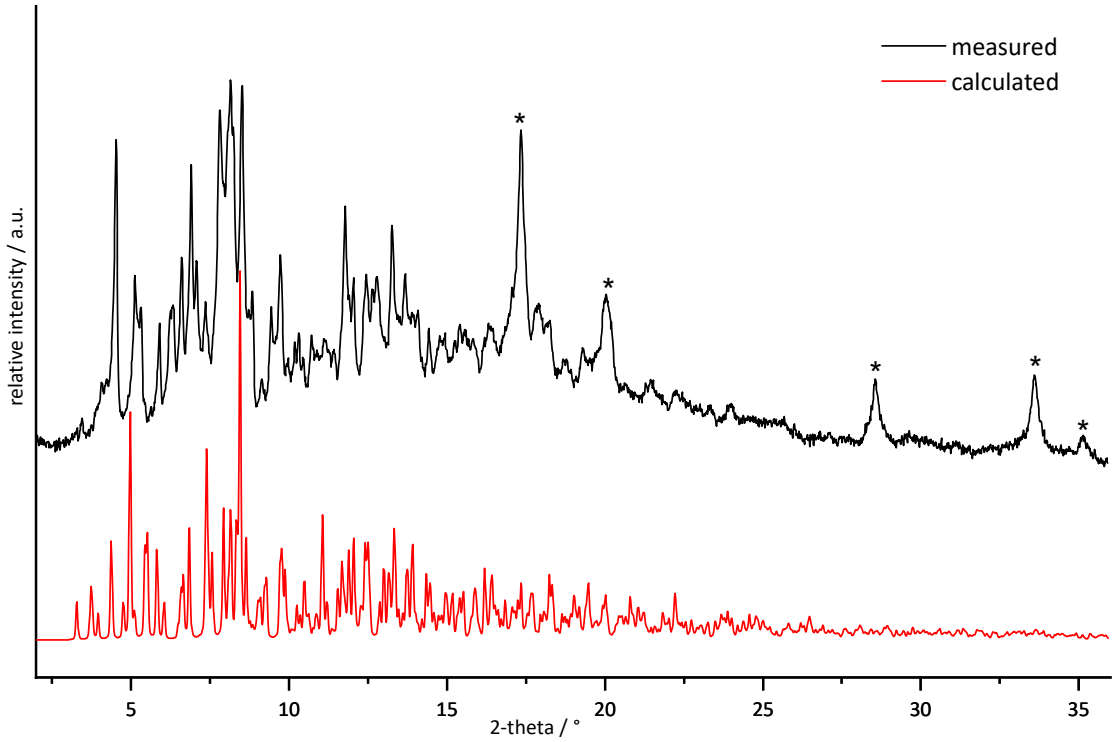


Figure S 36: Measured powder XRD data of bulk material of **4** at 100 K (black) and calculated powder diffraction pattern, simulated with single-crystal data of **4** (red). The measured and simulated powder XRD show some serious discrepancies, which are likely caused by the decomposition of compound during sample preparation at RT. The reflexes marked with an asterisk can be assigned to elemental gold (PDF-# 04-0784).

9. Quantum-Chemical Calculations

Table S 12: Summary of thermodynamic data calculated at the DLPNO-CCSD(T)/def2-QZVPP//r2scan-3c levels of theory.

	E^0 (r2scan–3c) / H	H^0(r2scan–3c)[a] / H	G^0(r2scan–3c)[a] / H	E^0(DLPNO–CCSD(T)) / H	T1 diag. (DLPNO–CCSD(T))
$[Cu]^0$	–1640.4553	–1640.4530	–1640.4712	–1639.7254	0.018
$[Cu]^+$	–1640.1696	–1640.1672	–1640.1854	–1639.4540	0.012
$[Ag]^0$	–147.0158	–147.0135	–147.0325	–146.8357	0.013
$[Ag]^+$	–146.7266	–146.7243	–146.7432	–146.5610	0.005
$[Au]^0$	–135.7550	–135.7526	–135.7725	–135.4254	0.012
$[Au]^+$	–135.4062	–135.4039	–135.4237	–135.0923	0.006
$[Cu(CO)_2)]^+$	–1866.8999	–1866.8775	–1866.9124	–1865.9368	0.019
$[Au(CO)_2)]^0$	–373.4156	–373.3936	–373.4299	–373.0155	0.015
$[Au(CO)_2)]^+$	–362.1715	–362.1488	–362.1840	–361.6226	0.016
CO	–113.2936	–113.2853	–113.3077	–113.1867	0.018
$[Cu(N_2)_2)]^+$	–1859.2805	–1859.2577	–1859.2928	–1858.3335	0.016
$[Ag(N_2)_2)]^+$	–365.7973	–365.7749	–365.8128	–365.4132	0.012
$[Au(N_2)_2)]^+$	–354.5235	–354.5006	–354.5365	–353.9898	0.013
N_2	–109.5071	–109.4982	–109.5199	–109.4033	0.013
Cl_2	–920.3153	–920.3106	–920.3360	–919.4795	0.009
$Cl^–$	–460.2381	–460.2357	–460.2532	–459.8229	0.003
Br_2	–5148.2626	–5148.2582	–5148.2861	–5146.0932	0.007
$Br^–$	–2574.2161	–2574.2138	–2574.2323	–2573.1302	0.005
I_2	–595.4866	–595.4823	–595.5119	–594.6012	0.007
$I^–$	–297.8279	–297.8255	–297.8447	–297.3827	0.006
$[Au(P_4)_2)]^0$ (0° angle)	–2866.6364	–2866.6088	–2866.6625	–2863.0042	0.017
$[Au(P_4)_2)]^+$ (0° angle)	–2866.41640	–2866.3884	–2866.4421	–2862.7933	0.015
$[Au(P_4)_2)]^+$ (90° angle)[b]	–2866.4150	–2866.3880	–2866.4405	–2862.7930	0.016
P_4	–1365.3954	–1365.3837	–1365.4155	–1363.7531	0.017
$[Au(P_4S_3)_2)]^+$ (apical)	–5255.6567	–5255.6084	–5255.6798	–5249.5420	0.018
$[Au(P_4S_3)_2)]^+$ (basal)	–5255.6547	–5255.6066	–5255.6786	–5249.5375	0.018
P_4S_3	–2560.0142	–2559.9927	–2560.0359	–2557.1217	0.020

a) E_{vrt} of a single atom equals $\frac{3}{2}RT$. The standard entropy of atoms was calculated with the Sackur-Tetrode equation.[37]
b) $[Au(P_4)_2)]^+$ (90° angle) is a transition state with one imaginary mode of –5.9 cm^{-1}.

Table S 13: Summary of thermodynamic data calculated at the B3LYP(D3BJ)/def2-TZVPP levels of theory.

	E_{SCF}(B3LYP) / H	E_{vrt}(B3LYP) / kJ mol^{-1}	$S°$(B3LYP) / kJ mol^{-1}K^{-1}	$G°$(B3LYP) / kJ mol^{-1}	$H°$(B3LYP) / kJ mol^{-1}	$E°$(B3LYP) / kJ mol^{-1}
[Au]$^{0\,a}$	–135.6905	3.7	0.1747	–356301.2	–356249.1	–356255.3
[Au]$^{+\,a}$	–135.3477	3.7	0.1747	–355401.2	–355349.1	–355355.3
[Au(CO)$_2$)]$^+$	–362.1309	57.3	0.3164	–950809.1	–950714.8	–950774.6
CO	–113.3111	19.4	0.1977	–297535.2	–297476.3	–297498.2
[Au(P$_4$)$_2$)]$^+$ (0° angle)	–2866.2690	70.66	0.5071	–7525465.9	–7525314.7	–7525387.8
[Au(P$_4$S$_3$)$_2$)]$^+$ (apical)	–5255.4712	124.6	0.6745	–13798311.0	–13798109.9	–13798237.0
[Au(P$_4$S$_3$)$_2$)]$^+$ (basal)	–5255.4690	124.3	0.6832	–13798308.1	–13798104.4	–13798231.1
[Au(C$_6$Me$_6$)$_2$)]$^+$	–1071.6348	1488.0	0.8717	–2812346.2	–2812086.3	–2813576.7
[Au(C$_6$Me$_6$)(CO)]$^+$	–716.8966041	770.92	0.59506	–1881615.69	–1881438.28	–1882211.68
C$_6$Me$_6$	–468.0395	736.1	0.4965	–1228246.8	–1228098.7	–1228837.4
[C$_6$Me$_6$]$^+$	–467.7664	732.1	0.4933	–1227533.0	–1227386.0	–1228120.5
[Au(Mes)$_2$)]$^+$	–835.8075	1025.3	0.7205	–2193599.2	–2193384.4	–2194412.2
[Au(Mes)(CO)]$^+$	–598.9815959	540.74	0.51988	–1572237.66	–1572082.66	–1572625.88
Mes	–350.1298	503.9	0.4187	–918884.1	–918759.2	–919265.6
[Mes]$^+$	–349.8323	499.0	0.4076	–918104.5	–917982.9	–918484.4
[Au(C$_6$H$_6$)$_2$)]$^+$	–599.9338	567.2	0.5038	–1574706.4	–1574556.2	–1575126.0
[Au(C$_6$H$_6$)(CO)]$^+$	–481.0406618	311.82	0.41369	–1262781.06	–1262657.72	–1262972.02
C$_6$H$_6$	–232.2050	275.1	0.2683	–609456.4	–609376.5	–609654.0
[C$_6$H$_6$]$^+$	–231.8733	270.2	0.3018	–608600.6	–608510.6	–608783.3
[Au(*o*–dfb)$_2$)]$^+$	–996.9063	489.2	0.5800	–2617058.3	–2616885.4	–2617377.1
[Au(*o*–dfb)(CO)]$^+$	–679.5250517	272.88	0.45012	–1783951.53	–1783817.32	–1784092.68
o–dfb	–430.6997	236.4	0.3206	–1130658.5	–1130562.9	–1130801.8
[*o*–dfb]$^+$	–430.3696	235.7	0.3253	–1129793.9	–1129696.9	–1129935.1
[Au(4FB)$_2$)]$^+$	–1393.8538	412.9	0.6569	–3659342.9	–3659147.0	–3659562.4
[Au(4FB)(CO)]$^+$	–877.9972723	234.62	0.48624	–2305089.27	–2304944.30	–2305181.4
4FB	–629.1838	198.4	0.3580	–1651827.7	–1651720.9	–1651921.8
[4FB]$^+$	–628.8459	198.3	0.3683	–1650943.5	–1650833.7	–1651034.5

a) E_{vrt} of a single atom equals $\frac{3}{2}RT$. The standard entropy of atoms was calculated with the Sackur-Tetrode equation.[37]

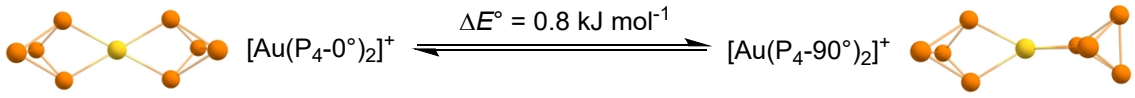


Figure S 37: Calculated structures and energy difference between two conformers of the $[Au(P_4)_2]^+$ cation with an torsion angle of 0° or 90° at the DLPNO-CCSD(T)/def2-QZVPP//r2scan-3c level of theory. The 90° structure has an imaginary mode of –6 cm^{-1}.

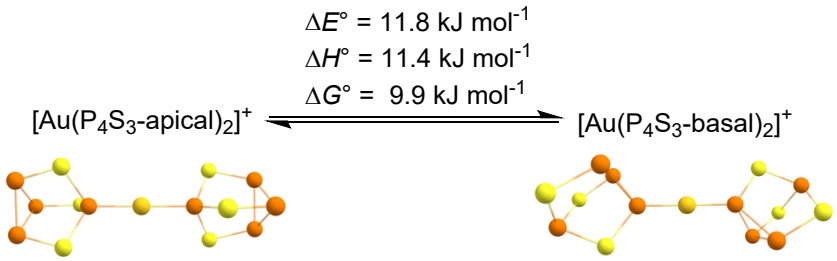


Figure S 38: Calculated structures and thermodynamics for the different coordination isomers of $[Au(P_4S_3)_2]^+$ at the DLPNO-CCSD(T)/def2-QZVPP//r2scan-3c level of theory.

Table S 14: Reaction energy, enthalpy, and Gibbs free energy for the dissociation of all ligands at the DLPNO-CCSD(T)/def2-QZVPP//r2scan-3c level of theory according to $[Au(L)_n]^m \longrightarrow [Au]^m + n\ L$.

	$\Delta_R G$ / kJ mol^{-1}	$\Delta_R H$ / kJ mol^{-1}	$\Delta_R E$ / kJ mol^{-1}
$[Au(CO)_2]^+$	324.7	402.3	412.0
$[Au(CO)_2]^0$	19.8	86.8	91.2
$[Au(P_4)_2]^+$	427.6	505.3	511.5
$[Au(P_4)_2]^0$	107.6	185.3	190.6

Table S 15: Reaction energy, enthalpy, and Gibbs free energy for the dissociation of all ligands at the DLPNO-CCSD(T)/def2-QZVPP//r2scan-3c level of theory according to $[M(N_2)_2]^+ \longrightarrow [M]^+ + 2\ N_2$.

	$\Delta_R G$ / kJ mol^{-1}	$\Delta_R H$ / kJ mol^{-1}	$\Delta_R E$ / kJ mol^{-1}
$[Au(N_2)_2]^+$	159.1	231.1	238.5
$[Ag(N_2)_2]^+$	49.1	113.5	119.6
$[Cu(N_2)_2]^+$	114.1	184.1	191.1

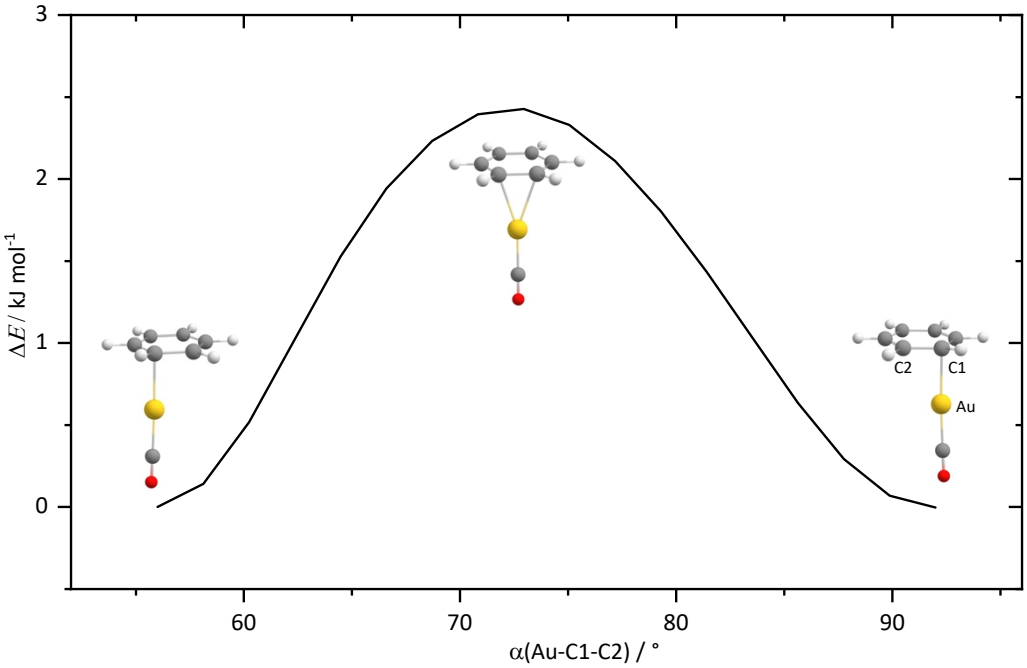


Figure S 39: Relaxed surface scan along the Au–C1–C2 angle at the B3LYP(D3BJ)/def2-TZVPP level of theory. This scan describes the transition $[Au(\eta^1\text{-}C_6H_6)(CO)]^+$ → $[Au(\eta^2\text{-}C_6H_6)(CO)]^+$ → $[Au(\eta^1\text{-}C_6H_6)(CO)]^+$.

Table S 16: Reaction energy, enthalpy, and Gibbs free energy for the exchange of CO versus one or two arene ligands at the B3LYP(D3BJ)/def2-TZVPP level of theory according to $[Au(CO)_2]^+ + n\ L \longrightarrow [Au(L)_2(CO)_{2-n}]^+ + n\ CO$.

	$\Delta_R G$ / kJ mol^{-1}	$\Delta_R H$ / kJ mol^{-1}	$\Delta_R E$ / kJ mol^{-1}
$[Au(C_6Me_6)(CO)]^{+}$[a]	–95.0	–101.0	–97.9
$[Au(Mes)(CO)]^+$	–79.7	–84.9	–83.8
$[Au(C_6H_6)(CO)]^+$	–50.7	–42.7	–41.5
[Au(*o*-dfb)(CO)]$^+$	–19.1	–15.9	–14.5
[Au(4FB)(CO)]$^+$	12.3	15.2	16.8
$[Au(C_6Me_6)_2]^+$	–113.9	–126.5	–123.7
$[Au(Mes)_2]^+$	–92.4	–103.7	–102.6
$[Au(C_6H_6)_2]^+$	–54.8	–41.0	–39.6
[Au(*o*-dfb)$_2$]$^+$	–2.6	2.7	4.7
[Au(4FB)$_2$]$^+$	51.2	51.2	51.2

a) The $[Au(C_6Me_6)(CO)]^+$ cation has one imaginary frequency of –15 cm^{-1}, which could not be removed.

Table S 17: Reaction energy, enthalpy, and Gibbs free energy for the decomposition of an $[Au(L)_n(CO)_m]^+$ cation at the B3LYP(D3BJ)/def2-TZVPP level of theory according to $[Au(L)_n(CO)_m]^+(g) \longrightarrow Au^0(s) + m\ CO + (n\text{-}1)\ L + [L]^+$.

	$\Delta_R G$ / kJ mol^{-1}	$\Delta_R H$ / kJ mol^{-1}	$\Delta_R E$ / kJ mol^{-1}
$[Au(CO)_2]^+$	468.5	504.3	879.7
$[Au(C_6Me_6)(CO)]^{+[a]}$	–80.0	–39.1	–28.4
$[Au(Mes)(CO)]^+$	–29.5	8.3	21.9
$[Au(C_6H_6)(CO)]^+$	17.8	55.7	69.2
$[Au(o\text{-dfb})(CO)]^+$	–5.1	28.9	38.1
$[Au(4FB)(CO)]^+$	–16.9	19.1	27.4
$[Au(C_6Me_6)_2]^+$	–61.2	–13.6	–2.5
$[Au(Mes)_2]^+$	–16.8	27.1	40.7
$[Au(C_6H_6)_2]^+$	21.9	54.0	67.3
$[Au(o\text{-dfb})_2]^+$	–21.6	10.4	18.9
$[Au(4FB)_2]^+$	–55.8	–22.8	–15.2

a) The $[Au(C_6Me_6)(CO)]^+$ cation has one imaginary frequency of –15 cm^{-1}, which could not be removed.

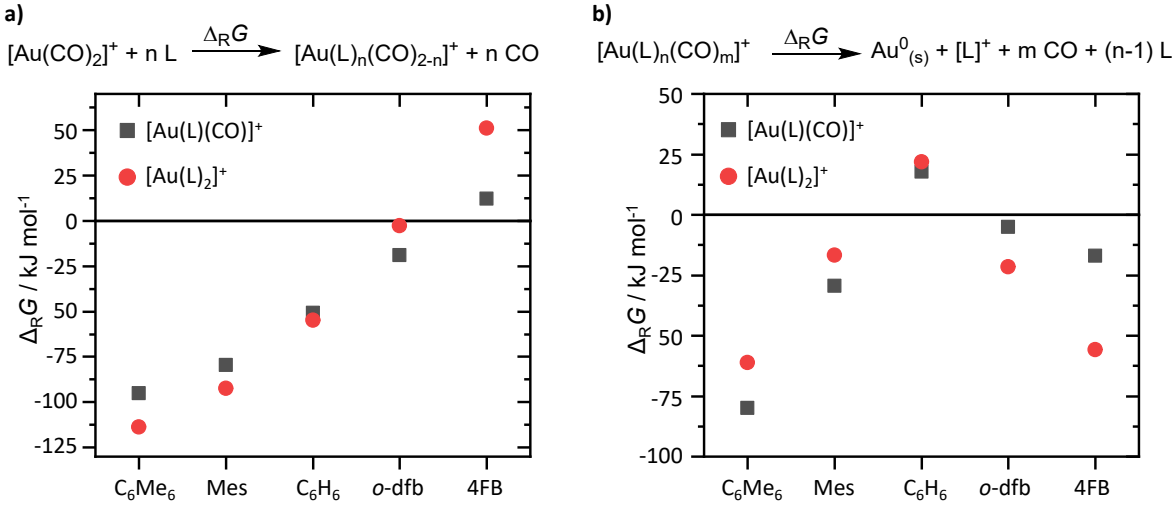


Figure S 40: Gibbs free energy $\Delta_R G$ for the formation (**a**) and decomposition (**b**) of a series of $[Au(arene)(CO)]^+$ and $[Au(arene)_2]^+$ (arene = C_6Me_6, Mes, C_6H_6, *o*-dfb, 4FB) cations. The calculations were performed at the B3LYP(D3BJ)/def2-TZVPP level of theory in the gas phase (Table S 16 and Table S 17).

Coordinates of the calculations at the r2scan-3c level of theory in Angstrom

$[Cu(CO)_2)]^+$

Cu	0.00000001883254	0.00000003344058	0.00000000079632
C	0.00000002463797	0.00000000185702	1.89086731160798
O	-0.00000002752923	-0.00000002276952	3.01212891813180
C	-0.00000000130734	0.00000001849931	-1.89086731201003
O	-0.00000001463394	-0.00000003102739	-3.01212891852607

$[Au(CO)_2)]^0$

Au	-0.04292640503050	-0.23322902013962	0.00000058286570
C	-0.04211104500482	-0.22809112444753	1.98111574806351
O	0.05414618283226	0.29577408584202	3.00495978737645
C	-0.04213524781025	-0.22808359727623	-1.98111571152581
O	0.05416251501331	0.29576945602137	-3.00496060677985

$[Au(CO)_2)]^+$

Au	-0.00000000040934	-0.00000000543655	-0.00000000043188
C	0.00000000122472	-0.00000000086769	1.98541379313191
O	-0.00000000245272	0.00000000201180	3.10589807333590
C	0.00000000698735	0.00000000546228	-1.98541379281168
O	-0.00000000535001	-0.00000000116984	-3.10589807322424

CO

C	0.00000000000000	0.00000000000000	0.56522576164065
O	0.00000000000000	0.00000000000000	-0.56522576164065

$[Cu(N_2)_2)]^+$

Cu	-0.00000000662707	0.00000003044051	-0.00000000170881
N	0.00000000284144	-0.00000000779087	1.87260767068466
N	0.00000000901772	-0.00000001837795	2.96873630569737
N	-0.00000003088247	0.00000003553297	-1.87260767069502
N	0.00000002565038	-0.00000003980464	-2.96873630397820

$[Ag(N_2)_2)]^+$

Ag	0.00000000105364	0.00000000528053	0.00000000505244
N	0.00000000195097	0.00000000235350	2.15487529520225
N	-0.00000000000100	-0.00000000662514	3.24878144747653
N	-0.00000000795522	0.00000000887854	-2.15487529816569
N	0.00000000495162	-0.00000000988743	-3.24878144956553

$[Au(N_2)_2)]^+$

Au	-0.00000000798200	0.00000000242801	-0.00000000205108
N	0.00000000010966	-0.00000000086428	2.00247092330053
N	0.00000000443951	-0.00000000032428	3.09800238018216
N	-0.00000000210572	-0.00000000098311	-2.00247092231050
N	0.00000000553853	-0.00000000025634	-3.09800237912112

N_2

N	0.00000000000000	0.00000000000000	0.54702974537322
N	0.00000000000000	0.00000000000000	-0.54702974537322

Cl_2

Cl	0.00000000000000	0.00000000000000	1.01574738242401
Cl	0.00000000000000	0.00000000000000	-1.01574738242401

Br_2

Br	0.00000000000000	0.00000000000000	1.15997713890191
Br	0.00000000000000	0.00000000000000	-1.15997713890191

I_2

I	0.00000000000000	0.00000000000000	1.35806078130238
I	0.00000000000000	0.00000000000000	-1.35806078130238

$[Au(P_4)_2)]^0$ (0° angle)

Au	0.00000001454608	0.00000334783030	-0.00000002689680
P	1.36615752742393	0.00000040438935	2.03526041993568
P	-1.36615747140014	0.00000025695255	2.03526033226083
P	0.00000004798278	-1.10400933619703	3.41019917286587
P	-0.00000007804418	1.10400702323391	3.41020156044764
P	1.36615749709645	0.00000021767670	-2.03526037072377

P	-1.36615751246987	0.00000037562060	-2.03526036833620
P	-0.00000006971510	-1.10400932122128	-3.41019919565452
P	0.00000004458006	1.10400703171490	-3.41020152389873

$[Au(P_4)_2)]^+$ (0° angle)

Au	0.00000003676125	0.00000290510306	-0.00000001309105
P	1.21699492093842	0.00000047659897	2.17226109599623
P	-1.21699492004377	0.00000042191305	2.17226108519602
P	0.00000001748807	-1.12531051039715	3.62726721346481
P	-0.00000004488430	1.12530822434178	3.62726970251915
P	1.21699494301215	0.00000033175295	-2.17226111475539
P	-1.21699492238820	0.00000039199474	-2.17226107845757
P	-0.00000004362083	-1.12531048956464	-3.62726729871524
P	0.00000001273720	1.12530824825722	-3.62726959215697

$[Au(P_4)_2)]^+$ (90° angle)

Au	-0.00280860007650	-0.00000077972670	-0.00000011092072
P	0.82372174277830	0.88943245933660	2.17415443437212
P	-0.82376171007885	-0.89143040732413	2.17462371998068
P	0.82600385031332	-0.76511955917702	3.63265265666611
P	-0.82463312132658	0.76215053544182	3.63394909965376
P	0.82382174909923	-0.88936564523402	-2.17414435982445
P	-0.82380708651313	0.89136295459407	-2.17463390094069
P	-0.82452465324673	-0.76221711402316	-3.63396018711273
P	0.82598782905094	0.76518755611253	-3.63264135187410

P_4

P	-0.78247246763482	-0.78247247060105	-0.78247246932416
P	0.78247246499008	0.78247246873128	-0.78247246480966
P	-0.78247246135615	0.78247246696711	0.78247246667943
P	0.78247246400088	-0.78247246509734	0.78247246745439

$[Au(P_4S_3)_2)]^+$ (apical)

Au	-0.00000004967256	-0.00000000117995	-0.00000004358517
P	-1.35776519465248	1.70805616211273	0.78142235167917
P	-2.46230808426457	4.70695843413859	0.95249804089254
P	-2.61017099541382	3.67081240269253	2.97707948538545
P	-4.13027392475051	3.20408495945590	1.34406588704414
S	-0.99341059529353	3.58566543628431	-0.09357884266910
S	-1.20835023399670	2.08123537241379	2.84562941437213
S	-3.41607869872617	1.40239556651215	0.47651927603122
P	1.35776509303498	-1.70805620108879	-0.78142240122795
P	2.46230826519786	-4.70695842543906	-0.95249796095670
P	2.61017106330758	-3.67081243855289	-2.97707943081591
P	4.13027394713471	-3.20408480371708	-1.34406585494670
S	0.99341067058440	-3.58566548948096	0.09357885809124
S	1.20835016011000	-2.08123553569846	-2.84562944400446
S	3.41607857740079	-1.40239543845281	-0.47651933528990

$[Au(P_4S_3)_2)]^+$ (basal)

Au	-0.00000009122717	-0.00000006021345	0.00000001510144
P	-4.05101046638529	3.35016371200490	1.28586525888478
P	-1.33902990771043	1.73130446531259	0.76256158369411
P	-1.08668434088973	2.80266925203549	2.71654752918836
P	-0.81045758223832	3.91110380638216	0.71820631110673
S	-3.37851220445243	1.52581565659739	0.36935197748399
S	-3.10476810136058	3.15562557584325	3.19747788723411
S	-2.71081990924448	4.73436135316131	0.34853029158071
P	4.05101085725416	-3.35016221060715	-1.28586771667059
P	1.33902979022888	-1.73130453633982	-0.76256156732965
P	1.08668185371723	-2.80267213765845	-2.71654566609513
P	0.81045938213140	-3.91110426189668	-0.71820253150901
S	3.37851258658902	-1.52581348569986	-0.36935573285913
S	3.10476510402855	-3.15562742212940	-3.19747899492608
S	2.71082302955919	-4.73435970679226	-0.34852864488464

P_4S_3

P	-0.00020169422279	-0.00000000434325	-1.74131912749463
S	0.93957557238030	1.62668090689678	-0.72817496293982
S	0.93957557647290	-1.62668091481982	-0.72817497078751
S	-1.87867395008695	0.00000000345431	-0.72804821925772
P	0.65349967257216	1.13211333662435	1.30854224125635

P 0.65349967510396 -1.13211332850255 1.30854223279368
P -1.30727485221958 0.00000000069018 1.30863300642966

Coordinates and frequencies of the calculations at the B3LYP(D3BJ)/def2-TZVPP of theory

$[Au(CO)_2)]^+$
Symmetry: d6h
Cartesian coordinates in Ångström:

Au	0.0000000	0.0000000	-0.0000000
C	0.0000000	0.0000000	2.0014701
O	0.0000000	0.0000000	3.1158141
C	0.0000000	0.0000000	-2.0014701
O	0.0000000	0.0000000	-3.1158141

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6	e1u	63.66	0.19334	YES	NO
7	e1u	63.66	0.19334	YES	NO
8	e1g	308.40	0.00000	NO	YES
9	e1g	308.40	0.00000	NO	YES
10	a2u	343.23	39.80471	YES	NO
11	a1g	385.76	0.00000	NO	YES
12	e1u	404.78	7.94325	YES	NO
13	e1u	404.78	7.94325	YES	NO
14	a2u	2296.79	504.63222	YES	NO
15	a1g	2331.49	0.00000	NO	YES

$raman spectrum

# mode	symmetry	wave number cm**(-1)	selection rule	derivative of isotropic a.u.	derivative of polarizability anisotropy a.u.	raman scattering cross sections bohr**2/sr T,T	II,II
1		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
2		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
3		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
4		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
5		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
6	e1u	63.66	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
7	e1u	63.66	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
8	e1g	308.40	YES	0.000000	0.011689	0.46573D-16	0.34930D-16
9	e1g	308.40	YES	0.000000	0.011689	0.46573D-16	0.34930D-16
10	a2u	343.23	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
11	a1g	385.76	YES	0.009897	0.012333	0.30278D-15	0.27540D-16
12	e1u	404.78	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
13	e1u	404.78	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
14	a2u	2296.79	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
15	a1g	2331.49	YES	0.117993	0.340160	0.34733D-14	0.11068D-14

CO
Symmetry: c6v
Cartesian coordinates in Ångström:

C	0.00000	0.00000	-0.56243
O	0.00000	0.00000	0.56243

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6	a1	2213.96	76.50678	YES	YES

$[Au(P_4)_2)]^+$ (0° angle)
Symmetry: d2h
Cartesian coordinates in Ångström:

Au	0.0000000	0.0000000	0.0000000
P	1.2154977	0.0000000	2.1941720
P	-1.2154977	0.0000000	2.1941720
P	0.0000000	-1.1189271	3.6396846

```
P     0.0000000    1.1189271    3.6396846
P     1.2154977    0.0000000   -2.1941720
P    -1.2154977    0.0000000   -2.1941720
P     0.0000000   -1.1189271   -3.6396846
P     0.0000000    1.1189271   -3.6396846

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        au            13.06         0.00000       NO      NO
     8        b2u           28.64         0.53748       YES     NO
     9        b3u           38.65         1.08510       YES     NO
    10        b3g           80.46         0.00000       NO      YES
    11        b1u          121.71         4.50578       YES     NO
    12        ag           123.01         0.00000       NO      YES
    13        b2u          127.86         1.29149       YES     NO
    14        b2g          166.90         0.00000       NO      YES
    15        b3u          175.39         1.28499       YES     NO
    16        b1u          367.91         4.56897       YES     NO
    17        b1g          373.24         0.00000       NO      YES
    18        ag           373.53         0.00000       NO      YES
    19        au           373.86         0.00000       NO      NO
    20        b1u          382.60        17.00145       YES     NO
    21        ag           391.24         0.00000       NO      YES
    22        b2g          457.56         0.00000       NO      YES
    23        b3g          462.27         0.00000       NO      YES
    24        b2u          462.27         0.66365       YES     NO
    25        b3u          465.65         0.27594       YES     NO
    26        b1u          583.75         0.03986       YES     NO
    27        ag           585.58         0.00000       NO      YES

$raman spectrum
# mode symmetry wave  selection  derivative of  derivative of     raman
#              number   rule       isotropic   polarizability   scattering
#                                polarizability   anisotropy   cross sections
#             cm**(-1)               a.u.          a.u.        bohr**2/sr
#                                                                T,T        II,II
    1            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    2            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    3            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    4            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    5            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    6            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    7    au     13.06   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
    8    b2u    28.64   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
    9    b3u    38.65   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   10    b3g    80.46   YES        0.000000     0.047663 0.78859D-14 0.59144D-14
   11    b1u   121.71   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   12    ag    123.01   YES       -0.014474     0.039821 0.63176D-14 0.19057D-14
   13    b2u   127.86   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   14    b2g   166.90   YES        0.000000     0.026774 0.67237D-15 0.50428D-15
   15    b3u   175.39   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   16    b1u   367.91   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   17    b1g   373.24   YES        0.000000     0.106284 0.28673D-14 0.21505D-14
   18    ag    373.53   YES       -0.028260     0.123750 0.61605D-14 0.29120D-14
   19    au    373.86   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   20    b1u   382.60   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   21    ag    391.24   YES       -0.007242     0.133109 0.43269D-14 0.31406D-14
   22    b2g   457.56   YES        0.000000     0.144015 0.38797D-14 0.29098D-14
   23    b3g   462.27   YES        0.000000     0.192148 0.68027D-14 0.51020D-14
   24    b2u   462.27   NO         0.000000     0.000000 0.52815D-34 0.39612D-34
   25    b3u   465.65   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   26    b1u   583.75   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   27    ag    585.58   YES       -0.183515     0.204585 0.54923D-13 0.40978D-14

[Au(P4S3)2)]+ (apical)
Symmetry: ci
Cartesian coordinates in Ångström:
Au    0.0000000    0.0000000    0.0000000
P    -1.3635262    1.7157194    0.7819417
P    -2.4640190    4.7016941    0.9564026
P    -2.6093383    3.6683465    2.9711605
P    -4.1240854    3.2049882    1.3466386
S    -1.0007927    3.5790434   -0.0877439
S    -1.2114262    2.0814786    2.8320427
```

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S    -3.4065532    1.4100160    0.4777511
P     1.3635262   -1.7157194   -0.7819417
P     2.4640190   -4.7016941   -0.9564026
P     2.6093383   -3.6683465   -2.9711605
P     4.1240854   -3.2049882   -1.3466386
S     1.0007927   -3.5790434    0.0877439
S     1.2114262   -2.0814786   -2.8320427
S     3.4065532   -1.4100160   -0.4777511

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        au             8.78         0.00003      YES     NO
     8        au            16.15         0.16212      YES     NO
     9        au            16.44         0.16150      YES     NO
    10        ag            61.80         0.00000      NO      YES
    11        ag            61.93         0.00000      NO      YES
    12        ag            97.98         0.00000      NO      YES
    13        au           106.33         0.04749      YES     NO
    14        au           106.37         0.04810      YES     NO
    15        au           145.62         1.48032      YES     NO
    16        ag           185.20         0.00000      NO      YES
    17        au           185.25         0.00004      YES     NO
    18        ag           222.05         0.00000      NO      YES
    19        ag           222.14         0.00000      NO      YES
    20        au           224.71         5.48542      YES     NO
    21        au           224.80         5.48180      YES     NO
    22        ag           284.22         0.00000      NO      YES
    23        ag           284.24         0.00000      NO      YES
    24        au           284.36         0.46566      YES     NO
    25        au           284.38         0.46698      YES     NO
    26        ag           332.90         0.00000      NO      YES
    27        au           332.97         0.13452      YES     NO
    28        ag           332.97         0.00000      NO      YES
    29        au           333.03         0.13542      YES     NO
    30        au           382.65        29.11226      YES     NO
    31        ag           390.51         0.00000      NO      YES
    32        au           423.49        70.31441      YES     NO
    33        ag           424.50         0.00000      NO      YES
    34        ag           454.00         0.00000      NO      YES
    35        ag           454.04         0.00000      NO      YES
    36        au           455.14         6.89265      YES     NO
    37        au           455.19         6.88379      YES     NO
    38        au           466.74         9.97513      YES     NO
    39        ag           470.29         0.00000      NO      YES
    40        au           489.32        43.33703      YES     NO
    41        ag           504.30         0.00000      NO      YES
    42        ag           504.33         0.00000      NO      YES
    43        au           510.04        22.46891      YES     NO
    44        au           510.07        22.48188      YES     NO
    45        ag           510.60         0.00000      NO      YES

$raman spectrum
# mode symmetry wave  selection  derivative of  derivative of     raman
#              number   rule       isotropic   polarizability   scattering
#                                polarizability   anisotropy   cross sections
#             cm**(-1)               a.u.           a.u.        bohr**2/sr
#                                                                 T,T        II,II
    1            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    2            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    3            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    4            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    5            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    6            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    7    au      8.78   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
    8    au     16.15   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
    9    au     16.44   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   10    ag     61.80   YES        0.000005     0.005540 0.17448D-15 0.13086D-15
   11    ag     61.93   YES        0.000011     0.005560 0.17507D-15 0.13129D-15
   12    ag     97.98   YES        0.028690     0.071881 0.34859D-13 0.93636D-14
   13    au    106.33   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   14    au    106.37   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   15    au    145.62   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   16    ag    185.20   YES       -0.000005     0.000168 0.22265D-19 0.16563D-19
   17    au    185.25   NO         0.000000     0.000000 0.23569D-34 0.92632D-35
```

18	ag	222.05	YES	0.000002	0.082537	0.39442D-14	0.29582D-14
19	ag	222.14	YES	-0.000004	0.082541	0.39419D-14	0.29564D-14
20	au	224.71	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
21	au	224.80	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
22	ag	284.22	YES	0.000007	0.118042	0.54041D-14	0.40531D-14
23	ag	284.24	YES	0.000004	0.118035	0.54029D-14	0.40522D-14
24	au	284.36	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
25	au	284.38	NO	0.000000	0.000000	0.11585D-34	0.45531D-35
26	ag	332.90	YES	-0.000003	0.130825	0.51786D-14	0.38840D-14
27	au	332.97	NO	0.000000	0.000000	0.93491D-33	0.69942D-33
28	ag	332.97	YES	0.000003	0.130814	0.51761D-14	0.38821D-14
29	au	333.03	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
30	au	382.65	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
31	ag	390.51	YES	-0.075768	0.058841	0.16128D-13	0.61544D-15
32	au	423.49	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
33	ag	424.50	YES	-0.054754	0.011144	0.70783D-14	0.19477D-16
34	ag	454.00	YES	-0.000014	0.050797	0.48829D-15	0.36621D-15
35	ag	454.04	YES	-0.000039	0.050774	0.48778D-15	0.36584D-15
36	au	455.14	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
37	au	455.19	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
38	au	466.74	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
39	ag	470.29	YES	0.091131	0.039033	0.17057D-13	0.20528D-15
40	au	489.32	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
41	ag	504.30	YES	-0.000274	0.065421	0.69415D-15	0.52051D-15
42	ag	504.33	YES	0.000432	0.065425	0.69438D-15	0.52053D-15
43	au	510.04	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
44	au	510.07	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
45	ag	510.60	YES	0.090183	0.158009	0.18546D-13	0.29819D-14

$[Au(P_4S_3)_2)]^+$ (basal)
Symmetry: c1
Cartesian coordinates in Ångström:

Au	0.0000003	0.0000006	-0.0000008
P	-4.0402537	3.3550317	1.2895128
P	-1.3502881	1.7298422	0.7662743
P	-1.0879255	2.7949696	2.7067205
P	-0.8123377	3.8923817	0.7148669
S	-3.3809302	1.5349735	0.3779506
S	-3.0973530	3.1596603	3.1895339
S	-2.7046264	4.7235577	0.3510972
P	4.0402386	-3.3550922	-1.2894033
P	1.3502885	-1.7298412	-0.7662760
P	1.0880372	-2.7948483	-2.7068032
P	0.8122604	-3.8923653	-0.7150335
S	3.3809078	-1.5350639	-0.3777868
S	3.0974889	-3.1595799	-3.1894849
S	2.7044932	-4.7236264	-0.3511675

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.29	0.01262	YES	YES
8	a	14.62	0.05972	YES	YES
9	a	15.55	0.04044	YES	YES
10	a	48.64	0.00000	YES	YES
11	a	60.39	0.00000	YES	YES
12	a	89.91	0.35542	YES	YES
13	a	92.54	0.00000	YES	YES
14	a	105.14	1.58332	YES	YES
15	a	139.07	1.17280	YES	YES
16	a	192.94	0.00000	YES	YES
17	a	197.27	0.00042	YES	YES
18	a	217.74	0.00000	YES	YES
19	a	217.96	5.39104	YES	YES
20	a	221.03	6.34284	YES	YES
21	a	221.23	0.00000	YES	YES
22	a	287.33	0.00000	YES	YES
23	a	287.92	0.00841	YES	YES
24	a	307.36	10.62525	YES	YES
25	a	308.55	0.00000	YES	YES
26	a	346.17	5.32581	YES	YES
27	a	346.22	0.00000	YES	YES
28	a	365.72	18.71689	YES	YES
29	a	370.51	0.00000	YES	YES
30	a	371.89	0.00000	YES	YES

31	a	374.30	0.15096	YES	YES
32	a	410.16	30.76558	YES	YES
33	a	410.54	0.00000	YES	YES
34	a	412.68	21.70624	YES	YES
35	a	412.94	0.00000	YES	YES
36	a	419.50	0.00000	YES	YES
37	a	420.80	17.01800	YES	YES
38	a	467.23	27.35607	YES	YES
39	a	468.34	0.00000	YES	YES
40	a	485.78	0.00001	YES	YES
41	a	485.81	5.46374	YES	YES
42	a	494.59	12.04321	YES	YES
43	a	509.89	0.00000	YES	YES
44	a	528.26	0.00000	YES	YES
45	a	533.17	3.42101	YES	YES

$raman spectrum

# mode	symmetry	wave number	selection rule	derivative of isotropic polarizability	derivative of polarizability anisotropy	raman scattering cross sections	
#		cm**(-1)		a.u.	a.u.	bohr**2/sr	
#						T,T	II,II
1		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
2		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
3		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
4		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
5		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
6		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
7	a	6.29	YES	0.000000	0.000001	0.45061D-21	0.32047D-21
8	a	14.62	YES	-0.000000	0.000001	0.54128D-22	0.31253D-22
9	a	15.55	YES	0.000000	0.000000	0.81399D-23	0.58498D-23
10	a	48.64	YES	-0.000041	0.030185	0.81578D-14	0.61182D-14
11	a	60.39	YES	0.007810	0.038287	0.12779D-13	0.65281D-14
12	a	89.91	YES	-0.000003	0.000007	0.42669D-21	0.10986D-21
13	a	92.54	YES	0.035313	0.097638	0.63203D-13	0.19179D-13
14	a	105.14	YES	0.000000	0.000001	0.92600D-24	0.61391D-24
15	a	139.07	YES	0.000000	0.000000	0.21405D-24	0.16049D-24
16	a	192.94	YES	0.000015	0.017610	0.22712D-15	0.17034D-15
17	a	197.27	YES	0.000000	0.000001	0.13013D-23	0.83930D-24
18	a	217.74	YES	0.000083	0.078806	0.37145D-14	0.27859D-14
19	a	217.96	YES	0.000001	0.000031	0.57588D-21	0.43054D-21
20	a	221.03	YES	-0.000002	0.000034	0.68890D-21	0.49240D-21
21	a	221.23	YES	-0.004338	0.064743	0.25652D-14	0.18314D-14
22	a	287.33	YES	-0.000001	0.121689	0.56448D-14	0.42336D-14
23	a	287.92	YES	-0.000000	0.000011	0.46855D-22	0.34961D-22
24	a	307.36	YES	-0.000000	0.000013	0.57060D-22	0.42700D-22
25	a	308.55	YES	-0.007328	0.123367	0.53900D-14	0.38882D-14
26	a	346.17	YES	-0.000016	0.000061	0.19159D-20	0.79025D-21
27	a	346.22	YES	-0.031722	0.117041	0.71250D-14	0.29258D-14
28	a	365.72	YES	0.000000	0.000004	0.38115D-23	0.24651D-23
29	a	370.51	YES	0.000400	0.138596	0.49311D-14	0.36980D-14
30	a	371.89	YES	-0.064477	0.101034	0.14543D-13	0.19541D-14
31	a	374.30	YES	-0.000003	0.000010	0.46649D-22	0.20341D-22
32	a	410.16	YES	-0.000000	0.000003	0.27740D-23	0.17592D-23
33	a	410.54	YES	-0.018535	0.034227	0.11071D-14	0.19313D-15
34	a	412.68	YES	0.000004	0.000007	0.49542D-22	0.79859D-23
35	a	412.94	YES	-0.060673	0.085888	0.10632D-13	0.12056D-14
36	a	419.50	YES	0.000355	0.101214	0.21805D-14	0.16352D-14
37	a	420.80	YES	0.000000	0.000009	0.18294D-22	0.13286D-22
38	a	467.23	YES	0.000000	0.000003	0.13017D-23	0.97514D-24
39	a	468.34	YES	-0.065916	0.056447	0.94107D-14	0.43191D-15
40	a	485.78	YES	-0.000036	0.051260	0.45008D-15	0.33756D-15
41	a	485.81	YES	0.000000	0.000085	0.12293D-20	0.92199D-21
42	a	494.59	YES	0.000000	0.000004	0.27620D-23	0.19671D-23
43	a	509.89	YES	-0.139806	0.240165	0.44291D-13	0.69028D-14
44	a	528.26	YES	-0.011280	0.087258	0.13708D-14	0.86541D-15
45	a	533.17	YES	0.000000	0.000004	0.22691D-23	0.16879D-23

$[Au(C_6Me_6)_2)]^+$
Symmetry: c1
Cartesian coordinates in Ångström:

C	2.5688950	0.9243150	0.8094283
C	2.4463260	0.4636975	-0.5383429
C	3.0896824	2.3206313	1.0335304
C	2.0019791	-0.8776254	-0.7919664
C	1.6923537	-1.7308483	0.3217892
C	1.8707805	-1.2700327	1.6205922
C	2.2581634	0.0742619	1.8655222
Au	0.0966794	0.3932093	-0.7495752
C	3.0194723	1.3165264	-1.6460323
C	2.2952989	0.5663423	3.2915186

```
C     1.6566296   -2.1931139    2.7944199
C     1.1967899   -3.1270612    0.0464987
C     2.1858606   -1.5109113   -2.1548550
C    -2.5465247   -0.8203259    1.0086815
C    -2.5609009   -0.6392655   -0.3698878
C    -3.0539986   -2.1062095    1.6129686
C    -2.1794770    0.6257083   -0.9334061
C    -1.7579757    1.6805866   -0.0545033
C    -1.6906839    1.4403575    1.3511566
C    -2.0527232    0.1979538    1.8639527
C    -3.0067452   -1.7418468   -1.2951212
C    -1.8970183   -0.0967634    3.3357089
C    -1.2508059    2.5703350    2.2453300
C    -1.5933572    3.0974236   -0.5525107
C    -2.5644894    0.9211582   -2.3675892
H     0.5317246   -3.1470997   -0.8137894
H     0.6440680   -3.5322087    0.8875495
H     2.0211745   -3.8118268   -0.1696548
H     2.7996517    2.3694098   -1.4944942
H     2.6478669    1.0422021   -2.6264150
H     4.1077400    1.2112049   -1.6649348
H     3.2673894    0.3861333    3.7577925
H     1.5502006    0.0612960    3.9006512
H     2.0950732    1.6313390    3.3575386
H    -1.3883310    3.1518315   -1.6150996
H    -0.7877746    3.6111641   -0.0353706
H    -2.5110451    3.6616455   -0.3647773
H    -2.7883701    0.1831413    3.9031594
H    -1.0565204    0.4420145    3.7635348
H    -1.7249579   -1.1549047    3.5115813
H    -2.8735327   -2.7218410   -0.8486143
H    -2.4451441   -1.7328349   -2.2257919
H    -4.0629910   -1.6388767   -1.5587640
H    -1.8215523    3.4754851    2.0397163
H    -0.1971821    2.8152157    2.0882688
H    -1.3840133    2.3423638    3.2959618
H    -3.7998939   -2.5807959    0.9832327
H    -3.5182785   -1.9303740    2.5798124
H    -2.2463489   -2.8282486    1.7669440
H    -2.3444706    0.0909057   -3.0313326
H    -2.0676792    1.7970997   -2.7672025
H    -3.6414696    1.1004465   -2.4202159
H     2.1993910   -0.7868567   -2.9607590
H     1.4094522   -2.2357381   -2.3788702
H     3.1404202   -2.0434238   -2.1749340
H     1.8111536   -3.2331128    2.5257952
H     0.6446856   -2.1023961    3.1996622
H     2.3468688   -1.9663981    3.6029689
H     4.0405567    2.4642417    0.5195269
H     3.2598838    2.5371938    2.0810756
H     2.4038669    3.0758709    0.6430016

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                      -0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a              9.67         0.00243      YES     YES
     8        a             16.15         0.19071      YES     YES
     9        a             29.48         0.15467      YES     YES
    10        a             37.57         0.07901      YES     YES
    11        a             42.61         0.09057      YES     YES
    12        a             51.41         0.07450      YES     YES
    13        a             65.08         0.05935      YES     YES
    14        a             68.30         0.08359      YES     YES
    15        a             74.31         0.22680      YES     YES
    16        a             86.72         0.29028      YES     YES
    17        a             90.98         0.19187      YES     YES
    18        a             95.88         0.69432      YES     YES
    19        a            101.42         0.08684      YES     YES
    20        a            103.50         0.14311      YES     YES
    21        a            105.08         0.04978      YES     YES
    22        a            112.09         0.13311      YES     YES
    23        a            116.75         0.26412      YES     YES
    24        a            119.98         0.35140      YES     YES
    25        a            126.83         0.97354      YES     YES
    26        a            138.16         0.04511      YES     YES
```

27	a	142.20	0.05626	YES	YES
28	a	147.77	0.10746	YES	YES
29	a	153.19	0.64184	YES	YES
30	a	159.86	0.28711	YES	YES
31	a	171.84	0.30306	YES	YES
32	a	176.73	0.01866	YES	YES
33	a	180.24	0.49146	YES	YES
34	a	239.48	14.89577	YES	YES
35	a	244.95	0.40301	YES	YES
36	a	335.17	0.56928	YES	YES
37	a	342.42	1.23340	YES	YES
38	a	347.27	0.38183	YES	YES
39	a	349.97	0.25019	YES	YES
40	a	359.58	0.61788	YES	YES
41	a	367.67	0.13130	YES	YES
42	a	375.15	0.50017	YES	YES
43	a	400.89	0.96224	YES	YES
44	a	420.30	0.07417	YES	YES
45	a	421.67	0.13608	YES	YES
46	a	427.37	0.01308	YES	YES
47	a	429.14	0.01110	YES	YES
48	a	452.48	0.40090	YES	YES
49	a	453.12	0.06293	YES	YES
50	a	458.07	0.05179	YES	YES
51	a	458.89	0.17650	YES	YES
52	a	468.12	0.02351	YES	YES
53	a	469.72	0.03366	YES	YES
54	a	556.45	2.21252	YES	YES
55	a	558.52	0.97208	YES	YES
56	a	572.84	2.04703	YES	YES
57	a	574.57	3.36401	YES	YES
58	a	584.88	1.43606	YES	YES
59	a	587.86	2.52125	YES	YES
60	a	590.26	2.21827	YES	YES
61	a	591.85	0.50500	YES	YES
62	a	592.35	0.69668	YES	YES
63	a	598.75	4.77719	YES	YES
64	a	731.16	0.38522	YES	YES
65	a	732.16	2.83534	YES	YES
66	a	802.02	2.09084	YES	YES
67	a	803.59	1.39234	YES	YES
68	a	804.75	1.57784	YES	YES
69	a	805.77	4.00250	YES	YES
70	a	982.72	0.70926	YES	YES
71	a	983.48	0.45696	YES	YES
72	a	984.76	1.09291	YES	YES
73	a	985.75	2.19960	YES	YES
74	a	1005.74	0.26942	YES	YES
75	a	1006.89	2.77854	YES	YES
76	a	1013.04	6.38331	YES	YES
77	a	1015.13	1.21660	YES	YES
78	a	1035.15	0.44139	YES	YES
79	a	1036.93	6.18700	YES	YES
80	a	1045.25	7.59020	YES	YES
81	a	1048.03	14.85315	YES	YES
82	a	1051.84	1.09765	YES	YES
83	a	1053.83	8.15542	YES	YES
84	a	1067.56	2.86391	YES	YES
85	a	1068.63	9.94243	YES	YES
86	a	1072.58	1.83919	YES	YES
87	a	1072.81	4.52366	YES	YES
88	a	1080.60	2.56444	YES	YES
89	a	1081.67	8.32783	YES	YES
90	a	1082.69	3.20383	YES	YES
91	a	1083.15	13.49301	YES	YES
92	a	1088.69	0.59815	YES	YES
93	a	1089.28	2.34258	YES	YES
94	a	1091.24	0.84928	YES	YES
95	a	1091.88	0.35367	YES	YES
96	a	1126.07	0.57343	YES	YES
97	a	1126.66	0.25909	YES	YES
98	a	1269.05	4.69188	YES	YES
99	a	1275.37	1.54252	YES	YES
100	a	1279.85	0.71040	YES	YES
101	a	1280.50	0.42031	YES	YES
102	a	1327.63	34.25337	YES	YES
103	a	1331.82	12.68977	YES	YES
104	a	1401.75	3.47703	YES	YES
105	a	1403.36	8.15526	YES	YES
106	a	1406.69	1.29917	YES	YES
107	a	1409.05	7.14714	YES	YES

108	a	1414.94	0.11761	YES	YES
109	a	1416.74	0.32639	YES	YES
110	a	1417.13	2.25761	YES	YES
111	a	1417.68	0.50452	YES	YES
112	a	1418.36	0.78088	YES	YES
113	a	1419.68	9.28826	YES	YES
114	a	1422.86	1.42768	YES	YES
115	a	1424.13	3.16939	YES	YES
116	a	1426.67	28.53613	YES	YES
117	a	1429.20	13.63515	YES	YES
118	a	1434.74	2.89192	YES	YES
119	a	1437.50	8.17178	YES	YES
120	a	1468.11	5.27617	YES	YES
121	a	1468.40	6.90923	YES	YES
122	a	1471.78	7.92001	YES	YES
123	a	1474.20	3.05358	YES	YES
124	a	1478.87	11.49052	YES	YES
125	a	1479.35	5.82074	YES	YES
126	a	1481.57	28.01760	YES	YES
127	a	1481.98	10.32553	YES	YES
128	a	1489.79	1.87182	YES	YES
129	a	1490.77	7.82975	YES	YES
130	a	1494.68	19.72434	YES	YES
131	a	1495.86	9.23847	YES	YES
132	a	1497.15	12.84151	YES	YES
133	a	1498.13	13.67916	YES	YES
134	a	1501.50	15.85350	YES	YES
135	a	1501.91	19.35409	YES	YES
136	a	1502.79	13.60096	YES	YES
137	a	1503.32	22.88500	YES	YES
138	a	1522.59	11.50743	YES	YES
139	a	1524.55	4.79796	YES	YES
140	a	1526.09	2.17819	YES	YES
141	a	1527.70	2.45328	YES	YES
142	a	1543.40	3.08639	YES	YES
143	a	1544.22	3.92365	YES	YES
144	a	1565.56	2.97200	YES	YES
145	a	1568.66	0.11569	YES	YES
146	a	1599.89	6.67412	YES	YES
147	a	1602.58	12.02636	YES	YES
148	a	3024.10	9.10746	YES	YES
149	a	3029.55	10.35504	YES	YES
150	a	3032.66	6.41581	YES	YES
151	a	3032.87	12.02241	YES	YES
152	a	3034.39	8.05612	YES	YES
153	a	3034.94	6.73402	YES	YES
154	a	3035.05	5.40082	YES	YES
155	a	3036.28	9.49750	YES	YES
156	a	3036.97	5.09717	YES	YES
157	a	3037.14	10.05048	YES	YES
158	a	3038.07	9.67029	YES	YES
159	a	3039.64	9.50707	YES	YES
160	a	3083.24	8.87557	YES	YES
161	a	3088.47	8.68790	YES	YES
162	a	3104.90	11.73753	YES	YES
163	a	3107.48	14.98363	YES	YES
164	a	3108.29	7.47424	YES	YES
165	a	3109.96	2.04923	YES	YES
166	a	3114.45	1.99567	YES	YES
167	a	3114.82	1.40618	YES	YES
168	a	3118.31	3.25620	YES	YES
169	a	3119.97	2.94253	YES	YES
170	a	3127.21	3.63871	YES	YES
171	a	3127.62	3.34902	YES	YES
172	a	3137.45	8.73006	YES	YES
173	a	3138.33	5.10996	YES	YES
174	a	3142.07	14.14351	YES	YES
175	a	3142.34	6.76430	YES	YES
176	a	3152.85	6.21024	YES	YES
177	a	3154.44	10.10724	YES	YES
178	a	3156.16	4.23729	YES	YES
179	a	3156.79	6.05291	YES	YES
180	a	3167.56	6.22548	YES	YES
181	a	3169.65	8.72514	YES	YES
182	a	3171.44	4.84798	YES	YES
183	a	3172.47	6.32892	YES	YES

$[Au(C_6Me_6)(CO)]^+$
Symmetry: c1
Cartesian coordinates in Ångström:
Au 2.1260484 0.9075466 -0.0293723

```
C    -0.3232963   -0.7865668   -1.2224574
C    -0.1700104    0.6119680   -1.2452447
C    -0.3694221   -1.5655312   -2.5129687
C    -0.0770135    1.3435880   -0.0047458
C    -0.1408342    0.6206250    1.2419892
C    -0.3169037   -0.7748939    1.2278036
C    -0.4701567   -1.4574588    0.0070128
C    -0.2481026    1.3725519   -2.5446112
C    -0.7996143   -2.9260996    0.0183214
C    -0.3921857   -1.5390004    2.5242747
C    -0.1496262    1.3594739    2.5560706
C    -0.3116749    2.8457193   -0.0154730
C     4.0577553    0.7357867   -0.0481126
O     5.1786646    0.6739593   -0.0590688
H    -0.0279663    3.2996316   -0.9576182
H     0.2261614    3.3662718    0.7699329
H    -1.3767343    3.0387856    0.1336206
H     0.0548409    2.4172452    2.4477543
H     0.5790504    0.9519800    3.2539223
H    -1.1298732    1.2612313    3.0276335
H     0.0901322   -2.5101925    2.4420229
H    -1.4313278   -1.7170003    2.8138207
H     0.0800609   -1.0065662    3.3426890
H    -1.4342501   -3.1965393   -0.8210183
H    -1.3195294   -3.2127963    0.9267776
H     0.1051025   -3.5378875   -0.0469061
H     0.3299269   -1.1671672   -3.2436425
H    -1.3636876   -1.5328714   -2.9656195
H    -0.1123859   -2.6085964   -2.3616885
H    -0.0495149    0.7424272   -3.4029599
H     0.4418690    2.2109068   -2.5845817
H    -1.2555022    1.7794694   -2.6675571

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1        a              -3.23         0.00000       YES     YES
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7                        0.00         0.00000        -       -
     8        a              37.52         0.03791       YES     YES
     9        a              42.92         0.00542       YES     YES
    10        a              54.06         0.14960       YES     YES
    11        a              62.58         0.40674       YES     YES
    12        a              73.61         0.20094       YES     YES
    13        a              93.76         0.12320       YES     YES
    14        a             102.66         0.22278       YES     YES
    15        a             117.62         0.47821       YES     YES
    16        a             120.58         0.03826       YES     YES
    17        a             128.43         0.74654       YES     YES
    18        a             135.97         0.06364       YES     YES
    19        a             156.29         0.47401       YES     YES
    20        a             168.38         0.04742       YES     YES
    21        a             244.45        10.13613       YES     YES
    22        a             333.03         0.18876       YES     YES
    23        a             351.76         2.23449       YES     YES
    24        a             362.22         1.47335       YES     YES
    25        a             373.27         9.96958       YES     YES
    26        a             396.32         3.54898       YES     YES
    27        a             399.68         7.56579       YES     YES
    28        a             415.92         1.07713       YES     YES
    29        a             421.57         9.40914       YES     YES
    30        a             426.84         1.70777       YES     YES
    31        a             453.74         0.04135       YES     YES
    32        a             454.54         0.64486       YES     YES
    33        a             464.82         0.01647       YES     YES
    34        a             560.31         3.27026       YES     YES
    35        a             579.83         0.55918       YES     YES
    36        a             588.02         1.18270       YES     YES
    37        a             590.15         3.02330       YES     YES
    38        a             598.75         1.76400       YES     YES
    39        a             723.34         8.15820       YES     YES
    40        a             801.69         2.02932       YES     YES
    41        a             806.44         3.22852       YES     YES
    42        a             984.30         1.09575       YES     YES
    43        a             985.19         0.49376       YES     YES
    44        a            1008.97         1.28661       YES     YES
    45        a            1011.97         2.93848       YES     YES
```

46	a	1036.24	6.74646	YES	YES
47	a	1046.95	1.34054	YES	YES
48	a	1051.66	11.05775	YES	YES
49	a	1063.63	1.03455	YES	YES
50	a	1071.74	9.90991	YES	YES
51	a	1077.13	5.12788	YES	YES
52	a	1082.86	13.17563	YES	YES
53	a	1090.30	5.93459	YES	YES
54	a	1092.02	1.99744	YES	YES
55	a	1128.10	0.23128	YES	YES
56	a	1278.59	4.02393	YES	YES
57	a	1291.16	23.74921	YES	YES
58	a	1307.26	6.91192	YES	YES
59	a	1399.47	11.72633	YES	YES
60	a	1410.19	19.68058	YES	YES
61	a	1416.59	0.21413	YES	YES
62	a	1417.31	3.80057	YES	YES
63	a	1419.31	2.80645	YES	YES
64	a	1426.84	10.00741	YES	YES
65	a	1428.59	12.49069	YES	YES
66	a	1435.75	3.71590	YES	YES
67	a	1462.72	3.19318	YES	YES
68	a	1471.26	0.51926	YES	YES
69	a	1476.74	14.76611	YES	YES
70	a	1482.97	5.16349	YES	YES
71	a	1489.02	19.49329	YES	YES
72	a	1492.89	13.27110	YES	YES
73	a	1496.23	22.45716	YES	YES
74	a	1503.14	17.24392	YES	YES
75	a	1507.10	2.21529	YES	YES
76	a	1522.36	12.77343	YES	YES
77	a	1526.05	20.97222	YES	YES
78	a	1539.47	7.88493	YES	YES
79	a	1563.18	1.74660	YES	YES
80	a	1574.22	17.80756	YES	YES
81	a	2240.87	649.75328	YES	YES
82	a	3030.64	1.92763	YES	YES
83	a	3037.14	2.77978	YES	YES
84	a	3038.26	1.88385	YES	YES
85	a	3039.68	3.23291	YES	YES
86	a	3044.33	2.85989	YES	YES
87	a	3047.27	2.18858	YES	YES
88	a	3104.65	1.45204	YES	YES
89	a	3108.18	6.81319	YES	YES
90	a	3112.08	4.09943	YES	YES
91	a	3116.45	4.08058	YES	YES
92	a	3117.73	1.06348	YES	YES
93	a	3131.34	1.78329	YES	YES
94	a	3148.06	7.66133	YES	YES
95	a	3154.61	10.54329	YES	YES
96	a	3157.64	0.73278	YES	YES
97	a	3166.27	8.23086	YES	YES
98	a	3172.72	4.83146	YES	YES
99	a	3177.51	4.21254	YES	YES

C_6Me_6
Symmetry: d3d
Cartesian coordinates in Ångström:

C	1.2138902	-0.7008398	0.0107135
C	1.2138902	0.7008398	-0.0107135
C	-1.2138902	0.7008398	-0.0107135
C	-1.2138902	-0.7008398	0.0107135
C	-0.0000000	-1.4016797	-0.0107135
C	2.5217589	-1.4559382	0.0808806
C	0.0000000	-2.9118763	-0.0808806
C	-0.0000000	1.4016797	0.0107135
C	2.5217589	1.4559382	-0.0808806
C	0.0000000	2.9118763	0.0808806
C	-2.5217589	1.4559382	-0.0808806
C	-2.5217589	-1.4559382	0.0808806
H	3.2832483	0.8862390	-0.6084250
H	2.9194253	1.6855310	0.9130768
H	2.4091296	2.4002570	-0.6084250
H	3.2832483	-0.8862390	0.6084250
H	2.9194253	-1.6855310	-0.9130768
H	2.4091296	-2.4002570	0.6084250
H	-0.8741187	-3.2864959	-0.6084250
H	0.0000000	-3.3710620	0.9130768
H	0.8741187	-3.2864959	-0.6084250
H	-3.2832483	-0.8862390	0.6084250
H	-2.4091296	-2.4002570	0.6084250

```
H    -2.9194253   -1.6855310   -0.9130768
H    -3.2832483    0.8862390   -0.6084250
H    -2.4091296    2.4002570   -0.6084250
H    -2.9194253    1.6855310    0.9130768
H     0.8741187    3.2864959    0.6084250
H    -0.8741187    3.2864959    0.6084250
H     0.0000000    3.3710620   -0.9130768

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        eu             85.02         0.00035       YES     NO
     8        eu             85.02         0.00035       YES     NO
     9        a2g            86.51         0.00000       NO      NO
    10        a1u            98.54         0.00000       NO      NO
    11        eg            104.15         0.00000       NO      YES
    12        eg            104.15         0.00000       NO      YES
    13        eu            131.45         0.06135       YES     NO
    14        eu            131.45         0.06135       YES     NO
    15        a1g           166.30         0.00000       NO      YES
    16        a2u           197.58         6.75120       YES     NO
    17        eu            348.45         1.16095       YES     NO
    18        eu            348.45         1.16095       YES     NO
    19        eg            354.67         0.00000       NO      YES
    20        eg            354.67         0.00000       NO      YES
    21        eg            415.20         0.00000       NO      YES
    22        eg            415.20         0.00000       NO      YES
    23        a1u           456.97         0.00000       NO      NO
    24        eg            460.32         0.00000       NO      YES
    25        eg            460.32         0.00000       NO      YES
    26        a1g           561.41         0.00000       NO      YES
    27        eu            592.19         1.60763       YES     NO
    28        eu            592.19         1.60763       YES     NO
    29        a2g           592.72         0.00000       NO      NO
    30        a2u           595.01         0.38288       YES     NO
    31        a1g           748.01         0.00000       NO      YES
    32        eu            814.61         0.60578       YES     NO
    33        eu            814.61         0.60578       YES     NO
    34        eg            992.77         0.00000       NO      YES
    35        eg            992.77         0.00000       NO      YES
    36        a1u           999.65         0.00000       NO      NO
    37        a2u          1012.34         0.69413       YES     NO
    38        eg           1037.59         0.00000       NO      YES
    39        eg           1037.59         0.00000       NO      YES
    40        eu           1067.15         7.77466       YES     NO
    41        eu           1067.15         7.77466       YES     NO
    42        a1g          1074.08         0.00000       NO      YES
    43        eu           1081.78        11.66672       YES     NO
    44        eu           1081.78        11.66672       YES     NO
    45        eg           1090.03         0.00000       NO      YES
    46        eg           1090.03         0.00000       NO      YES
    47        a2g          1122.76         0.00000       NO      NO
    48        a2u          1271.22         0.01202       YES     NO
    49        a1u          1311.47         0.00000       NO      NO
    50        a1g          1328.27         0.00000       NO      YES
    51        eg           1412.12         0.00000       NO      YES
    52        eg           1412.12         0.00000       NO      YES
    53        a2u          1412.61         0.53244       YES     NO
    54        eu           1419.42         1.50491       YES     NO
    55        eu           1419.42         1.50491       YES     NO
    56        a1g          1427.38         0.00000       NO      YES
    57        eu           1445.00         1.13057       YES     NO
    58        eu           1445.00         1.13057       YES     NO
    59        eg           1475.63         0.00000       NO      YES
    60        eg           1475.63         0.00000       NO      YES
    61        a2u          1484.55        34.19450       YES     NO
    62        a1u          1486.82         0.00000       NO      NO
    63        a2g          1499.25         0.00000       NO      NO
    64        eg           1502.14         0.00000       NO      YES
    65        eg           1502.14         0.00000       NO      YES
    66        eu           1508.53        31.29921       YES     NO
    67        eu           1508.53        31.29921       YES     NO
    68        eu           1528.24         0.61344       YES     NO
    69        eu           1528.24         0.61344       YES     NO
    70        a1g          1541.84         0.00000       NO      YES
```

71	eg	1616.41	0.00000	NO	YES
72	eg	1616.41	0.00000	NO	YES
73	eu	3012.34	85.35179	YES	NO
74	eu	3012.34	85.35179	YES	NO
75	eg	3012.55	0.00000	NO	YES
76	eg	3012.55	0.00000	NO	YES
77	a2u	3013.10	32.93508	YES	NO
78	a1g	3013.49	0.00000	NO	YES
79	a2u	3088.31	81.74306	YES	NO
80	eg	3090.29	0.00000	NO	YES
81	eg	3090.29	0.00000	NO	YES
82	eu	3096.00	7.33856	YES	NO
83	eu	3096.00	7.33856	YES	NO
84	a1g	3100.91	0.00000	NO	YES
85	a2g	3114.06	0.00000	NO	NO
86	eu	3120.38	60.31859	YES	NO
87	eu	3120.38	60.31859	YES	NO
88	eg	3127.78	0.00000	NO	YES
89	eg	3127.78	0.00000	NO	YES
90	a1u	3130.32	0.00000	NO	NO

$[C_6Me_6]^+$
Symmetry: c1
Cartesian coordinates in Ångström:

C	3.7447557	1.3903158	0.1458403
C	2.3317578	1.5898861	0.0250469
C	2.1514527	-0.7342625	-0.6623159
C	3.5643441	-0.9338683	-0.5412767
C	4.3625149	0.1399510	-0.2107144
C	4.5896404	2.4839294	0.6942592
C	5.8596883	0.0351707	-0.2044021
C	1.5336567	0.5162241	-0.3059893
C	1.7541205	2.9532796	0.2810736
C	0.0364695	0.6205283	-0.3131291
C	1.3061151	-1.8275238	-1.2107291
C	4.1423350	-2.2972475	-0.7965633
H	2.4277514	3.7389171	-0.0532550
H	1.5686683	3.1147519	1.3469671
H	0.8117190	3.0893639	-0.2400087
H	4.0358894	3.1302371	1.3690703
H	4.9478591	3.1182348	-0.1284334
H	5.4708924	2.1059009	1.2044929
H	6.2065018	-0.7482293	-0.8707259
H	6.2370652	-0.1929372	0.7971893
H	6.3254473	0.9659494	-0.5200950
H	3.4685354	-3.0829242	-0.4626956
H	5.0842829	-2.4330092	-0.2745408
H	4.3289013	-2.4588836	-1.8622429
H	1.8605862	-2.4776358	-1.8811449
H	0.4280443	-1.4484100	-1.7257963
H	0.9420896	-2.4577318	-0.3874371
H	-0.3110878	1.4061665	0.3500937
H	-0.4288625	-0.3093975	0.0058430
H	-0.3406839	0.8444840	-1.3157305

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	63.16	0.45929	YES	YES
8	a	84.59	0.05201	YES	YES
9	a	105.73	0.00065	YES	YES
10	a	114.08	0.00008	YES	YES
11	a	121.87	1.55405	YES	YES
12	a	133.64	0.00009	YES	YES
13	a	145.35	0.03158	YES	YES
14	a	147.63	0.00010	YES	YES
15	a	153.38	0.46471	YES	YES
16	a	180.11	0.00003	YES	YES
17	a	201.25	4.59352	YES	YES
18	a	337.19	0.57870	YES	YES
19	a	356.42	0.19834	YES	YES
20	a	363.23	0.00000	YES	YES
21	a	371.99	0.00000	YES	YES
22	a	402.59	0.00001	YES	YES
23	a	405.21	0.00000	YES	YES

24	a	441.73	0.20622	YES	YES
25	a	448.75	0.00000	YES	YES
26	a	553.66	0.00000	YES	YES
27	a	576.10	2.15230	YES	YES
28	a	582.52	4.00251	YES	YES
29	a	589.78	2.14574	YES	YES
30	a	592.99	0.00035	YES	YES
31	a	706.22	0.00001	YES	YES
32	a	810.02	3.83623	YES	YES
33	a	812.27	0.41456	YES	YES
34	a	857.95	0.00007	YES	YES
35	a	968.49	19.83305	YES	YES
36	a	981.12	0.00001	YES	YES
37	a	1000.74	0.00149	YES	YES
38	a	1008.74	0.00006	YES	YES
39	a	1014.01	5.74312	YES	YES
40	a	1036.61	67.84909	YES	YES
41	a	1061.68	7.41626	YES	YES
42	a	1072.16	0.00001	YES	YES
43	a	1086.75	0.00539	YES	YES
44	a	1091.52	19.26711	YES	YES
45	a	1093.32	39.30604	YES	YES
46	a	1105.90	0.00015	YES	YES
47	a	1127.42	0.00017	YES	YES
48	a	1263.10	0.00191	YES	YES
49	a	1289.85	0.73704	YES	YES
50	a	1320.44	0.00100	YES	YES
51	a	1327.33	204.01416	YES	YES
52	a	1346.12	106.55491	YES	YES
53	a	1387.69	0.00727	YES	YES
54	a	1388.92	39.62255	YES	YES
55	a	1415.01	0.00020	YES	YES
56	a	1418.44	20.99184	YES	YES
57	a	1421.11	19.63629	YES	YES
58	a	1424.28	0.00011	YES	YES
59	a	1444.79	0.68422	YES	YES
60	a	1448.55	0.00114	YES	YES
61	a	1460.71	0.00006	YES	YES
62	a	1466.42	0.39650	YES	YES
63	a	1480.31	60.98460	YES	YES
64	a	1483.62	0.02283	YES	YES
65	a	1487.68	66.46315	YES	YES
66	a	1495.36	0.00057	YES	YES
67	a	1498.04	0.00002	YES	YES
68	a	1516.42	4.64376	YES	YES
69	a	1517.74	49.71075	YES	YES
70	a	1532.49	48.93172	YES	YES
71	a	1535.17	0.00102	YES	YES
72	a	1640.70	0.00012	YES	YES
73	a	2987.92	48.63101	YES	YES
74	a	2988.90	0.00122	YES	YES
75	a	3026.88	0.00241	YES	YES
76	a	3027.70	0.77169	YES	YES
77	a	3031.06	0.00089	YES	YES
78	a	3031.71	0.43453	YES	YES
79	a	3106.20	5.93714	YES	YES
80	a	3107.22	0.01177	YES	YES
81	a	3107.91	0.00277	YES	YES
82	a	3110.06	2.96084	YES	YES
83	a	3111.36	4.70894	YES	YES
84	a	3112.34	0.00232	YES	YES
85	a	3143.77	0.04353	YES	YES
86	a	3144.58	4.04560	YES	YES
87	a	3154.16	7.40378	YES	YES
88	a	3156.22	0.02062	YES	YES
89	a	3156.27	0.00410	YES	YES
90	a	3157.98	0.31671	YES	YES

$[Au(Mes)_2)]^+$
Symmetry: c2
Cartesian coordinates in Ångström:

C	2.9790619	0.8416479	0.3301836
C	2.6720287	0.5491209	-0.9909386
H	3.4088739	1.8059018	0.5697234
C	2.0922902	-0.7238523	-1.2892103
C	1.9231516	-1.6986733	-0.2572480
C	2.2496972	-1.3454486	1.0449843
C	2.7775310	-0.0889780	1.3536635
Au	-0.0000000	0.0000000	-1.1617563
C	3.0235500	1.4979395	-2.0991897
C	3.1069026	0.2660395	2.7724593

```
H     2.1162986   -2.0717674    1.8365002
C     1.4932487   -3.0957146   -0.5980742
H     2.1030265   -1.0638253   -2.3202232
C    -2.9790619   -0.8416479    0.3301836
C    -2.6720287   -0.5491209   -0.9909386
H    -3.4088739   -1.8059018    0.5697234
C    -2.0922902    0.7238523   -1.2892103
C    -1.9231516    1.6986733   -0.2572480
C    -2.2496972    1.3454486    1.0449843
C    -2.7775310    0.0889780    1.3536635
C    -3.0235500   -1.4979395   -2.0991897
C    -3.1069026   -0.2660395    2.7724593
H    -2.1162986    2.0717674    1.8365002
C    -1.4932487    3.0957146   -0.5980742
H    -2.1030265    1.0638253   -2.3202232
H     0.9856186   -3.1418528   -1.5595213
H     0.8352987   -3.5072792    0.1659364
H     2.3711652   -3.7437353   -0.6549981
H     2.8800582    2.5342738   -1.7971564
H     2.4383433    1.3100642   -2.9972691
H     4.0778710    1.3781303   -2.3604554
H     3.9370481    0.9687880    2.8247819
H     3.3572550   -0.6173053    3.3575394
H     2.2459610    0.7424939    3.2493905
H    -0.9856186    3.1418528   -1.5595213
H    -0.8352987    3.5072792    0.1659364
H    -2.3711652    3.7437353   -0.6549981
H    -3.9370481   -0.9687880    2.8247819
H    -3.3572550    0.6173053    3.3575394
H    -2.2459610   -0.7424939    3.2493905
H    -2.8800582   -2.5342738   -1.7971564
H    -2.4383433   -1.3100642   -2.9972691
H    -4.0778710   -1.3781303   -2.3604554

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                       0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a              4.60         0.00940      YES     YES
     8        a             24.63         0.09075      YES     YES
     9        b             31.39         0.31892      YES     YES
    10        b             41.65         0.10346      YES     YES
    11        a             45.36         0.00014      YES     YES
    12        b             56.04         0.94264      YES     YES
    13        a             67.55         0.17461      YES     YES
    14        b             70.52         0.03632      YES     YES
    15        a             80.75         2.36508      YES     YES
    16        a             97.94         0.00133      YES     YES
    17        b            103.37         1.88093      YES     YES
    18        a            112.57         0.09352      YES     YES
    19        b            113.41         0.66451      YES     YES
    20        a            128.35         0.01960      YES     YES
    21        b            150.31         1.50523      YES     YES
    22        a            185.03         0.45194      YES     YES
    23        b            186.36         4.99854      YES     YES
    24        a            206.70         0.06499      YES     YES
    25        b            209.61         0.54121      YES     YES
    26        b            272.99         0.07989      YES     YES
    27        a            274.17         0.00330      YES     YES
    28        a            277.10         0.01110      YES     YES
    29        b            277.22         0.25166      YES     YES
    30        b            352.43        36.27245      YES     YES
    31        a            380.18         0.50495      YES     YES
    32        b            462.73         0.24944      YES     YES
    33        a            462.97         0.02010      YES     YES
    34        a            507.23         0.00118      YES     YES
    35        b            507.36         0.01780      YES     YES
    36        b            514.30         6.10801      YES     YES
    37        a            515.99         0.01046      YES     YES
    38        a            544.64         0.03510      YES     YES
    39        b            544.79         0.07974      YES     YES
    40        b            549.31        12.77103      YES     YES
    41        a            553.34         0.90646      YES     YES
    42        a            581.18         0.18817      YES     YES
    43        b            581.33         0.01283      YES     YES
    44        b            714.52         1.03977      YES     YES
```

45	a	719.35	4.53615	YES	YES
46	b	876.86	98.97473	YES	YES
47	a	878.63	2.14027	YES	YES
48	b	914.95	69.41851	YES	YES
49	a	920.46	0.00000	YES	YES
50	b	920.97	0.69705	YES	YES
51	a	933.82	17.03453	YES	YES
52	a	940.46	0.00110	YES	YES
53	b	940.78	0.04243	YES	YES
54	b	943.72	6.92082	YES	YES
55	a	944.59	1.57815	YES	YES
56	b	1002.97	10.63250	YES	YES
57	a	1004.52	0.33833	YES	YES
58	a	1030.60	0.14598	YES	YES
59	b	1030.95	2.94462	YES	YES
60	a	1039.86	0.37147	YES	YES
61	b	1039.92	11.18032	YES	YES
62	a	1042.11	0.07425	YES	YES
63	b	1042.80	0.44319	YES	YES
64	a	1057.36	2.86743	YES	YES
65	b	1057.43	25.68567	YES	YES
66	b	1058.74	20.20087	YES	YES
67	a	1060.03	0.73582	YES	YES
68	b	1064.58	14.99578	YES	YES
69	a	1065.14	11.38696	YES	YES
70	a	1179.87	0.05155	YES	YES
71	b	1179.89	0.66455	YES	YES
72	b	1186.63	4.04197	YES	YES
73	a	1187.25	4.40552	YES	YES
74	b	1316.56	53.98389	YES	YES
75	a	1317.71	1.79384	YES	YES
76	b	1318.76	11.85347	YES	YES
77	a	1320.93	2.08588	YES	YES
78	a	1353.18	1.78026	YES	YES
79	b	1359.22	23.45402	YES	YES
80	b	1416.98	5.06647	YES	YES
81	a	1417.51	17.60854	YES	YES
82	a	1419.15	4.79949	YES	YES
83	b	1419.93	26.48556	YES	YES
84	b	1420.68	6.47653	YES	YES
85	a	1421.49	0.37818	YES	YES
86	b	1433.58	21.15246	YES	YES
87	a	1436.79	3.83216	YES	YES
88	b	1451.18	1.03675	YES	YES
89	a	1451.63	0.01695	YES	YES
90	b	1483.95	1.19428	YES	YES
91	a	1484.03	0.19341	YES	YES
92	b	1489.34	44.76977	YES	YES
93	a	1489.41	4.90996	YES	YES
94	a	1490.15	5.54727	YES	YES
95	b	1490.61	4.75668	YES	YES
96	b	1491.95	0.39536	YES	YES
97	a	1492.17	2.47577	YES	YES
98	b	1499.91	5.61920	YES	YES
99	a	1502.04	46.44285	YES	YES
100	a	1508.09	6.59251	YES	YES
101	b	1508.38	79.96858	YES	YES
102	a	1580.36	5.93641	YES	YES
103	b	1581.31	59.12532	YES	YES
104	b	1631.88	59.17792	YES	YES
105	a	1634.69	160.08470	YES	YES
106	b	3031.01	1.63445	YES	YES
107	a	3031.12	4.20964	YES	YES
108	a	3036.75	2.64524	YES	YES
109	b	3036.75	1.84569	YES	YES
110	a	3037.40	0.69627	YES	YES
111	b	3037.40	3.90681	YES	YES
112	b	3092.26	13.67008	YES	YES
113	a	3092.35	4.21672	YES	YES
114	a	3096.00	0.94527	YES	YES
115	b	3096.14	6.36383	YES	YES
116	b	3096.27	8.41320	YES	YES
117	a	3096.40	1.07274	YES	YES
118	b	3126.46	4.25011	YES	YES
119	a	3126.48	0.02032	YES	YES
120	b	3126.62	2.91783	YES	YES
121	a	3126.66	12.23258	YES	YES
122	b	3127.03	7.50437	YES	YES
123	a	3127.04	6.52120	YES	YES
124	a	3136.91	0.00314	YES	YES
125	b	3136.93	0.02052	YES	YES

126	a	3173.49	0.71269	YES	YES
127	b	3173.56	7.38202	YES	YES
128	b	3174.79	2.09088	YES	YES
129	a	3174.91	1.71867	YES	YES

[Au(Mes)(CO)]⁺
Symmetry: c1
Cartesian coordinates in Ångström:

Au	1.9964238	0.6373212	-0.8722370
C	-0.2874998	-0.8160908	-1.1003981
C	-0.1929572	0.6158102	-1.0635041
C	-0.2722732	-1.5424114	-2.4122472
C	-0.4188396	1.3256873	0.1635987
C	-0.5984089	0.5878306	1.3245330
C	-0.6265583	-0.8117987	1.3103614
C	-0.4707993	-1.4923272	0.0969726
H	-0.3244965	1.1581274	-1.9961267
H	-0.5279013	-2.5730631	0.0876317
C	-0.8131265	-1.5750192	2.5846263
H	-0.7537833	1.1087172	2.2604336
C	-0.5398227	2.8203884	0.1623279
C	3.9458754	0.7049756	-0.7850701
O	5.0653367	0.7547659	-0.7546965
H	-0.0604289	3.2711625	-0.7045227
H	-0.1188490	3.2573451	1.0662919
H	-1.5977055	3.0932984	0.1309508
H	-1.2960160	-2.5345372	2.4083885
H	-1.3998908	-1.0094302	3.3063524
H	0.1595403	-1.7775805	3.0417592
H	0.1969600	-0.9574176	-3.2009303
H	-1.3011049	-1.7439247	-2.7211660
H	0.2363255	-2.5018292	-2.3333292

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	42.52	0.08255	YES	YES
8	a	51.09	0.01839	YES	YES
9	a	55.71	0.36284	YES	YES
10	a	69.83	0.79428	YES	YES
11	a	80.21	0.00087	YES	YES
12	a	104.57	0.78883	YES	YES
13	a	116.88	0.53265	YES	YES
14	a	141.31	0.36417	YES	YES
15	a	183.56	3.03609	YES	YES
16	a	205.81	0.12626	YES	YES
17	a	272.01	0.16250	YES	YES
18	a	278.33	0.18588	YES	YES
19	a	376.50	10.18507	YES	YES
20	a	379.06	4.44527	YES	YES
21	a	385.77	0.42864	YES	YES
22	a	398.80	21.50098	YES	YES
23	a	464.38	0.09148	YES	YES
24	a	507.47	0.00031	YES	YES
25	a	513.15	1.87500	YES	YES
26	a	549.76	0.01677	YES	YES
27	a	552.98	4.94079	YES	YES
28	a	579.69	0.09213	YES	YES
29	a	716.40	3.89533	YES	YES
30	a	883.27	40.52255	YES	YES
31	a	928.56	0.25575	YES	YES
32	a	934.07	38.93681	YES	YES
33	a	942.39	0.01867	YES	YES
34	a	944.99	16.16949	YES	YES
35	a	1001.76	3.16583	YES	YES
36	a	1031.07	2.19748	YES	YES
37	a	1039.52	5.04365	YES	YES
38	a	1044.19	0.01565	YES	YES
39	a	1056.41	16.65696	YES	YES
40	a	1057.59	6.23749	YES	YES
41	a	1065.29	15.91064	YES	YES
42	a	1177.83	0.36615	YES	YES
43	a	1185.58	5.36008	YES	YES
44	a	1316.76	26.78441	YES	YES

45	a	1320.58	7.05928	YES	YES
46	a	1357.70	15.16219	YES	YES
47	a	1417.05	15.06108	YES	YES
48	a	1420.46	11.48130	YES	YES
49	a	1421.48	8.00636	YES	YES
50	a	1431.08	4.40034	YES	YES
51	a	1447.29	0.58851	YES	YES
52	a	1481.51	0.17684	YES	YES
53	a	1488.23	27.51233	YES	YES
54	a	1488.97	1.48210	YES	YES
55	a	1491.46	1.41425	YES	YES
56	a	1499.02	23.43571	YES	YES
57	a	1506.78	57.99469	YES	YES
58	a	1571.86	40.62627	YES	YES
59	a	1628.26	126.90015	YES	YES
60	a	2255.83	508.47170	YES	YES
61	a	3032.66	0.43023	YES	YES
62	a	3037.59	0.03111	YES	YES
63	a	3037.61	0.63172	YES	YES
64	a	3095.70	5.82272	YES	YES
65	a	3098.06	3.58493	YES	YES
66	a	3098.28	3.05566	YES	YES
67	a	3126.66	3.18740	YES	YES
68	a	3129.94	0.84499	YES	YES
69	a	3130.25	5.81627	YES	YES
70	a	3131.70	3.62004	YES	YES
71	a	3179.19	1.41852	YES	YES
72	a	3180.37	0.63080	YES	YES

Mes
Symmetry: c3
Cartesian coordinates in Ångström:

C	-0.35733	1.33627	0.01041
C	-1.35418	0.36822	0.00934
C	0.99598	0.98864	0.00934
C	1.33591	-0.35868	0.01041
C	0.35820	-1.35686	0.00934
C	-0.97858	-0.97760	0.01041
C	-2.81002	0.75173	-0.00385
H	-1.74706	-1.74222	0.01816
H	2.38233	-0.64189	0.01816
C	0.75399	-2.80941	-0.00385
H	-0.63527	2.38411	0.01816
C	2.05603	2.05768	-0.00385
H	2.09823	2.55569	-0.97566
H	3.04238	1.64129	0.19817
H	1.85269	2.82652	0.74343
H	1.52150	-3.01774	0.74343
H	1.16417	-3.09496	-0.97566
H	-0.09979	-3.45543	0.19817
H	-2.94259	1.81414	0.19817
H	-3.37419	0.19122	0.74343
H	-3.26240	0.53928	-0.97566

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	19.81	0.29056	YES	YES
8	e	33.32	0.07823	YES	YES
9	e	33.32	0.07823	YES	YES
10	a	172.95	5.37880	YES	YES
11	e	222.57	0.00648	YES	YES
12	e	222.57	0.00648	YES	YES
13	e	272.38	0.48467	YES	YES
14	e	272.38	0.48467	YES	YES
15	a	463.76	0.00013	YES	YES
16	e	522.83	0.41800	YES	YES
17	e	522.83	0.41800	YES	YES
18	e	534.02	0.21570	YES	YES
19	e	534.02	0.21570	YES	YES
20	a	580.91	0.00117	YES	YES
21	a	712.03	12.51074	YES	YES
22	a	861.66	23.34008	YES	YES
23	e	902.16	0.02286	YES	YES

24	e	902.16	0.02286	YES	YES
25	e	948.87	2.34661	YES	YES
26	e	948.87	2.34661	YES	YES
27	a	1017.81	0.08937	YES	YES
28	e	1034.50	2.82421	YES	YES
29	e	1034.50	2.82421	YES	YES
30	a	1040.02	0.02059	YES	YES
31	e	1064.44	2.00890	YES	YES
32	e	1064.44	2.00890	YES	YES
33	a	1066.02	6.88396	YES	YES
34	e	1190.11	0.19043	YES	YES
35	e	1190.11	0.19043	YES	YES
36	a	1302.94	0.03947	YES	YES
37	a	1326.28	0.09192	YES	YES
38	a	1348.21	0.03679	YES	YES
39	e	1413.64	1.21082	YES	YES
40	e	1413.64	1.21082	YES	YES
41	a	1417.16	0.07464	YES	YES
42	e	1460.62	0.56194	YES	YES
43	e	1460.62	0.56194	YES	YES
44	a	1487.22	15.97275	YES	YES
45	e	1488.20	0.02720	YES	YES
46	e	1488.20	0.02720	YES	YES
47	a	1494.95	1.51599	YES	YES
48	e	1515.08	21.06179	YES	YES
49	e	1515.08	21.06179	YES	YES
50	e	1644.85	27.88868	YES	YES
51	e	1644.85	27.88868	YES	YES
52	e	3024.77	46.82572	YES	YES
53	e	3024.77	46.82572	YES	YES
54	a	3025.39	1.89106	YES	YES
55	e	3073.51	2.13337	YES	YES
56	e	3073.51	2.13337	YES	YES
57	a	3073.67	47.85160	YES	YES
58	a	3102.84	0.01737	YES	YES
59	e	3103.12	24.33670	YES	YES
60	e	3103.12	24.33670	YES	YES
61	e	3149.86	26.92904	YES	YES
62	e	3149.86	26.92904	YES	YES
63	a	3152.71	0.01344	YES	YES

$[Mes]^+$
Symmetry: c1
Cartesian coordinates in Ångström:

C	-0.3488824	1.3004297	-0.0466429
C	-1.3938633	0.3081259	0.0030968
C	1.0260796	0.9740758	-0.0498712
C	1.3453229	-0.3596444	-0.0023749
C	0.3308288	-1.3800078	0.0486926
C	-1.0279729	-1.0152012	0.0498165
C	-2.8098901	0.7600707	0.0017988
H	-1.7823122	-1.7886290	0.0878462
H	2.3819110	-0.6712089	-0.0026615
C	0.7493554	-2.7955260	0.0998950
H	-0.6405371	2.3438646	-0.0834495
C	2.0574146	2.0585352	-0.1025157
H	1.9239240	2.6737614	-0.9941855
H	3.0650351	1.6502614	-0.1148414
H	1.9645870	2.7192403	0.7615461
H	1.3873672	-2.9641581	0.9757494
H	1.3839098	-3.0296993	-0.7629716
H	-0.0895160	-3.4844431	0.1284054
H	-2.9996860	1.4164824	0.8565897
H	-3.5056974	-0.0736492	0.0373611
H	-3.0173782	1.3573198	-0.8912834

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	78.96	2.40811	YES	YES
8	a	89.11	0.51692	YES	YES
9	a	117.57	1.21508	YES	YES
10	a	154.49	0.61243	YES	YES
11	a	176.13	0.00245	YES	YES

12	a	203.76	0.14167	YES	YES
13	a	250.77	15.23399	YES	YES
14	a	269.74	0.92723	YES	YES
15	a	312.37	23.89026	YES	YES
16	a	452.31	6.79659	YES	YES
17	a	465.73	0.12321	YES	YES
18	a	498.35	0.68002	YES	YES
19	a	510.72	0.08598	YES	YES
20	a	574.32	0.05736	YES	YES
21	a	595.76	8.47012	YES	YES
22	a	850.42	8.05917	YES	YES
23	a	892.70	0.02954	YES	YES
24	a	904.23	34.08899	YES	YES
25	a	931.32	0.79716	YES	YES
26	a	933.94	5.94325	YES	YES
27	a	958.01	36.13171	YES	YES
28	a	994.98	3.58954	YES	YES
29	a	1021.03	11.01630	YES	YES
30	a	1030.87	31.27297	YES	YES
31	a	1048.12	3.85174	YES	YES
32	a	1050.72	1.86565	YES	YES
33	a	1071.33	5.50165	YES	YES
34	a	1171.09	73.50053	YES	YES
35	a	1179.14	17.32840	YES	YES
36	a	1254.42	100.41560	YES	YES
37	a	1331.86	14.14331	YES	YES
38	a	1336.21	2.07649	YES	YES
39	a	1372.34	93.14190	YES	YES
40	a	1390.59	35.26349	YES	YES
41	a	1404.55	10.15594	YES	YES
42	a	1422.89	22.42188	YES	YES
43	a	1428.72	71.68363	YES	YES
44	a	1442.25	13.22487	YES	YES
45	a	1458.30	11.34749	YES	YES
46	a	1470.45	29.32805	YES	YES
47	a	1477.75	12.35096	YES	YES
48	a	1481.22	29.26582	YES	YES
49	a	1496.26	66.31373	YES	YES
50	a	1554.39	121.24591	YES	YES
51	a	1643.47	50.63341	YES	YES
52	a	2999.12	63.76367	YES	YES
53	a	3015.79	19.58910	YES	YES
54	a	3032.92	1.46680	YES	YES
55	a	3038.46	0.77289	YES	YES
56	a	3059.13	0.00514	YES	YES
57	a	3091.59	0.71836	YES	YES
58	a	3135.83	5.14081	YES	YES
59	a	3142.93	7.88435	YES	YES
60	a	3149.29	10.54449	YES	YES
61	a	3173.26	0.07768	YES	YES
62	a	3186.53	0.02012	YES	YES
63	a	3198.33	0.07038	YES	YES

$[Au(C_6H_6)_2)]^+$
Symmetry: c2
Cartesian coordinates in Ångström:

C	2.4554167	2.5216722	-0.7542212
C	2.3298853	1.3109409	-1.4043256
H	2.5705402	3.4302648	-1.3285172
C	2.2095960	0.1180192	-0.6552057
C	2.2054968	0.1832646	0.7644371
C	2.3215092	1.4355905	1.4030116
C	2.4530296	2.5833461	0.6472303
Au	0.0000000	-0.0000000	-0.0113113
H	2.3560880	1.2586699	-2.4833893
H	2.5671536	3.5393740	1.1389480
H	2.3396734	1.4814518	2.4825173
H	2.2826780	-0.7258265	1.3460979
H	2.3131592	-0.8386334	-1.1509277
C	-2.4554167	-2.5216722	-0.7542212
C	-2.3298853	-1.3109409	-1.4043256
H	-2.5705402	-3.4302648	-1.3285172
C	-2.2095960	-0.1180192	-0.6552057
C	-2.2054968	-0.1832646	0.7644371
C	-2.3215092	-1.4355905	1.4030116
C	-2.4530296	-2.5833461	0.6472303
H	-2.3560880	-1.2586699	-2.4833893
H	-2.5671536	-3.5393740	1.1389480
H	-2.3396734	-1.4814518	2.4825173
H	-2.2826780	0.7258265	1.3460979

H   -2.3131592   0.8386334   -1.1509277

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.82	0.07887	YES	YES
8	a	17.48	1.57773	YES	YES
9	b	42.88	1.03037	YES	YES
10	b	72.35	0.15819	YES	YES
11	a	81.52	0.00998	YES	YES
12	a	87.21	0.00002	YES	YES
13	b	121.14	1.34069	YES	YES
14	b	243.03	0.30820	YES	YES
15	a	247.66	0.00006	YES	YES
16	b	418.30	0.14515	YES	YES
17	a	420.19	0.29760	YES	YES
18	b	425.55	0.10634	YES	YES
19	a	430.51	0.02510	YES	YES
20	a	611.81	0.37962	YES	YES
21	b	613.35	0.01714	YES	YES
22	a	615.70	0.00146	YES	YES
23	b	615.78	2.43261	YES	YES
24	a	699.55	1.08531	YES	YES
25	b	700.89	0.93424	YES	YES
26	b	739.67	185.78512	YES	YES
27	a	740.73	0.00149	YES	YES
28	b	880.63	0.11501	YES	YES
29	a	883.52	0.04074	YES	YES
30	b	918.69	3.31265	YES	YES
31	a	923.87	0.00611	YES	YES
32	b	980.26	16.72997	YES	YES
33	a	983.96	0.09808	YES	YES
34	b	986.28	0.06431	YES	YES
35	a	994.16	3.92630	YES	YES
36	b	1014.78	0.80031	YES	YES
37	a	1015.20	0.00795	YES	YES
38	a	1032.31	2.32694	YES	YES
39	b	1033.10	0.20157	YES	YES
40	b	1042.58	5.12174	YES	YES
41	a	1043.16	0.01933	YES	YES
42	a	1045.16	0.31112	YES	YES
43	b	1045.35	0.03035	YES	YES
44	a	1058.89	0.59961	YES	YES
45	b	1059.84	0.00150	YES	YES
46	a	1180.74	0.00146	YES	YES
47	b	1180.99	3.83880	YES	YES
48	b	1201.80	0.72881	YES	YES
49	a	1202.96	0.02476	YES	YES
50	a	1204.52	0.58746	YES	YES
51	b	1204.76	0.08343	YES	YES
52	b	1353.01	50.69624	YES	YES
53	a	1357.94	0.19286	YES	YES
54	a	1387.61	0.32148	YES	YES
55	b	1387.67	0.00017	YES	YES
56	b	1497.71	0.17123	YES	YES
57	a	1497.92	32.22095	YES	YES
58	b	1500.43	27.96802	YES	YES
59	a	1502.77	0.16014	YES	YES
60	b	1591.68	6.88075	YES	YES
61	a	1594.21	0.00326	YES	YES
62	a	1623.42	7.66740	YES	YES
63	b	1623.76	0.67815	YES	YES
64	a	3174.48	1.30957	YES	YES
65	b	3175.03	0.17290	YES	YES
66	b	3185.94	1.60276	YES	YES
67	a	3186.38	0.03230	YES	YES
68	a	3190.63	0.81424	YES	YES
69	b	3190.64	0.01186	YES	YES
70	b	3199.33	0.01902	YES	YES
71	a	3199.44	0.00002	YES	YES
72	a	3207.04	0.01647	YES	YES
73	b	3207.05	0.00286	YES	YES
74	b	3211.74	0.61368	YES	YES
75	a	3211.75	0.00020	YES	YES

$[Au(C_6H_6)(CO)]^+$
Symmetry: cs
Cartesian coordinates in Ångström:

Au	1.6248796	0.9752988	0.0000000
C	-0.8861318	-0.9362261	-1.2133500
C	-0.6967617	0.4404167	-1.2268573
H	-0.9748632	-1.4755500	-2.1455883
C	-0.5910721	1.1528656	0.0000000
C	-0.6967617	0.4404167	1.2268573
C	-0.8861318	-0.9362261	1.2133500
C	-0.9939581	-1.6133231	0.0000000
H	-0.6732179	0.9835547	-2.1614538
H	-1.1666666	-2.6808427	0.0000000
H	-0.9748632	-1.4755500	2.1455883
H	-0.6732179	0.9835547	2.1614538
H	-0.6888007	2.2337771	0.0000000
C	3.5785146	0.9509576	0.0000000
O	4.6984203	0.9570350	0.0000000

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a'	54.32	0.30287	YES	YES
8	a"	62.42	0.56156	YES	YES
9	a"	74.74	0.04311	YES	YES
10	a'	85.33	0.84140	YES	YES
11	a'	266.10	0.64975	YES	YES
12	a'	370.50	7.58624	YES	YES
13	a"	374.00	4.92248	YES	YES
14	a'	392.95	14.57594	YES	YES
15	a"	408.78	0.01104	YES	YES
16	a'	451.37	4.18934	YES	YES
17	a"	613.66	0.17607	YES	YES
18	a'	615.61	0.75109	YES	YES
19	a'	698.65	20.40698	YES	YES
20	a'	748.22	83.30846	YES	YES
21	a"	887.68	0.03217	YES	YES
22	a'	932.93	18.40690	YES	YES
23	a'	978.97	24.36198	YES	YES
24	a'	1005.47	1.08550	YES	YES
25	a"	1022.17	0.31905	YES	YES
26	a'	1036.70	5.50669	YES	YES
27	a'	1046.19	0.01321	YES	YES
28	a"	1050.80	1.58076	YES	YES
29	a'	1055.86	0.51605	YES	YES
30	a"	1180.73	0.16864	YES	YES
31	a"	1204.63	0.78729	YES	YES
32	a'	1205.53	0.78829	YES	YES
33	a"	1355.90	6.94906	YES	YES
34	a"	1386.90	0.22842	YES	YES
35	a"	1500.48	26.93093	YES	YES
36	a'	1501.11	15.33322	YES	YES
37	a"	1594.91	0.92895	YES	YES
38	a'	1612.35	16.96574	YES	YES
39	a'	2265.13	476.77056	YES	YES
40	a'	3148.44	4.99749	YES	YES
41	a'	3191.44	0.57086	YES	YES
42	a"	3194.90	1.26887	YES	YES
43	a'	3199.23	0.97134	YES	YES
44	a"	3208.70	1.40657	YES	YES
45	a'	3213.27	0.04202	YES	YES

$raman spectrum

# mode	symmetry	wave number cm**(-1)	selection rule	derivative of isotropic polarizability a.u.	derivative of polarizability anisotropy a.u.	raman scattering cross sections bohr**2/sr T,T	II,II
1		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
2		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
3		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
4		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
5		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
6		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
7	a'	54.32	YES	-0.006007	0.062203	0.31021D-13	0.21056D-13

8	a"	62.42	YES	0.000000	0.020466	0.23366D-14	0.17525D-14
9	a"	74.74	YES	0.000000	0.082751	0.27261D-13	0.20446D-13
10	a'	85.33	YES	-0.007120	0.031010	0.47703D-14	0.22458D-14
11	a'	266.10	YES	-0.003620	0.071567	0.22708D-14	0.16554D-14
12	a'	370.50	YES	-0.008993	0.028261	0.43858D-15	0.15377D-15
13	a"	374.00	YES	0.000000	0.012299	0.38275D-16	0.28706D-16
14	a'	392.95	YES	0.022312	0.042142	0.17319D-14	0.31274D-15
15	a"	408.78	YES	0.000000	0.013635	0.41132D-16	0.30849D-16
16	a'	451.37	YES	0.011759	0.030042	0.46915D-15	0.12920D-15
17	a"	613.66	YES	0.000000	0.060614	0.44829D-15	0.33622D-15
18	a'	615.61	YES	-0.003142	0.057529	0.41546D-15	0.30148D-15
19	a'	698.65	YES	0.000416	0.037121	0.13968D-15	0.10462D-15
20	a'	748.22	YES	0.004099	0.033538	0.12046D-15	0.77348D-16
21	a"	887.68	YES	0.000000	0.000193	0.26579D-20	0.19934D-20
22	a'	932.93	YES	-0.015087	0.041938	0.28667D-15	0.87544D-16
23	a'	978.97	YES	0.088260	0.048041	0.55532D-14	0.10687D-15
24	a'	1005.47	YES	0.059159	0.040597	0.24324D-14	0.73299D-16
25	a"	1022.17	YES	0.000000	0.002747	0.43648D-18	0.32736D-18
26	a'	1036.70	YES	-0.009062	0.019391	0.73572D-16	0.15961D-16
27	a'	1046.19	YES	0.033885	0.036284	0.79442D-15	0.55111D-16
28	a"	1050.80	YES	0.000000	0.020226	0.22679D-16	0.17010D-16
29	a'	1055.86	YES	-0.020921	0.013926	0.28163D-15	0.80046D-17
30	a"	1180.73	YES	0.000000	0.048320	0.10787D-15	0.80902D-16
31	a"	1204.63	YES	0.000000	0.047700	0.10180D-15	0.76352D-16
32	a'	1205.53	YES	-0.009683	0.066958	0.24749D-15	0.15027D-15
33	a"	1355.90	YES	0.000000	0.018011	0.11950D-16	0.89627D-17
34	a"	1386.90	YES	0.000000	0.013805	0.67574D-17	0.50680D-17
35	a"	1500.48	YES	0.000000	0.046677	0.67405D-16	0.50554D-16
36	a'	1501.11	YES	0.014515	0.043564	0.13194D-15	0.44003D-16
37	a"	1594.91	YES	0.000000	0.094653	0.24845D-15	0.18634D-15
38	a'	1612.35	YES	-0.011350	0.113274	0.38821D-15	0.26161D-15
39	a'	2265.13	YES	-0.112297	0.351384	0.36159D-14	0.12620D-14
40	a'	3148.44	YES	0.056748	0.204126	0.45007D-15	0.18056D-15
41	a'	3191.44	YES	-0.045183	0.147898	0.24863D-15	0.90964D-16
42	a"	3194.90	YES	0.000000	0.282433	0.44083D-15	0.33063D-15
43	a'	3199.23	YES	-0.036156	0.258181	0.44779D-15	0.27514D-15
44	a"	3208.70	YES	0.000000	0.180596	0.17788D-15	0.13341D-15
45	a'	3213.27	YES	0.190271	0.241545	0.25284D-14	0.23761D-15

C_6H_6
Symmetry: d6h
Cartesian coordinates in Ångström:

H	2.1415748	1.2364388	0.0000000
H	2.1415748	-1.2364388	0.0000000
H	0.0000000	-2.4728776	0.0000000
C	1.2045212	-0.6954306	0.0000000
C	-0.0000000	-1.3908612	0.0000000
C	-1.2045212	-0.6954306	0.0000000
H	-2.1415748	-1.2364388	0.0000000
C	-1.2045212	0.6954306	0.0000000
C	-0.0000000	1.3908612	0.0000000
C	1.2045212	0.6954306	0.0000000
H	0.0000000	2.4728776	0.0000000
H	-2.1415748	1.2364388	0.0000000

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	e2u	412.73	0.00000	NO	NO
8	e2u	412.73	0.00000	NO	NO
9	e2g	624.82	0.00000	NO	YES
10	e2g	624.82	0.00000	NO	YES
11	a2u	689.35	110.95090	YES	NO
12	b1g	725.05	0.00000	NO	NO
13	e1g	866.29	0.00000	NO	YES
14	e1g	866.29	0.00000	NO	YES
15	e2u	988.44	0.00000	NO	NO
16	e2u	988.44	0.00000	NO	NO
17	a1g	1017.81	0.00000	NO	YES
18	b1g	1019.70	0.00000	NO	NO
19	b2u	1029.77	0.00000	NO	NO
20	e1u	1061.83	5.10307	YES	NO
21	e1u	1061.83	5.10307	YES	NO
22	b1u	1176.21	0.00000	NO	NO

23	e2g	1199.63	0.00000	NO	YES
24	e2g	1199.63	0.00000	NO	YES
25	b1u	1336.99	0.00000	NO	NO
26	a2g	1387.06	0.00000	NO	NO
27	e1u	1518.27	7.44664	YES	NO
28	e1u	1518.27	7.44664	YES	NO
29	e2g	1636.74	0.00000	NO	YES
30	e2g	1636.74	0.00000	NO	YES
31	b2u	3161.01	0.00000	NO	NO
32	e2g	3170.68	0.00000	NO	YES
33	e2g	3170.68	0.00000	NO	YES
34	e1u	3186.10	36.34559	YES	NO
35	e1u	3186.10	36.34559	YES	NO
36	a1g	3195.98	0.00000	NO	YES

$[C_6H_6]^+$
Symmetry: c1
Cartesian coordinates in Ångström:

H	2.1638118	1.2548143	0.0000615
H	2.1314898	-1.2299778	0.0000833
H	-0.0055775	-2.4967428	-0.0001611
C	1.1953779	-0.6858719	-0.0000018
C	-0.0328818	-1.4162565	-0.0000614
C	-1.2160855	-0.7356267	0.0000684
H	-2.1638118	-1.2548141	0.0001074
C	-1.1953778	0.6858718	0.0000300
C	0.0328819	1.4162565	-0.0000336
C	1.2160856	0.7356267	0.0000140
H	0.0055774	2.4967428	-0.0000990
H	-2.1314898	1.2299777	-0.0000078

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	236.87	0.00001	YES	YES
8	a	289.81	2.66351	YES	YES
9	a	344.34	0.05222	YES	YES
10	a	415.57	0.00000	YES	YES
11	a	604.96	0.00000	YES	YES
12	a	684.87	83.75739	YES	YES
13	a	800.01	0.00000	YES	YES
14	a	909.78	0.00000	YES	YES
15	a	953.11	0.00000	YES	YES
16	a	964.97	28.59086	YES	YES
17	a	981.48	0.00000	YES	YES
18	a	1013.36	5.05950	YES	YES
19	a	1018.76	0.06286	YES	YES
20	a	1033.41	0.03048	YES	YES
21	a	1045.49	0.00000	YES	YES
22	a	1071.77	11.47474	YES	YES
23	a	1205.83	2.89091	YES	YES
24	a	1220.78	0.00000	YES	YES
25	a	1373.31	0.00000	YES	YES
26	a	1396.32	0.00000	YES	YES
27	a	1403.30	34.71736	YES	YES
28	a	1461.13	116.90904	YES	YES
29	a	1548.92	47.28058	YES	YES
30	a	1670.18	0.00000	YES	YES
31	a	3192.11	1.92887	YES	YES
32	a	3195.44	0.00000	YES	YES
33	a	3206.78	0.00000	YES	YES
34	a	3209.83	8.59029	YES	YES
35	a	3217.89	16.21074	YES	YES
36	a	3220.53	0.00000	YES	YES

$[Au(o\text{-}dfb)_2)]^+$
Symmetry: c2
Cartesian coordinates in Ångström:

C	2.52021	2.52022	-0.74336
C	2.36880	1.32936	-1.40780
F	2.67255	3.65397	-1.41036
C	2.21264	0.13726	-0.66153

```
C          2.21733        0.19075        0.75787
C          2.36936        1.42677        1.41445
C          2.52330        2.56809        0.66491
Au         0.00000       -0.00000       -0.07317
H          2.39945        1.31290       -2.48764
F          2.67888        3.74385        1.25094
H          2.39723        1.49030        2.49262
H          2.27400       -0.72359        1.33219
H          2.31802       -0.81447       -1.16571
C         -2.52021       -2.52022       -0.74336
C         -2.36880       -1.32936       -1.40780
F         -2.67255       -3.65397       -1.41036
C         -2.21264       -0.13726       -0.66153
C         -2.21733       -0.19075        0.75787
C         -2.36936       -1.42677        1.41445
C         -2.52330       -2.56809        0.66491
H         -2.39945       -1.31290       -2.48764
F         -2.67888       -3.74385        1.25094
H         -2.39723       -1.49030        2.49262
H         -2.27400        0.72359        1.33219
H         -2.31802        0.81447       -1.16571

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                      -0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a              5.44         0.56684      YES     YES
     8        a             21.40         4.09066      YES     YES
     9        b             27.62         0.93269      YES     YES
    10        b             48.67         0.53117      YES     YES
    11        a             54.22         0.04085      YES     YES
    12        a             57.40         0.01518      YES     YES
    13        b             98.92         1.60425      YES     YES
    14        b            182.44         0.73667      YES     YES
    15        a            186.22         0.03670      YES     YES
    16        a            209.87         0.04251      YES     YES
    17        b            216.63         0.78392      YES     YES
    18        b            293.34         0.65842      YES     YES
    19        a            293.69         0.00413      YES     YES
    20        b            364.31         0.36449      YES     YES
    21        a            374.78         0.00001      YES     YES
    22        a            443.39         0.37176      YES     YES
    23        b            443.94         0.35198      YES     YES
    24        b            452.00         1.83407      YES     YES
    25        a            455.04         0.00576      YES     YES
    26        a            551.85         8.75181      YES     YES
    27        b            552.39         0.03536      YES     YES
    28        a            569.24         1.90103      YES     YES
    29        b            573.65         9.39961      YES     YES
    30        a            577.66         0.09619      YES     YES
    31        b            579.30        13.45896      YES     YES
    32        a            718.29         0.06362      YES     YES
    33        b            718.67         0.37453      YES     YES
    34        a            779.39         0.13648      YES     YES
    35        b            779.41        43.93371      YES     YES
    36        b            849.48       141.26855      YES     YES
    37        a            853.79         0.90496      YES     YES
    38        b            860.19         1.03317      YES     YES
    39        a            862.04        30.63776      YES     YES
    40        b            874.14         4.35358      YES     YES
    41        a            875.63         0.17436      YES     YES
    42        b            951.55        13.03913      YES     YES
    43        a            954.79         0.00075      YES     YES
    44        b            987.87         8.36950      YES     YES
    45        a            992.10         3.32190      YES     YES
    46        b           1008.26        30.49719      YES     YES
    47        a           1011.93         0.06632      YES     YES
    48        a           1111.10        14.69402      YES     YES
    49        b           1111.59         0.52945      YES     YES
    50        b           1175.36        13.60819      YES     YES
    51        a           1175.64         0.04573      YES     YES
    52        b           1251.72         0.71595      YES     YES
    53        a           1251.99        69.14729      YES     YES
    54        b           1299.26        33.18403      YES     YES
    55        a           1299.57        17.68841      YES     YES
    56        b           1307.01       296.56074      YES     YES
```

57	a	1310.32	1.08622	YES	YES
58	b	1373.42	89.64604	YES	YES
59	a	1377.15	0.45371	YES	YES
60	a	1468.59	29.52632	YES	YES
61	b	1468.63	0.25548	YES	YES
62	b	1537.95	744.36495	YES	YES
63	a	1541.83	0.62326	YES	YES
64	b	1583.39	64.47100	YES	YES
65	a	1587.32	0.00001	YES	YES
66	b	1633.71	1.93232	YES	YES
67	a	1634.15	49.17207	YES	YES
68	a	3180.93	2.27380	YES	YES
69	b	3181.37	1.60378	YES	YES
70	b	3195.78	3.74287	YES	YES
71	a	3196.14	0.16451	YES	YES
72	a	3213.35	21.57955	YES	YES
73	b	3213.37	0.19093	YES	YES
74	b	3214.88	2.63626	YES	YES
75	a	3214.95	0.75688	YES	YES

[Au(o-dfb)(CO)]$^+$
Symmetry: c1
Cartesian coordinates in Ångström:

Au	1.6780005	1.0381383	0.0506780
C	-0.9446913	-0.9076500	-1.2020267
C	-0.7066372	0.4487857	-1.2292015
F	-1.0972362	-1.5917888	-2.3234416
C	-0.5340900	1.1527985	-0.0022612
C	-0.6524808	0.4471294	1.2275968
C	-0.8903396	-0.9203529	1.2307066
C	-1.0475568	-1.5837816	0.0230625
H	-0.6881030	0.9668078	-2.1779772
F	-1.2906668	-2.8770954	0.0063418
H	-0.9820375	-1.4789974	2.1513343
H	-0.6001430	0.9885324	2.1615253
H	-0.6372966	2.2335872	-0.0052464
C	3.6370126	1.0348691	0.0455151
O	4.7562655	1.0490177	0.0433941

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	41.41	0.18377	YES	YES
8	a	55.53	0.23474	YES	YES
9	a	67.72	1.47300	YES	YES
10	a	74.10	0.78316	YES	YES
11	a	167.31	0.63582	YES	YES
12	a	253.56	0.52669	YES	YES
13	a	293.93	0.35766	YES	YES
14	a	360.13	0.15434	YES	YES
15	a	369.93	7.22056	YES	YES
16	a	373.19	5.95074	YES	YES
17	a	389.35	14.56849	YES	YES
18	a	444.72	1.27093	YES	YES
19	a	465.25	2.76657	YES	YES
20	a	553.62	6.87950	YES	YES
21	a	573.31	11.35834	YES	YES
22	a	598.14	5.26224	YES	YES
23	a	732.00	2.78516	YES	YES
24	a	781.77	18.47536	YES	YES
25	a	848.13	76.54458	YES	YES
26	a	867.69	21.25344	YES	YES
27	a	890.95	22.96250	YES	YES
28	a	961.98	25.02090	YES	YES
29	a	994.60	27.05698	YES	YES
30	a	1021.36	2.73145	YES	YES
31	a	1112.06	10.09235	YES	YES
32	a	1176.78	4.43954	YES	YES
33	a	1254.11	30.00958	YES	YES
34	a	1296.14	35.05243	YES	YES
35	a	1325.82	140.66743	YES	YES
36	a	1374.69	6.24248	YES	YES
37	a	1469.38	30.82930	YES	YES
38	a	1538.47	254.59402	YES	YES

39	a	1590.81	100.08664	YES	YES
40	a	1620.30	50.53258	YES	YES
41	a	2269.60	448.21116	YES	YES
42	a	3145.38	9.06225	YES	YES
43	a	3201.61	2.02940	YES	YES
44	a	3206.46	11.94538	YES	YES
45	a	3214.12	8.84219	YES	YES

o-dfb
Symmetry: c2v
Cartesian coordinates in Ångström:

H	1.2390071	0.0000000	-2.1769595
H	2.4758962	0.0000000	-0.0113956
F	1.3492114	0.0000000	2.3225347
C	1.3954532	0.0000000	-0.0412187
C	0.6943789	0.0000000	1.1502596
C	-0.6943789	0.0000000	1.1502596
F	-1.3492114	0.0000000	2.3225347
C	-1.3954532	0.0000000	-0.0412187
C	-0.6948598	0.0000000	-1.2431320
C	0.6948598	0.0000000	-1.2431320
H	-1.2390071	0.0000000	-2.1769595
H	-2.4758962	0.0000000	-0.0113956

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a2	188.40	0.00000	NO	YES
8	a1	288.40	0.22991	YES	YES
9	b2	292.75	0.01938	YES	YES
10	b1	444.75	0.07729	YES	YES
11	b2	463.70	3.68288	YES	YES
12	b1	552.90	3.67970	YES	YES
13	a2	565.47	0.00000	NO	YES
14	a1	584.99	4.84546	YES	YES
15	a2	704.45	0.00000	NO	YES
16	b2	767.10	80.37443	YES	YES
17	a1	778.51	33.79457	YES	YES
18	a2	857.84	0.00000	NO	YES
19	b1	865.07	19.60648	YES	YES
20	b2	948.91	4.77600	YES	YES
21	a2	972.97	0.00000	NO	YES
22	a1	1050.18	6.55896	YES	YES
23	b1	1125.87	21.07062	YES	YES
24	a1	1178.64	1.18617	YES	YES
25	b1	1222.85	40.61803	YES	YES
26	b1	1292.49	3.69984	YES	YES
27	a1	1297.08	142.56419	YES	YES
28	a1	1335.99	0.05318	YES	YES
29	b1	1494.70	11.16537	YES	YES
30	a1	1544.94	182.15826	YES	YES
31	b1	1643.72	8.40292	YES	YES
32	a1	1648.22	21.81101	YES	YES
33	b1	3183.93	1.01254	YES	YES
34	a1	3195.05	7.92313	YES	YES
35	b1	3203.23	3.02252	YES	YES
36	a1	3208.85	1.93719	YES	YES

[o-dfb]$^+$
Symmetry: c2v
Cartesian coordinates in Ångström:

H	1.2376139	0.0000000	-2.1659502
H	2.5217220	0.0000000	-0.0198233
F	1.3147935	0.0000000	2.2998106
C	1.4411946	0.0000000	-0.0425829
C	0.7265965	0.0000000	1.1449965
C	-0.7265965	0.0000000	1.1449965
F	-1.3147935	0.0000000	2.2998106
C	-1.4411946	0.0000000	-0.0425829
C	-0.7199454	0.0000000	-1.2164506
C	0.7199454	0.0000000	-1.2164506
H	-1.2376139	0.0000000	-2.1659502
H	-2.5217220	0.0000000	-0.0198233

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a2	149.23	0.00000	NO	YES
8	b2	260.72	0.07748	YES	YES
9	a1	298.91	1.80515	YES	YES
10	b1	395.28	4.27031	YES	YES
11	a2	421.66	0.00000	NO	YES
12	b2	452.04	0.17637	YES	YES
13	b1	533.14	12.60357	YES	YES
14	a1	572.99	3.19278	YES	YES
15	a2	732.76	0.00000	NO	YES
16	a1	763.77	11.12891	YES	YES
17	b2	780.44	80.45664	YES	YES
18	b1	857.50	5.38045	YES	YES
19	a2	877.99	0.00000	NO	YES
20	a1	982.11	12.37555	YES	YES
21	b2	992.64	7.59263	YES	YES
22	a2	1010.80	0.00000	NO	YES
23	b1	1125.77	24.99350	YES	YES
24	a1	1196.51	2.50523	YES	YES
25	b1	1206.64	6.09384	YES	YES
26	b1	1345.26	11.99666	YES	YES
27	a1	1364.36	50.77697	YES	YES
28	a1	1400.83	4.89016	YES	YES
29	b1	1473.32	81.74663	YES	YES
30	a1	1515.64	606.20521	YES	YES
31	b1	1534.74	8.25084	YES	YES
32	a1	1576.76	12.20859	YES	YES
33	b1	3202.14	0.07421	YES	YES
34	a1	3209.34	3.89564	YES	YES
35	b1	3216.97	43.73246	YES	YES
36	a1	3219.51	6.34992	YES	YES

$[Au(4FB)_2)]^+$
Symmetry: c2
Cartesian coordinates in Ångström:

H	-2.31510	1.13454	-0.97894
C	0.86050	-2.63678	-1.39455
F	-1.05345	2.61288	-2.70610
C	1.54447	-1.76796	-0.56412
F	1.05345	-2.61288	-2.70610
C	1.30224	-1.79349	0.84197
C	0.40243	-2.75877	1.35567
C	-0.26957	-3.62487	0.51136
F	0.67819	4.38879	-1.66153
C	-0.03451	-3.56580	-0.86648
Au	0.00000	-0.00000	0.57424
C	-0.86050	2.63678	-1.39455
H	2.31510	-1.13454	-0.97894
C	0.03451	3.56580	-0.86648
C	0.26957	3.62487	0.51136
F	1.12107	4.51141	0.98930
C	-0.40243	2.75877	1.35567
C	-1.30224	1.79349	0.84197
C	-1.54447	1.76796	-0.56412
F	-0.67819	-4.38879	-1.66153
H	-2.03321	1.37594	1.52551
F	-0.22525	2.85664	2.66078
F	-1.12107	-4.51141	0.98930
F	0.22525	-2.85664	2.66078
H	2.03321	-1.37594	1.52551

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	2.70	0.41176	YES	YES

8	a	25.68	0.00163	YES	YES
9	b	26.42	0.23565	YES	YES
10	b	32.26	1.79660	YES	YES
11	a	39.25	1.01631	YES	YES
12	a	50.58	0.07382	YES	YES
13	b	83.45	0.74054	YES	YES
14	a	117.09	0.04492	YES	YES
15	b	130.34	1.30257	YES	YES
16	a	151.06	0.00101	YES	YES
17	b	151.11	0.79433	YES	YES
18	a	234.91	0.17571	YES	YES
19	b	240.24	2.08583	YES	YES
20	b	280.79	0.13903	YES	YES
21	a	280.90	0.02494	YES	YES
22	b	287.41	0.69243	YES	YES
23	a	287.64	1.35271	YES	YES
24	b	324.93	3.59131	YES	YES
25	a	325.25	0.01321	YES	YES
26	b	331.42	0.66759	YES	YES
27	a	332.17	0.16071	YES	YES
28	b	396.62	28.26889	YES	YES
29	a	412.57	0.02999	YES	YES
30	a	456.92	0.41167	YES	YES
31	b	457.22	1.99875	YES	YES
32	a	486.93	0.06471	YES	YES
33	b	487.16	2.63078	YES	YES
34	b	565.64	22.56099	YES	YES
35	a	572.00	0.52853	YES	YES
36	b	609.90	4.73815	YES	YES
37	a	611.43	1.74288	YES	YES
38	a	651.35	0.51722	YES	YES
39	b	651.85	2.87532	YES	YES
40	a	694.19	0.58563	YES	YES
41	b	695.41	30.25530	YES	YES
42	b	740.86	4.38457	YES	YES
43	a	741.86	2.31848	YES	YES
44	b	759.77	0.45340	YES	YES
45	a	761.03	19.44334	YES	YES
46	b	869.00	133.20553	YES	YES
47	a	870.99	1.21653	YES	YES
48	b	930.09	96.36516	YES	YES
49	a	946.37	21.41899	YES	YES
50	b	1015.92	7.55522	YES	YES
51	a	1016.34	180.74232	YES	YES
52	b	1066.55	134.71660	YES	YES
53	a	1067.67	2.10248	YES	YES
54	b	1188.82	66.68657	YES	YES
55	a	1190.04	2.02189	YES	YES
56	b	1257.08	18.45081	YES	YES
57	a	1258.47	152.58998	YES	YES
58	b	1310.77	157.77858	YES	YES
59	a	1316.65	21.08864	YES	YES
60	b	1321.81	54.53107	YES	YES
61	a	1326.28	0.37633	YES	YES
62	b	1359.02	18.54915	YES	YES
63	a	1362.74	10.34417	YES	YES
64	b	1511.32	93.79311	YES	YES
65	a	1515.26	515.35769	YES	YES
66	b	1531.08	694.19151	YES	YES
67	a	1537.36	60.92493	YES	YES
68	b	1608.50	35.38119	YES	YES
69	a	1609.71	84.70087	YES	YES
70	b	1630.34	15.82832	YES	YES
71	a	1632.07	114.94274	YES	YES
72	a	3163.96	9.74795	YES	YES
73	b	3164.02	17.26386	YES	YES
74	b	3210.76	21.35363	YES	YES
75	a	3210.79	0.87156	YES	YES

[Au(4FB)(CO)]⁺
Symmetry: c1
Cartesian coordinates in Ångström:

Au	1.7337163	1.0673226	0.0596135
C	-0.9948095	-0.9348934	-1.2130310
C	-0.7131586	0.4235704	-1.2252479
F	-1.1883481	-1.5946065	-2.3355897
C	-0.4763676	1.1309794	-0.0177880
C	-0.6240921	0.4324207	1.2221203
C	-0.9019125	-0.9154654	1.2181766
C	-1.0950765	-1.6000081	0.0103767

```
F    -0.6986207    1.0677638   -2.3741236
F    -1.3642503   -2.8803331    0.0221363
F    -1.0122254   -1.5948832    2.3473318
H    -0.5602299    0.9616548    2.1621662
H    -0.6142587    2.2085432   -0.0407222
C     3.6956774    1.0982572    0.0795544
O     4.8139563    1.1296778    0.0850266

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             38.34         0.07708       YES     YES
     8        a             46.13         0.12883       YES     YES
     9        a             66.67         0.64593       YES     YES
    10        a             73.13         0.25615       YES     YES
    11        a            124.76         0.40460       YES     YES
    12        a            150.27         0.21049       YES     YES
    13        a            249.88         1.67460       YES     YES
    14        a            280.79         0.09942       YES     YES
    15        a            288.57         0.64238       YES     YES
    16        a            326.22         0.99878       YES     YES
    17        a            327.73         1.10100       YES     YES
    18        a            368.79         5.83817       YES     YES
    19        a            369.45         6.23216       YES     YES
    20        a            384.60        11.23649       YES     YES
    21        a            427.83         7.00202       YES     YES
    22        a            457.29         1.81446       YES     YES
    23        a            487.95         1.07963       YES     YES
    24        a            574.74         9.90095       YES     YES
    25        a            614.39         2.50247       YES     YES
    26        a            659.01         1.15111       YES     YES
    27        a            695.17        12.52021       YES     YES
    28        a            747.50         5.55508       YES     YES
    29        a            761.95         9.44558       YES     YES
    30        a            874.09        79.99588       YES     YES
    31        a            934.93        68.95944       YES     YES
    32        a           1018.94        94.96313       YES     YES
    33        a           1067.68        57.93478       YES     YES
    34        a           1192.80        41.67182       YES     YES
    35        a           1259.49        74.21409       YES     YES
    36        a           1316.36        65.80889       YES     YES
    37        a           1326.98        12.57306       YES     YES
    38        a           1373.73        11.61917       YES     YES
    39        a           1514.03       312.51245       YES     YES
    40        a           1535.49       376.31045       YES     YES
    41        a           1605.33        98.15560       YES     YES
    42        a           1626.84        27.50599       YES     YES
    43        a           2274.79       427.41074       YES     YES
    44        a           3141.21        22.92612       YES     YES
    45        a           3210.36        16.67091       YES     YES


4FB
Symmetry: c2v
Cartesian coordinates in Ångström:
H          1.25576        0.00000       -2.16986
F          2.71867        0.00000       -0.02178
F          1.35683        0.00000        2.32039
C          1.37829        0.00000       -0.04564
C          0.69418        0.00000        1.16376
C         -0.69418        0.00000        1.16376
F         -1.35683        0.00000        2.32039
C         -1.37829        0.00000       -0.04564
C         -0.69546        0.00000       -1.24673
C          0.69546        0.00000       -1.24673
H         -1.25576        0.00000       -2.16986
F         -2.71867        0.00000       -0.02178

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
```

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a2	155.58	0.00000	NO	YES
8	b2	156.12	1.47479	YES	YES
9	a1	278.75	0.03725	YES	YES
10	b1	284.71	0.30491	YES	YES
11	b2	288.84	0.01737	YES	YES
12	a1	324.54	1.98548	YES	YES
13	a2	374.73	0.00000	NO	YES
14	a1	461.99	0.05570	YES	YES
15	b1	491.79	0.01339	YES	YES
16	a2	550.23	0.00000	NO	YES
17	b2	609.40	7.87094	YES	YES
18	b1	610.85	1.88768	YES	YES
19	a1	694.72	20.33590	YES	YES
20	a2	715.09	0.00000	NO	YES
21	b1	756.50	19.00484	YES	YES
22	b2	817.37	42.44647	YES	YES
23	a2	928.22	0.00000	NO	YES
24	b1	999.65	150.93449	YES	YES
25	a1	1066.96	73.68524	YES	YES
26	a1	1182.91	24.61319	YES	YES
27	b1	1257.14	71.04232	YES	YES
28	b1	1282.93	28.93074	YES	YES
29	a1	1325.68	0.85646	YES	YES
30	a1	1348.25	33.04320	YES	YES
31	a1	1536.73	171.82431	YES	YES
32	b1	1542.24	290.10518	YES	YES
33	a1	1657.46	5.80957	YES	YES
34	b1	1657.53	14.09743	YES	YES
35	b1	3207.42	0.61940	YES	YES
36	a1	3218.88	0.63538	YES	YES

$[4FB]^+$
Symmetry: c1
Cartesian coordinates in Ångström:

H	1.2606955	-0.0000878	-2.1835324
F	2.6479095	0.0000544	-0.0046948
F	1.3617135	0.0000375	2.3303407
C	1.3553906	0.0000122	-0.0284140
C	0.6724076	0.0000332	1.2234954
C	-0.6992791	0.0000010	1.2200219
F	-1.3942224	-0.0001650	2.3235705
C	-1.3746931	0.0000552	-0.0351729
C	-0.6865290	0.0000206	-1.2783633
C	0.6745721	-0.0000415	-1.2749898
H	-1.2679654	-0.0000139	-2.1899416
F	-2.6673698	0.0000941	-0.0198797

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	128.57	3.58609	YES	YES
8	a	134.84	0.00004	YES	YES
9	a	271.93	0.07496	YES	YES
10	a	277.60	0.17145	YES	YES
11	a	286.49	1.76158	YES	YES
12	a	328.04	0.00002	YES	YES
13	a	341.63	5.64354	YES	YES
14	a	409.16	16.65370	YES	YES
15	a	453.44	0.94840	YES	YES
16	a	566.74	0.00013	YES	YES
17	a	603.57	4.73985	YES	YES
18	a	606.67	0.00424	YES	YES
19	a	683.60	20.75113	YES	YES
20	a	723.41	0.00000	YES	YES
21	a	748.54	18.51985	YES	YES
22	a	831.08	46.37591	YES	YES
23	a	982.94	0.00007	YES	YES
24	a	1010.54	11.59141	YES	YES
25	a	1104.52	65.82208	YES	YES
26	a	1223.37	52.27512	YES	YES
27	a	1227.08	10.97479	YES	YES
28	a	1349.89	157.60202	YES	YES

29	a	1363.53	21.60245	YES	YES
30	a	1383.64	252.69671	YES	YES
31	a	1440.77	1.87827	YES	YES
32	a	1491.43	604.62316	YES	YES
33	a	1597.22	181.24968	YES	YES
34	a	1686.08	45.48198	YES	YES
35	a	3209.30	7.33274	YES	YES
36	a	3218.64	44.38766	YES	YES

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