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Halogen bonding between entirely negative fluorine atoms? Evidence from the crystal packing of some gold(I) and gold(III) complexes with extensively fluorinated *m*-terphenyl ligands and triphenylphosphane

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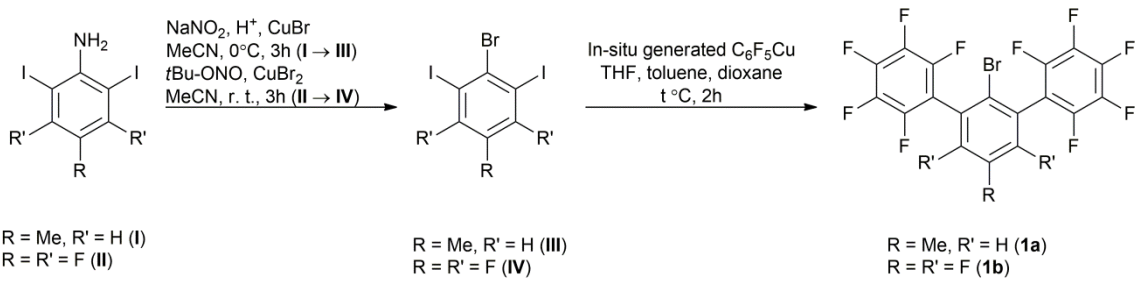
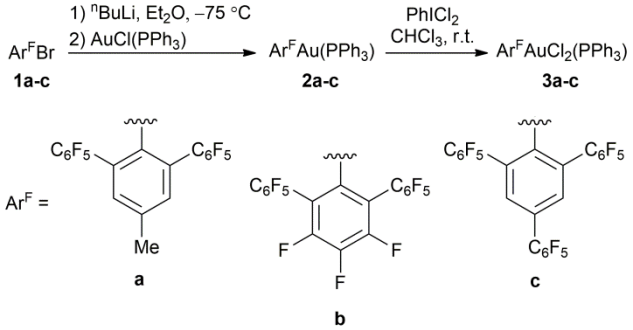


Scheme S1. Synthesis of proligands **1a** and **1b** starting from the corresponding iodo-substituted anilines **I** and **II**.



Scheme S2. Synthesis of the gold complexes 2a-c and 3a-c.

General experimental details

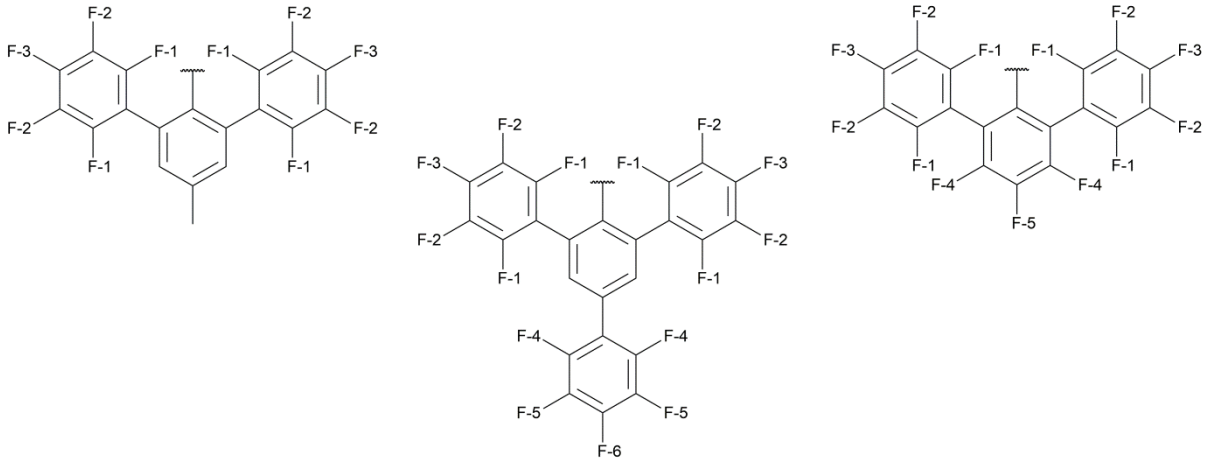
Compounds **I**, **II**, **III** and **3a-3c,** were prepared in air, while the syntheses of **IV**, **1a-c** and **2a-c** were performed under argon using standard Schlenk techniques, with work-up carried out in air. Where required, solvents were dried by standard procedures and were freshly distilled under argon prior to use. Bromopentafluorobenzene, 3,4,5-trifluoroaniline, *p*-toluidine, *tert*-butyl nitrite (90%), butyllithium (1.6M in hexanes) and triphenylphosphane were purchased from commercial suppliers and used without further purification. Aniline was distilled before it was used. The other starting materials were prepared according to known (**1c**,[1] AuCl(tht),[2] $PhICl_2$;[3]) or modified literature procedures (2,6-I_2-4-$MeC_6H_2NH_2$ (**I**),[4] 2,6-$I_2C_6F_3NH_2$ (**II**),[5] $AuCl(PPh_3)$[6]). Syntheses of the unreported aryl bromides, 2,6-I_2-4-MeC_6H_2Br (**III**) and 2,6-$I_2C_6F_3Br$ (**IV**), were also carried out by adapting literature procedures.[7,8]

The melting points are not corrected. MS/HRMS spectra were recorded on a Thermo Scientific Orbitrap XL mass spectrometer equipped with a standard ESI/APCI source. Data analysis and calculations of the theoretical isotopic patterns were carried out with the Xcalibur software package.[9] The ^{1}H, ^{13}C, ^{31}P and ^{19}F NMR spectra were recorded at room temperature on Bruker Avance III 400 or Bruker Avance III 600 instruments, while 2D ^{1}H–^{19}F HOESY experiments were recorded on a Bruker AM-400 instrument. The ^{1}H chemical shifts are reported in δ units (ppm) relative to the residual peak of the deuterated solvent ($CHCl_3$, 7.26 ppm; CHD_2CN, 1.94 ppm). The ^{13}C chemical shifts are reported in δ units (ppm) relative to the peak of the deuterated solvent ($CDCl_3$, 77.16 ppm; CD_3CN, 1.32 ppm).[10] Where possible, the ^{1}H, ^{13}C and ^{19}F resonances were assigned using 2D correlation NMR experiments (COSY, HSQC, HMBC, HOESY). The ^{31}P and ^{19}F NMR chemical shifts are reported in *δ* units (ppm) relative to H_3PO_4 (0 ppm) and $CFCl_3$ (0 ppm), respectively, using the chemical shift of the lock solvent as a reference. The NMR spectra were processed using the MestReNova software.[11] For proligands **1a**-**1b** and gold(I) complexes ^{19}F were assigned according to numbering in Scheme S3. For gold(III) species, numbering in Scheme S4 was used, in accordance with the restricted rotation around C–C bonds connecting the flanking C_6F_5 rings to the central aromatic ring (*vide infra*). ^{1}H and ^{13}C resonances for the triphenylphosphane in gold(I) complexes were attributed using *o,m,p,i*-nomenclature and for gold(III) complexes the unequivalence of the phenyl rings was indicated according to Figure S1 as Ph^a and Ph^b.

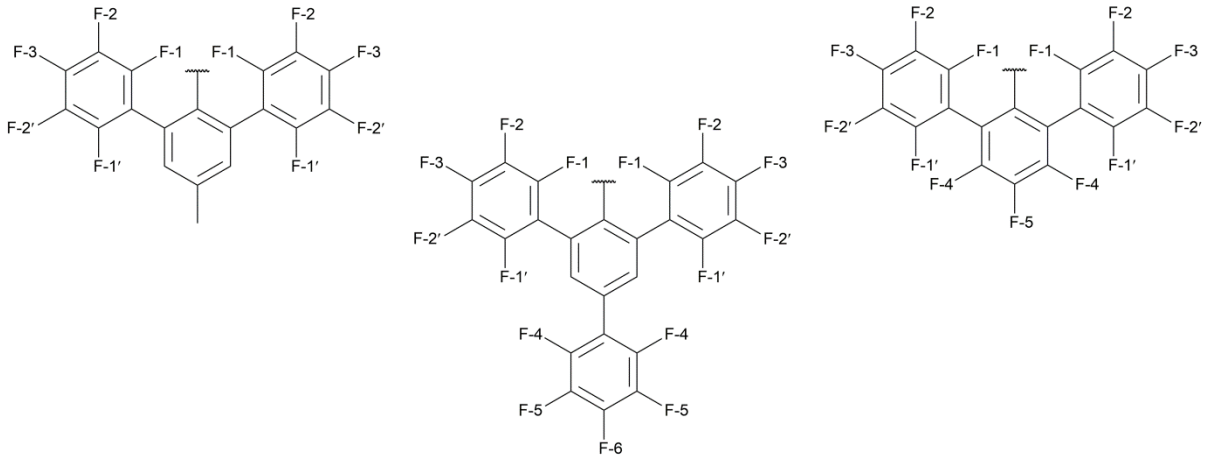
The details of the crystal structure determination and refinement for compounds **2a**-**2c** and **3a**-**3c** are given in Table S1. Data were collected on Bruker SMART APEX (**2a-2c**, **3a** and **3c**) and Agilent Technologies XCalibur (**3b**)

diffractometers, using graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å). For this purpose the crystals were attached with Paratone oil to a cryo-loop. The structures were refined with anisotropic thermal parameters. All hydrogen atoms were refined with a riding model and a mutual isotropic thermal parameter. For structure solving and refinement the SHELXL-2018 software package were used.[12] The drawings were created with the Diamond program.[13] CCDC reference numbers: 1985132 (**2a**), 1981844 (**2b**), 1985133 (**2c**), 1981845 (**3a**), 1981847 (**3b**·$CHCl_3$), 1981846 (**3c**·$CHCl_3$).

Numbering schemes for NMR assignments



Scheme S3. Numbering scheme for assignments of ^{19}F NMR resonances of the proligands and gold(I) complexes.



Scheme S4. Numbering scheme for assignments of ^{19}F NMR resonances of gold(III) complexes; ”prime” denotes atoms pointing away from the bulky triphenylphosphane group.

Synthetic procedures

Synthesis of AuCl(PPh$_3$).[14] A 50 ml round bottom flask was charged with AuCl(tht) (1.27 g, 4 mmol) and triphenylphosphane (1.05 g, 4 mmol). Toluene (40 mL) was added and the mixture stirred for 2h at room temperature. The solid was filtered off, washed with diethyl ether (3 x 5 mL) and dried at reduced pressure to yield AuCl(PPh$_3$) (1.64 g, 84%) as a white solid. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 7.44–7.55 (m, 15H). **^{31}P{^{1}H} NMR** ($CDCl_3$, 243 MHz): δ 33.17 (s).

Synthesis of 2,6-I$_2$-4-MeC$_6$H$_2$NH$_2$ (I). To a solution of *p*-toluidine (8 g, 74.66 mmol) in glacial acetic acid (250 mL) was added potassium iodide (16.52 g, 99.51 mmol) and potassium iodate (10.544 g, 49.27 mmol). The reaction mixture was stirred in an oil bath at 50 °C for 3.5 h. More potassium iodide (4.12 g, 24.88 mmol) and potassium iodate (2.64 g, 12.32 mmol) were added and stirred at 50 °C for another 1.5 h. The mixture was poured into a solution of sodium sulfite (24 g, 190.41 mmol) in water (300 mL). The brown precipitate was filtered off and dried at reduced pressure. Sublimation at 100 °C (9×10^{-3} mbar) afforded the desired aniline as a slightly yellow solid (19.95 g, 74%), m.p. 118-119 °C (lit.[15] 123.5–125 °C). **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 7.46 (s, 2H, C$_6$*H*$_2$), 4.45 (s, 2H, N*H*$_2$), 2.17 (s, 3H, Me). **^{13}C{^{1}H} NMR** ($CDCl_3$, 101 MHz): δ 143.92 (s), 139.88 (s), 131.11 (s), 81.60 (s), 19.38 (s).

Synthesis of 2,6-I$_2$C$_6$F$_3$NH$_2$ (II).[16] A 250 mL round-bottom flask was charged with glacial acetic acid (120 mL) and water (13.3 mL). Sodium chloride (23.87 g, 408.16 mmol), potassium iodide (33.87 g, 204.06 mmol), sodium *meta*-periodate (43.65 g, 204.08 mmol) and 3,4,5-trifluoroaniline (10 g, 68.02 mmol) were added under vigorous stirring. The reaction mixture was heated at 50 °C for 12 h on an oil bath. Afterward, the dark brown mixture was poured into a solution of sodium sulfite (21.71 g, 172.27 mmol) in water (270 mL) and the brown precipitate was filtered off and dried at reduced pressure to obtain the desired aniline as a slightly brown solid (25.61 g, 97%), m.p. 65-66 °C. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 4.77 (s, 2H, N*H*$_2$). **^{13}C{^{1}H} NMR** ($CDCl_3$, 151 MHz): δ 151.38 (ddd, $J_{C,F}$ = 244, 12, 6 Hz), 143.10 (m), 131.05 (dt, $J_{C,F}$ = 248, 19 Hz), 63.17 (m). **^{19}F{^{1}H} NMR** ($CDCl_3$, 565 MHz): δ −109.31 (d, $J_{F,F}$ = 24 Hz, 2F), −167.16 (t, $J_{F,F}$ = 23 Hz, 1F).

Synthesis of 2,6-I$_2$-4-MeC$_6$H$_2$Br (III). A suspension of 2,6-I$_2$-4-MeC$_6$H$_2$NH$_2$ (**I**, 1.436 g, 4 mmol) and *p*-toluenesulfonic acid monohydrate (2.283 g, 12 mmol) in acetonitrile (60 mL) was cooled to 0 °C. A solution of sodium nitrite (0.552 g, 8 mmol) in water (2 mL) was added dropwise *via* syringe. The reaction mixture was stirred at 0 °C for 30 min, then copper(I) bromide (1.435 g, 10 mmol) was added portion-wise and the mixture stirred for another 3 h at 0 °C. The suspension was taken out from the ice bath and after reaching room temperature, distilled water was added (50 mL). The aqueous phase was extracted with dichloromethane (3×50 mL). The combined organic phases were dried over anhydrous $MgSO_4$ and filtered, followed by removal of the solvents using a rotary evaporator. The crude product was partially purified by column chromatography (silica gel, hexane) yielding **III** in a mixture with an unidentified impurity (5-10%) as a white solid (0.90 g), m.p. 110-111 °C. The product was used without further purification for the synthesis of the proligand **1a**. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 7.67 (s, 2H, C$_6$*H*$_2$), 2.20 (s, 3H, Me). **^{13}C{^{1}H} NMR** ($CDCl_3$, 101 MHz): δ 140.99 (s), 140.37 (s), 132.64 (s), 99.70 (s), 19.89 (s). **HRMS** (APCI+, MeCN), *m/z* : [M$^+$] calcd. for $C_7H_5BrI_2$, 421.76585; Found, 421.76495.

Synthesis of 2,6-I$_2$C$_6$F$_3$Br (IV). A 100 mL three-necked round-bottom flask fitted with argon inlet and dropping funnel was charged with copper(II) bromide (4.45 g, 19.92 mmol). Acetonitrile (42 mL) was collected in the dropping funnel and part of it (15 mL) was introduced into the flask. *tert*-Butyl nitrite (90%, 2.60 g, 22.69 mmol) was added into the flask and the solution introduced in a water bath at room temperature. 2,6-I$_2$C$_6$F$_3$NH$_2$ (**II**, 6.57 g, 16.47 mmol) was added over the remaining acetonitrile (27 mL) from the dropping funnel and the resulting solution added dropwise over 1 h. The reaction mixture was stirred for further 2 h at room temperature. Water was added (60 mL) and the mixture extracted with diethyl ether (3 × 40 mL). The combined organic fractions were washed with brine (40 mL), dried over anhydrous Na_2SO_4, filtered and the solvent removed using a rotary evaporator to afford **IV** as an orange solid (6.93 g, 91%), m.p. 66-67 °C. **^{13}C{^{1}H} NMR** ($CDCl_3$, 151 MHz): δ 151.90 (ddd, $J_{C,F}$ = 250, 11, 5 Hz), 137.02 (dt, $J_{C,F}$ = 261, 19 Hz), 130.88 (d, $J_{C,F}$ = 5 Hz), 84.27 (m). **^{19}F{^{1}H} NMR** ($CDCl_3$, 376 MHz): δ −99.75 (d, $J_{F,F}$ = 22 Hz, 2F), −152.97 (t, $J_{F,F}$ = 22 Hz, 1F). **HRMS** (APCI+, MeCN), *m/z* : [M$^+$] calcd. for $C_6F_3BrI_2$, 461.72193; Found, 461.72144.

Synthesis of 2,6-(C$_6$F$_5$)$_2$-4-MeC$_6$H$_2$Br (1a). A 100 mL three-necked round-bottom flask fitted with argon inlet, dropping funnel and reflux condenser was charged with magnesium turnings (0.53 g, 22 mmol). THF (25 mL) was collected in the dropping funnel and a part of it (10 mL) was added into the flask. C_6F_5Br (4.94 g, 20 mmol) was

added to the remaining solvent in the dropping funnel. 1,2-$Br_2C_2H_4$ (0.37 g, 2 mmol) was introduced in the flask and the content carefully heated to reflux. Under vigorous stirring and gentle heating, the content of the dropping funnel was added dropwise into the flask. The reaction mixture was stirred at 86 °C for 1.5 h and then allowed to reach room temperature. Another 100 mL three-necked round-bottom flask fitted with argon inlet, dropping funnel and reflux condenser was charged with anhydrous copper(I) bromide (3.012 g, 21 mmol) and the dark brown solution of C_6F_5MgBr in THF (25 mL) was added *via* syringe . The resulting brown suspension was stirred at room temperature for 20 min and dioxane (7 mL) was added. After 30 min of stirring, a solution of 2,6-I_2-4-MeC_6H_2Br (**III**, 2.513 g, 6 mmol) in toluene (25 mL) was added dropwise from the dropping funnel. The reaction mixture was stirred at 75 °C on an oil bath for 2 h, allowed to reach room temperature and filtered through a pad of silica and washed with diethyl ether. The solvents were removed from the filtrate using a rotary evaporator. The remaining solid was heated 50-75 °C (9×10^{-3} mbar) for 3-4 hours in a sublimation apparatus to remove decafluorobiphenyl and other oily impurities. Further sublimation at 80 °C afforded **1a** as a white solid (2.02 g, 67%), m.p. 105-106 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 7.23 (s, 2H, C_6H_2), 2.43 (s, 3H, Me). **^{13}C{^{1}H} NMR** ($CDCl_3$, 101 MHz): δ 144.25 (dm, $^1J_{C,F}$ = 249 Hz), 141.53 (dm, $^1J_{C,F}$ = 257 Hz), 138.37 (s), 137.85 (dm, $^1J_{C,F}$ = 255 Hz), 133.96 (s), 129.46 (s), 122.95 (s), 115.30 (td, $J_{C,F}$ = 19 and 4 Hz), 20.92 (s). **^{19}F{^{1}H} NMR** ($CDCl_3$, 376 MHz): δ −129.48 (m, 4F, F-1), −153.63 (t, $J_{F,F}$ = 21 Hz, 2F, F-3), −161.77 (tt, $J_{F,F}$ = 21 and 5 Hz, 4F, F-2). **HRMS** (APCI+, MeCN), *m/z* : [M^+] calcd. for $C_{19}H_5F_{10}Br$, 501.94095; Found, 501.94133.

Synthesis of 2,6-(C_6F_5)$_2$$C_6F_3Br$ (1b). The procedure was similar to **1a**. Amounts used: magnesium turnings (1.85 g, 76.13 mmol), THF (80 mL, of which 20 mL were added into the flask); C_6F_5Br (18.4 g, 74.51 mmol), 1,2-$Br_2C_2H_4$ (0.3 g, 1.6 mmol), anhydrous copper(I) bromide (11.8 g, 82.26 mmol), dioxane (25 mL), 2,6-$I_2C_6F_3Br$ (**IV**, 11 g, 23.77 mmol), toluene (80 mL). Comments: The solution of C_6F_5MgBr was transferred *via* cannula over 5 min. The reaction mixture was stirred at 60 °C for 2 h, allowed to reach room temperature and quenched with methanol (6 mL). For the sublimation, the temperature was slowly increased up to 85 °C to obtain **1b** as a white solid (7.4 g, 58%), m.p. 109-111 °C (lit.[17] 99-100 °C) . **^{13}C{^{1}H} NMR** ($CDCl_3$, 101 MHz): δ 150.61 (dm, $^1J_{C,F}$ = 260 Hz), 144.48 (dm, $^1J_{C,F}$ = 253), 142.69 (dm, $^1J_{C,F}$ = 259), 139.89 (dt, $J_{C,F}$ = 259 and 16 Hz), 138.06 (dm, $^1J_{C,F}$ = 252 Hz), 121.76 (s), 115.46 (m), 107.61 (m). **^{19}F{^{1}H} NMR** ($CDCl_3$, 376 MHz): δ −123.93 (d, $J_{F,F}$ = 22 Hz, 2F, F-4), −137.66 (m, 4F, F-1), −150.19 (tt, $J_{F,F}$ = 21 and 3 Hz, 2F, F-3), −155.59 (t, $J_{F,F}$ = 22 Hz, 1F, F-5), −160.44 (m, 4F, F-2).

Synthesis of 2,6-(C_6F_5)$_2$-4-$MeC_6H_2Au(PPh_3)$ (2a). A 25 mL Schlenk flask was charged with 2,6-(C_6F_5)$_2$-4-MeC_6H_2Br (**1a**, 503 mg, 1 mmol) and diethyl ether (10 mL) was added. The colorless solution was cooled to −75 °C, using a liquid nitrogen-ethanol bath, and kept for 15 minutes. A solution of *n*-BuLi (1.6 M in hexane, 0.63 mL, 1 mmol) was added dropwise *via* syringe. The temperature was maintained between −70 and −75 °C for 1h. Solid $AuCl(PPh_3)$ (495 mg, 1 mmol) was added and the mixture was left to slowly warm up to −25 °C, then taken out from the bath and kept for 30 minutes at room temperature. The yellow suspension was filtered over a pad of anhydrous Na_2SO_4, in air. The pad was washed with freshly distilled diethyl ether (3 x 5 mL) and the organic fractions combined. Removal of solvent at reduced pressure gave a slightly yellow solid. The crude product was purified by column chromatography (alumina, petroleum ether until organic impurities started to be collected and then petroleum ether/ethyl acetate: 9/1). Removal of the volatiles at reduced pressure gave **2a** as a white solid (446 mg, 50%), m.p. 185-187 °C. Suitable crystals for structure determination were obtained by heptane diffusion into a solution of the compound in $CHCl_3$ (heptane/$CHCl_3$: 2/1, v/v). **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 7.49 (td, *J* = 7, 2 Hz, 3H, *p*-H), 7.41 (td, *J* = 8, 2 Hz, 6H, *m*-H), 7.29-7.23 (m, 6H, *o*-H), 7.22 (2H, C_6H_2), 2.42 (s, 3H, Me). **^{13}C{^{1}H} NMR** ($CDCl_3$, 151 MHz): δ 174.70 (d, $^2J_{C,P}$ = 113 Hz), 144.60 (dm, $^1J_{C,F}$ = 245 Hz), 139.81 (dm, $^1J_{C,F}$ = 251 Hz), 137.44 (dm, $^1J_{C,F}$ = 250 Hz), 135.58 (s), 135.40 (s), 133.99 (d, $^2J_{C,P}$ = 14 Hz, *o*-C), 131.48 (d, $^4J_{C,P}$ = 3 Hz, *p*-C), 130.47 (d, $^4J_{C,P}$ = 5.5 Hz), 130.35 (d, $^1J_{C,P}$ = 52 Hz, *i*-C), 129.15 (d, $^3J_{C,P}$ = 11 Hz, *m*-C), 121.79 (t, *J* = 18 Hz), 21.26 (s). **^{19}F{^{1}H} NMR** ($CDCl_3$, 565 MHz): δ −139.55 (dd, $J_{F,F}$ = 24 and 8 Hz, F-1), −158.11 (t, $J_{F,F}$ = 21 Hz, F-3), −163.69 (ddd, $J_{F,F}$ = 24, 20 and 8 Hz, F-2). **^{31}P{^{1}H} NMR** ($CDCl_3$, 243 MHz): δ 43.21(s). **MS** (APCI+, MeCN), *m/z* (relative intensity, %): 1341.14 (35) [M^+ + $Au(PPh_3)$)], 721.15 (11) [$Au(PPh_3)_2^+$], 500.09 (100) [$Au(PPh_3)^+$ + MeCN], 459.06 (19) [$Au(PPh_3)^+$]. **HRMS** (APCI+, MeCN), *m/z* : [M^+ + $Au(PPh_3)$)] calcd. for $C_{55}H_{35}F_{10}P_2Au_2$, 1341.13799; Found, 1341.14600. **MS** (APCI−, MeCN), *m/z* (relative intensity, %): 732.97 (30) [$C_{21}H_5F_{13}O_2Au^-$], 651.98 (29) [$C_{19}H_5F_{10}O_2Au^-$], 619.99 (100) [$C_{19}H_5F_{10}Au^-$], 600.99 (47) [$C_{19}H_5F_9Au^-$], 416.01 (45) [$C_{19}H_4F_8O_2^-$]. **HRMS** (APCI−, MeCN), *m/z* : [M^- − PPh_3] calcd. for $C_{19}H_5F_{10}Au$, 619.98916; Found, 619.99011.

Synthesis of 2,6-(C_6F_5)$_2$$C_6F_3Au(PPh_3)$ (2b). A 25 mL Schlenk flask was charged with 2,6-(C_6F_5)$_2$$C_6F_3Br$ (**1b**, 542 mg, 1 mmol) and diethyl ether (10 mL) was added. The colorless solution was cooled to −75 °C and kept for 15 minutes. A solution of *n*-BuLi (1.6 M in hexane, 0.64 mL, 1.02 mmol) was added dropwise *via* syringe. After the last drops, the solution suddenly changed color from yellow to dark green. The temperature was maintained

between −70 °C and −75 °C for 30 minutes. Solid AuCl(PPh_3) (505 mg, 1.02 mmol) was added and the mixture was left to slowly warm up to −25 °C, taken out from the bath and kept for 30 minutes at room temperature. The slightly yellow suspension was filtered over a pad of anhydrous Na_2SO_4, in air. The pad was washed with freshly distilled diethyl ether (3 x 5 mL) and the organic fractions combined. Removal of solvent at reduced pressure gave slightly yellow solid. The crude product was purified by column chromatography (alumina, heptane/ethyl acetate: 9/1). The solvent was removed using a rotary evaporator, yielding a slightly yellow oil which solidified upon addition of pentane (3 mL). Removal of the volatiles at reduced pressure gave **2b** as a white solid (800 mg, 87%), m.p. 133-135 °C. Suitable crystals for structure determination were obtained by slow evaporation of the solvent from a concentrated heptane solution. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 7.51 (td, J = 7 and 2 Hz, 3H, *p*-H), 7.42 (td, J = 8 and 2 Hz, 6H, *m*-H), 7.21 (ddd, J = 12, 8 and 1 Hz, 6H, *o*-H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 101 MHz): δ 176.30 (d, $^2J_{C,P}$ = 114 Hz), 150.13 (dt, $J_{C,F}$ = 272 and 13 Hz), 144.78 (dm, $^1J_{C,F}$ = 249 Hz), 140.81 (dm, $^1J_{C,F}$ = 256 Hz), 138.40 (dt, $J_{C,F}$ = 249 and 16 Hz), 137.57 (dm, $^1J_{C,F}$ = 252 Hz), 133.88 (d, $^2J_{C,P}$ = 14 Hz, *o*-C), 131.79 (d, $^4J_{C,P}$ = 3 Hz, *p*-C), 129.60 (d, $^1J_{C,P}$ = 53 Hz, *i*-C), 129.31 (d, $^3J_{C,P}$ = 11 Hz, *m*-C), 118.34 (s), 114.26 (t, $J_{C,F}$ = 18 Hz). **^{19}F{^{1}H} NMR** ($CDCl_3$, 376 MHz): δ −131.06 (dd, $J_{F,F}$ = 21 and 6 Hz, 2F, F-4), −138.03 (dd, $J_{F,F}$ = 23 and 8 Hz, 4F, F-1), −155.05 (t, $J_{F,F}$ = 21 Hz, 2F, F-3), −162.23 (t, $J_{F,F}$ = 21 Hz, 1F, F-5), −162.63 (td, $J_{F,F}$ = 22 and 8 Hz, 4F, F-2). **^{31}P{^{1}H} NMR** ($CDCl_3$, 162 MHz): δ 42.25 (t, $^5J_{P,F}$ = 6 Hz). **MS** (APCI+, MeCN), *m/z* (relative intensity, %): 1381.09 (19) [M^+ + Au(PPh_3)], 721.15 (9) [Au(PPh_3)$_2^+$], 500.09 (100) [Au(PPh_3)$^+$ + MeCN], 459.06 (21) [Au(PPh_3)$^+$]. **HRMS** (APCI+, MeCN), *m/z* : [M^+ + Au(PPh_3)] calcd. for $C_{54}H_{30}F_{13}P_2Au_2$, 1381.09407; Found, 1381.09651. **MS** (APCI−, MeCN), *m/z* (relative intensity, %): 772.93 (23) [$C_{20}F_{16}O_2Au^-$], 678.94 (17) [$C_{18}F_{14}Au^-$], 659.95 (100) [$C_{18}F_{13}Au^-$], 640.95 (14) [$C_{18}F_{12}Au^-$], 475.97 (23) [$C_{18}F_{12}O_2^-$]. **HRMS** (APCI−, MeCN), *m/z* : [M^- − PPh_3] calcd. for $C_{18}F_{13}Au$, 659.94525; Found, 659.94520.

Synthesis of 2,4,6-(C_6F_5)$_3$$C_6H_2$Au($PPh_3$) (2c). A 25 mL Schlenk flask was charged with 2,4,6-(C_6F_5)$_3$$C_6H_2$Br (**1c**, 655 mg, 1 mmol) and anhydrous diethyl ether (10 mL) was added. The solution was cooled to −85 °C and kept for 15 minutes. A white precipitate formed. A solution of *n*-BuLi (1.6 M in hexane, 0.62 mL, 1 mmol) was added dropwise *via* syringe. The suspension was left to warm up to −70 °C and stirred for 1h between −70 °C and −75 °C. During this time, it turned into a slightly yellow solution and then suddenly a white precipitate formed. The suspension was cooled to −80 °C and solid AuCl(PPh_3) (495 mg, 1 mmol) was added. The mixture was left to slowly warm up to room temperature overnight. The colorless suspension was filtered over a pad of anhydrous Na_2SO_4, in air. The pad was washed with freshly distilled diethyl ether (3 x 5 mL) and the organic fractions combined. Removal of solvent at reduced pressure gave **2c** as a white solid (935 mg, 89%), m.p 189-191 °C. Suitable crystals for structure determination were obtained by slow evaporation of solvent from a concentrated heptane solution. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 7.51 (td, J = 7 and 2 Hz, 3H, *p*-H), 7.46 (s, 2H, C_6H_2), 7.42 (td, J = 8 and 2 Hz, 6H, *m*-H), 7.29-7.22 (m, 6H, *o*-H). **^{13}C{^{1}H} NMR** ($CDCl_3$, 151 MHz): δ 180.60 (d, $^2J_{C,P}$ = 112 Hz), 144.59 (dm, $^1J_{C,F}$ = 246 Hz), 144.25 (dm, $^1J_{C,F}$ = 249 Hz), 140.35 (dm, $^1J_{C,F}$ = 254 Hz), 140.15 (dm, $^1J_{C,F}$ = 252 Hz), 137.90 (dm, $^1J_{C,F}$ = 252 Hz), 137.55 (dm, $^1J_{C,F}$ = 250 Hz), 136.27 (s), 133.97 (d, $^2J_{C,P}$ = 14 Hz, *o*-C), 131.63 (d, $^4J_{C,P}$ = 2 Hz, *p*-C), 130.91 (d, $^4J_{C,P}$ = 5 Hz), 130.05 (d, $^1J_{C,P}$ = 52 Hz, *i*-C), 129.25 (d, $^3J_{C,P}$ = 11 Hz, *m*-C), 123.92 (s) , 120.93 (t, J = 18 Hz), 115.39 (td, J = 16, 3 Hz). **^{19}F{^{1}H} NMR** ($CDCl_3$, 565 MHz): δ −139.32 (dd, $J_{F,F}$ = 24 and 8 Hz, 4F, F-1), −142.92 (dd, $J_{F,F}$ = 23 and 8 Hz, 2F, F-4), −155.48 (t, $J_{F,F}$ = 21 Hz, 1F, F-6), −157.00 (t, $J_{F,F}$ = 21 Hz, 2F, F-3), −162.17 (td, $J_{F,F}$ = 22 and 8 Hz, 2F, F-5), −163.12 (td, $J_{F,F}$ = 23 and 8 Hz, 4F, F-2). **^{31}P{^{1}H} NMR** ($CDCl_3$, 243 MHz): δ 42.86 (s). **MS** (APCI+, MeCN), *m/z* (relative intensity, %): 1493.11 (35) [M^+ + Au(PPh_3)], 721.15 (10) [Au(PPh_3)$_2^+$], 500.09 (100) [Au(PPh_3)$^+$ + MeCN], 459.06 (14) [Au(PPh_3)$^+$]. **HRMS** (APCI+, MeCN), *m/z*: [M^+ + Au(PPh_3)] calcd. for $C_{60}H_{32}F_{15}P_2Au_2$, 1493.10653; Found, 1493.11211. **MS** (APCI−, MeCN), *m/z* (relative intensity, %): 884.94 (21) [$C_{26}H_2F_{18}O_2Au^-$], 865.94 (10) [$C_{26}H_2F_{17}O_2Au^-$], 803.95 (18) [$C_{24}H_2F_{15}O_2Au^-$], 771.96 (33) [$C_{24}H_2F_{15}Au^-$], 606.98 (12) [$C_{24}H_2F_{15}O_2^-$], 587.98 (15) [$C_{24}H_2F_{14}O_2^-$], 567.98 (100) [$C_{24}HF_{13}O_2^-$], 547.97 (54) [$C_{24}F_{12}O^-_2$]. **HRMS** (APCI−, MeCN), *m/z*: [M^- − PPh_3] calcd. for $C_{24}H_2F_{15}Au$, 771.95770; Found, 771.95815.

Synthesis of 2,6-(C_6F_5)$_2$-4-MeC_6H_2AuCl_2(PPh_3) (3a). A 10 mL round bottom flask was charged with 2,6-(C_6F_5)$_2$-4-MeC_6H_2Au(PPh_3) (**2a**, 132 mg, 0.15 mmol) and chloroform (7 mL) was added. While stirring continuously, $PhICl_2$ (48 mg, 0.17 mmol) was added portionwise over 5 min. The mixture was stirred for 2h at room temperature and then petroleum ether (30 mL) was added until no further precipitation was observed. The crude product was collected by filtration, washed with pentane (3 x 5 mL) and dried at reduced pressure to give **3a** as a white solid (95 mg, 66%), m.p. 165 °C (dec). Suitable crystals for structure determination were obtained by heptane diffusion into a solution of the compound in CH_2Cl_2 (heptane/CH_2Cl_2 : 2/1, v/v). **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 7.61-7.57 (m, 2H, *p*-H^b), 7.51 (t, J = 8 Hz and 1H, *p*-H^a), 7.41 (td, J = 8 and 3 Hz, 6H, *m*-H^a, *m*-H^b), 7.21 (dd, J = 13 and 8 Hz, 4H, *o*-H^b), 7.05 (s, 2H, C_6H_2), 6.73 (dd, J = 13 and 8 Hz, 2H, *o*-H^a), 2.40 (s, 3H, Me). **^{13}C{^{1}H} NMR** ($CDCl_3$, 151 MHz): δ 145.28 (dm, $^1J_{C,F}$ = 248 Hz), 143.66 (dm, $^1J_{C,F}$ = 240 Hz), 141.59 (s), 141.20 (dm, $^1J_{C,F}$ = 250 Hz), 138.27 (dm, $^1J_{C,F}$ =

254 Hz), 137.28 (s), 137.08 (dm, $^{1}J_{C,F}$ = 251 Hz), 135.37 (s), 134.61 (dt, *J* = 10 and 4 Hz, *o*-C^{a}), 134.27 (d, $^{2}J_{C,P}$ = 11 Hz, *o*-C^{b}), 133.15 (d, $^{4}J_{C,P}$ = 3 Hz, *p*-C^{a}), 133.10 (d, $^{4}J_{C,P}$ = 3 Hz, *p*-C^{b}), 130.82 (s), 129.14 (d, $^{3}J_{C,P}$ = 13 Hz, *m*-C^{b}), 129.05 (d, $^{3}J_{C,P}$ = 14 Hz, *m*-C^{a}), 125.47 (d, $^{1}J_{C,P}$ = 68 Hz, *i*-C^{b}), 123.45 (d, $^{1}J_{C,P}$ = 64 Hz, *i*-C^{a}), 117.77 – 117.08 (m), 20.49 (s). **^{19}F{^{1}H} NMR** ($CDCl_3$, 565 MHz): *δ* −130.47 (dd, $J_{F,F}$ = 24 and 8 Hz, 2F, F-1'), −138.01 (dd, *J* = 22, 6 Hz, 2F, F-1), −153.50 (t, *J* = 21 Hz, 2F, F-3), −160.00 (td, *J* = 23, 7 Hz, 2F, F-2'), −162.33 (td, $J_{F,F}$ = 23 and 8 Hz, 2F, F-2). **^{31}P{^{1}H} NMR** ($CDCl_3$, 243 MHz): *δ* 30.05 (s). **MS** (ESI+, MeCN), *m/z* (relative intensity, %): 1929.02 (100) [2M^{+} + Na], 975.01 (54) [M^{+} + Na]. **HRMS** (ESI+, MeCN), *m/z*: [M^{+} + Na] calcd. for $C_{37}H_{20}F_{10}Cl_2PAuNa$, 975.00777; Found, 975.00821.

Synthesis of 2,6-$(C_6F_5)_2C_6F_3AuCl_2(PPh_3)$ (3b). A 10 mL round bottom flask was charged with 2,6-$(C_6F_5)_2C_6F_3Au(PPh_3)$ (**2b**, 380 mg, 0.41 mmol) and chloroform (5 mL) was added. While stirring continuously, $PhICl_2$ (115 mg, 0.41 mmol) was added portionwise over 5 min. The mixture was stirred for 2h at room temperature and then precipitated with pentane (25 mL). The crude product was collected by filtration, washed with pentane (2 x 5 mL) and dried at reduced pressure to give **3b** as a white solid (373 mg, 91%), m.p. 210 °C (dec.). Suitable crystals for structure determination were obtained by heptane diffusion into a solution of the compound in $CHCl_3$ (heptane/$CHCl_3$: 2/1, v/v). **^{1}H NMR** ($CDCl_3$, 600 MHz): *δ* 7.67-7.57 (m, 3H, *p*-H^{a}, *p*-H^{b}), 7.44 (td, *J* = 8 and 3 Hz, 4H, *m*-H^{b}), 7.35 (td, *J* = 8 and 3 Hz, 2H, *m*-H^{a}), 7.17 (ddd, *J* = 14, 8 and 1 Hz, 4H, *o*-H^{b}), 6.80 (ddd, *J* = 13, 8 and 1 Hz, 2H, *o*-H^{a}). **^{13}C{^{1}H} NMR** ($CDCl_3$, 151 MHz): *δ* 150.71 (dm, $^{1}J_{C,F}$ = 261 Hz), 145.46 (dm, $^{1}J_{C,F}$ = 258 Hz), 144.07 (dm, $^{1}J_{C,F}$ = 252 Hz), 142.30 (dm, $^{1}J_{C,F}$ = 258 Hz), 142.29 (s), 138.82 (dm, $^{1}J_{C,F}$ = 255 Hz), 138.45 (dm, $^{1}J_{C,F}$ = 254 Hz), 137.18 (dm, $^{1}J_{C,F}$ = 252 Hz), 134.31 (m, *o*-C^{a}), 134.22 (d, *J* = 11 Hz,*o*-C^{b}), 133.96 (d, $^{4}J_{C,P}$ = 3 Hz, *p*-C^{a}), 133.53 (d, $^{4}J_{C,P}$ = 3 Hz, *p*-C^{b}), 129.58 (d, *J* = 12.1 Hz, *m*-C^{a}), 129.36 (d, *J* = 12.8 Hz, *m*-C^{b}), 124.78 (d, $^{1}J_{C,P}$ = 69 Hz, *i*-C^{b}), 123.12 (d, $^{1}J_{C,P}$ = 63 Hz, *i*-C^{a}), 116.00 (s), 109.85 (t, *J* = 17 Hz). **^{19}F{^{1}H} NMR** ($CDCl_3$, 565 MHz): *δ* −124.31 (d, $J_{F,F}$ = 16 Hz, 2F, F-4), −129.14 (d, $J_{F,F}$ = 22 Hz, 2F, F-2'), −135.75 (d, $J_{F,F}$ = 18 Hz, 2F, F-2), −150.48 (t, $J_{F,F}$ = 21 Hz, 2F, F-3), −158.17 (t, $J_{F,F}$ = 21 Hz, 1F, F-5), −159.09 (td, $J_{F,F}$ = 22 and 7 Hz, 2F, F-1'), −161.34 (td, $J_{F,F}$ = 23 and 8 Hz, 2F, F-1). **^{31}P{^{1}H} NMR** ($CDCl_3$, 243 MHz): *δ* 31.67 (s). MS (ESI+, MeCN), *m/z* (relative intensity, %): 2008.93 (56) [2M^{+} + Na], 1014.96 (100) [M^{+} + Na]. HRMS (ESI+, MeCN), *m/z*: [M^{+} + Na] calcd. for $C_{36}H_{15}F_{13}Cl_2PAuNa$, 1014.96386; Found, 1014.96354.

Synthesis of 2,4,6-$(C_6F_5)_3C_6H_2AuCl_2(PPh_3)$ (3c). A 10 mL round bottom flask was charged with 2,4,6-$(C_6F_5)_3C_6H_2AuPPh_3$ (**2c**, 510 mg, 0.5 mmol) and chloroform (7 mL) was added. While stirring continuously, $PhICl_2$ (150 mg, 0.55 mmol) was added portionwise over 5 min. The mixture was stirred for 2h at room temperature and then petroleum ether (50 mL) was added until no further precipitation was observed. The crude product was collected by filtration, washed with pentane (2 x 20 mL) and dried at reduced pressure to give **3c** as a white solid (440 mg, 80%), m.p. 209 °C (dec.). Suitable crystals for structure determination were obtained after adding petroleum ether over a solution of the compound in $CHCl_3$ (petroleum ether/$CHCl_3$: 4/3, v/v). **^{1}H NMR** (CD_3CN, 600 MHz): *δ* 7.68 (tdd, *J* = 6, 3 and 1 Hz, 2H, *p*-H^{b}), 7.57 (tdt, *J* = 7, 2 and 1Hz, 1H, *p*-H^{a}), 7.53-7.47 (m, 4H, *m*-H^{b}), 7.45 (s, 2H, C_6H_2), 7.30-7.23 (m, 2H, *m*-H^{a}), 7.21-7.10 (m, 4H, *o*-H^{b}), 6.78-6.70 (m, 2H, *o*-H^{a}). **^{13}C{^{1}H} NMR** (CD_3CN, 151 MHz): *δ* 147.67 (s), 146.07 (dm, $^{1}J_{C,F}$ = 249 Hz), 145.26 (dm, $^{1}J_{C,F}$ = 246 Hz), 144.92 (dm, $^{1}J_{C,F}$ = 248 Hz), 142.44 (dm, $^{1}J_{C,F}$ = 254 Hz), 142.02 (dm, $^{1}J_{C,F}$ = 252 Hz), 139.03 (dm, $^{1}J_{C,F}$ = 251 Hz), 138.32 (dm, $^{1}J_{C,F}$ = 251 Hz), 136.83 (s), 135.31 (dt, *J* = 10 and 4 Hz, *o*-C^{a}), 135.09 (d, $^{2}J_{C,P}$ = 1, *o*-C^{b} Hz), 134.39 (d, $^{4}J_{C,P}$ = 3 Hz, *p*-C^{a}), 134.31 (d, $^{4}J_{C,P}$ = 3 Hz, *p*-C^{b}), 132.58 (s), 130.23 (d, $^{3}J_{C,P}$ = 13 Hz, *m*-C^{a}, *m*-C^{b}), 127.00 (s), 125.95 (d, $^{1}J_{C,P}$ = 69 Hz, *i*-C^{b}), 123.89 (d, $^{1}J_{C,P}$ = 64 Hz, *i*-C^{a}), 117.46 (td, *J* = 18, 4 Hz), 114.36 (td, *J* = 18, 4 Hz). **^{19}F{^{1}H} NMR** (CD_3CN, 565 MHz): *δ* −132.93 (dd, $J_{F,F}$ = 23 and 7 Hz, 2F, F-1'), −137.99 (dd, $J_{F,F}$ = 24 and 7 Hz, 2F, F-1), −144.55 (dd, $J_{F,F}$ = 22 and 8 Hz, 2F, F-4), −154.81 (t, $J_{F,F}$ = 20 Hz, 2F, F-3), −156.27 (t, $J_{F,F}$ = 20 Hz, 1F, F-6), −162.82 (td, $J_{F,F}$ = 22 and 8 Hz, 2F, F-2'), −163.53 (td, $J_{F,F}$ = 22 and 7 Hz, 2F, F-2), −164.01 (td, $J_{F,F}$ = 22 and 8 Hz, 2F, F-5). **^{31}P{^{1}H} NMR** (CD_3CN, 243 MHz): *δ* 31.82 (s). MS (ESI+, MeCN), *m/z* (relative intensity, %): 2232.96 (61) [2M^{+} + Na], 1563.05 (28) [M^{+} + Au(PPh_3)], 1126.98 (19) [M^{+} + Na], 953.08 (100) [$Au_2Cl(PPh_3)_2^{+}$]. HRMS (ESI+, MeCN), *m/z*: [M^{+} + Na] calcd. for $C_{42}H_{17}F_{15}Cl_2PAuNa$, 1126.97631; Found, 1126.97914.

Through space coupling

For gold(III) complexes **3a-c** the ^{1}H NMR and ^{13}C NMR spectra reveal a 2:1 (Ph^{b} : Ph^{a}) ratio for the phenyl rings of the phosphane, while $^{19}F\{^{1}H\}$ NMR spectra show that fluorine atoms in *ortho* and *meta* positions belonging to the flanking C_6F_5 groups become unequivalent. Another remarkable feature in their ^{13}C NMR spectra is the presence of a complex multiplet, instead of a simple doublet, for the carbon atom in *ortho* position of the phenyl lying above the fluorinated ligand (Ph^{a}). Thus, for example, the multiplet at δ 135.4 ppm observed for **3b**, in CD_3CN (Figure S1), is in fact a doublet of triplets revealing the expected $^{2}J_{CP}$ coupling (9.9 Hz) and an additional $^{8}J_{CF}$ through-space coupling (4.4 Hz). A similar behavior was also observed for **3a** ($^{8}J_{CF}$ 3.8 Hz) and **3c** ($^{8}J_{CF}$ 3.8 Hz). The absence of the coupling between fluorine atoms and the *ipso* carbon atom or the phosphorous atom excludes a classical through-bond transmission pathway or *via* intramolecular Au···F contact. Through-space ^{13}C–^{19}F coupling up to six bonds have been observed before.[18] However, this is the first report of such coupling occurring between atoms linked through eight covalent bonds. Coupling is most probably transmitted through the intermediate C_o–H bond.[19] Short contact distances between one of the two (F,H-*ortho*) pairs have been observed in the crystal structures [2.46 Å, **3a**; 2.29 Å, **3b**; 2.64 Å, **3c**]. In solution, the close proximity between the hydrogen atoms attached to C_o atoms and the fluorine atoms was confirmed by 2D ^{1}H–^{19}F HOESY experiments (*vide infra* Figure S42 and Figure S47).

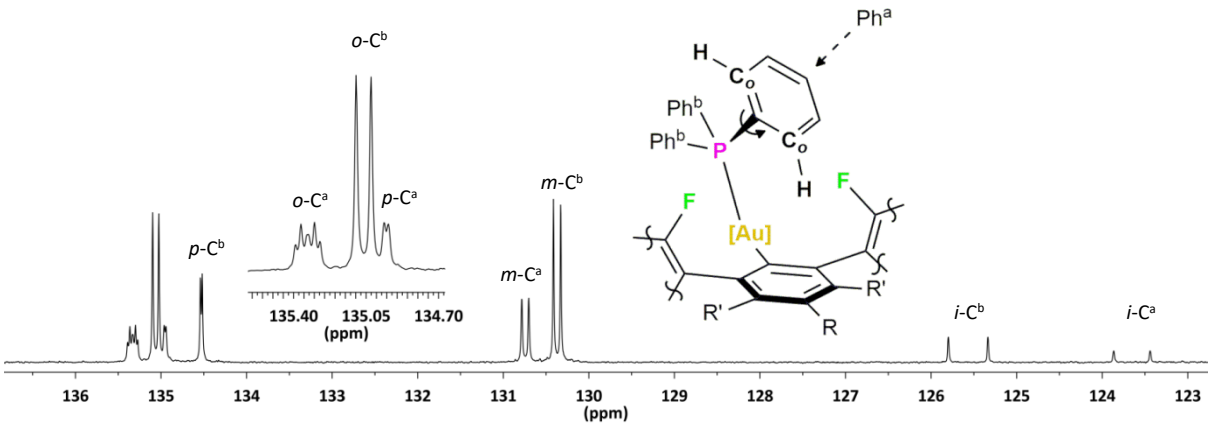


Figure S1. Detail from the ^{13}C-NMR spectrum of **3b** (CD_3CN, 151 MHz) showing the unequivalence of the phenyl rings Ph^{a} and Ph^{b}, in a 1:2 ratio, which results in two sets of corresponding ^{13}C resonances.

Crystallographic data

Tables S1-S6

Table S1. Crystal data and structure refinement details for compounds **2a-c** and **3a-c**.

Compound	**2a**	**2b**	**2c**	**3a**	**3b**·$CHCl_3$	**3c**·$CHCl_3$
CCDC no.	1985132	1981844	1985133	1981845	1981847	1981846
Formula	$C_{37}H_{20}AuF_{10}P$	$C_{36}H_{15}AuF_{13}P$	$C_{42}H_{17}AuF_{15}P$	$C_{37}H_{20}AuCl_2F_{10}P$	$C_{36}H_{15}AuCl_2F_{13}P{\cdot}CHCl_3$	$C_{42}H_{17}AuCl_2F_{15}P{\cdot}CHCl_3$
Formula weight	882.47	922.42	1034.49	953.37	1112.68	1224.76
Crystal system	triclinic	triclinic	monoclinic	trigonal	monoclinic	monoclinic
Space group / No.	$P\bar{1}$	$P\bar{1}$	*C*2/*c*	$R\bar{3}$	$P2_1/c$	$P2_1/c$
a [Å]	8.861(3)	13.8553(13)	22.855(6)	29.979(5)	10.3840(4)	14.723(2)
b [Å]	9.823(4)	14.7279(14)	18.306(5)	29.979(5)	15.1675(6)	12.1740(18)
c [Å]	19.310(7)	17.3368(16)	18.308(5)	23.525(9)	24.3914(10)	24.203(4)
α [°]	83.090(6)	77.107(2)	90	90	90	90
β [°]	89.197(7)	69.802(2)	107.093(5)	90	96.950(4)	99.761(3)
γ [°]	77.683(7)	85.275(2)	90	120	90	90
V [Å^3]	1630.0(10)	3236.4(5)	7401(3)	18310(11)	3813.4(3)	4275.3(11)
Z	2	4	8	18	4	4
D(calc) [g/cm^3]	1.798	1.893	1.857	1.556	1.938	1.903
μ(MoKα) [mm^{-1}]	4.646	4.697	4.126	3.855	4.343	3.890
F(000)	852	1768	3984	8280	2136	2360
Crystal size [mm]	0.25 x 0.32 x 0.38	0.34 x 0.39 x 0.40	0.34 x 0.39 x 0.42	0.29 x 0.33 x 0.38	0.04 x 0.20 x 0.30	0.08 x 0.20 x 0.42
Temperature (K)	294(2)	294(2)	293(2)	294(2)	200(2)	295(2)
Radiation [Å]	MoKα / 0.71073	MoKα / 0.71073	MoKα / 0.71073	MoKα / 0.71073	MoKα / 0.71073	MoKα / 0.71073
Theta min-max [°]	1.1, 25.0	1.6, 25.1	1.5, 25.1	1.2, 25.1	1.7, 25.1	1.5, 25.1
Dataset	±10; ±11; ±22	±16; ±17; ±20	±27; ±21; ±22	±35; ±35; ±28	−6: 12; ±18; −28:29	±17; ±14; ±28
Tot., Uniq. data, R(int)	15854, 5736, 0.049	31938, 11567, 0.049	35305, 6634, 0.073	60731, 7291, 0.186	16225, 6834, 0.042	41023, 7654, 0.088
Observed data [I > 2.0 σ(I)]	4936	9488	4920	3830	5806	6554
N_{ref}, N_{par}	5736, 443	11567, 919	6634, 532	7291, 461	6834, 514	7654, 586
R, wR_2, S	0.0392, 0.1016, 1.03	0.0406, 0.1032, 1.00	0.0593, 0.1164, 1.09	0.0595, 0.1475, 0.90	0.0355, 0.0733, 1.03	0.0392, 0.0976, 1.00
Max. and av. shift/error	0.00, 0.00	0.00, 0.00	0.00, 0.00	0.00, 0.00	0.00, 0.00	0.00, 0.00
Min. and max. resd. dens. [e/Å^3]	−0.43, 1.32	−0.73, 3.28	−1.01, 1.15	−0.48, 2.14	−1.34, 0.97	−0.92, 0.97

Table S2. Molecular parameters (bond lengths in Å and angles in deg) for **3a-c** and related Au(III) complexes.

Compound	**3a**	**3b**·$CHCl_3$	**3c**·$CHCl_3$	*cis*-[Au(2,4,6-$C_6F_3H_2$)Cl_2(PPh_3)]	*cis*-[Au(C_6F_5)Cl_2(PPh_3)]	*cis*-[Au(C_6F_5)Cl_2(P*t*Bu)$_3$}]
Au(1)–C(19)	2.035(8)	2.040(5)	2.047(4)	2.016(5)	2.019(4)	2.033(3)
Au(1)–P(1)	2.321(3)	2.325(1)	2.339(2)	2.308(1)	2.304(1)	2.416(1)
Au(1)–Cl(1)	2.363(3)	2.335(1)	2.352(1)	2.343(1)	2.328(1)	2.324(1)
Au(1)–Cl(2)	2.315(3)	2.327(1)	2.327(2)	2.334(1)	2.314(1)	2.346(1)
C(19)–Au(1)–P(1)	96.6(2)	97.2(1)	95.4(1)	91.4(1)	91.8(1)	98.8(1)
P(1)–Au(1)–Cl(1)	87.3(1)	86.6(1)	88.4(1)	89.2(1)	87.8(1)	94.5(1)
Cl(1)–Au(1)–Cl(2)	90.0(1)	89.2(1)	88.9(1)	92.2(1)	92.1(1)	85.4(1)
Cl(2)–Au(1)–C(19)	86.4(3)	87.2(1)	87.9(1)	87.2(1)	88.3(1)	81.4(1)
C(19)–Au(1)–Cl(1)	175.4(2)	175.6(1)	174.5(1)	178.7(1)	177.7(1)	165.8(1)
P(1)–Au(1)–Cl(2)	174.7(1)	173.6(1)	173.0(1)	177.6(1)	178.6(1)	177.4(1)
Au(1)–P(1)–C(1)	119.6(4)	120.2(2)	119.5(2)	113.4(2)	113.2(1)	112.2(1)

Table S3. Intermolecular C–X···H–C (X = F, Cl) and Au–Cl···H–C contacts below Σr_{vdW}(H,F) = 2.57 Å and Σr_{vdW}(H,Cl) = 2.85 Å.

Compound	**interaction***	**X···H (Å)**	**Y–X···H (deg)**	**C–H···X (deg)**	**symmetry operation**
2a	C–F···H–C	2.547(5)	136.2(4)	138.0(6)	1−x, −y, 1−z
	C–F···H–C	2.588(6)**	135.3(4)	173.0(6)	x, −1+y, z
3a	C–F···H–C	2.472(7)	140.4(8)	137.1(10)	1/3+y, 2/3−x, 2/3−z
	C–F···H–C	2.524(11)	114.2(9)	150.5(10)	2/3−x, 1/3−y, 4/3−z
2b	C–F···H–C	2.490(4)	122.5(3)	141.0(5)	1−x, 1−y, 1−z
	C–F···H–C	2.534(3)	153.9(3)	134.8(5)	−x, −y, 1−z
3b·$CHCl_3$	C–F···H–C	2.444(3)	147.0(3)	136.3(3)	1+x, y, z
	C–F···H–C	2.462(3)	121.2(3)	139.2(4)	1−x, 1−y, 1−z
	Au–Cl···H–C	2.750(1)	157.2(1)	152.3(4)	3/2−x, −1/2+y, 1/2−z
2c	C–F···H–C	2.572(8)	155.1(7)	142.2(6)	x, 1−y, 1/2+z
3c·$CHCl_3$	C–F···H–C	2.564(6)	148.2(5)	161.5(3)	−1/2+x, −1/2+y, 1/2−z
	Au–Cl···H–C	2.581(1)	92.8(1)	153.7(4)	x, y, z
	Au–Cl···H–C	2.807(2)	86.7(1)	131.6(4)	x, y, z
	C–Cl···H–C	2.940(1)**	104.6(2)	165.0(5)	1−x, −y, 1−z

* The atoms on the left side of the interaction belong to the (x,y,z) molecule, while the atoms on the right side of the interaction belong to the molecule generated by the symmetry operation listed on the last column of the table.

** Interactions at distances slightly larger than Σr_{vdW} were included if they had very good geometrical arrangements.

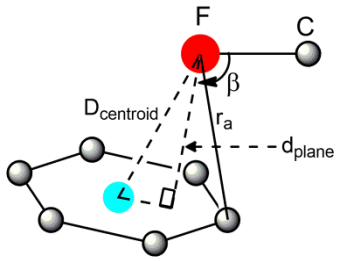


Figure S2. Definition of geometrical C–F···π_F parameters.

Table S4. Intermolecular C–F···π_F interactions having at least one F···C(r_a) contact below Σr_{vdW}(C,F) = 3.17 Å.

Compound	interaction type	d_{plane} (Å)	contact* (Å)	r_a (Å)	$D_{centroid}$ (Å)	β(deg)	symmetry operation
2a	paralell offset	2.927(7)	F(4)···C(30)	3.113(11)	3.440(5)	89.4(5)	−x, 2−y, −z
			C(30)···F(4)	3.113(11)			
2b	vertex to face	3.066(4)	F(8)···C(72)	3.204(9)	3.098(4)	31.6(3)	−x, 1−y, 1−z
	vertex to face	2.913(5)	F(16)···C(28)	2.997(8)	3.569(5)	52.4(3)	1−x, −y, −z
	paralell offset	2.797(4)	F(7)···C(63)	3.135(8)	3.766(4)	89.2(3)	−1+x, y, z
			C(33)···F(15)	3.171(7)			
	paralell offset	2.580(4)	F(11)···C(59)	3.175(6)	3.881(3)	83.8(3)	x, y, −1+z
			F(11)···C(58)	3.156(7)			
	edge to face	2.916(3)	F(13)···C(36)	3.076(6)	3.707(3)	34.6(3)	−x, 1−y, −z
		2.884(3)	F(12)···C(35)	3.024(7)	3.692(3)	34.3(3)	
3b·$CHCl_3$	vertex to face	2.982(3)	F(9)···C(28)	2.992(7)	3.216(4)	32.1(4)	1−x, 1−y, 1−z
2c	paralell offset	2.729(6)	F(10)···C(29)	3.121(14)	3.748(7)	83.7(4)	1−x, y, ½−z
3c·$CHCl_3$	paralell offset	2.669(5)	F(9)···C(35)	3.137(8)	3.891(5)	89.5(4)	−x, −y, 1−z

* The atoms on the left side of the interaction belong to the (x,y,z) molecule, while the atoms on the right side of the interaction belong to the molecule generated by the symmetry operation listed on the last column of the table.

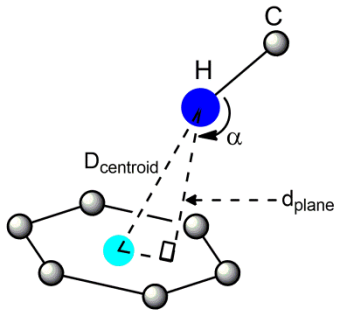


Figure S3. Definition of geometrical C–H···π parameters.

Table S5. Intermolecular C–H···π interactions ($D_{centroid}$ < 3 Å).

compound	interaction*	d_{plane} (Å)	$D_{centroid}$ (Å)	α(deg)	symmetry operation
2b	C(4)–H(4)···$Ph_{(C54–C60)}$	2.84	2.85	160	−x, −y, 1−z
	C(40)–H(40)···$Ph_{(C19–C24)}$	2.84	2.96	139	1−x, 1−y, −z
3a	C(23)–H(23)···$Ph_{(C1–C6)}$	2.94	2.98	123	2/3−y, 1/3+x−y, 1/3−z

* The atoms on the left side of the interaction belong to the (x,y,z) molecule, while the phenyl rings on the right side of the belong to the molecule generated by the symmetry operation listed on the last column of the table.

Table S6. Intermolecular π···π stacking interactions, not included among C–F···π_F (interplanar distance < 3.8 Å, slippage < 2 Å).

compound	interaction*	$Ph_{centroid}$···$Ph_{centroid}$ (Å)	interplanar distance (Å)	Slippage (Å)	symmetry operation
2c	$Ph_{(C37-C42)}$···$Ph_{(C37-C42)}$	3.480(7)	3.467(5)	0.306	1−x, y, 1/2−z

* The phenyl ring on the left side of the interaction belongs to the (x,y,z) molecule, while the phenyl rings on the right side of the interaction belong to the molecule generated by the symmetry operation listed on the last column of the table.

Figures S4-S12

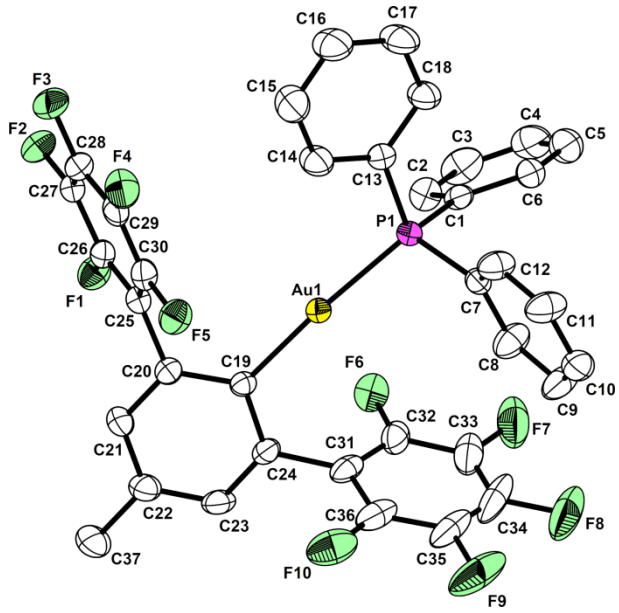


Figure S4. Molecular structure of **2a**. Thermal ellipsoid are shown at 25% probability level. Hydrogen atoms have been omitted for clarity

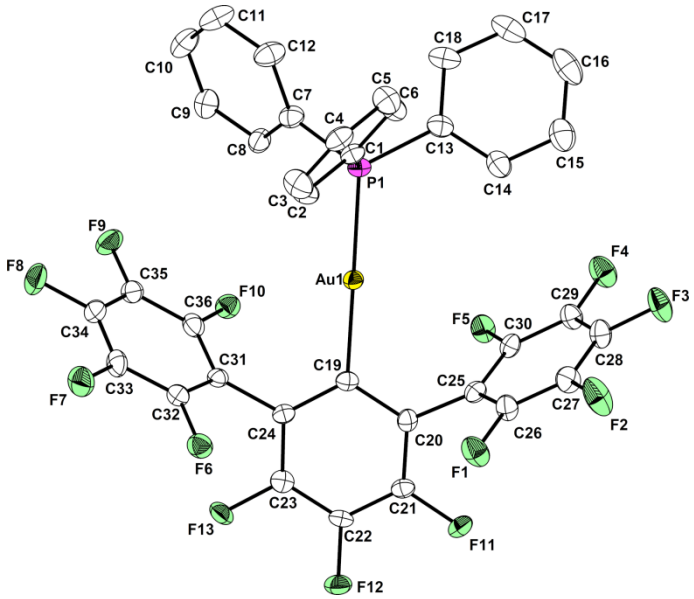


Figure S5. Molecular structure of **2b**. Thermal ellipsoid are shown at 25% probability level. Hydrogen atoms have been ommited for clarity.

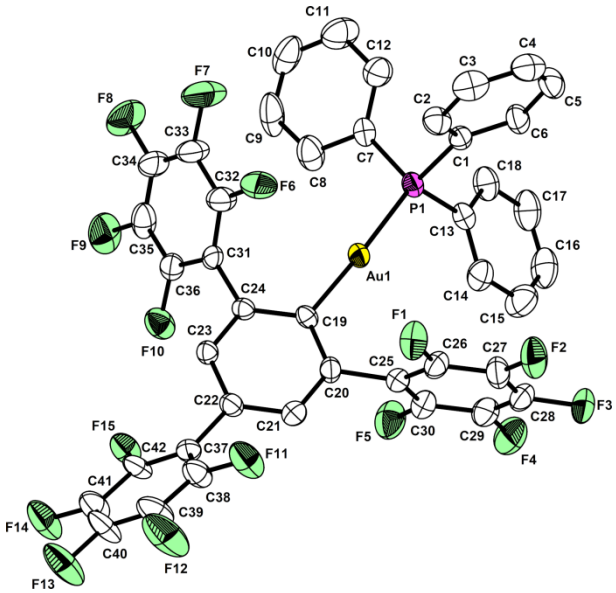


Figure S6. Molecular structure of **2c**. Thermal ellipsoid are shown at 25% probability level. Hydrogen atoms have been ommited for clarity.

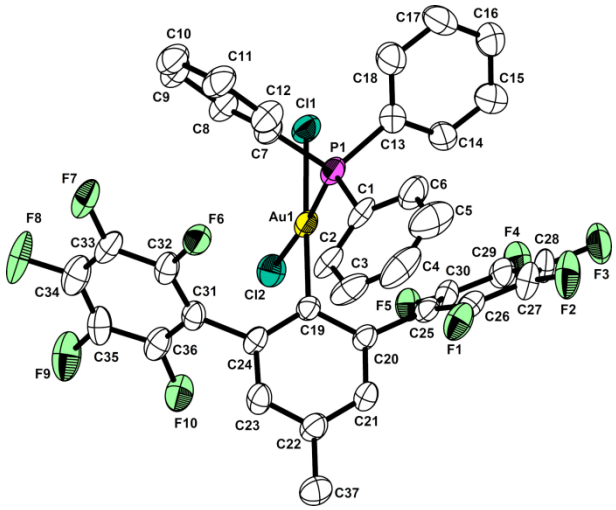


Figure S7. Molecular structure of **3a**. Thermal ellipsoid are shown at 25% probability level. Hydrogen atoms have been ommited for clarity.

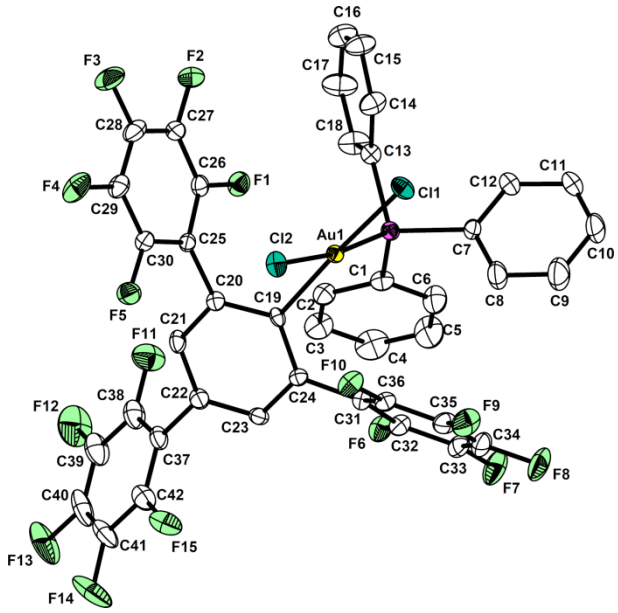


Figure S8. Molecular structure of **3c**·$CHCl_3$. Thermal ellipsoid are shown at 25% probability level. Hydrogen atoms and the solvent molecule have been ommited for clarity.

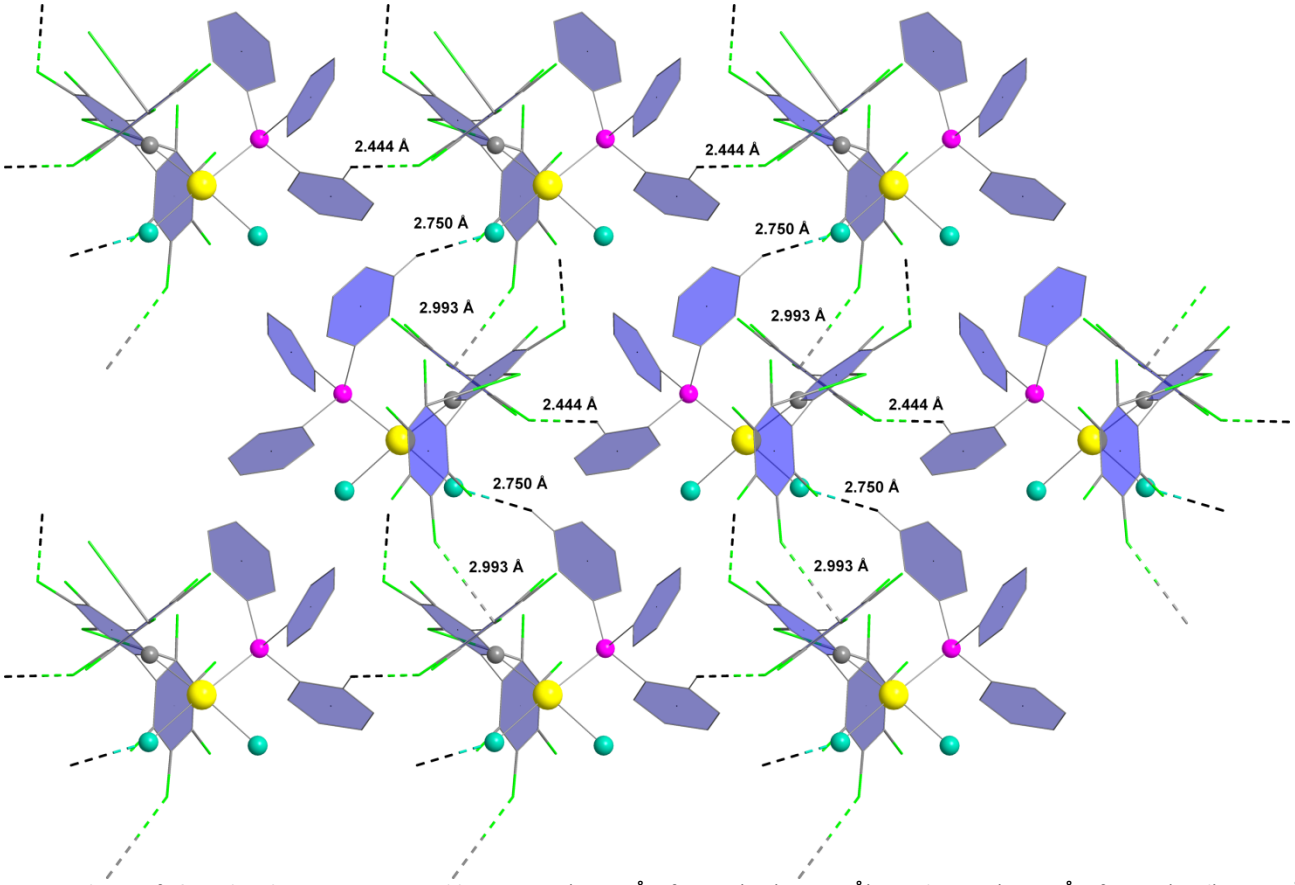


Figure S9. One layer of **3b** molecules interconnected by C–F···π_F (2.993 Å, cf. Σr_{vdW}(C,F) = 3.17 Å), C–Cl···H–C (2.750 Å, cf. Σr_{vdW}(H,Cl) = 2.85 Å) and C–F···H–C (2.444 Å, cf. Σr_{vdW}(F,H) 2.57 Å) interactions. Colour coding: Au = yellow, C = grey, Cl = turquoise, P = pink.

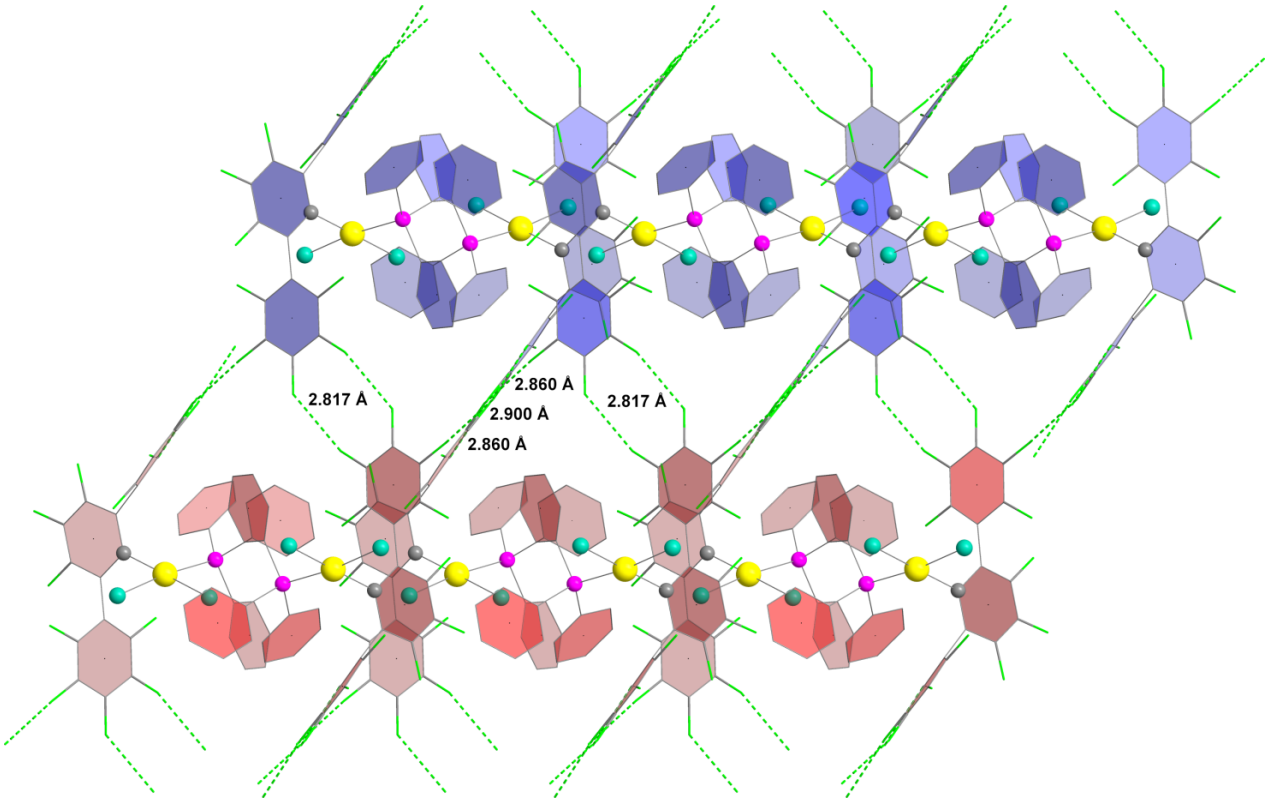


Figure S10. Two layers of **3b** molecules (red and blue phenyl rings for different layers) connected by three cooperative F···F interactions (one at 2.817 Å and two coplanar at 2.860 Å and 2.900 Å; cf. Σr_{vdW}(F,F) 2.94 Å, view along *b* axis). Colour coding: Au = yellow, C = grey, Cl = turquoise, P = pink.

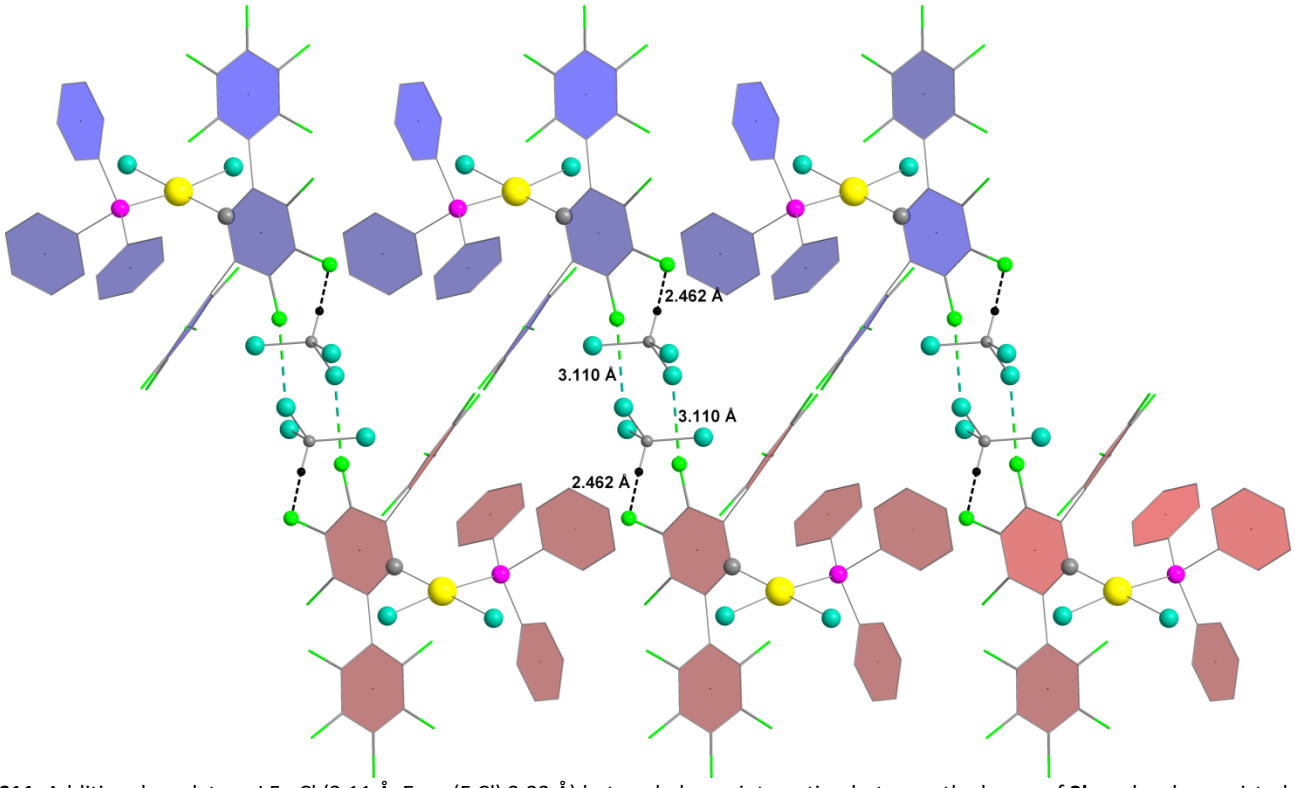


Figure S11. Additional weak type I F···Cl (3.11 Å; Σr_{vdW}(F,Cl) 3.22 Å) hetero-halogen interaction between the layers of **3b** molecules, assisted by a C–F···H–C interaction (2.462 Å, cf. Σr_{vdW}(F,H) 2.57 Å). Colour coding: Au = yellow, C = grey, F = green, Cl = turquoise, P = pink.

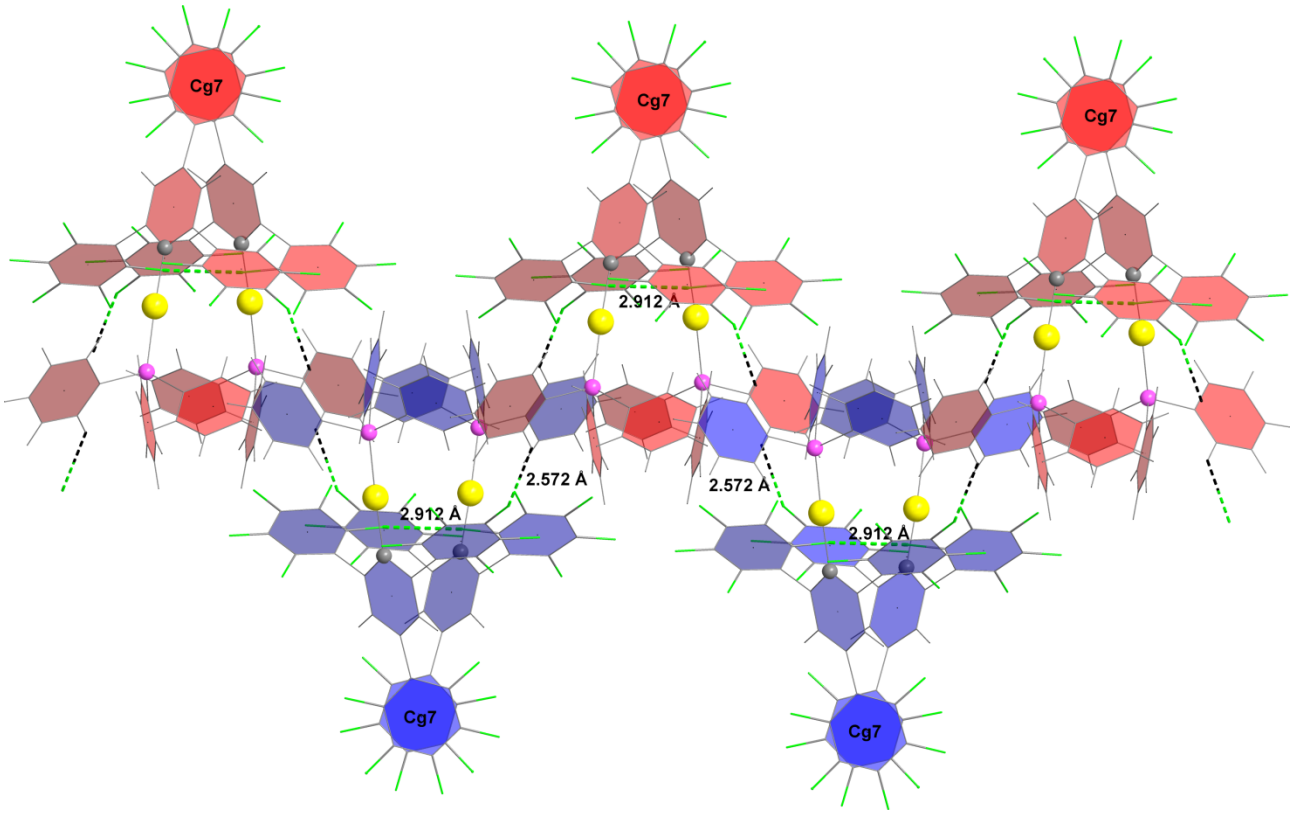


Figure S12. Weakly bound supramolecula chains built from dimer pairs of **2c** molecules connected by weak π···π stacking (staggered Cg7···Cg7 = 3.48 Å), further linked by C–F···H–C (2.572 Å; cf. Σr_{vdW}(F,H) 2.57 Å) and F···F (2.912 Å; cf. Σr_{vdW}(F,F) 2.94 Å) interactions. Colour coding: Au = yellow, C = grey, P = pink.

NMR spectra

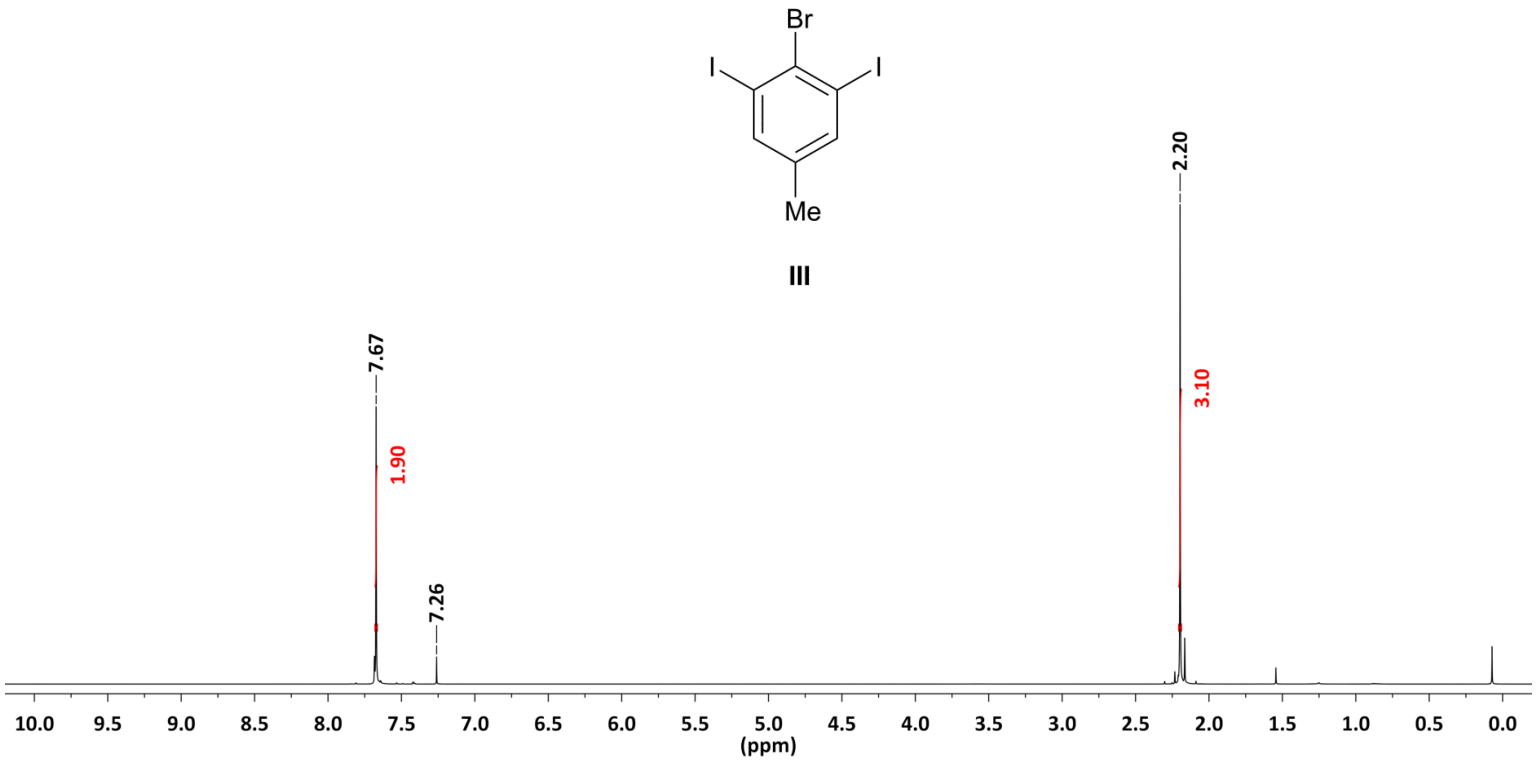


Figure S13. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of 2,6-I_2-4-MeC_6H_2Br (**III**).

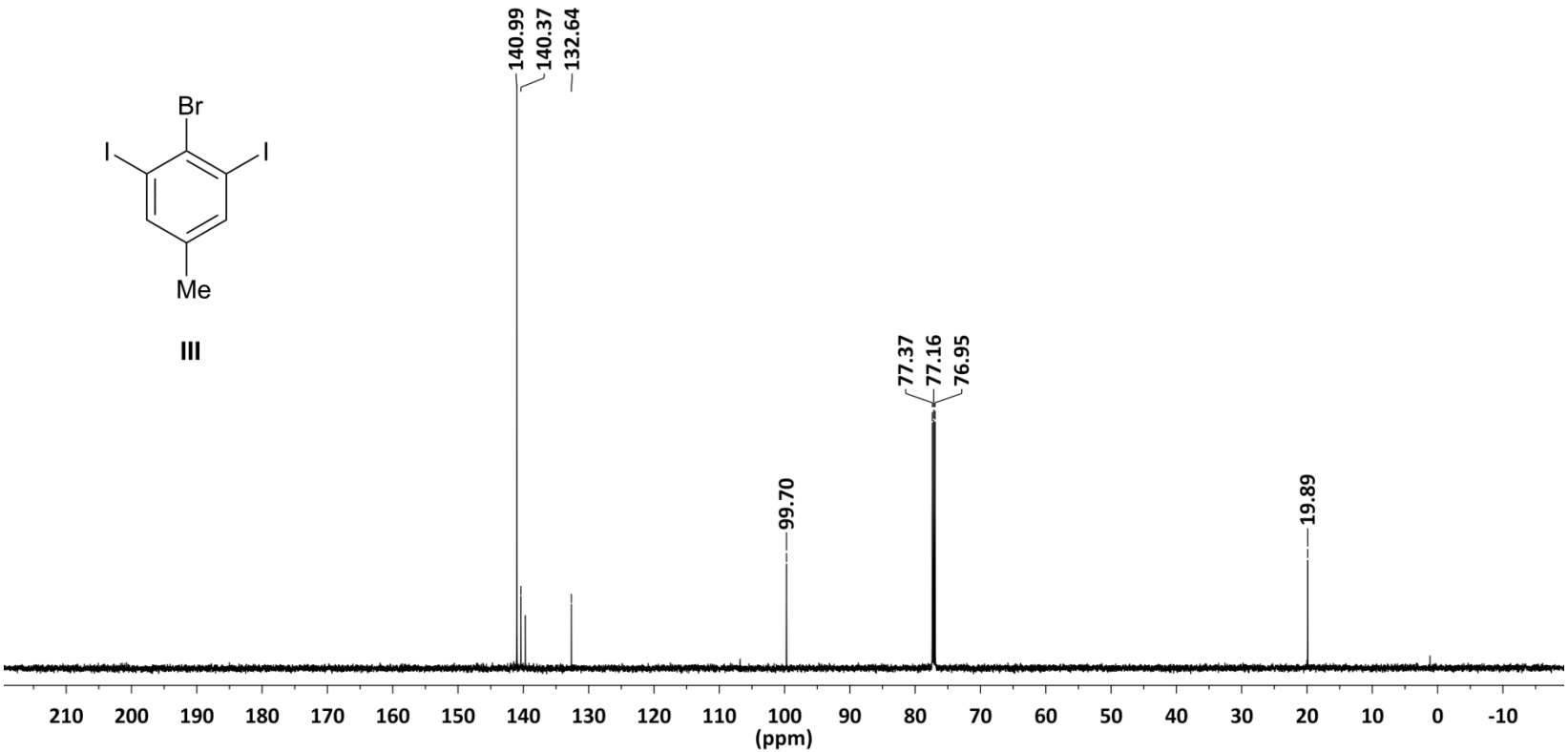


Figure S14. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz) spectrum of 2,6-I_2-4-MeC_6H_2Br (**III**).

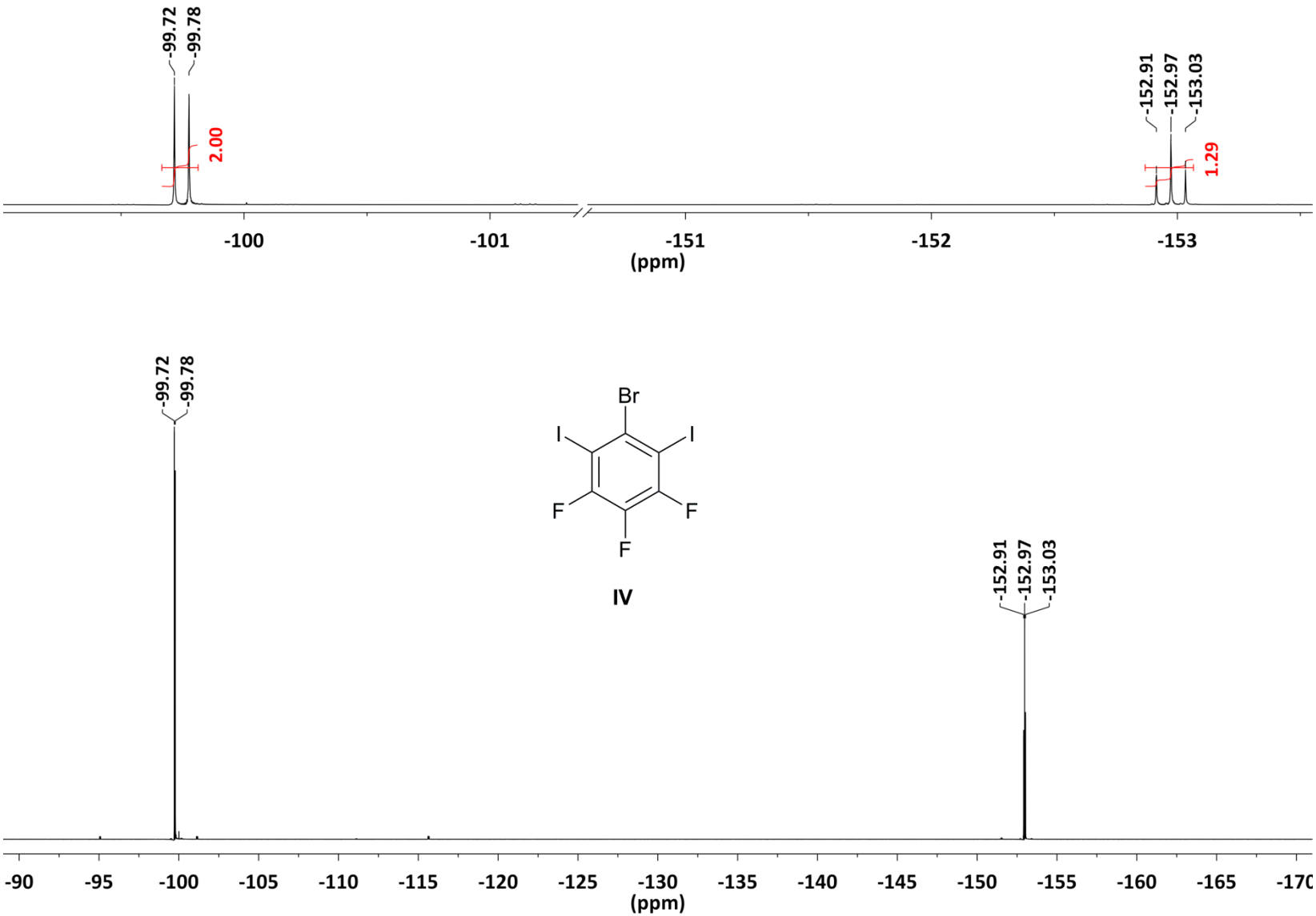


Figure S15. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 376 MHz) spectrum of 2,6-I_2-C_6F_3Br (**IV**).

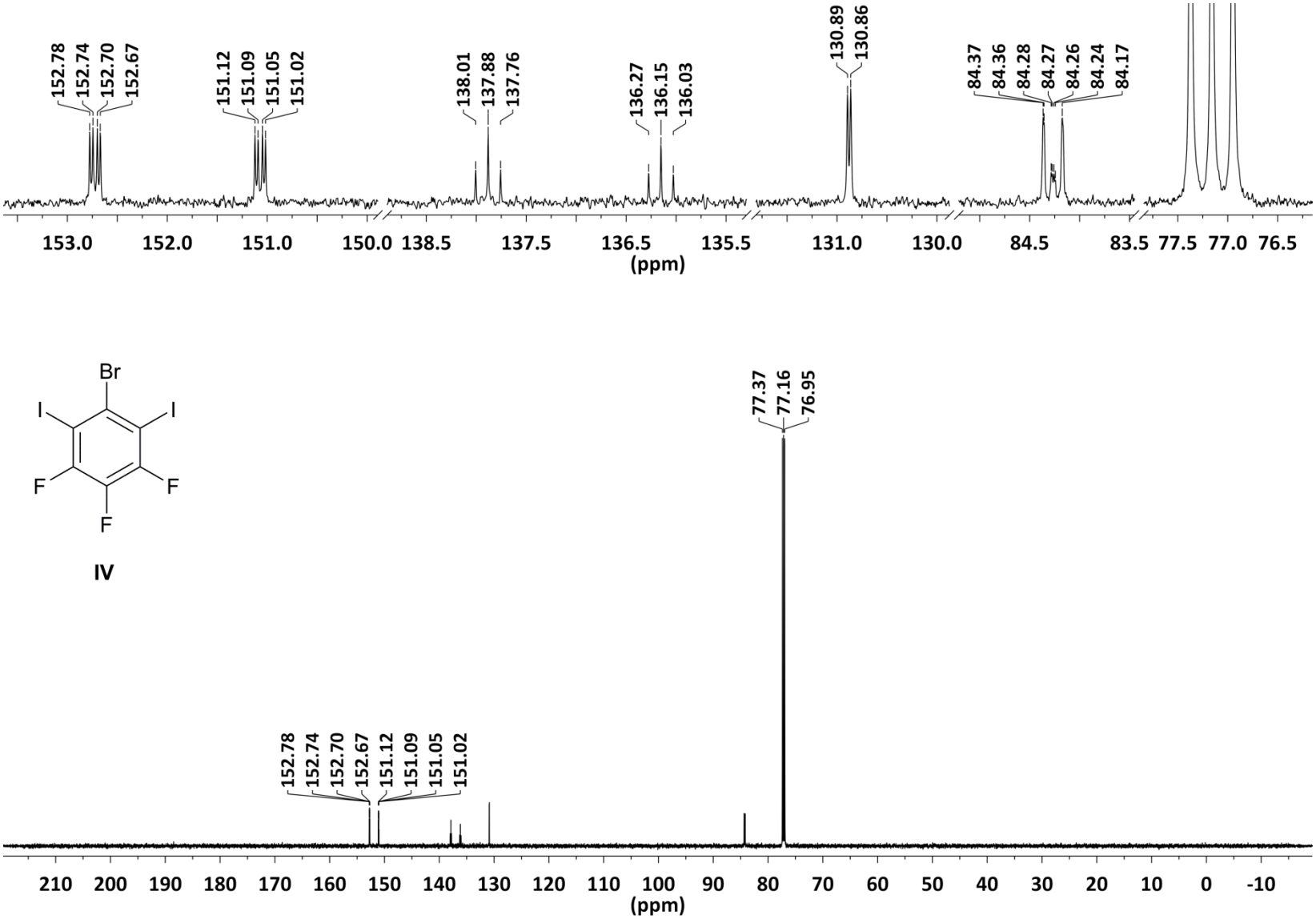


Figure S16. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 151 MHz) spectrum of 2,6-I_2-C_6F_3Br (**IV**).

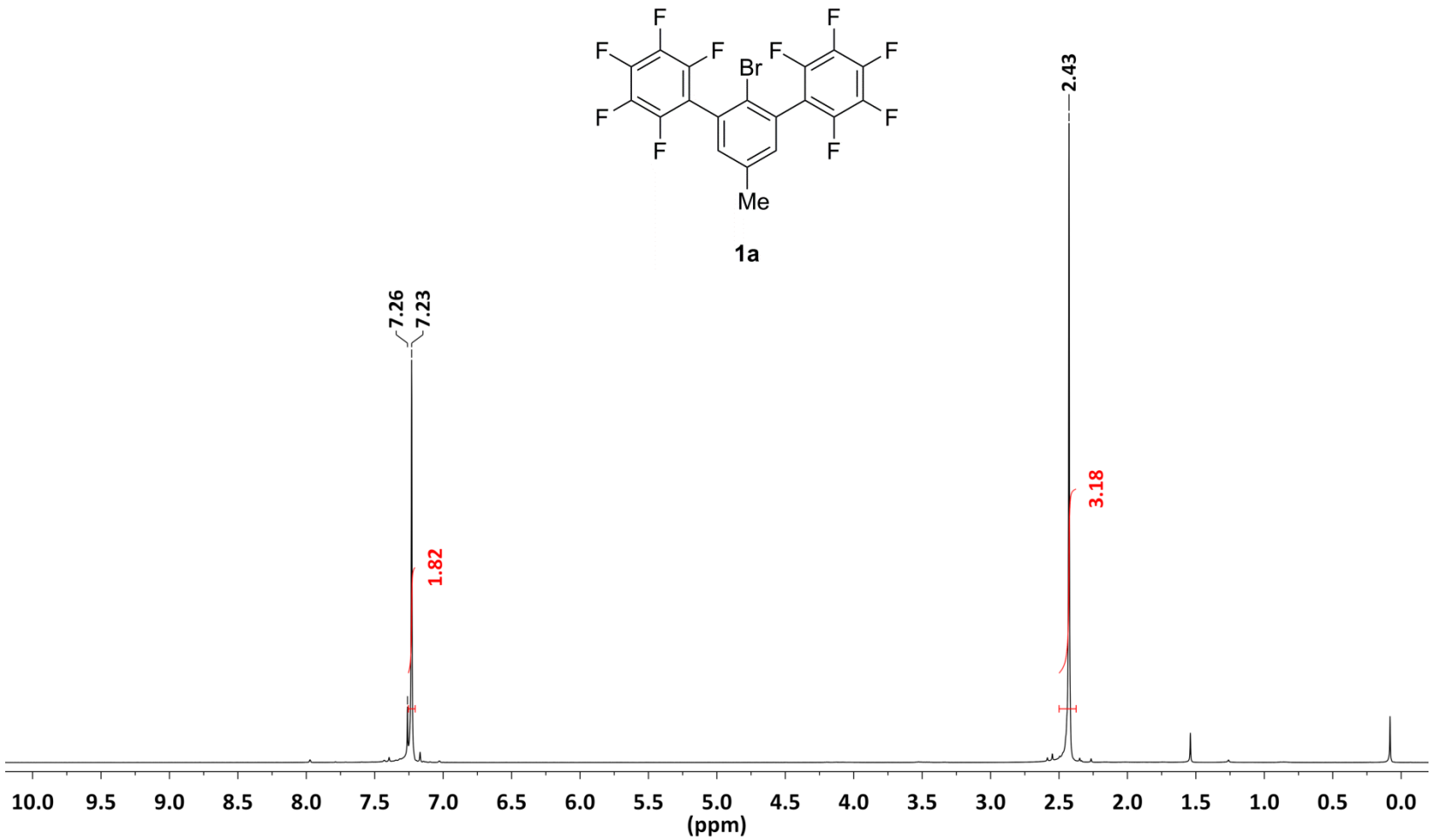


Figure S17. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of 2,6-(C_6F_5)-4-MeC_6H_2Br (**1a**).

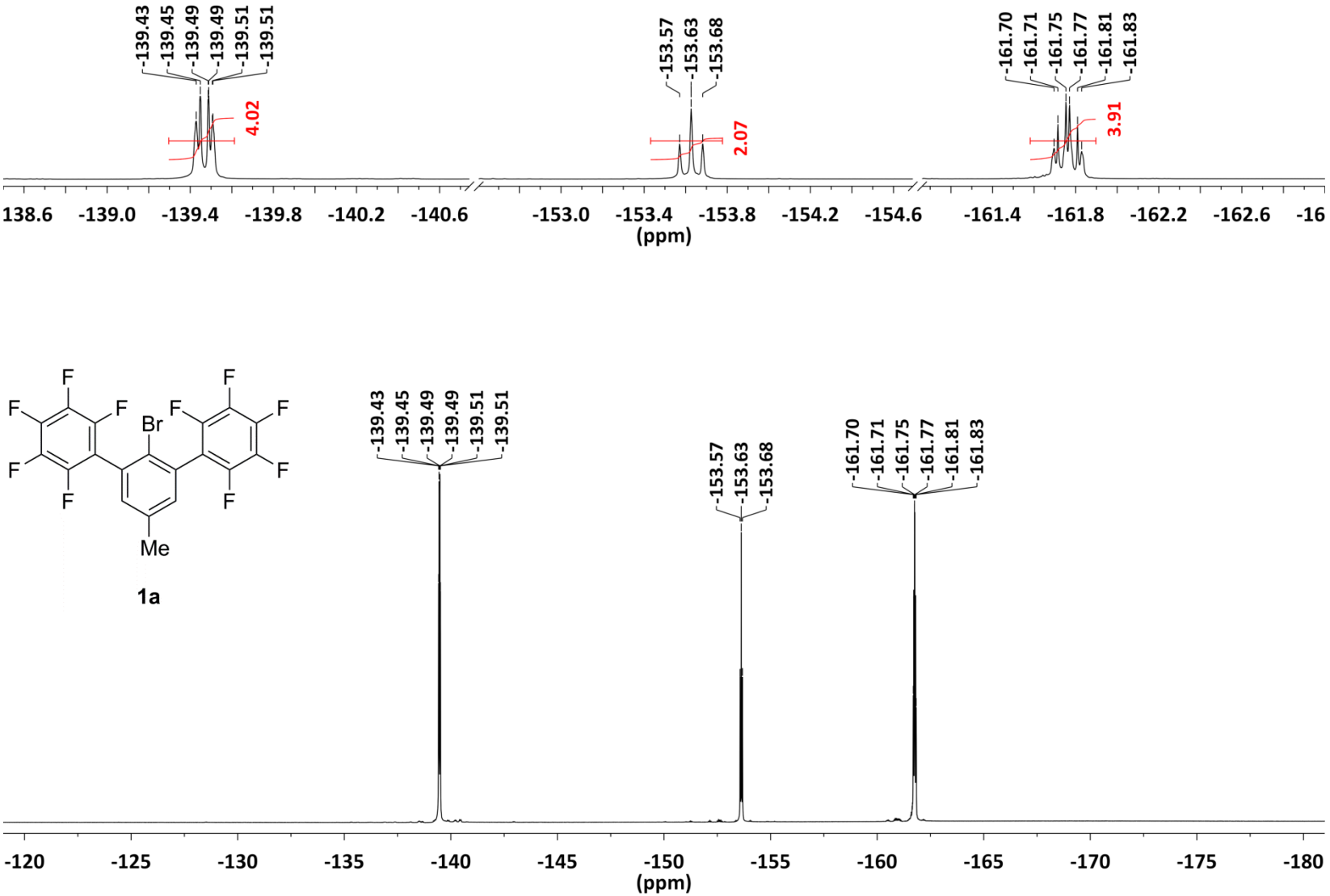


Figure S18. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 376 MHz) spectrum of 2,6-(C_6F_5)-4-MeC_6H_2Br (**1a**).

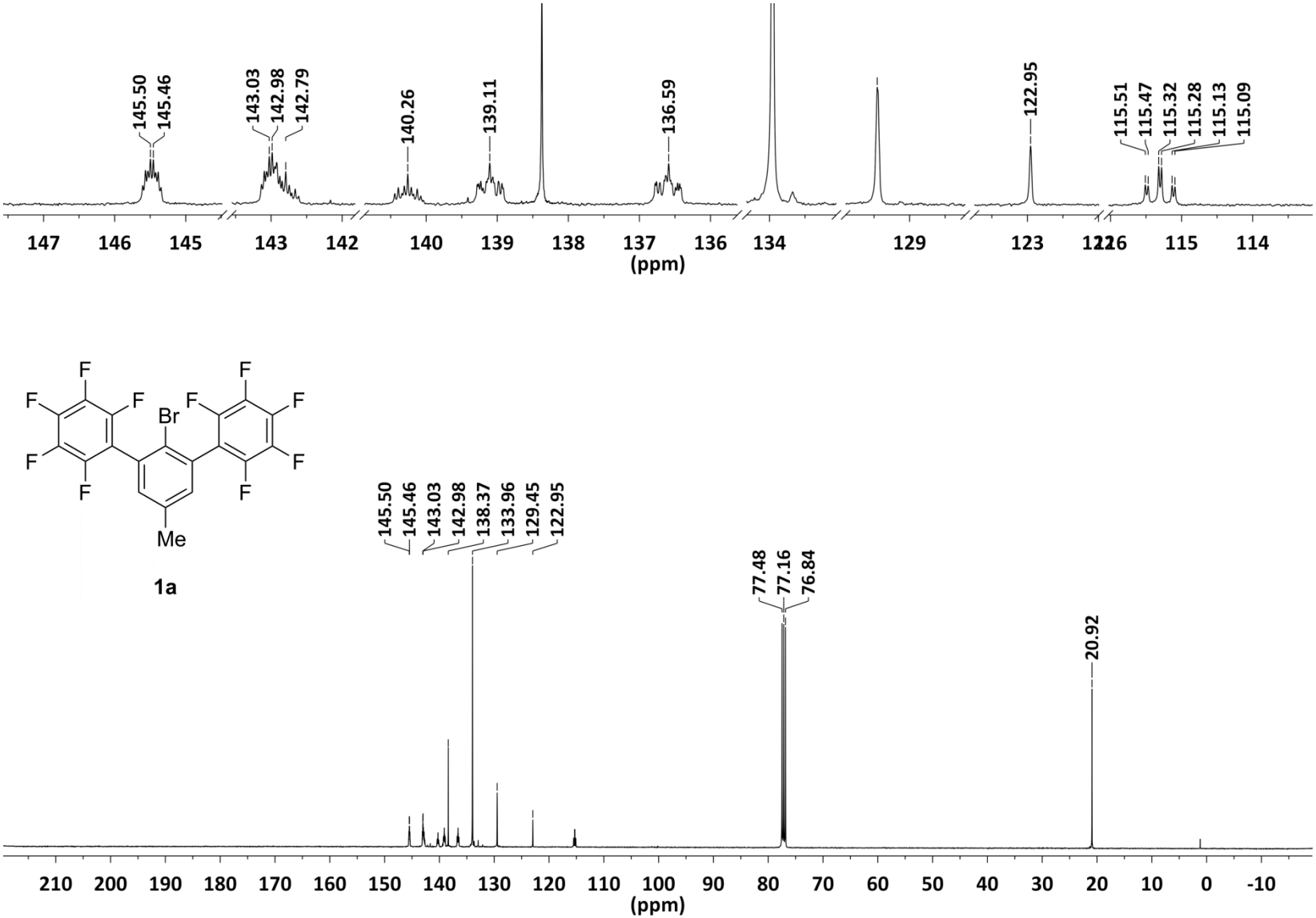


Figure S19. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz) spectrum of 2,6-(C_6F_5)-4-MeC_6H_2Br (**1a**).

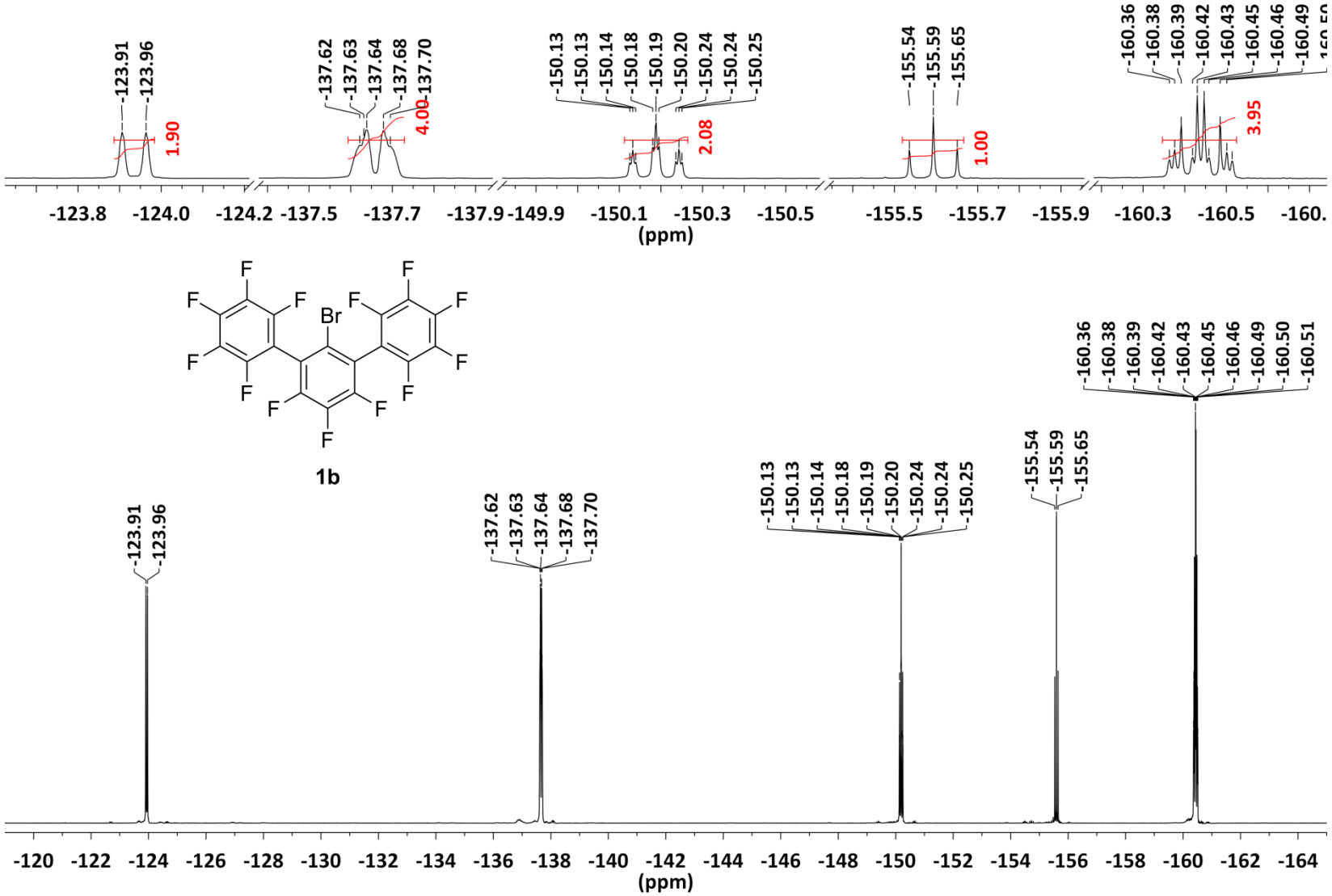


Figure S20. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 376 MHz) spectrum of 2,6-(C_6F_5)-C_6F_3Br (**1b**).

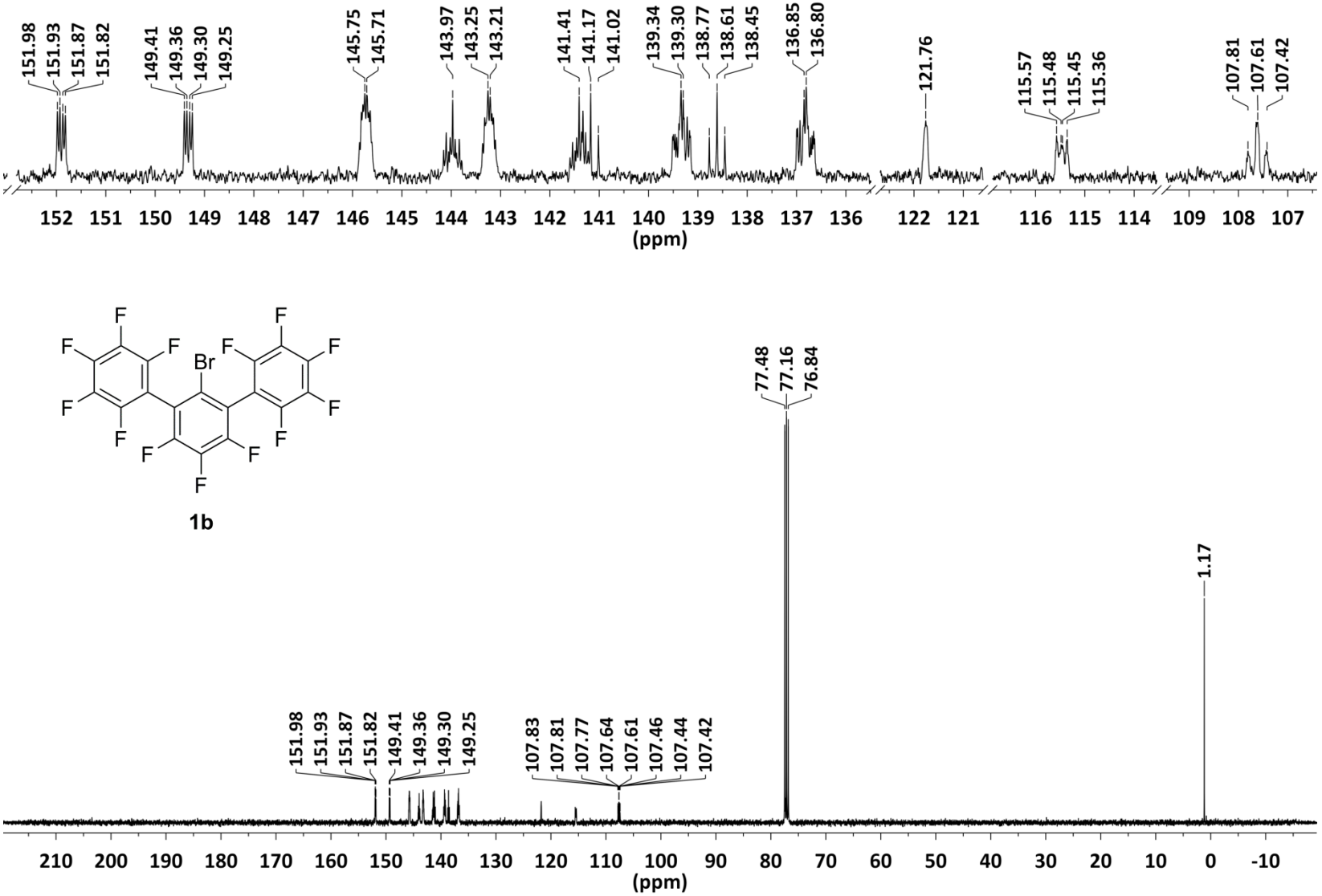


Figure S21. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz) spectrum of 2,6-(C_6F_5)-C_6F_3Br (**1b**).

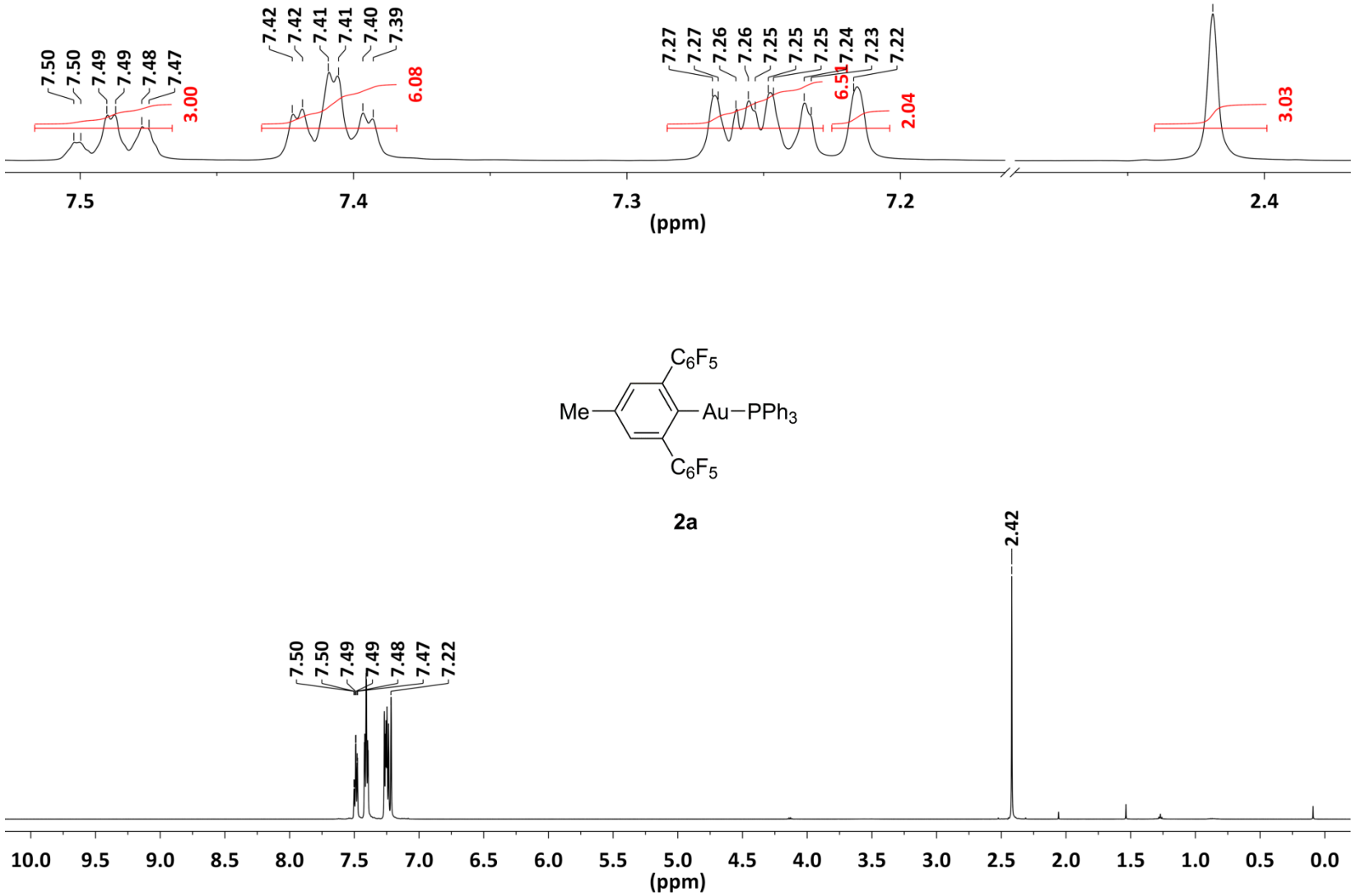


Figure S22. ^{1}H NMR ($CDCl_3$, 600 MHz) spectrum of 2,6-$(C_6F_5)_2$-4-$MeC_6H_2Au(PPh_3)$ (**2a**).

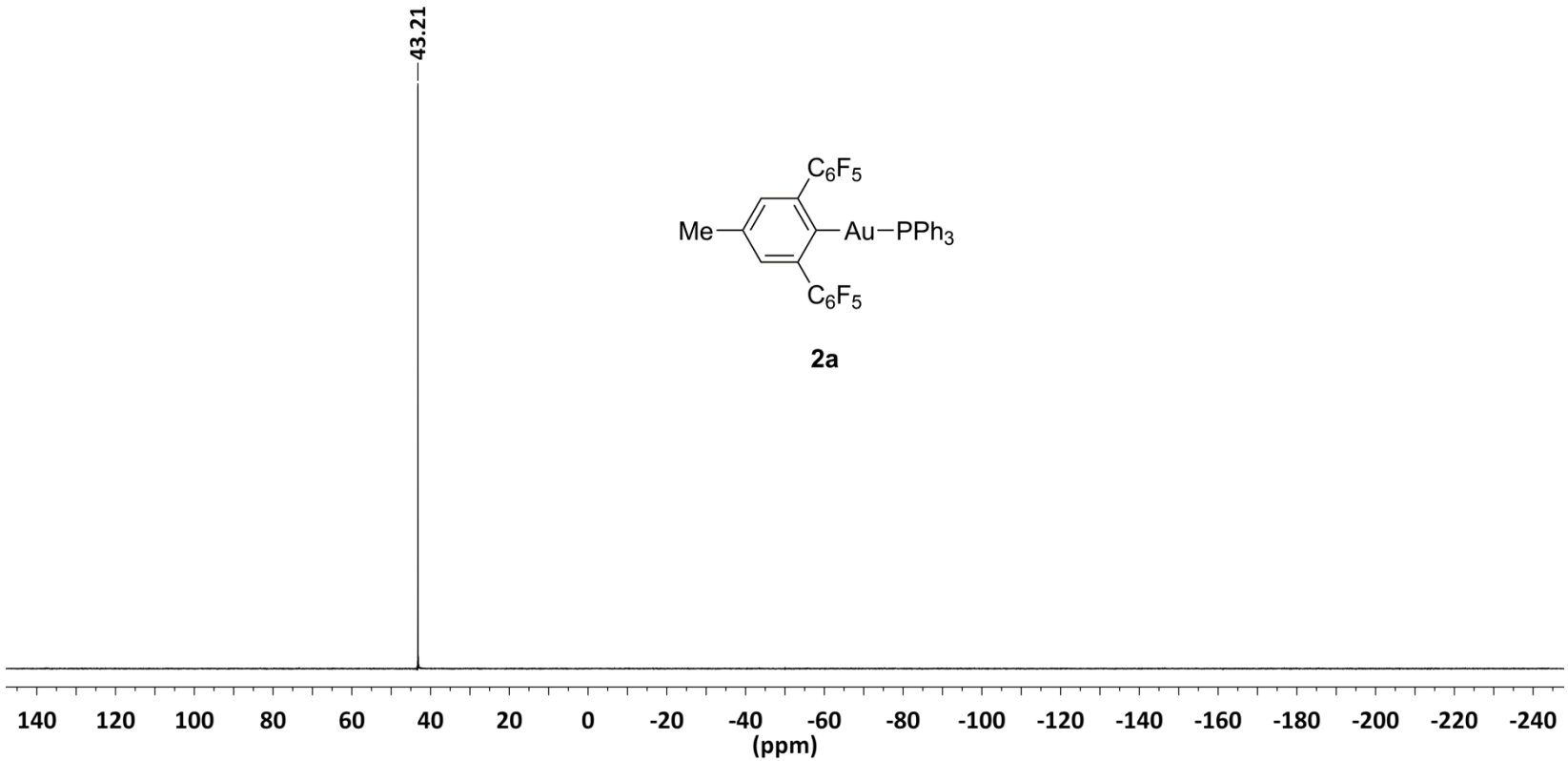


Figure S23. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 243 MHz) spectrum of 2,6-$(C_6F_5)_2$-4-$MeC_6H_2Au(PPh_3)$ (**2a**).

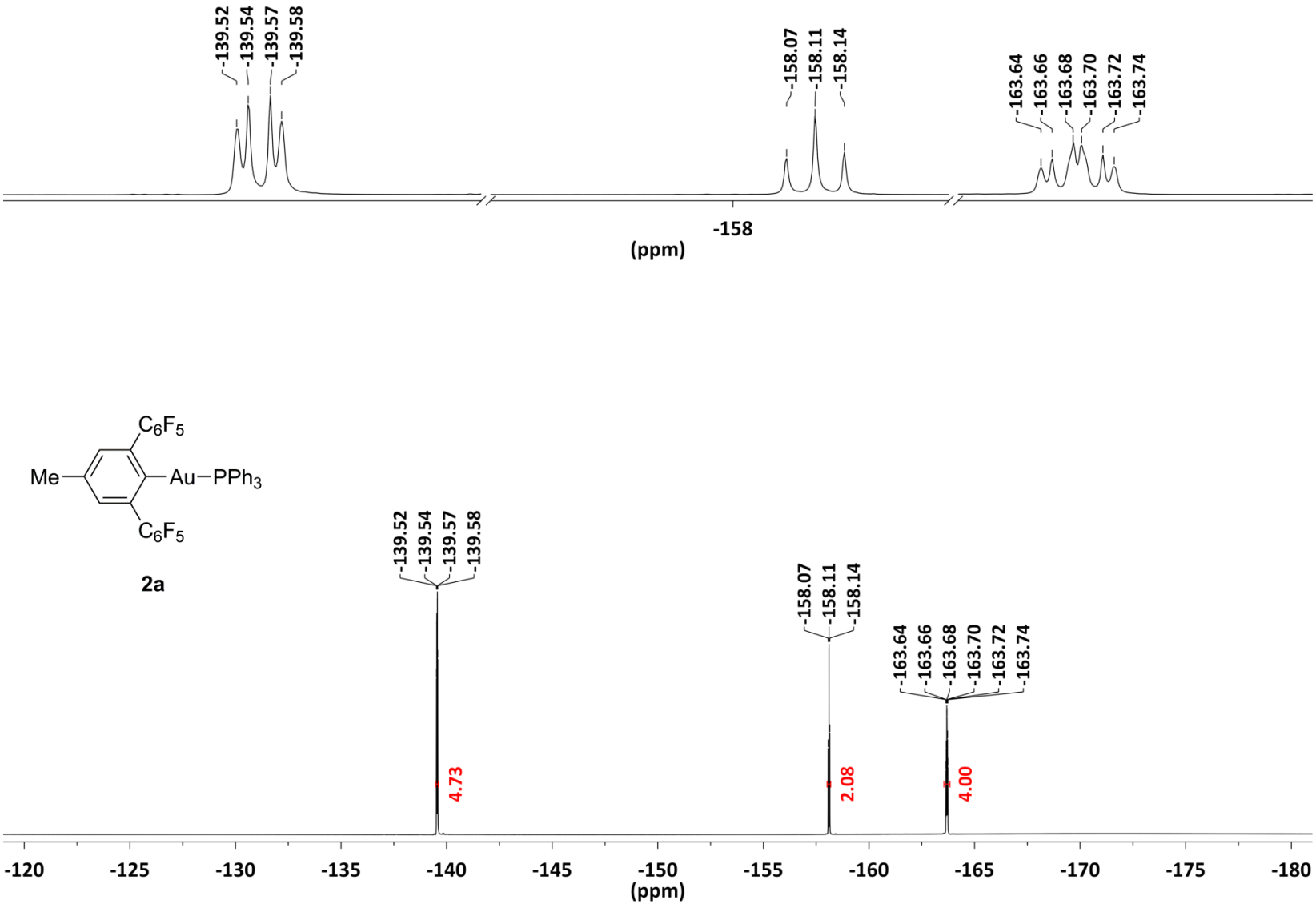


Figure S24. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 565 MHz) spectrum of 2,6-$(C_6F_5)_2$-4-$MeC_6H_2Au(PPh_3)$ (**2a**).

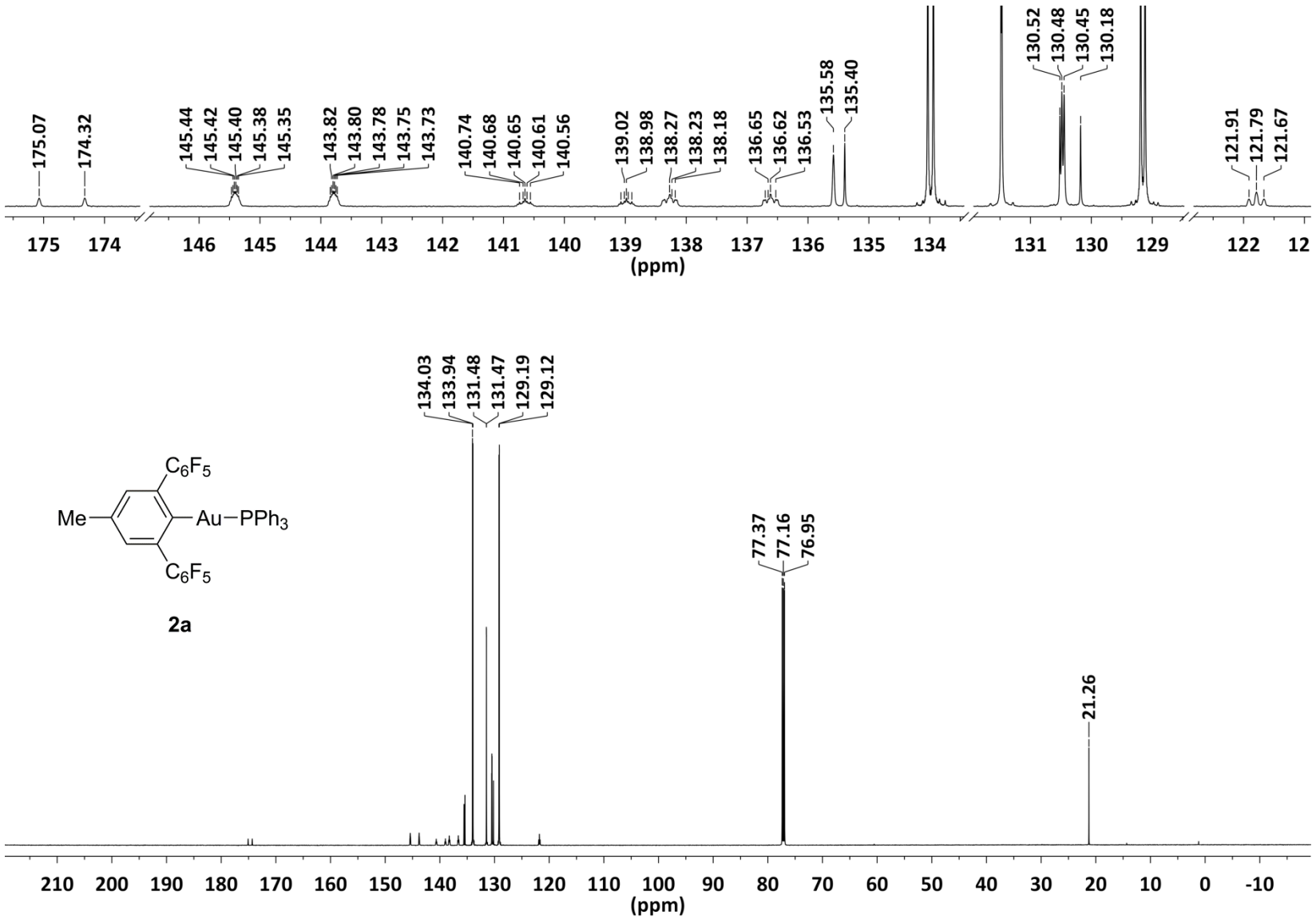


Figure S25. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 151 MHz) spectrum of 2,6-$(C_6F_5)_2$-4-$MeC_6H_2Au(PPh_3)$ (**2a**).

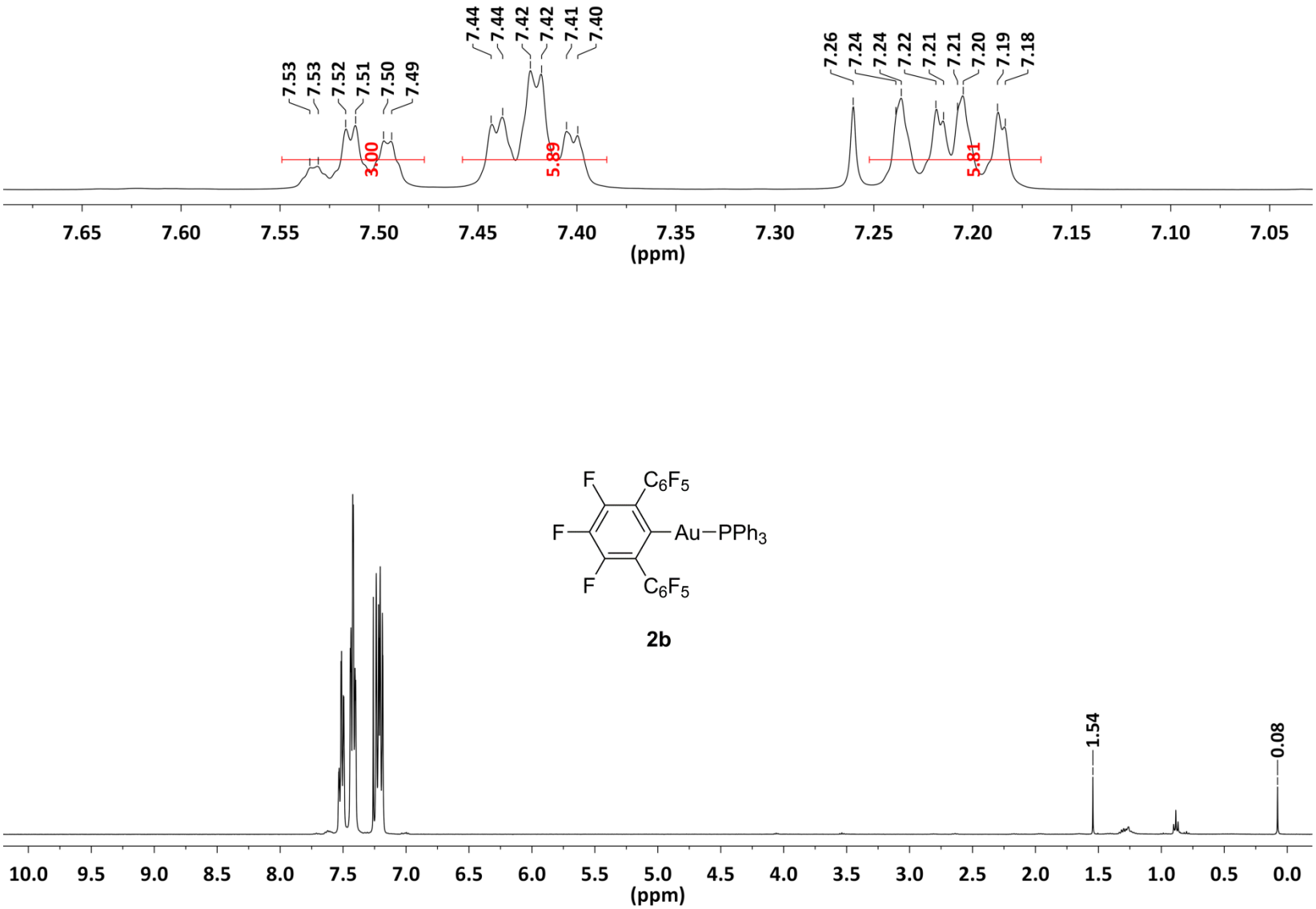


Figure S26. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3Au(PPh_3)$ (**2b**).

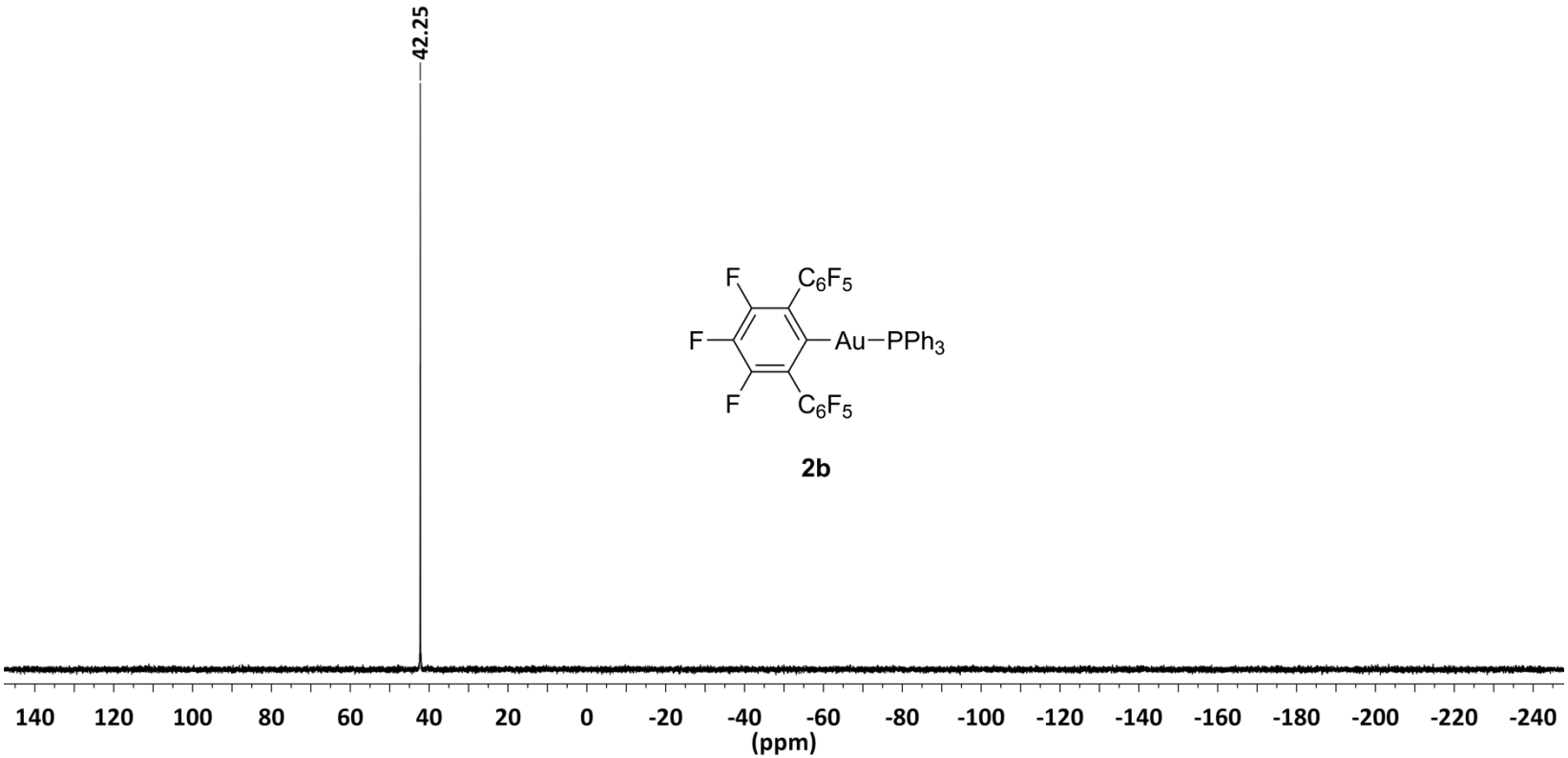


Figure S27. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 162 MHz) spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3Au(PPh_3)$ (**2b**).

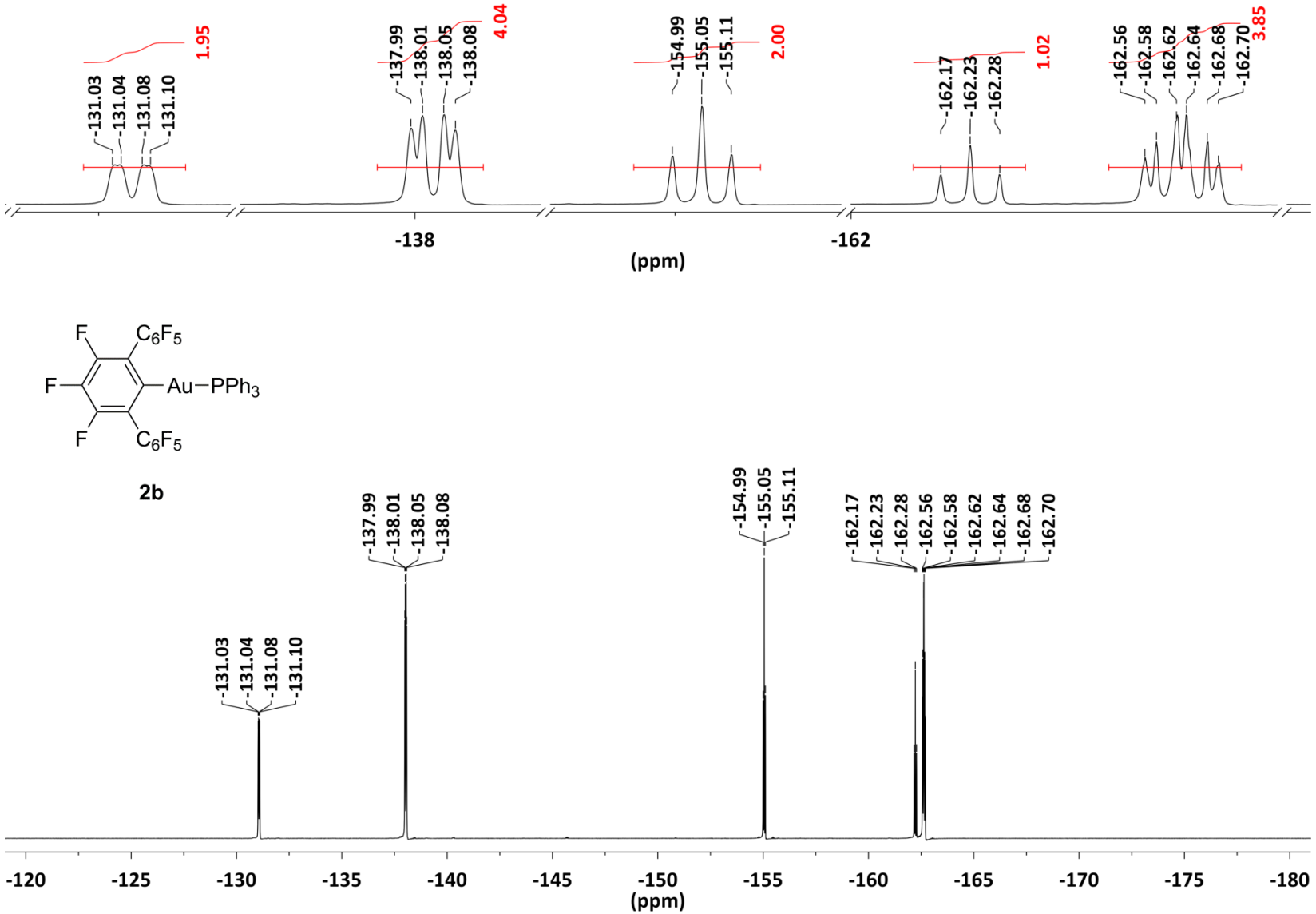


Figure S28. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 376 MHz) spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3Au(PPh_3)$ (**2b**).

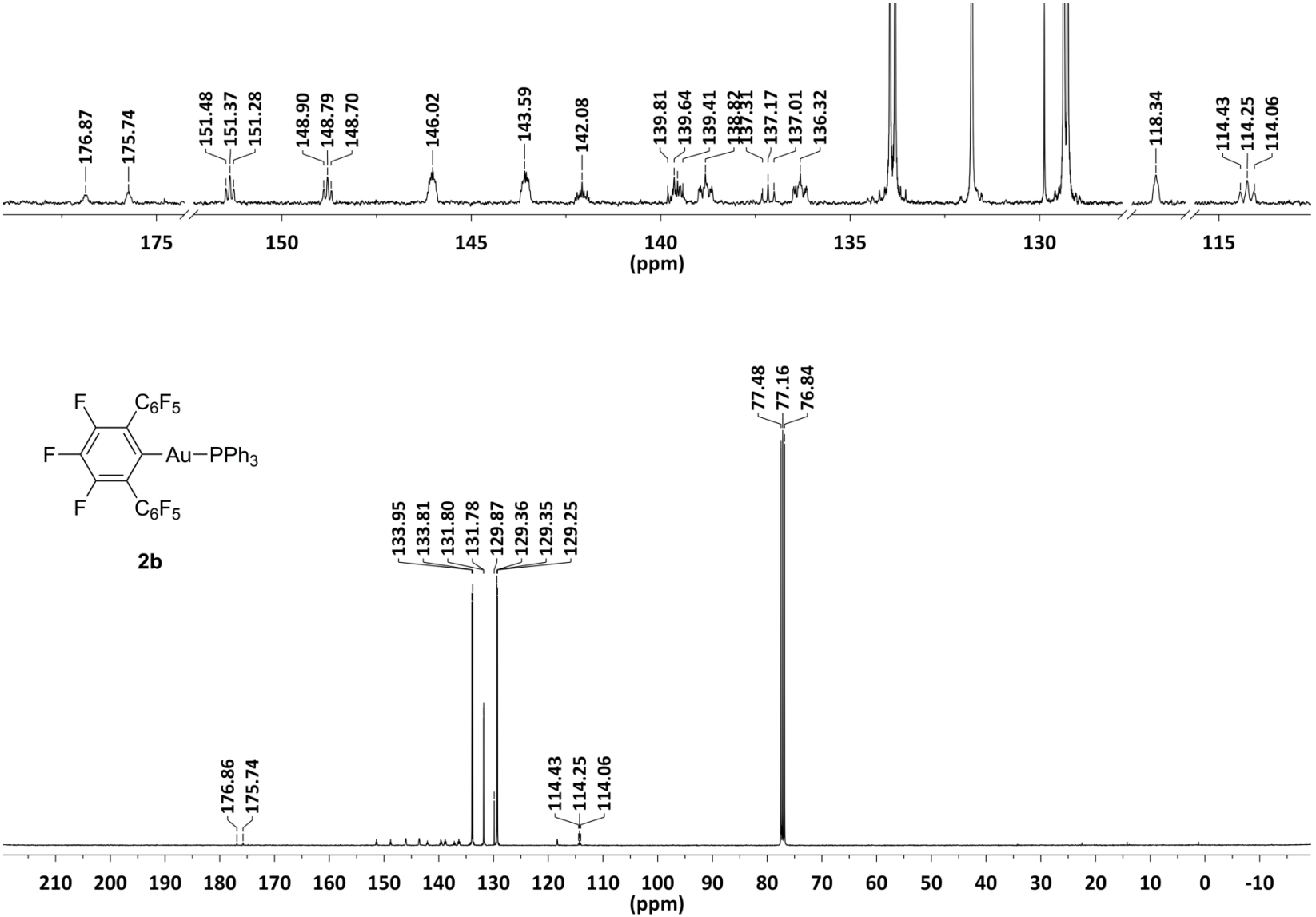


Figure S29. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz) spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3Au(PPh_3)$ (**2b**).

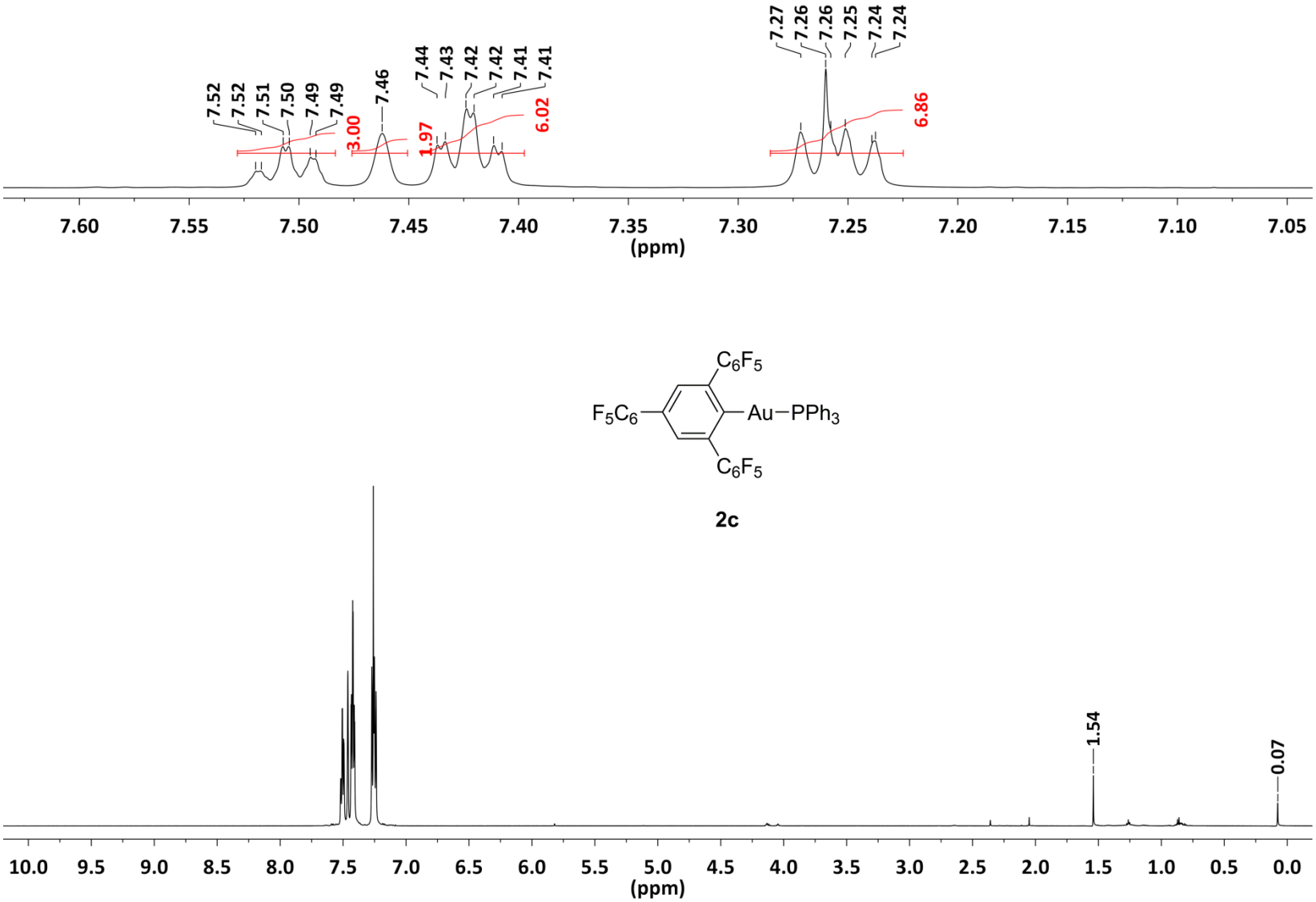


Figure S30. ^{1}H NMR ($CDCl_3$, 600 MHz) spectrum of 2,4,6-$(C_6F_5)_3$-$C_6H_2Au(PPh_3)$ (**2c**).

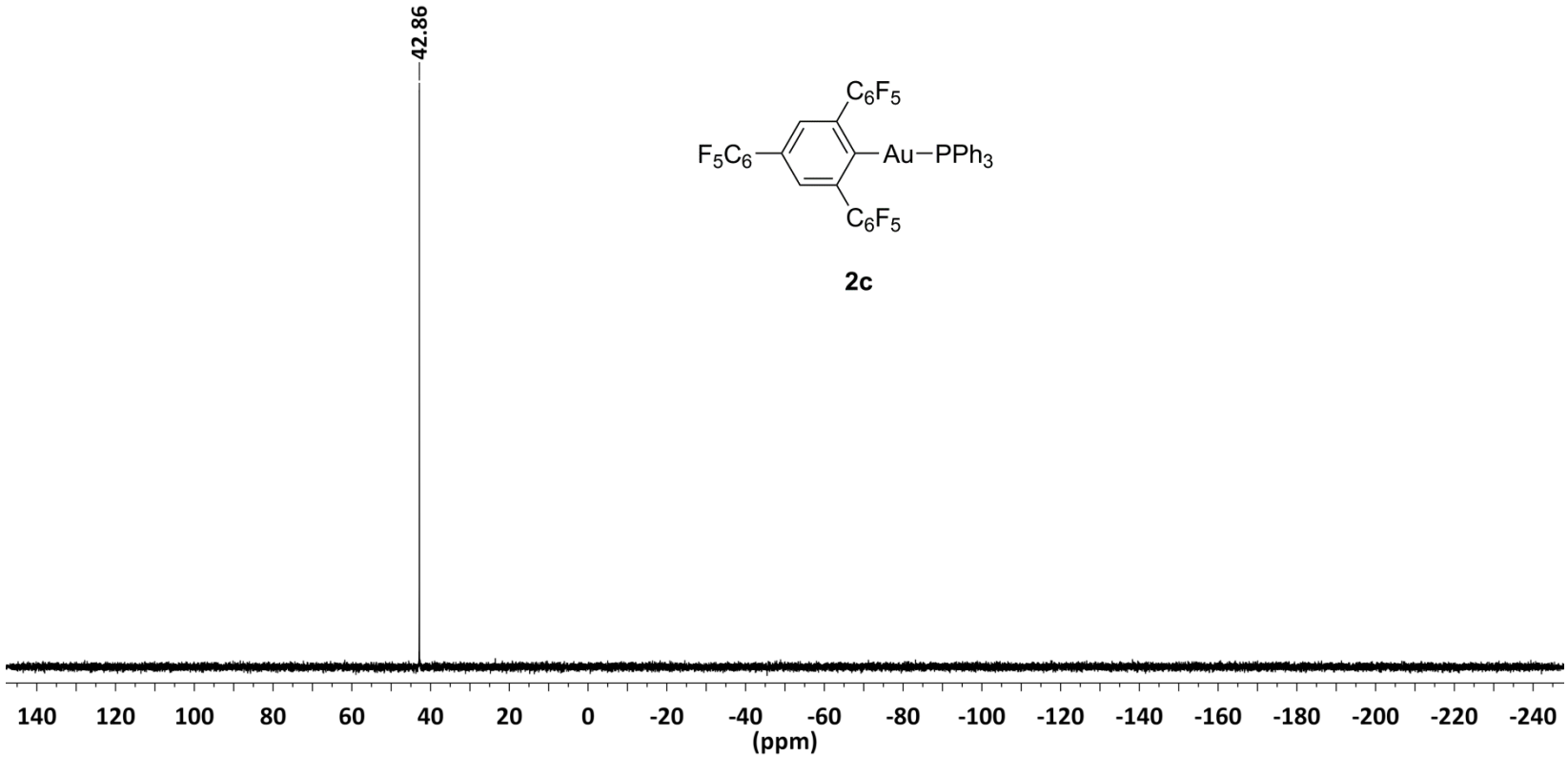


Figure S31. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 243 MHz) spectrum of 2,4,6-$(C_6F_5)_3$-$C_6H_2Au(PPh_3)$ (**2c**).

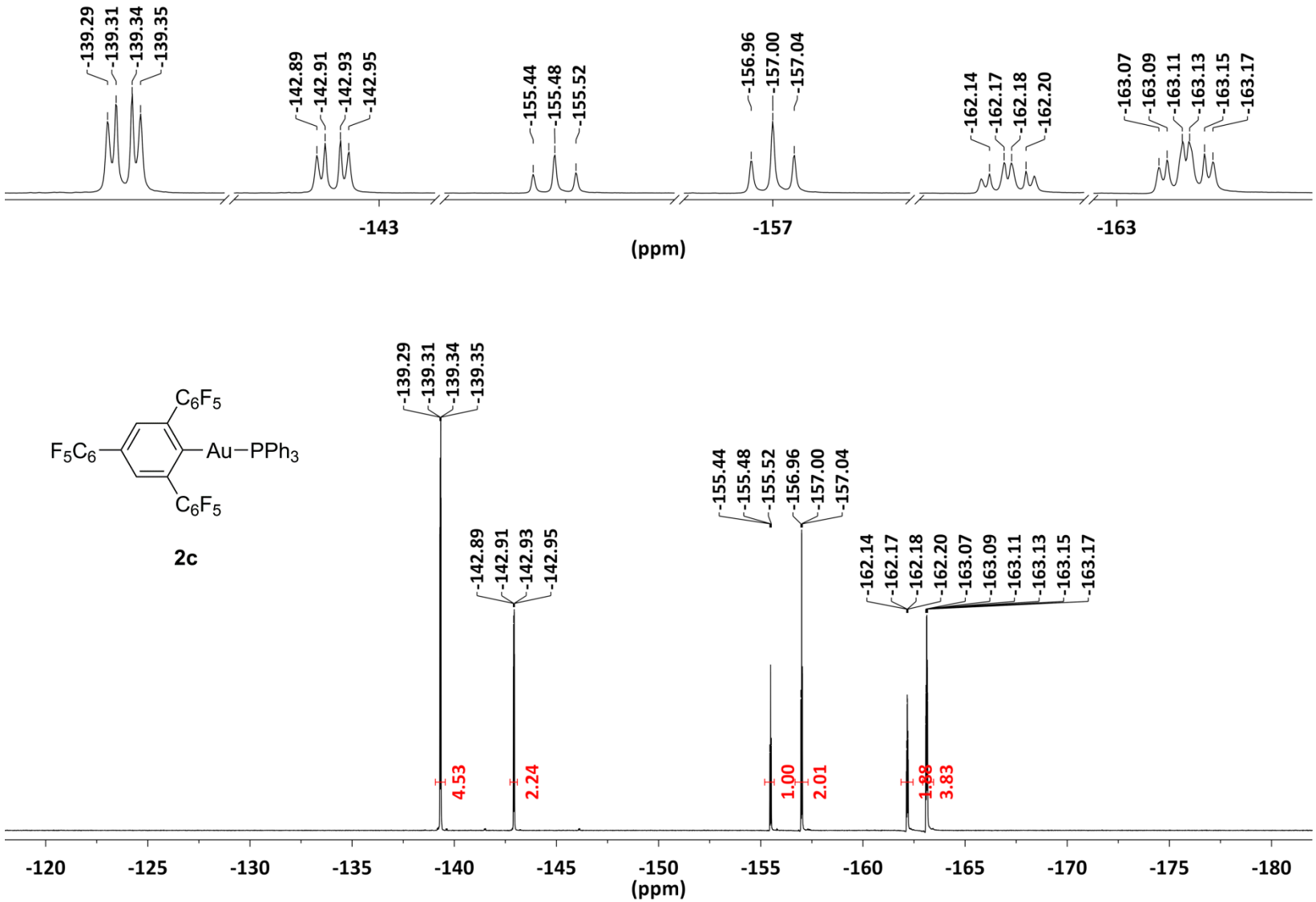


Figure S32. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 565 MHz) spectrum of 2,4,6-$(C_6F_5)_3$-$C_6H_2Au(PPh_3)$ (**2c**).

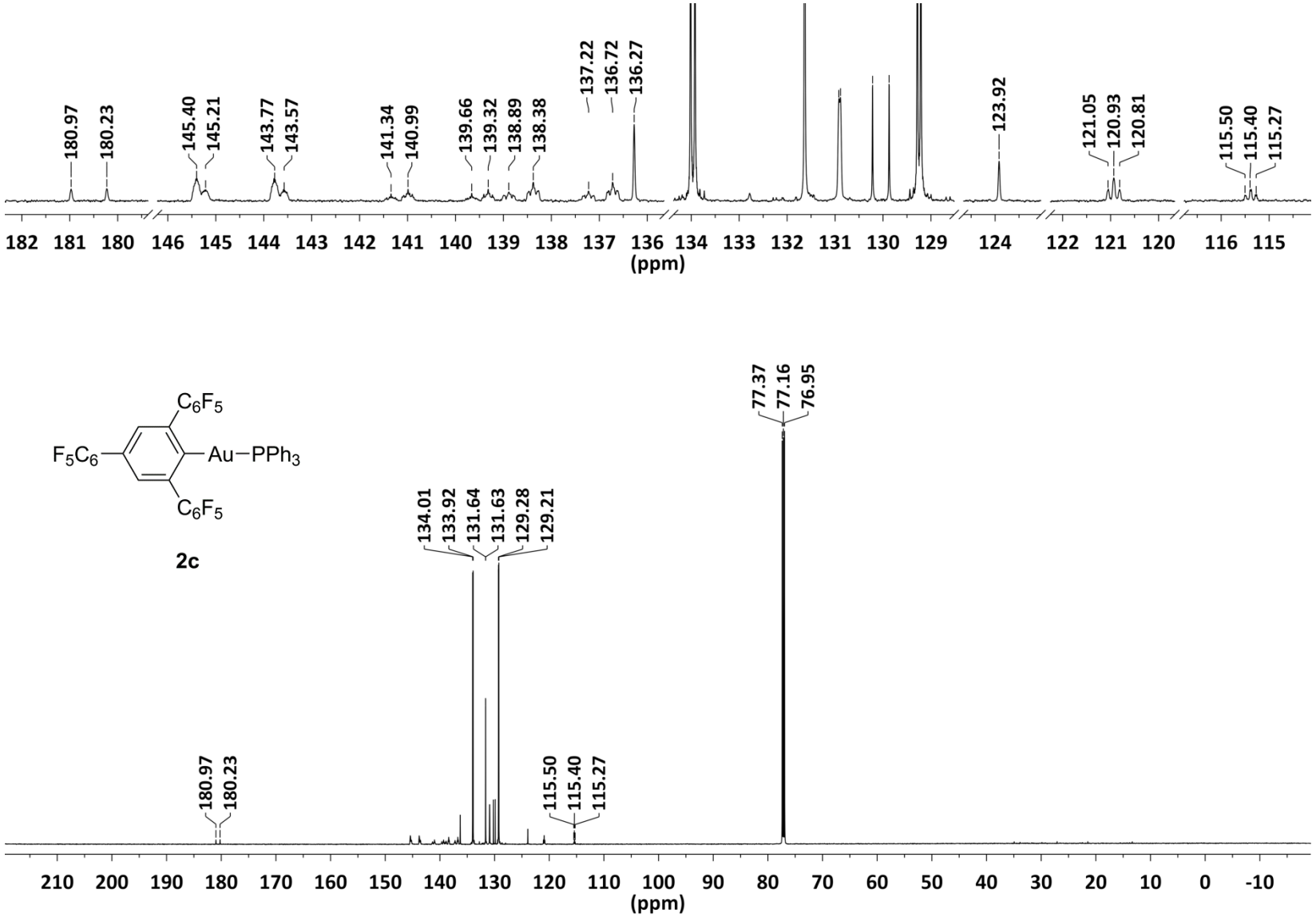


Figure S33. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 151 MHz) spectrum of 2,4,6-$(C_6F_5)_3$-$C_6H_2Au(PPh_3)$ (**2c**).

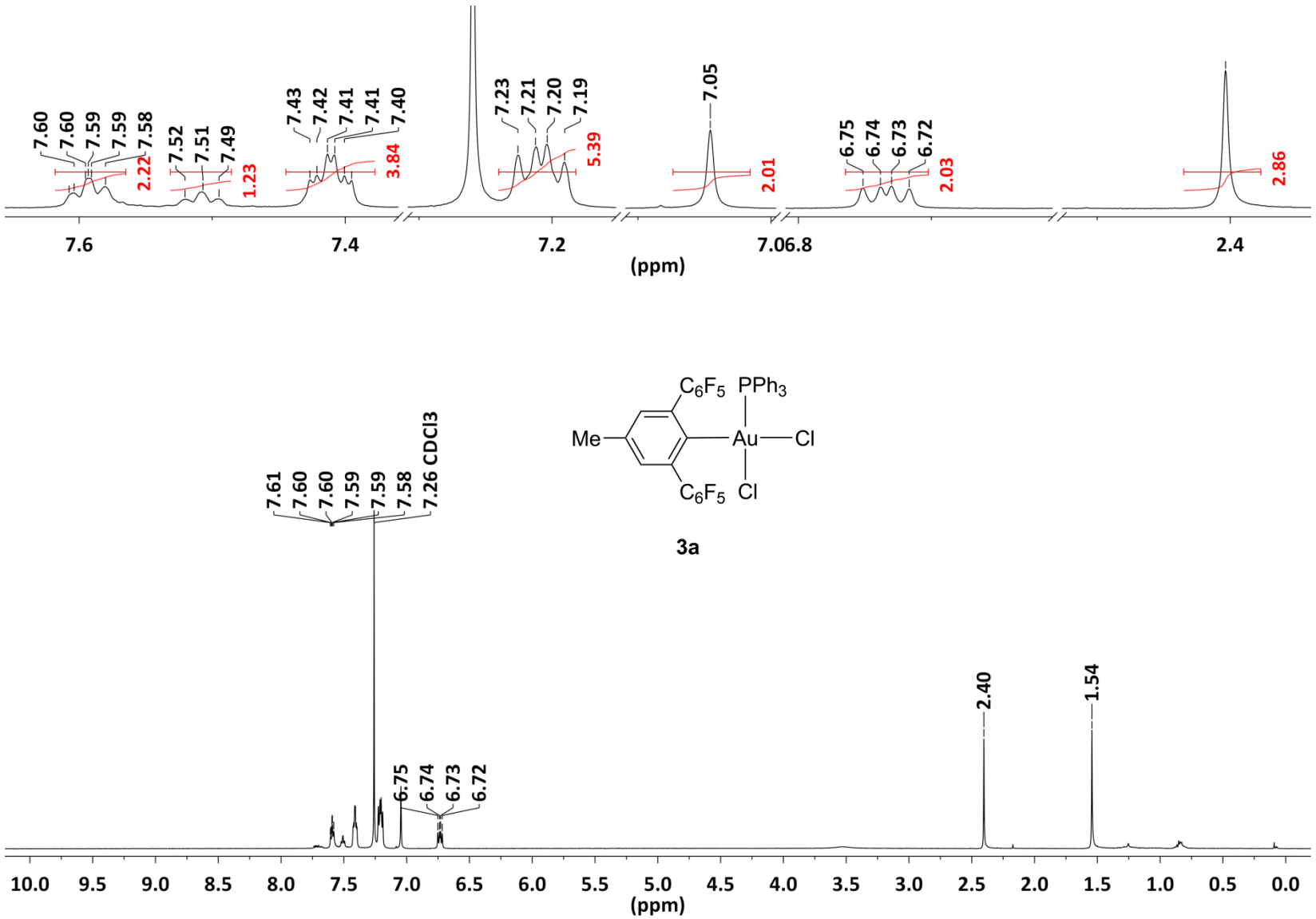


Figure S34. ^{1}H NMR ($CDCl_3$, 600 MHz) spectrum of 2,6-$(C_6F_5)_2$-4-$CH_3C_6H_2AuCl_2(PPh_3)$ (**3a**).

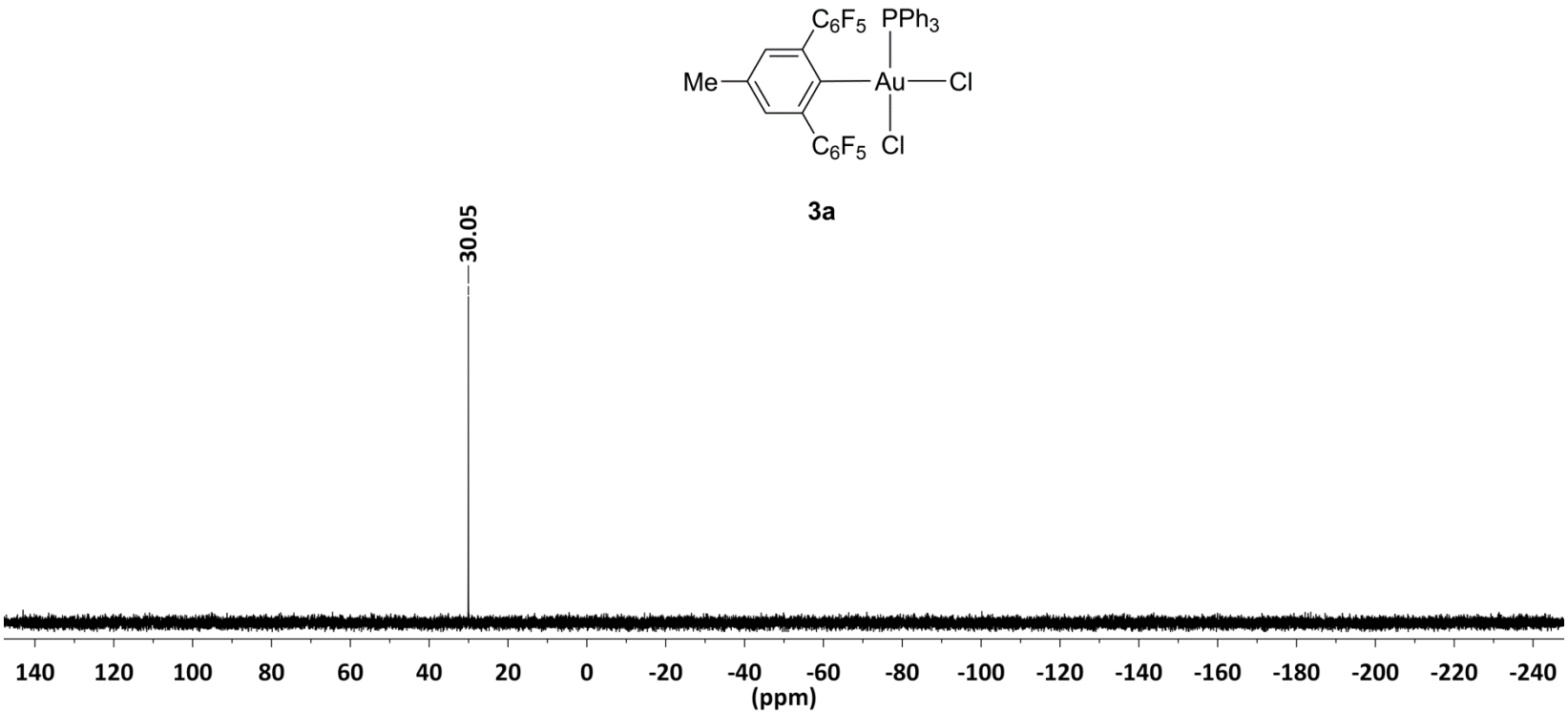


Figure S35. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 243 MHz) spectrum of 2,6-$(C_6F_5)_2$-4-$CH_3C_6H_2AuCl_2(PPh_3)$ (**3a**).

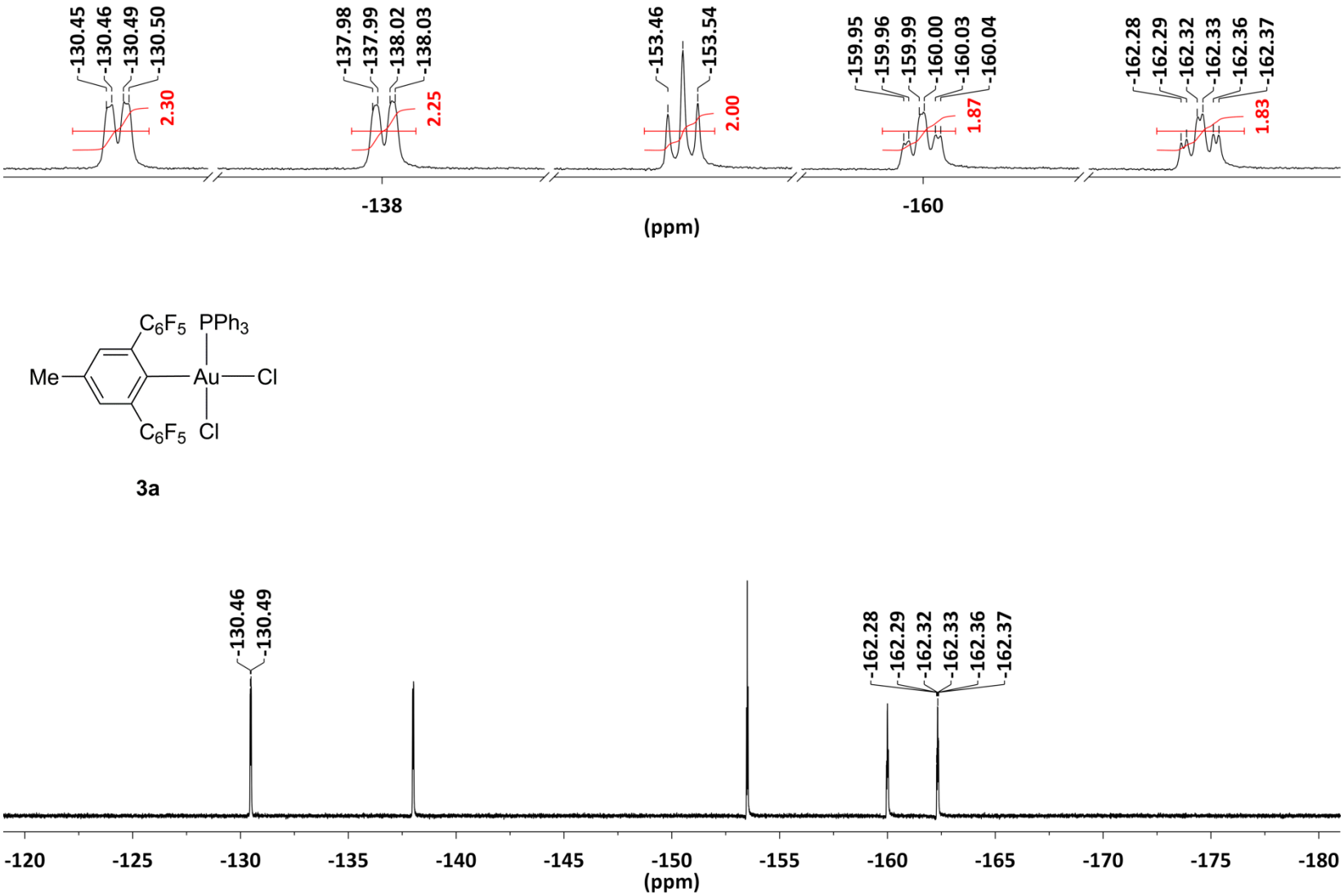


Figure S36. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 565 MHz) spectrum of 2,6-$(C_6F_5)_2$-4-$CH_3C_6H_2AuCl_2(PPh_3)$ (**3a**).

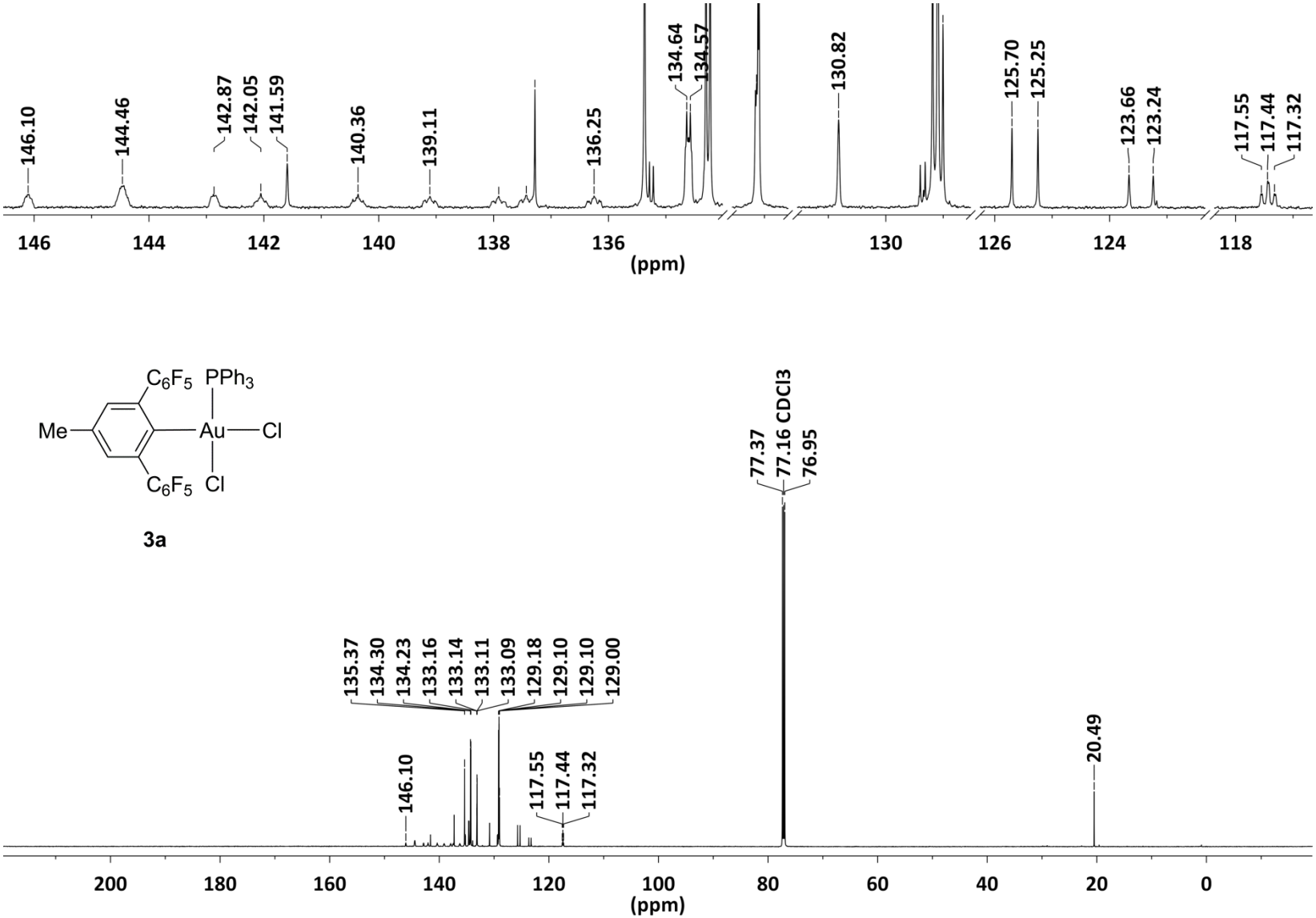


Figure S37. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 151 MHz) spectrum of 2,6-$(C_6F_5)_2$-4-$CH_3C_6H_2AuCl_2(PPh_3)$ (**3a**).

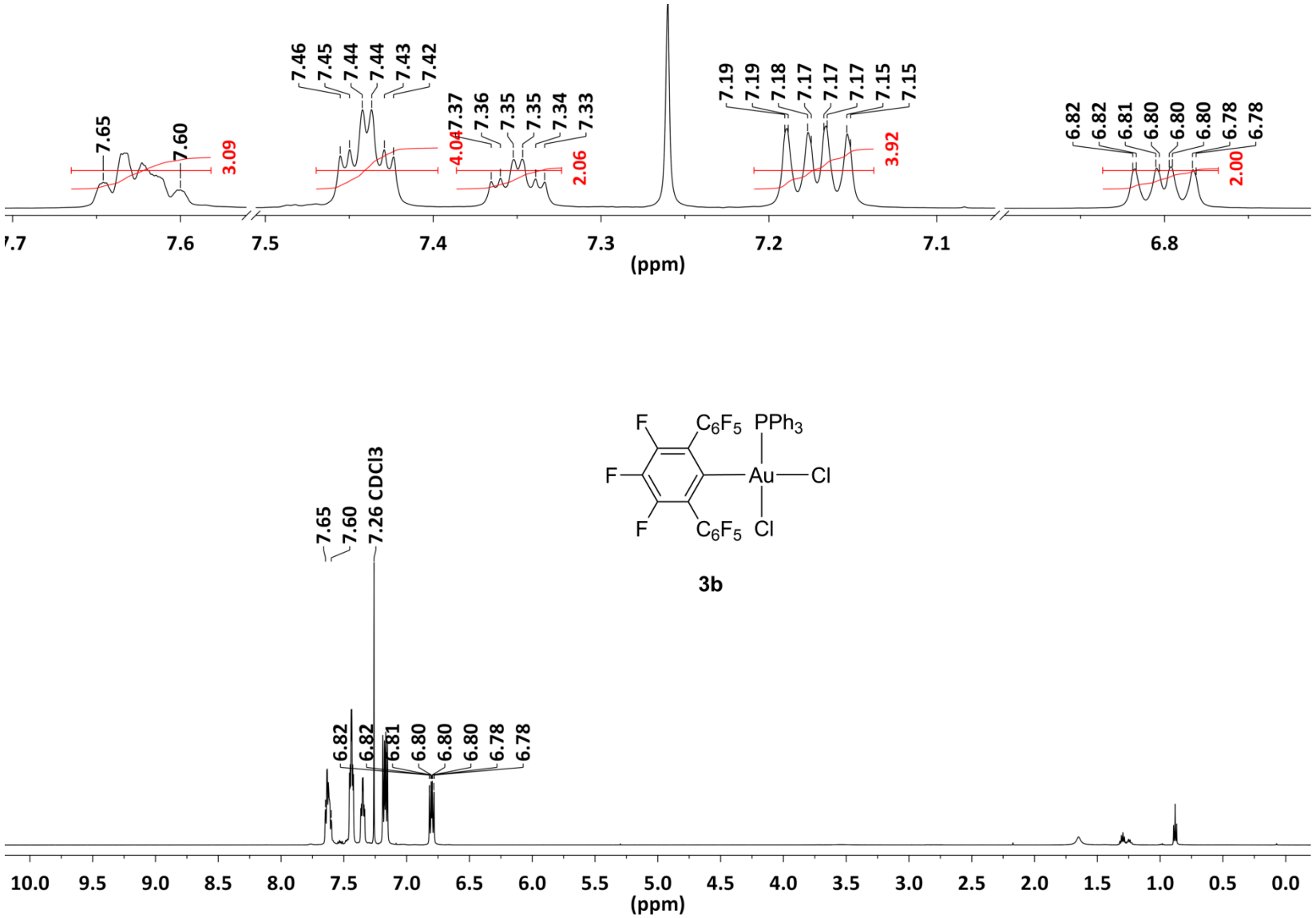


Figure S38. ^{1}H NMR ($CDCl_3$, 600 MHz) spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3AuCl_2(PPh_3)$ (**3b**).

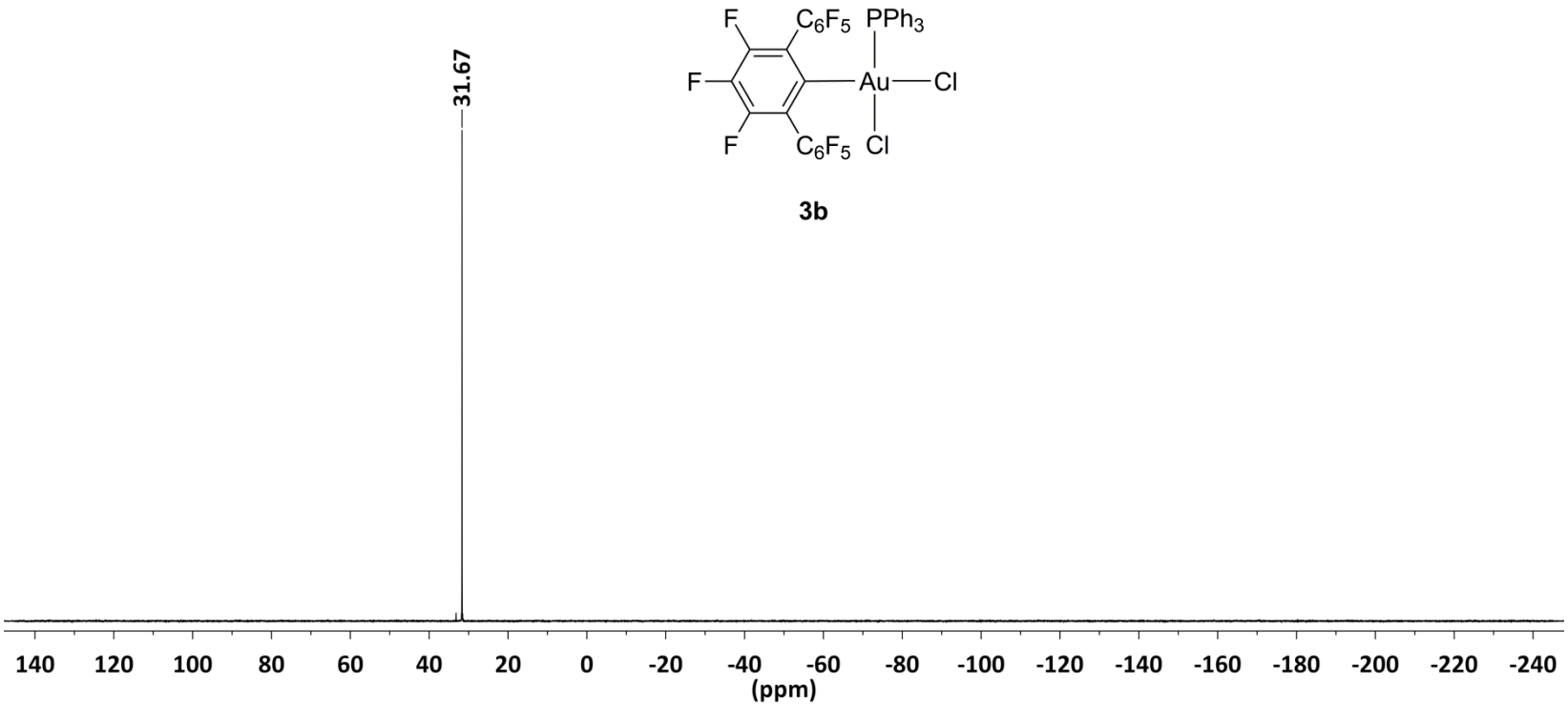


Figure S39. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 243 MHz) spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3AuCl_2(PPh_3)$ (**3b**).

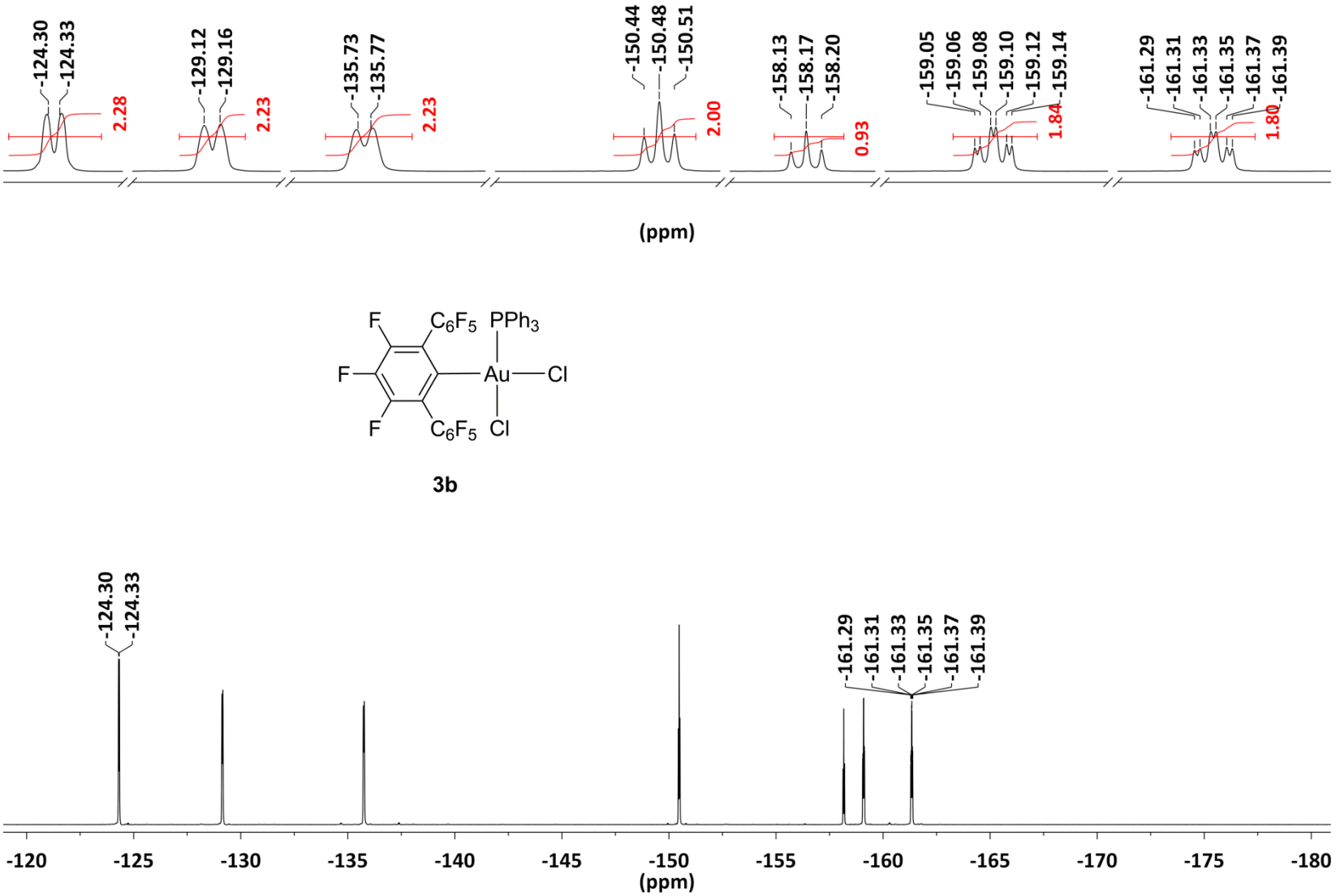


Figure S40. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 565 MHz) spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3AuCl_2(PPh_3)$ (**3b**).

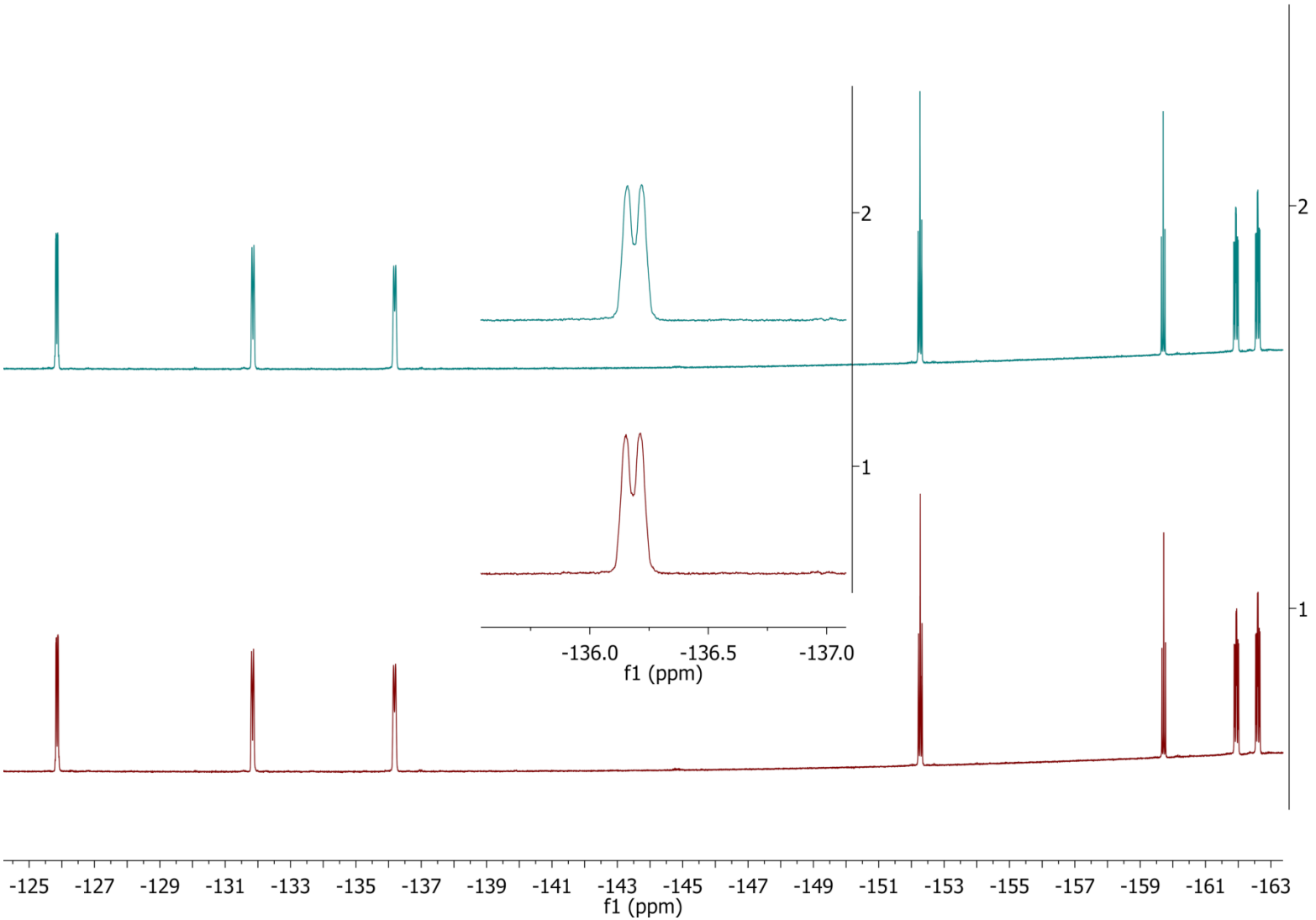


Figure S41. $^{19}F\{^{1}H\}$ NMR (below) and ^{19}F NMR (above) (CD_3CN, 376 MHz) spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3AuCl_2(PPh_3)$ (**3b**).

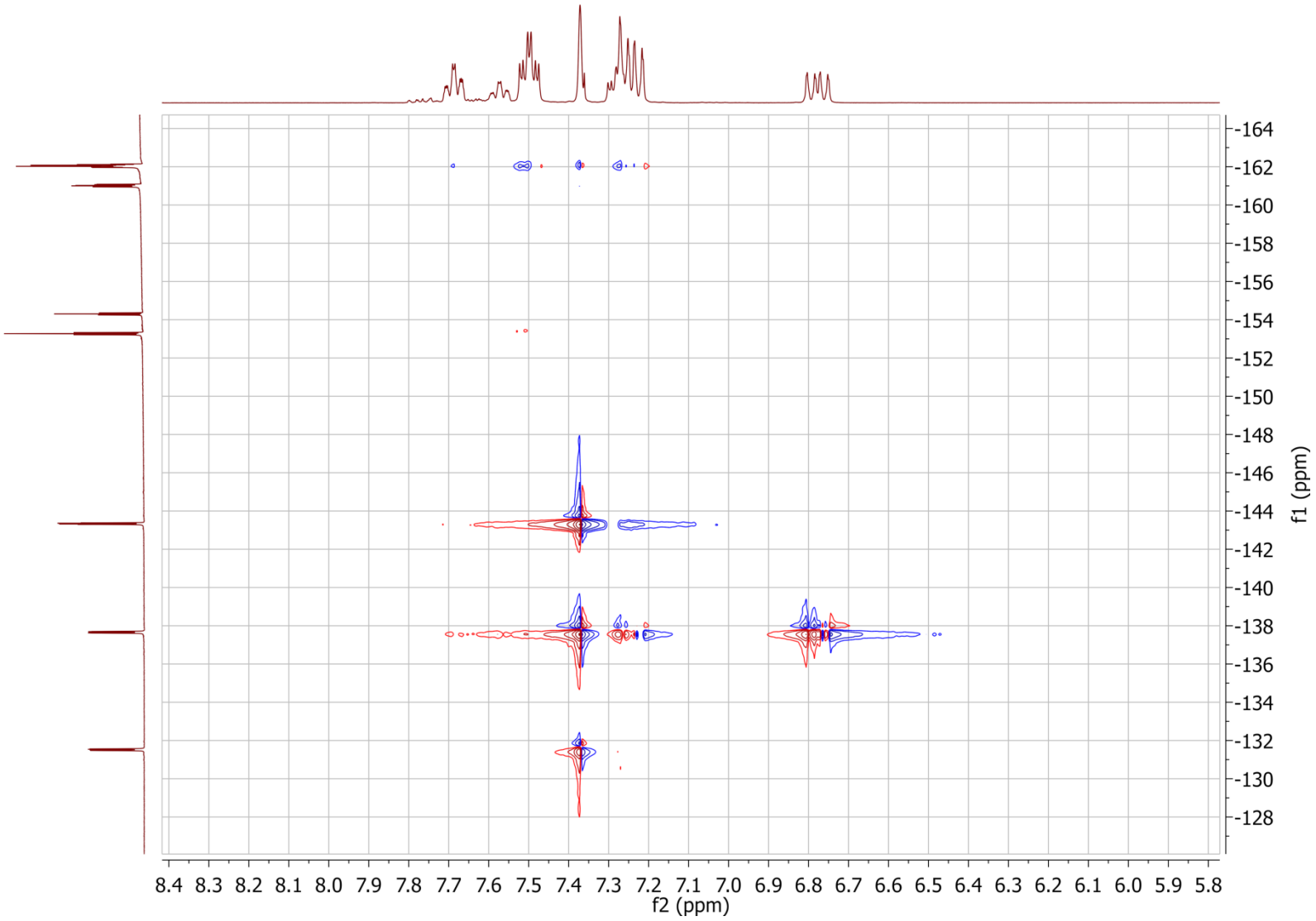


Figure S42. ^{1}H – ^{19}F HOESY ($CDCl_3$, 400 MHz and 376 MHz) spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3AuCl_2(PPh_3)$ (**3b**).

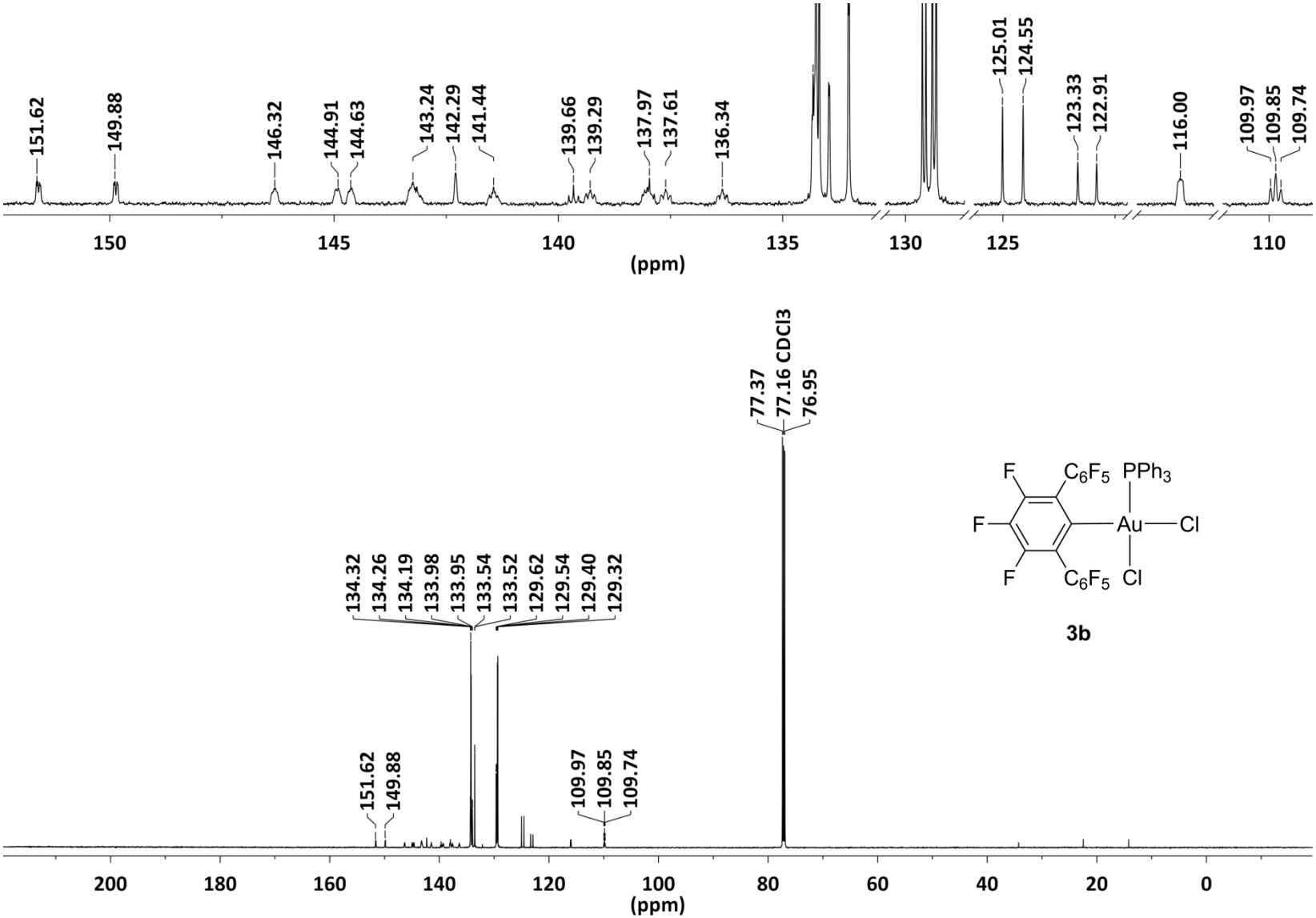


Figure S43. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 151 MHz) spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3AuCl_2(PPh_3)$ (**3b**).

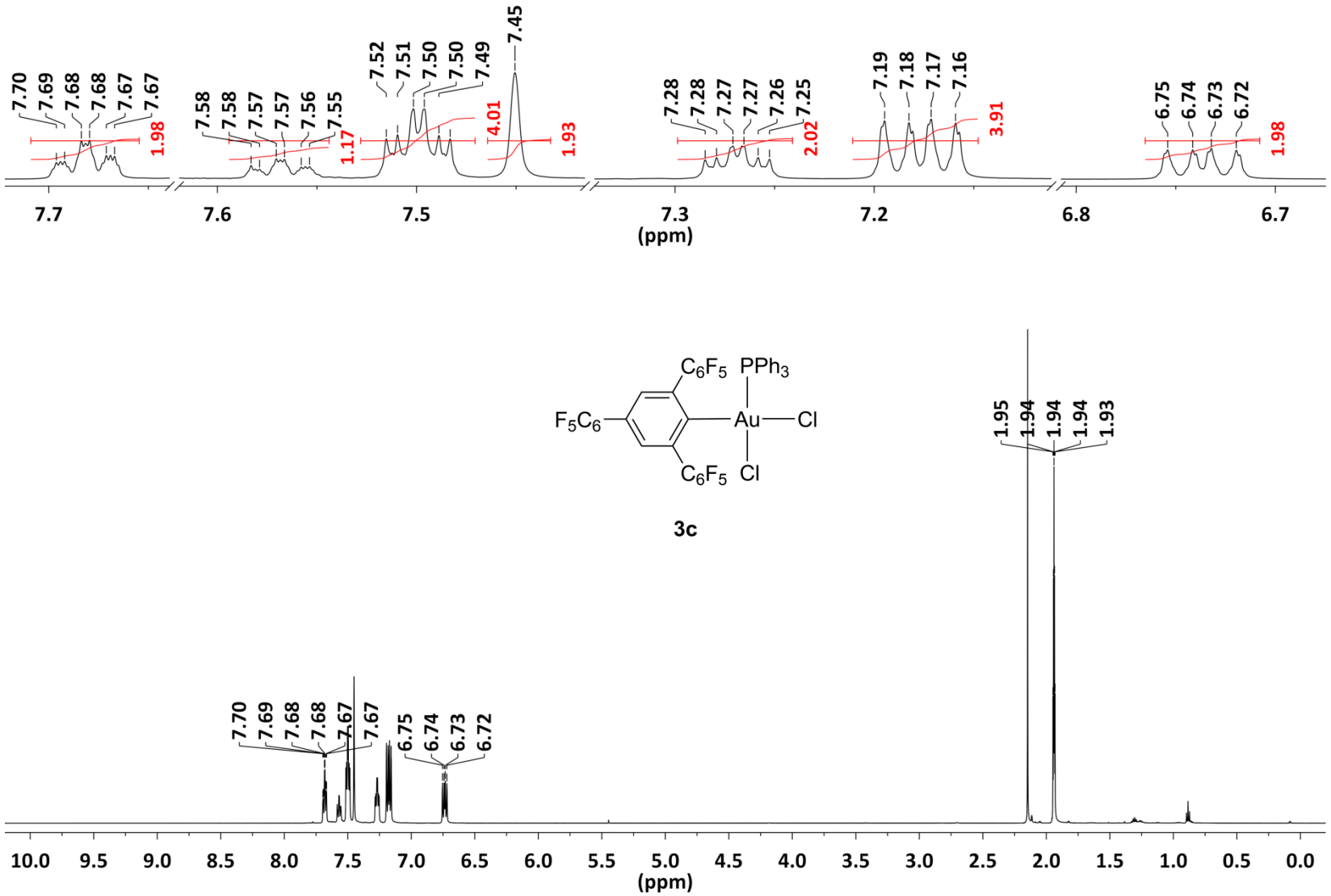


Figure S44. ^{1}H NMR (CD_3CN, 600 MHz) spectrum of 2,4,6-$(C_6F_5)_3$-$C_6H_2AuCl_2(PPh_3)$ (**3c**).

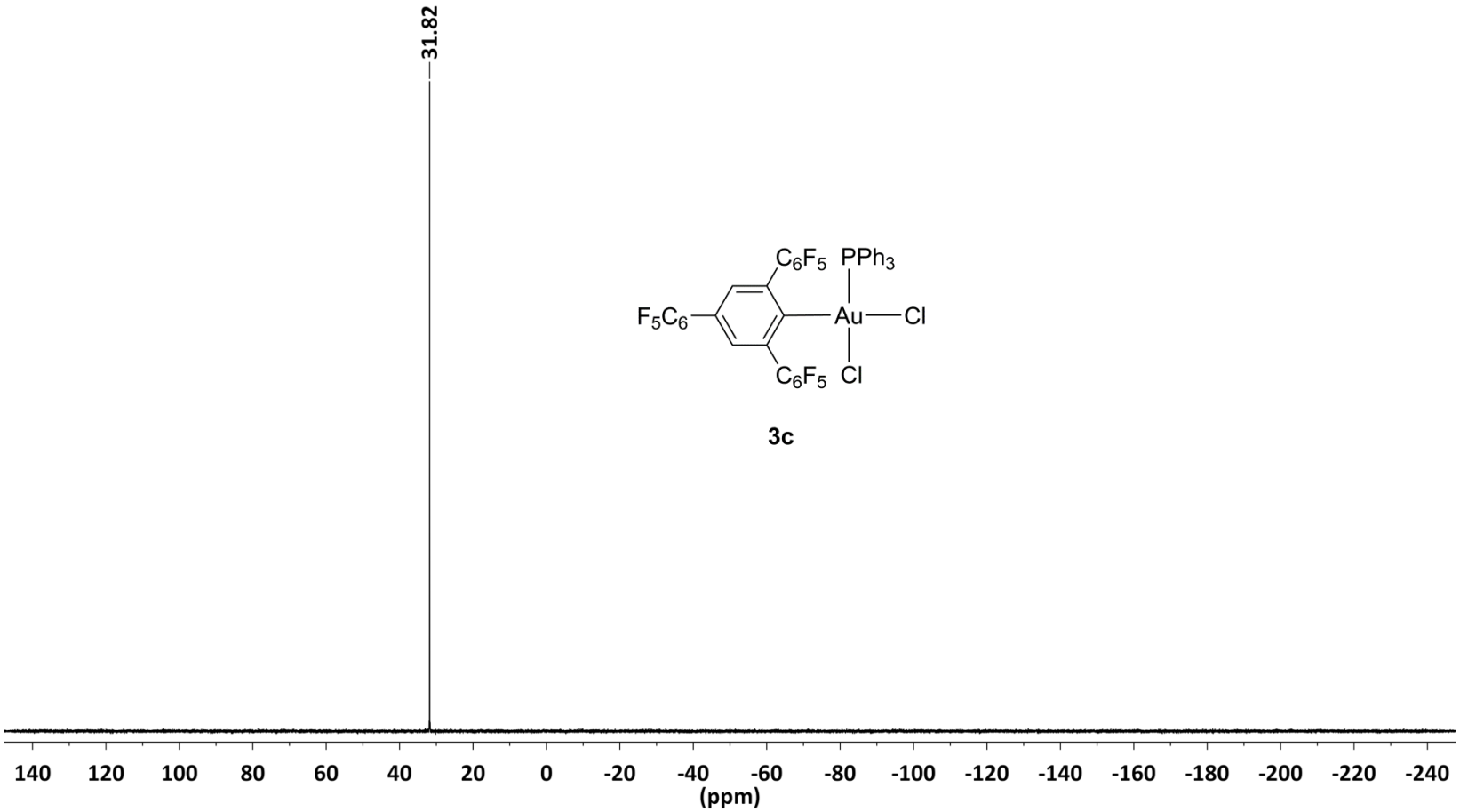


Figure S45. $^{31}P\{^{1}H\}$ NMR (CD_3CN, 243 MHz) spectrum of 2,4,6-$(C_6F_5)_3$-$C_6H_2AuCl_2(PPh_3)$ (**3c**).

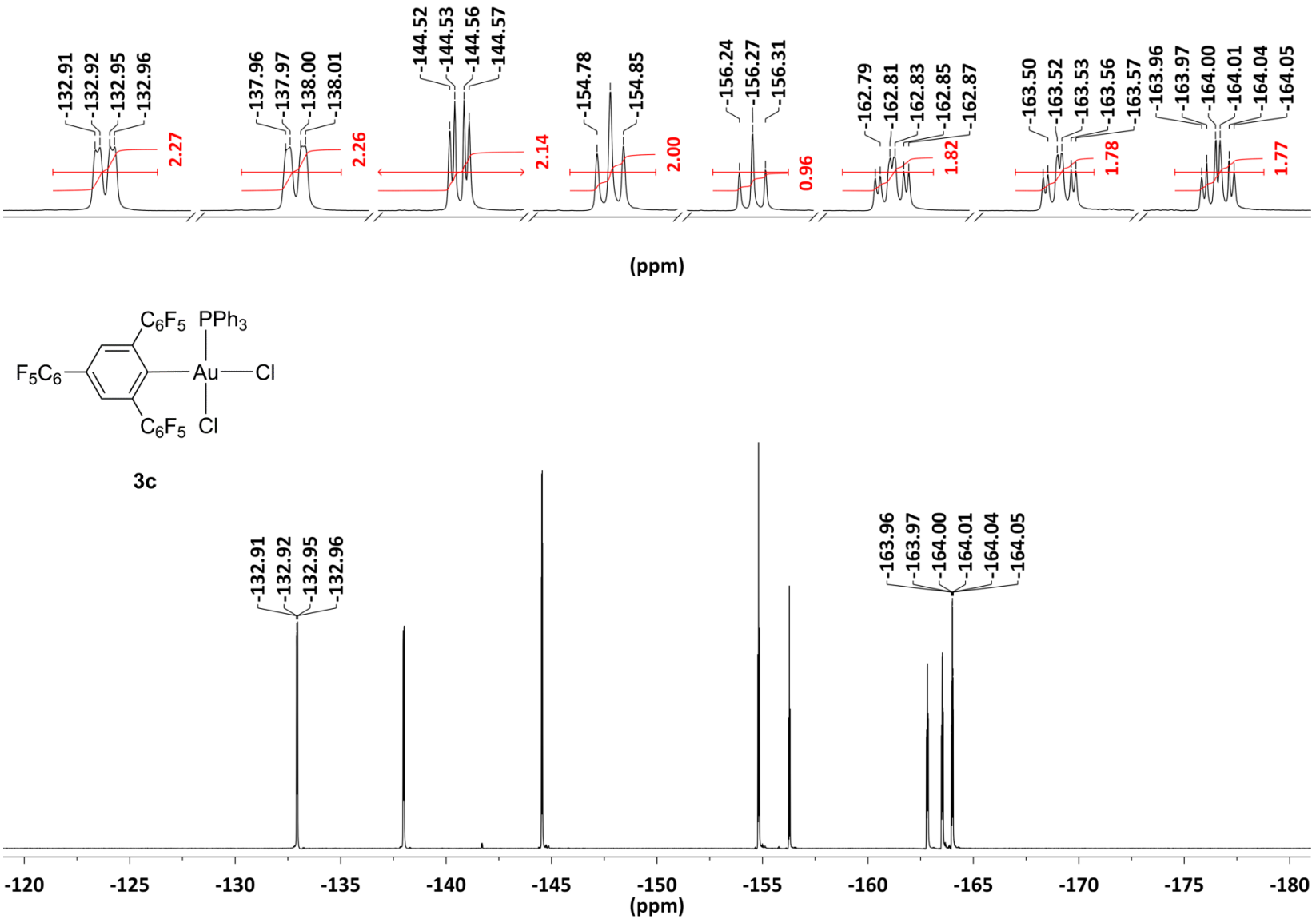


Figure S46. $^{19}F\{^{1}H\}$ NMR (CD_3CN, 565 MHz) spectrum of 2,4,6-$(C_6F_5)_3$-$C_6H_2AuCl_2(PPh_3)$ (**3c**).

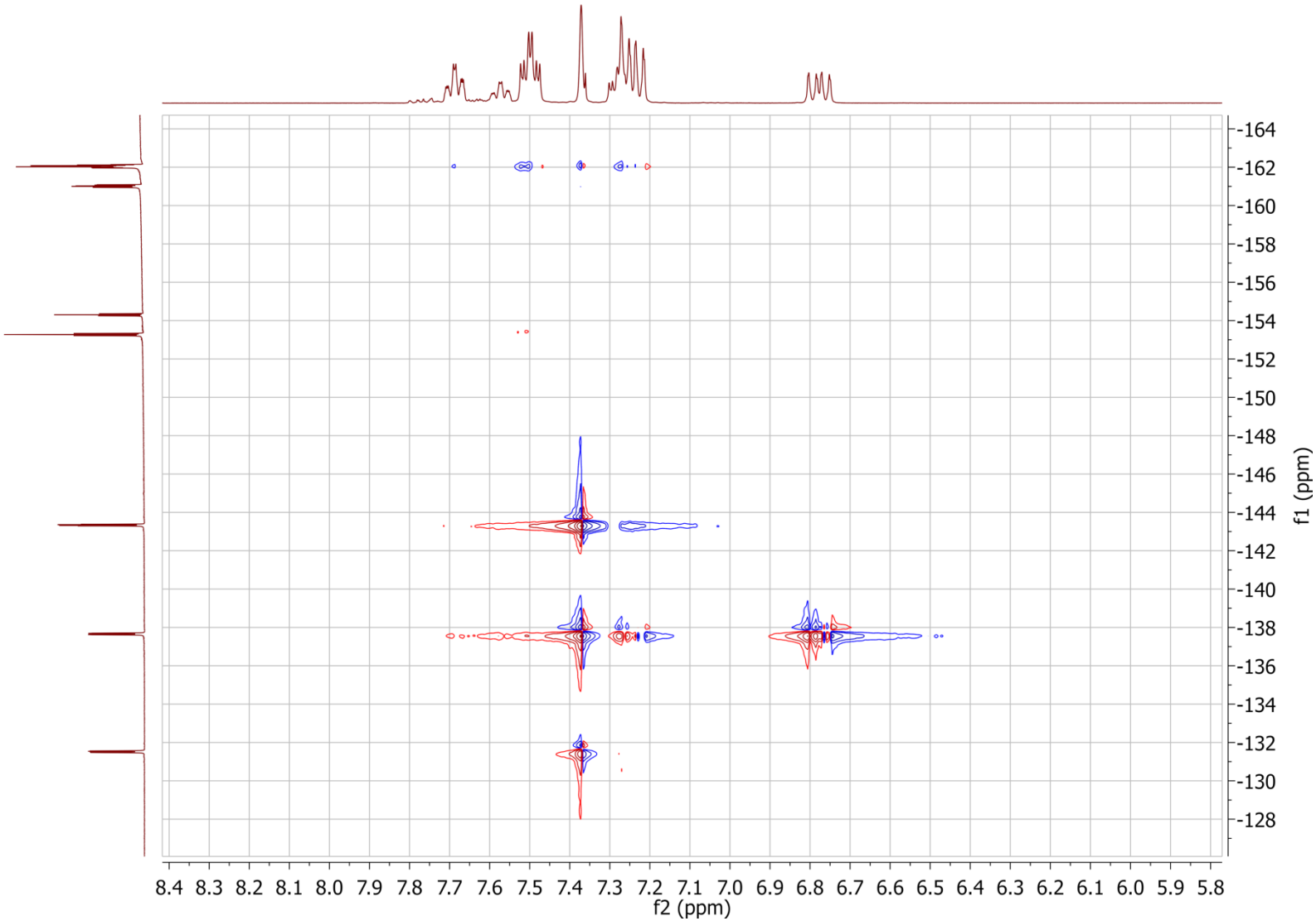


Figure S47. ^{1}H – ^{19}F HOESY ($CDCl_3$, 400 MHz and 376 MHz) spectrum of 2,4,6-$(C_6F_5)_3$-$C_6H_2AuCl_2(PPh_3)$ (**3c**).

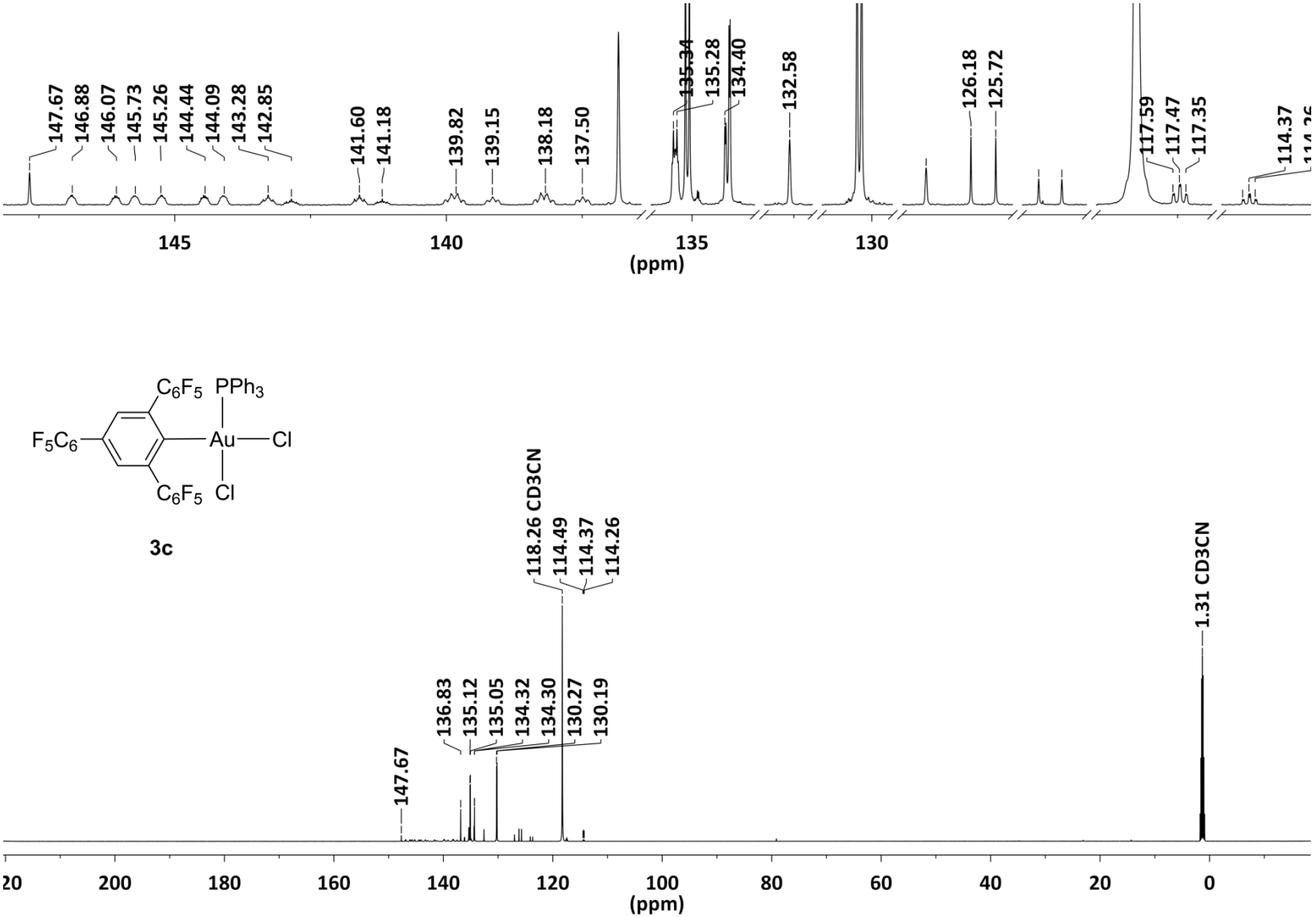


Figure S48. $^{13}C\{^{1}H\}$ NMR (CD_3CN, 151 MHz) spectrum of 2,4,6-$(C_6F_5)_3$-$C_6H_2AuCl_2(PPh_3)$ (**3c**).

MS data

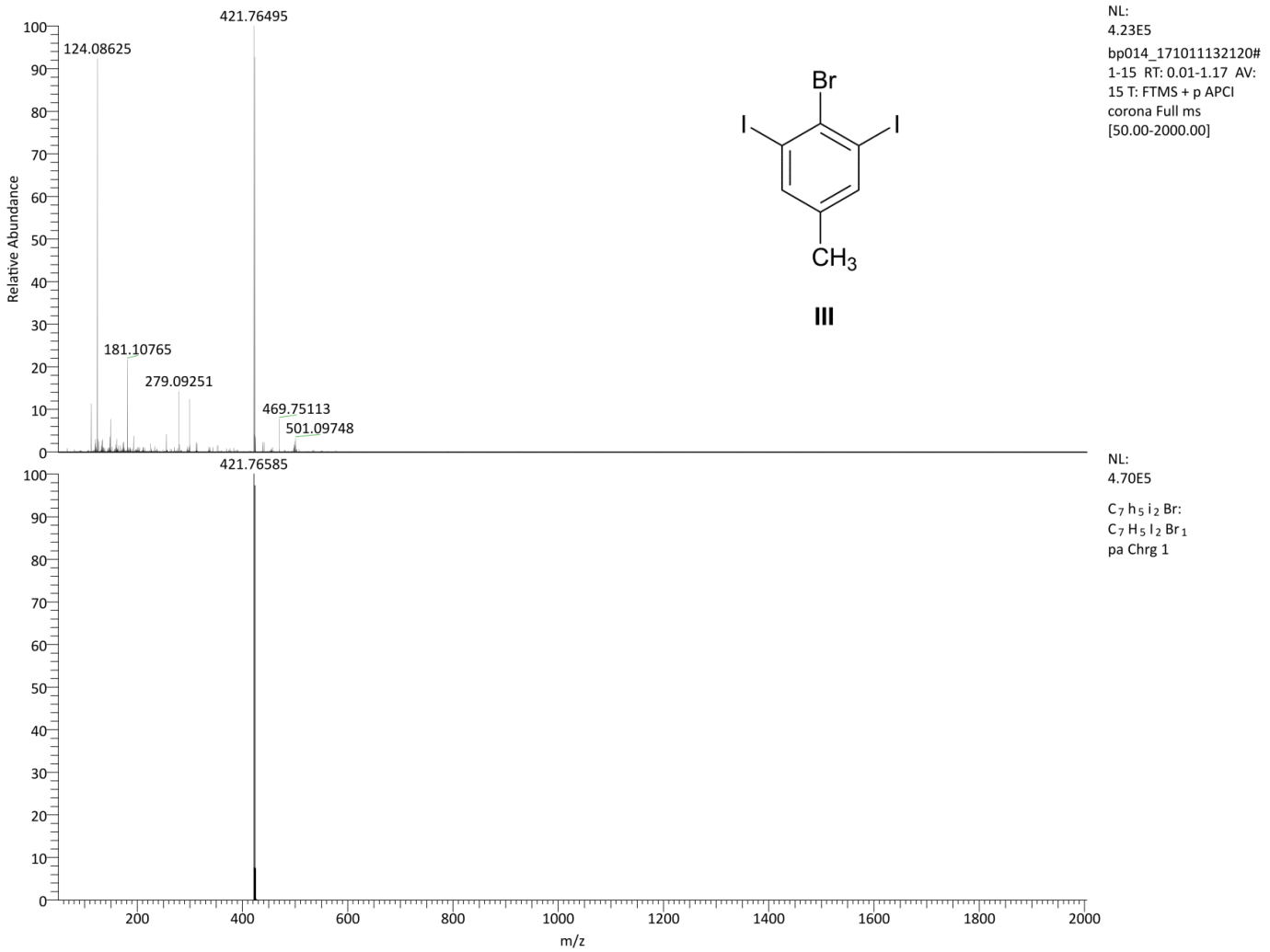


Figure S49. APCI(+) mass spectrum of 2,6-I_2-4-$CH_3C_6H_2Br$ (**III**) (top) and calculated peak of $[M]^+$ (bottom).

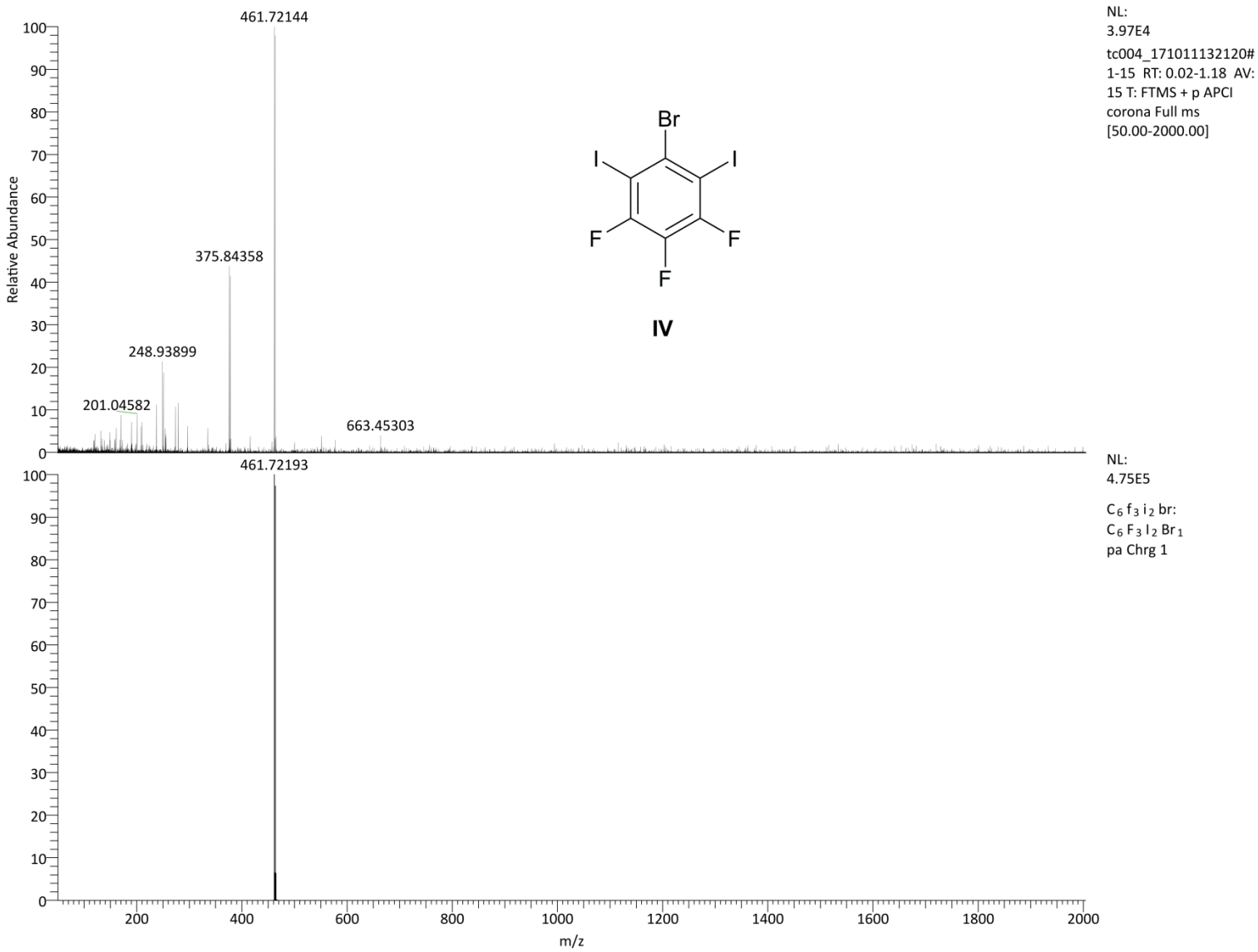


Figure S50. APCI(+) mass spectrum of 2,6-I_2-C_6F_3Br (**IV**) (top) and calculated peak of $[M]^+$ (bottom).

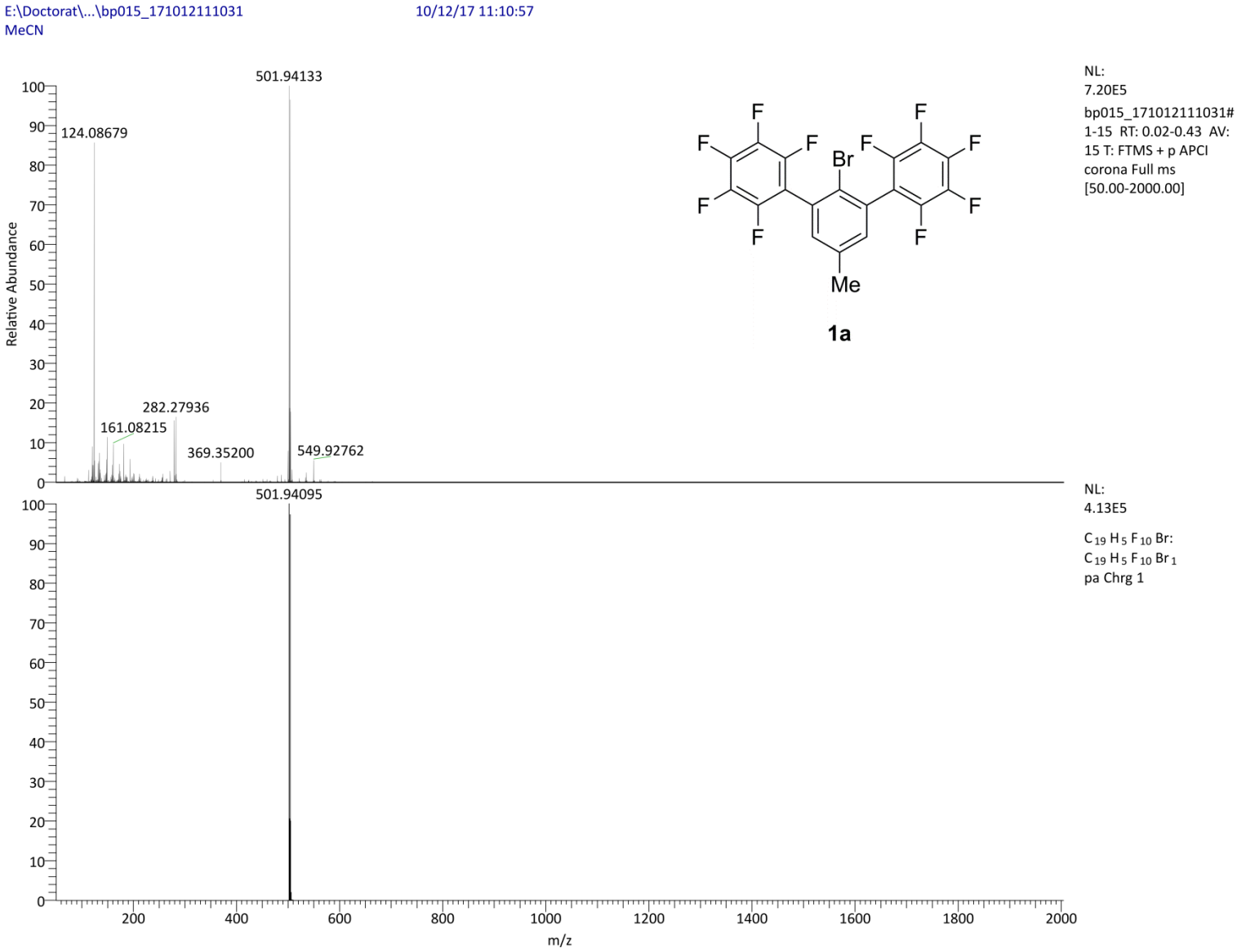


Figure S51. APCI(+) mass spectrum of 2,6-$(C_6F_5)_2$-4-$CH_3C_6H_2Br$ (**1a**) (top) and calculated peak of $[M]^+$ (bottom).

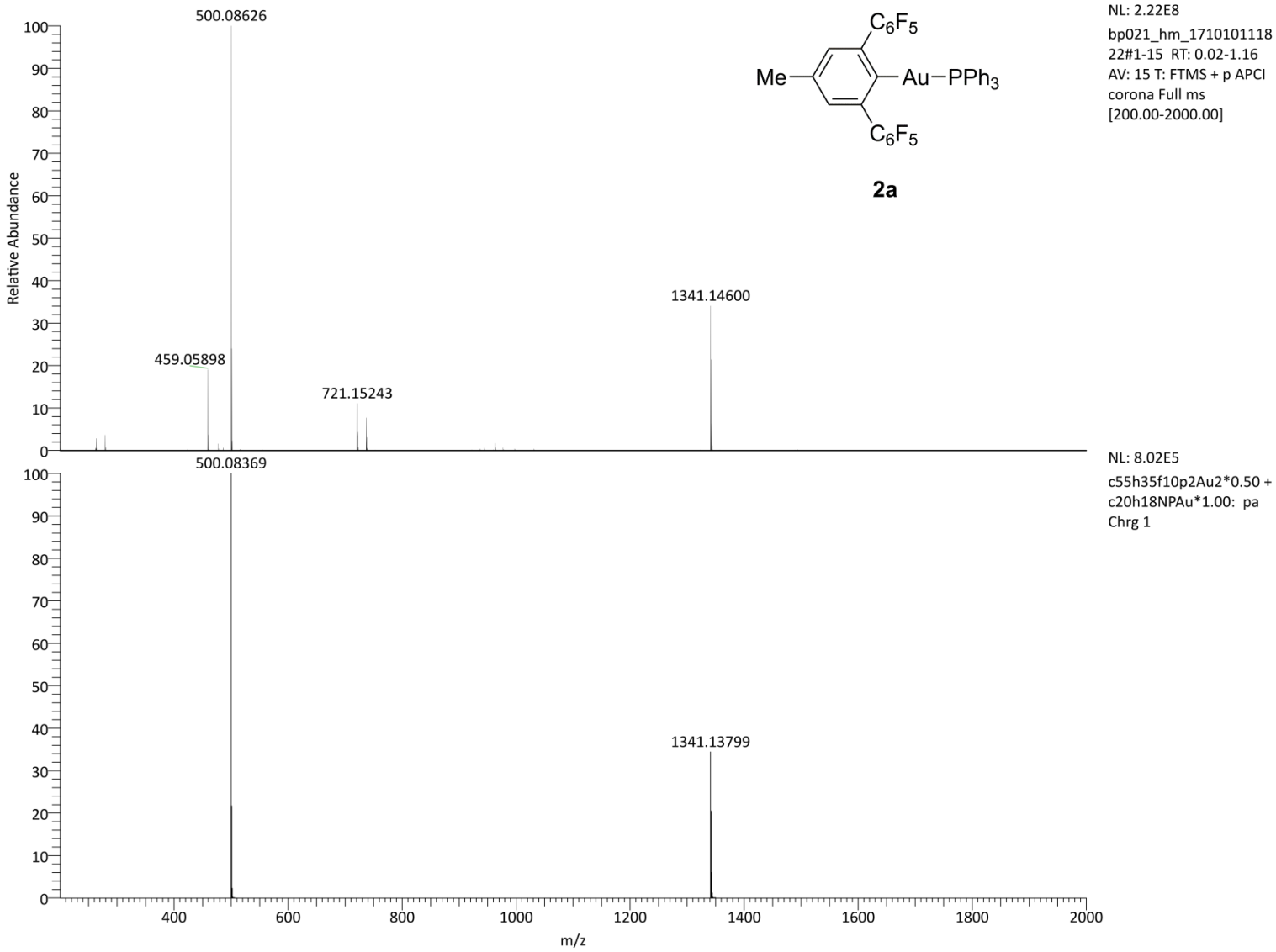


Figure S52. APCI(+) mass spectrum of 2,6-$(C_6F_5)_2$-4-$CH_3C_6H_2Au(PPh_3)$ (**2a**) (top) and calculated peak of $[M + Au(PPh_3)]^+$ and $[Au(PPh_3)_2]^+$ (bottom).

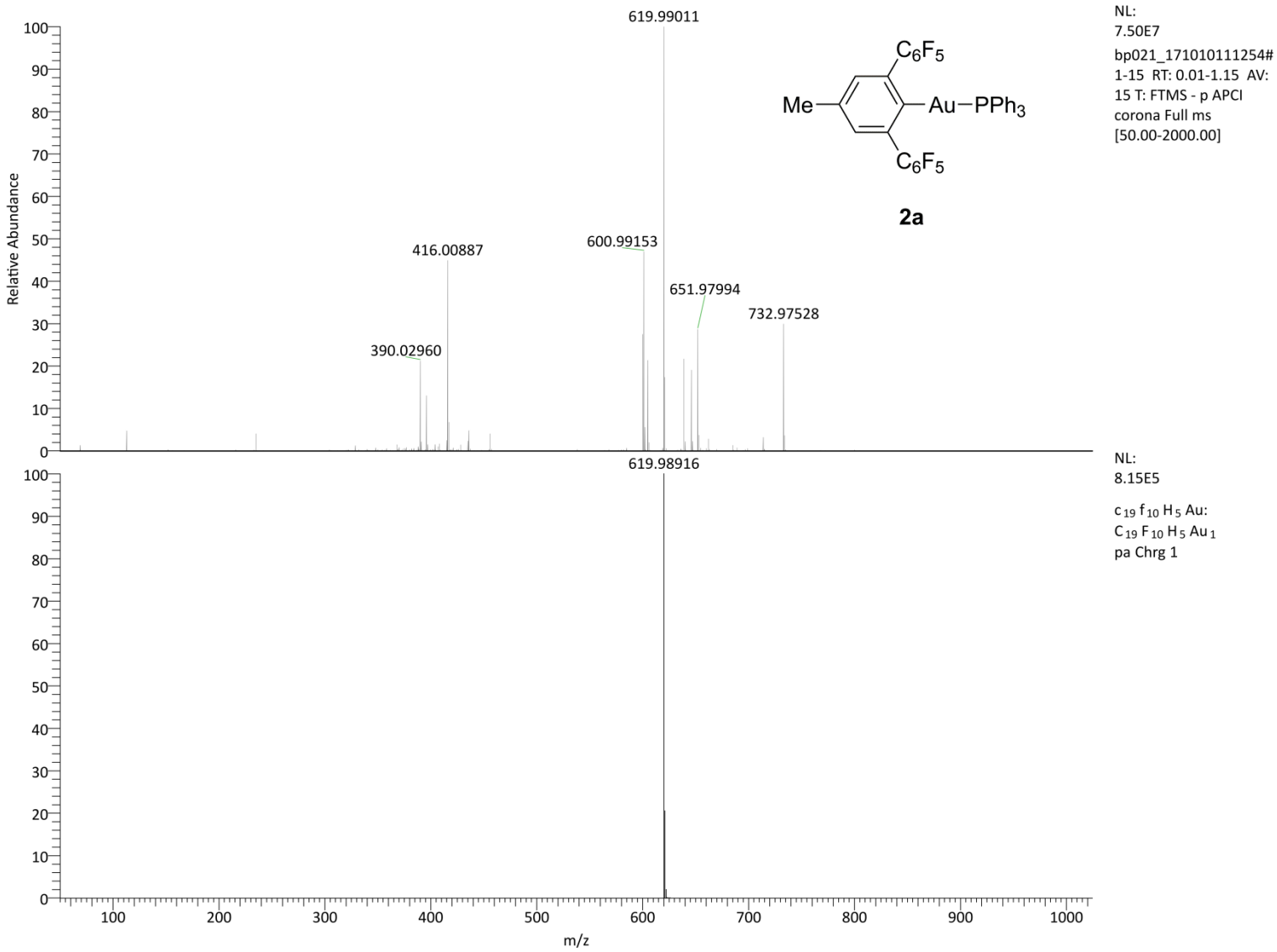


Figure S53. APCI(−) mass spectrum of 2,6-$(C_6F_5)_2$-4-$CH_3C_6H_2Au(PPh_3)$ (**2a**) (top) and calculated peak of $[M - PPh_3]^-$ (bottom).

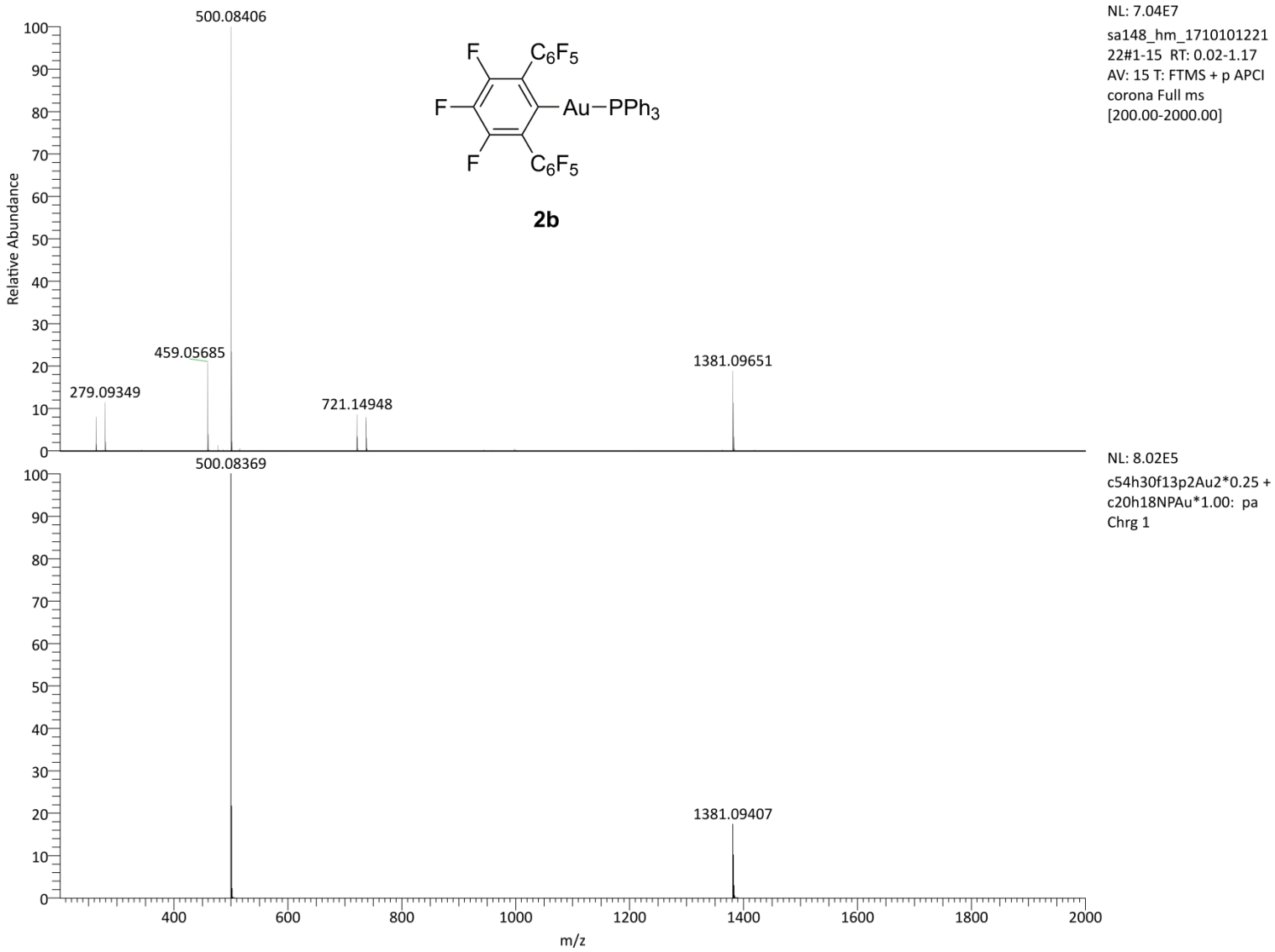


Figure S54. APCI(+) mass spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3Au(PPh_3)$ (**2b**) (top) and calculated peak of $[M + Au(PPh_3)]^+$ and $[Au(PPh_3)_2]^+$ (bottom).

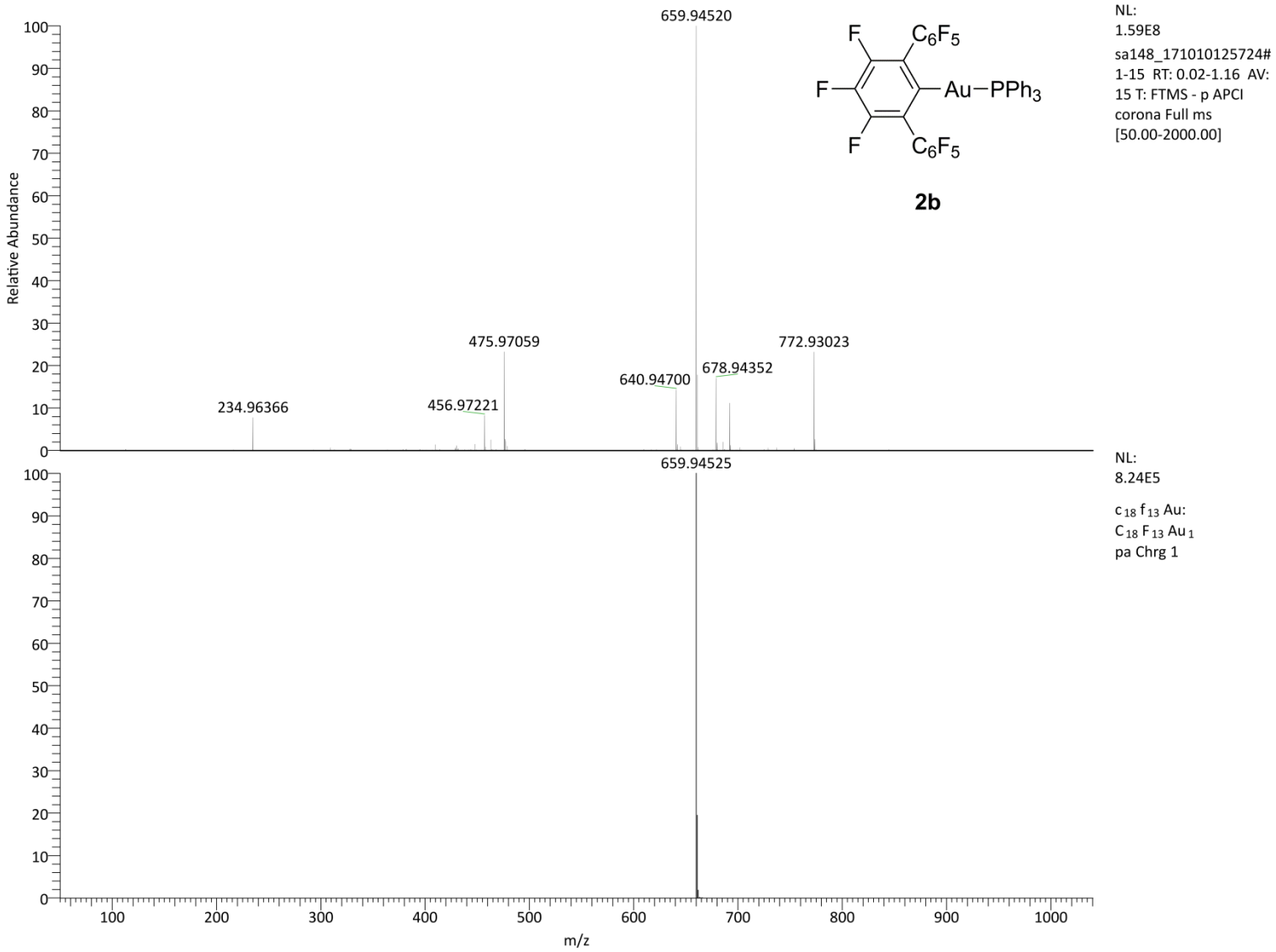


Figure S55. APCI(−) mass spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3Au(PPh_3)$ (**2b**) (top) and calculated peak of $[M - PPh_3]^-$ (bottom).

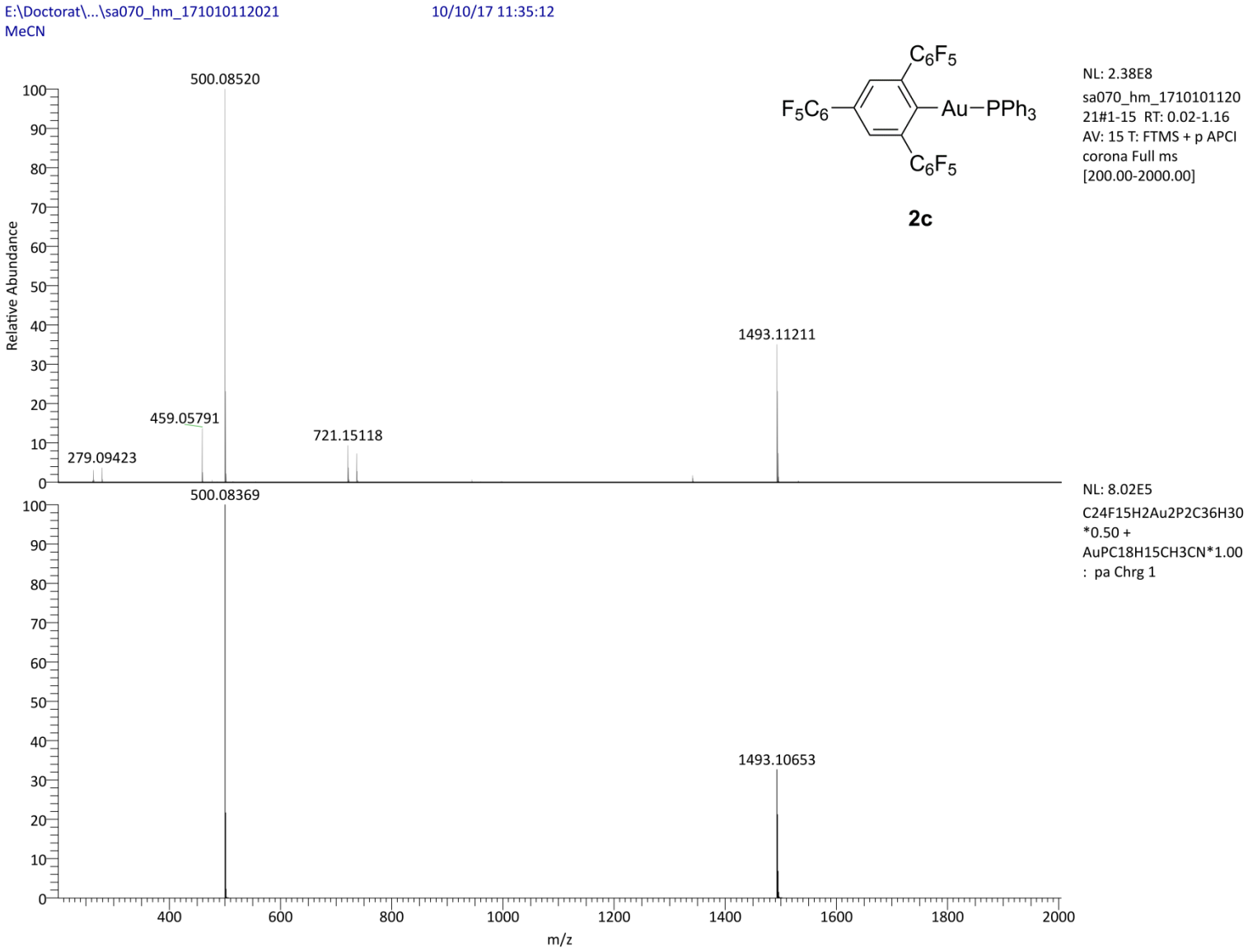


Figure S56. APCI(+) mass spectrum of 2,4,6-$(C_6F_5)_3$-$C_6H_2Au(PPh_3)$ (**2c**) (top) and calculated peak of $[M + Au(PPh_3)]^+$ and $[Au(PPh_3)_2]^+$ (bottom).

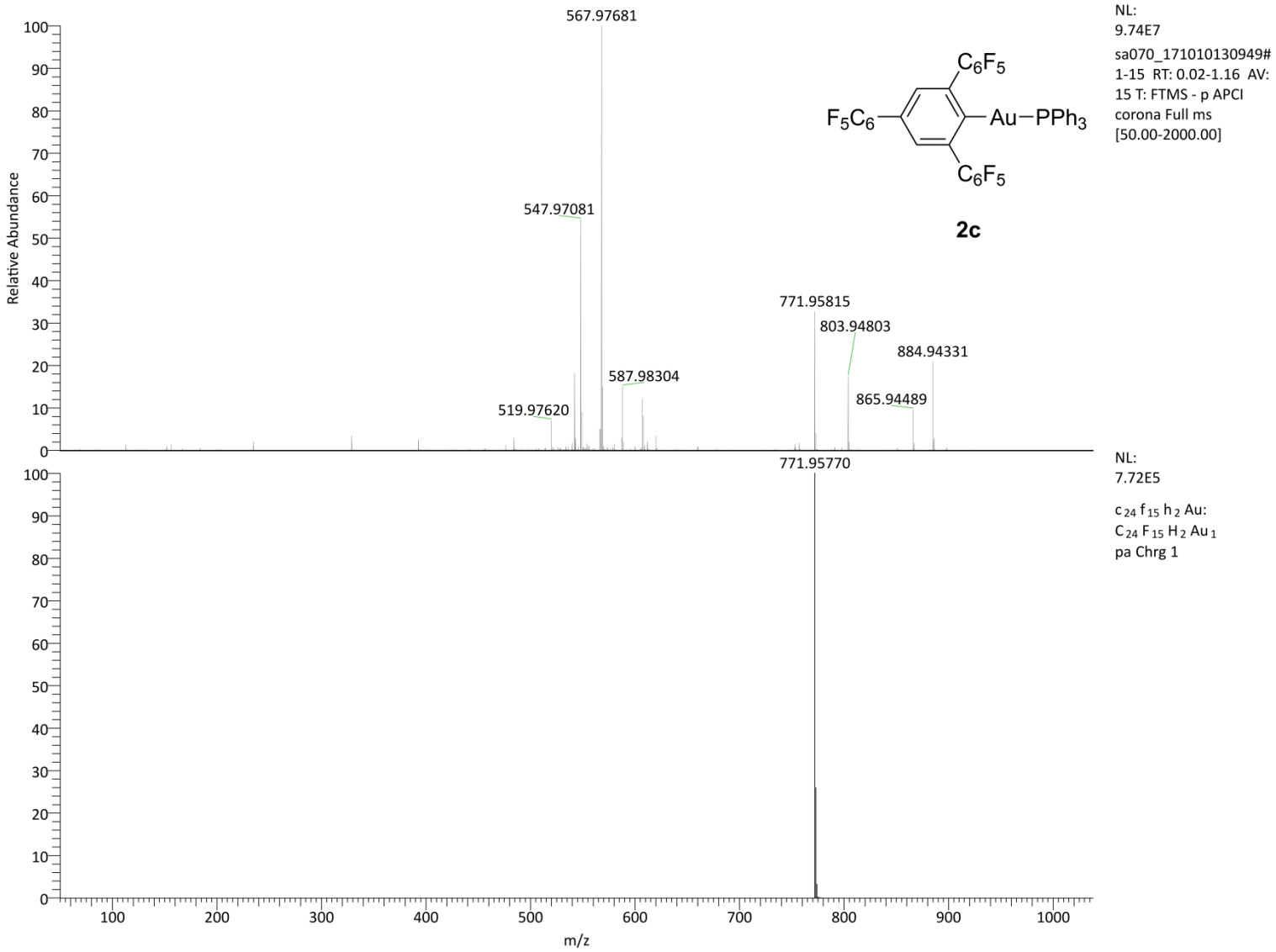


Figure S57. APCI(–) mass spectrum of 2,4,6-(C_6F_5)$_3$-$C_6H_2Au(PPh_3)$ (**2c**) (top) and calculated peak of $[M - PPh_3]^-$ (bottom).

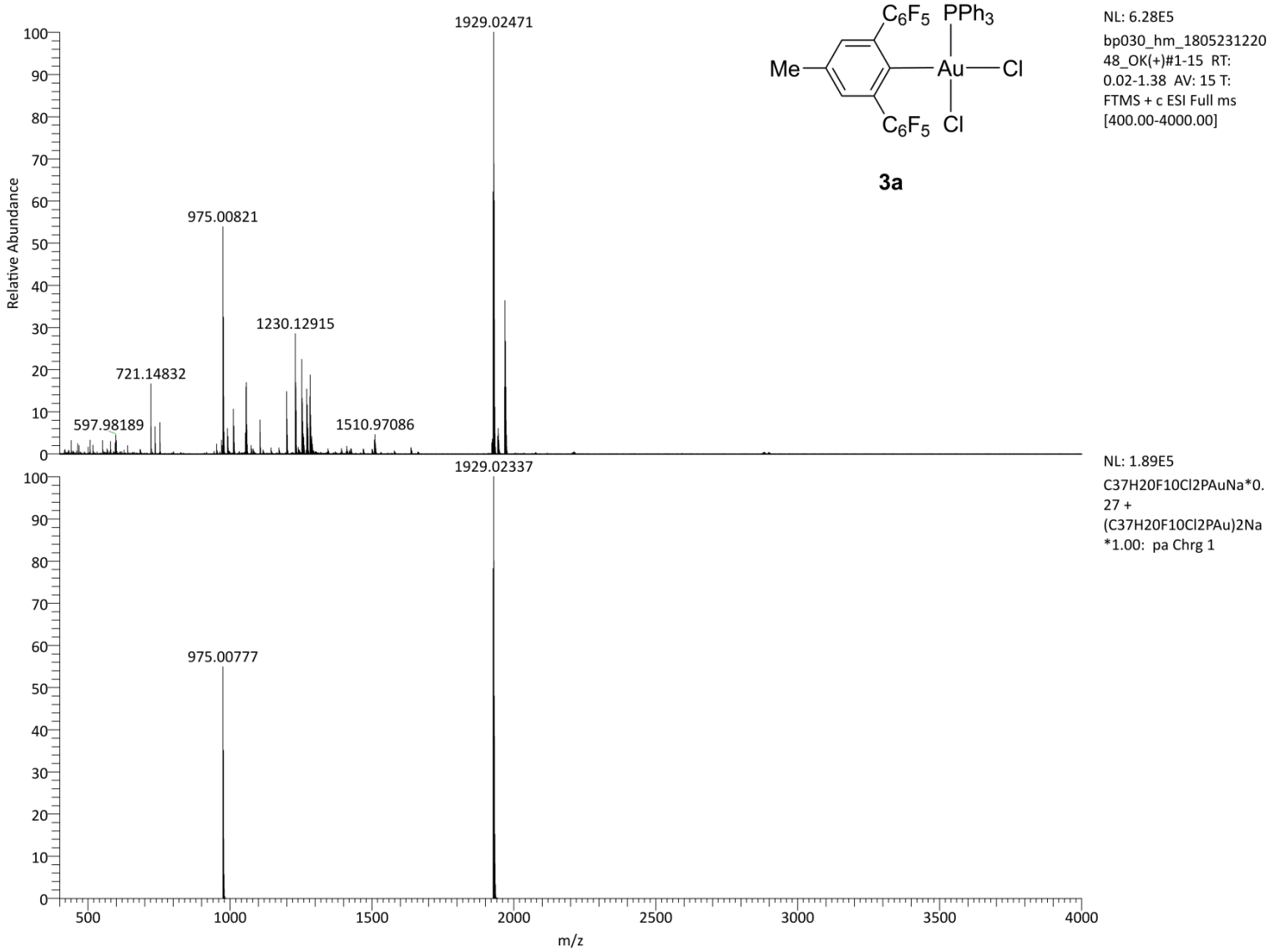


Figure S58. ESI(+) mass spectrum of 2,6-$(C_6F_5)_2$-4-$CH_3C_6H_2AuCl_2(PPh_3)$ (**3a**) (top) and calculated peak of $[M_2^+ + Na]$ and $[M^+ + Na]$ (bottom).

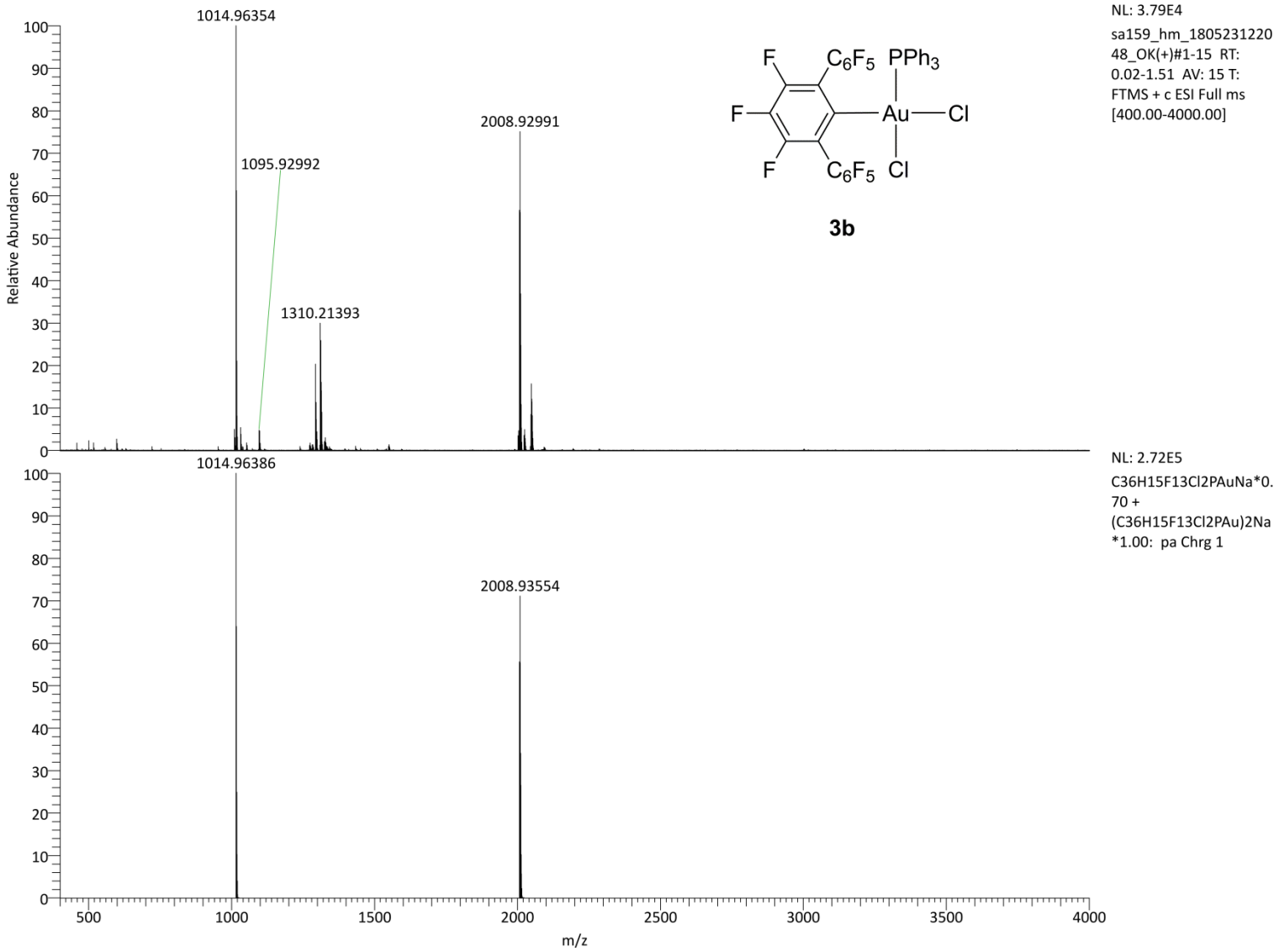


Figure S59. ESI(+) mass spectrum of 2,6-$(C_6F_5)_2$-$C_6F_3AuCl_2(PPh_3)$ (**3b**) (top) and calculated peak of $[M_2^+ + Na]$ and $[M^+ + Na]$ (bottom).

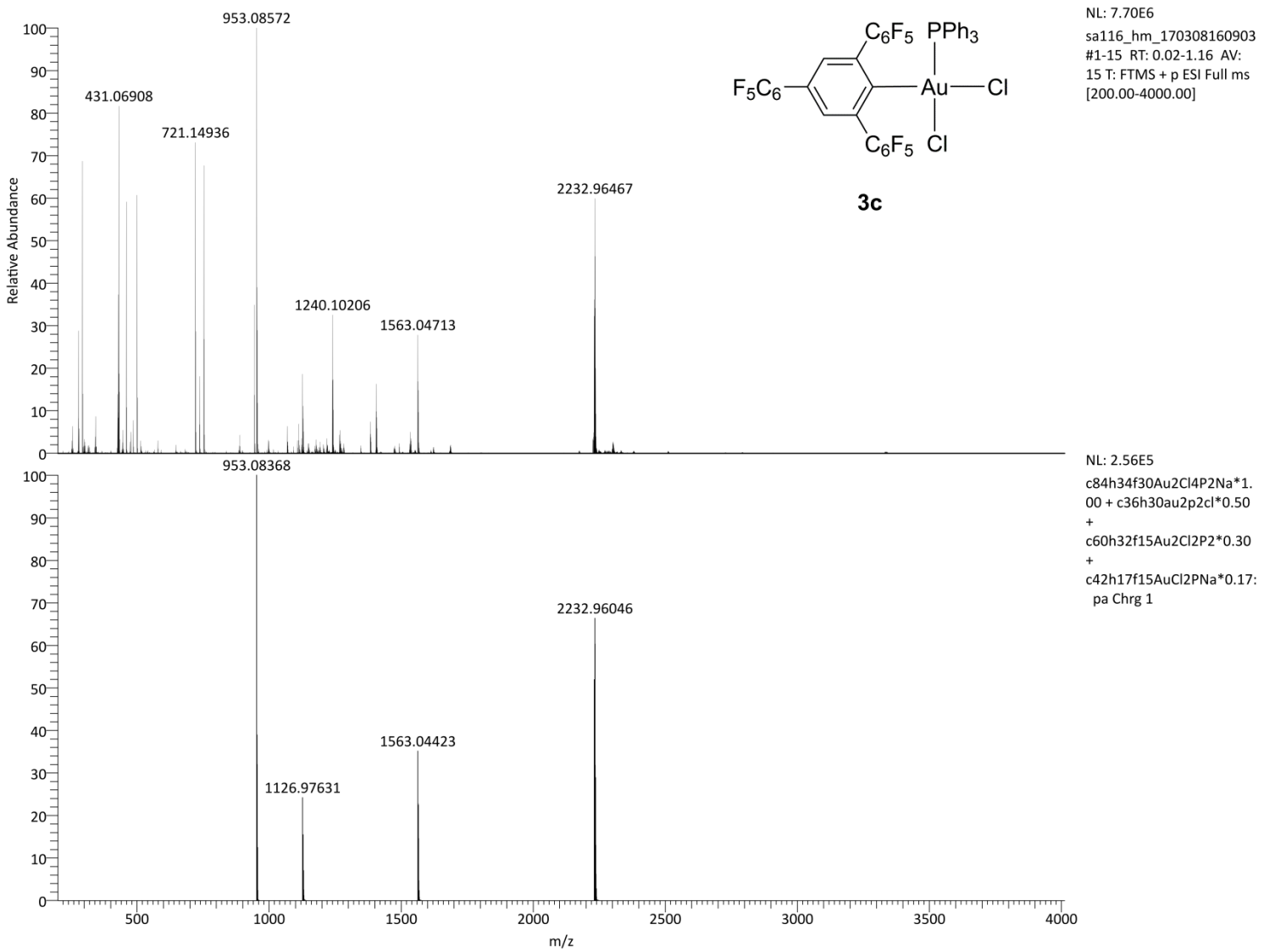


Figure S60. ESI(+) mass spectrum of 2,4,6-$(C_6F_5)_3$-$C_6H_2AuCl_2(PPh_3)$ (**3c**) (top) and calculated peak of $[M_2^+ + Na]$, $[M^+ + Au(PPh_3)]$, $[M^+ + Na]$ and $[Au_2Cl(PPh_3)_2^+]$ (100) (bottom).

Computational study

In order to evaluate the interactions energies between the molecules in the crystals, counterpoise corrected calculations were performed on pairs of molecules, generated using CrystalExplorer 17.5 running on an Ubuntu 16.04 virtual machine,[20] and the script for HPC computing with Tonto.[21]

In order to obtain the Gaussian input files with CrystalExplorer, in the crystallographic files the gold atoms were replaced with cooper atoms, element for which 6-31G basis set is available. These new crystallographic files were loaded into CrystalExplorer. The molecules within a radius of 3.8 Å around the molecule of interest were generated. Then using the tonto_hpc.py script the generation of the Gaussian input files was possible. In CrystalExplorer, the X–H bonds normalization was used.

In the Gaussian input files generated with CrystalExplorer, the copper atoms were replaced with gold atoms. Calculations were performed with Gaussian 09 rev. E01 using B3LYP functional,[22] LANL2DZ basis set with pseudopotentials for gold and 6-31G(d,p) 6d 10f basis set for all the other atoms.[23-25] Dispersion effects were accounted using D3 version of Grimme's dispersion with Becke-Johnson damping.[26]

Compact archive entries resulting from the single point calculations are provided as supporting info (*vide infra*). Corrected complexation energies of the pairs of molecules generated with CrystalExplorer are listed in Table S7.

Quantum theory of atoms in molecules was used to evaluate the local properties at the bond critical points (BCP) of the F···F interactions (see Tables S8 and S9). Wave functions used in the QTAIM study were obtained using Gaussian 09 rev. E01,[22] with M06-2X fuctional,[27] def2-SVP basis set,[28] and D3 version of Grimme's dispersion.[29] Analysis of the wave functions was performed with AIMALL 19.10.12.[30]

Table S7. Corrected complexation energies (in kcal/mole) of pairs of molecules generated with CrystalExplorer. The values in bold correspond to the pairs of molecules that exhibit F···F contacts.

Compound / Pair	**2a**	**2b(1)**[†]	**2b(2)**[†]	**2c**	**3a**	**3b**	**3c**
1	-4.09	**-15.03**[‡]	-3.64	-2.26	-6.93	-11.79	-2.32
2	-13.48	-7.88	-3.37	**-15.20**	-15.02	-13.57	**-4.46**
3	-6.11	-5.57	-7.18	-12.19	-20.26	-1.61	-16.65
4	-9.18	**-5.75**[‡]	-5.89	-3.38	-20.25	-10.21	-5.53
5	-8.31	**-10.44**	-4.32	-10.98	-3.57	-1.33	-3.9
6	-10.89	-3.37	**-10.44**	**-23.56**	-3.57	**-4.15**[‡]	-0.77
7	-4.53	-3.64	-19.14	-2.04	**-15.35**[‡]	-1.02	-3.6
8	-2.92[#]	-4.32	**-4.67**[§]	-3.59	-1.48	-1.98	-12.02
9	-3.70	-4.51	-5.35	-1.79	-0.43	-3.89	-1.08
10	-12.13	-7.18	-10.8	**-1.94**[‡]	-6.93	-10.18	-9.02
11	-1.42	-2.84	-2.98	-1.27		-2.67	-1.66
12		-2.90	-5.57			**-1.10**	-4.35
13		-5.35	-2.84			**-4.88**[‡]	-19.59
14		-19.14	-12.77				-9.03
15							-0.84
16							-0.92

[†] Compound 2b contains two molecules in the asymmetric unit. [‡] There are two contacts F···F between the calculated molecules. [§] There are four F···F contacts between the calculated molecules. [#] There is only a F···F contact of 2.987 Å [Σr_{vdW}(F,F) 2.94 Å].

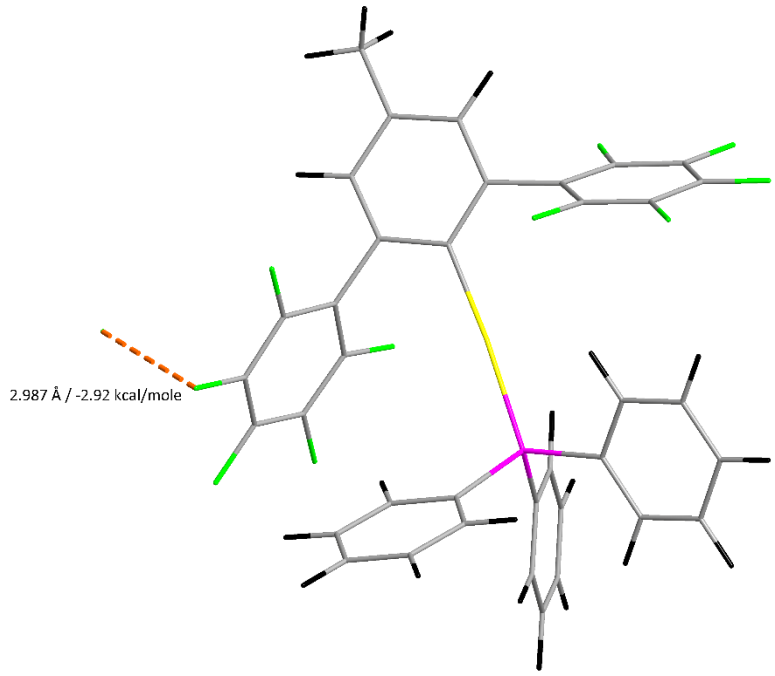


Figure S61. F···F contacts in **2a**. The complexation corrected energies are listed after the interatomic distances. These values correspond to the complexation energy between pairs of molecules, not only to the F···F interactions.

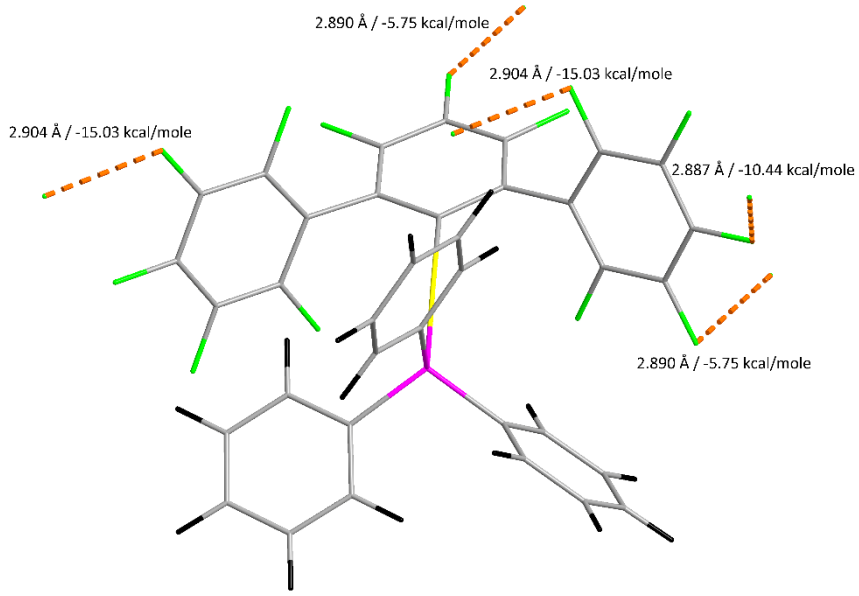


Figure S62. F···F contacts in **2b**, molecule 1. The complexation corrected energies are listed after the interatomic distances. These values correspond to the complexation energy between pairs of molecules, not only to the F···F interactions.

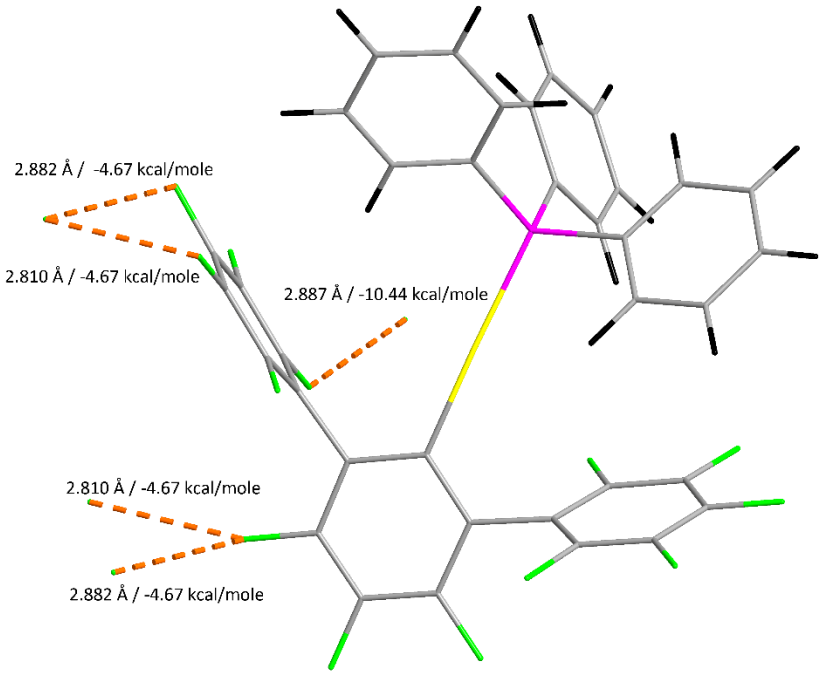


Figure S63. F···F contacts in **2b**, molecule 2. The complexation corrected energies are listed after the interatomic distances. These values correspond to the complexation energy between pairs of molecules, not only to the F···F interactions.

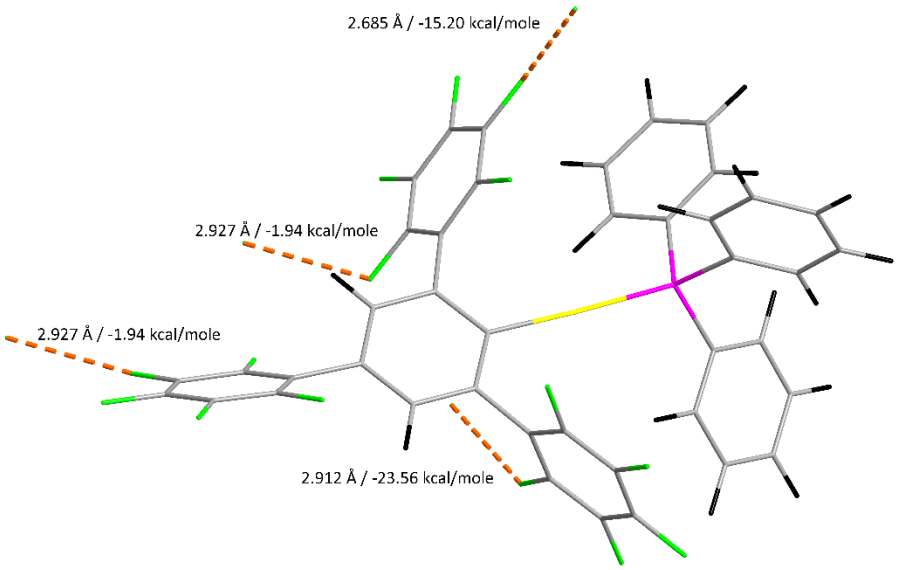


Figure S64. F···F contacts in **2c**. The complexation corrected energies are listed after the interatomic distances. These values correspond to the complexation energy between pairs of molecules, not only to the F···F interactions.

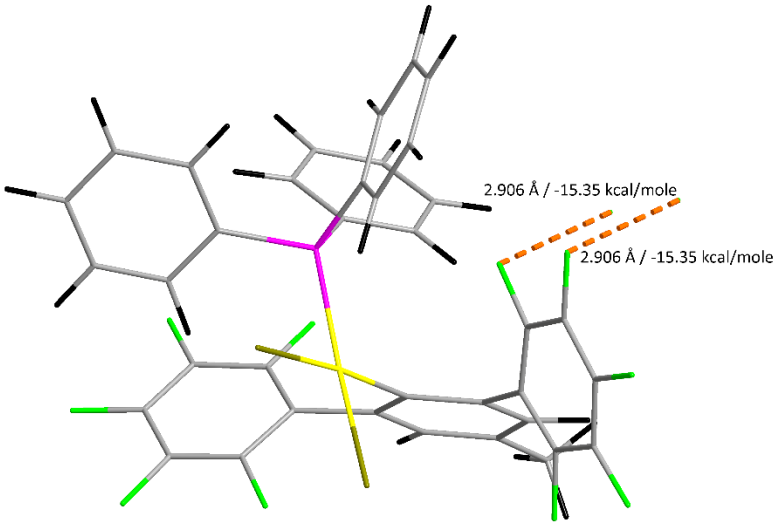


Figure S65. F···F contacts in **3a**. The complexation corrected energies are listed after the interatomic distances. These values correspond to the complexation energy between pairs of molecules, not only to the F···F interactions.

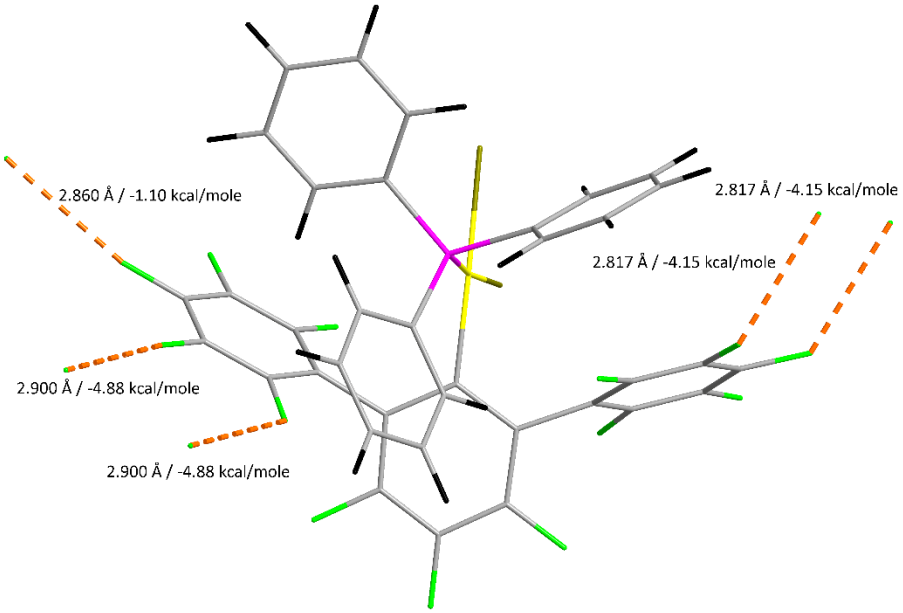


Figure S66. F···F contacts in **3b**. The complexation corrected energies are listed after the interatomic distances. These values correspond to the complexation energy between pairs of molecules, not only to the F···F interactions.

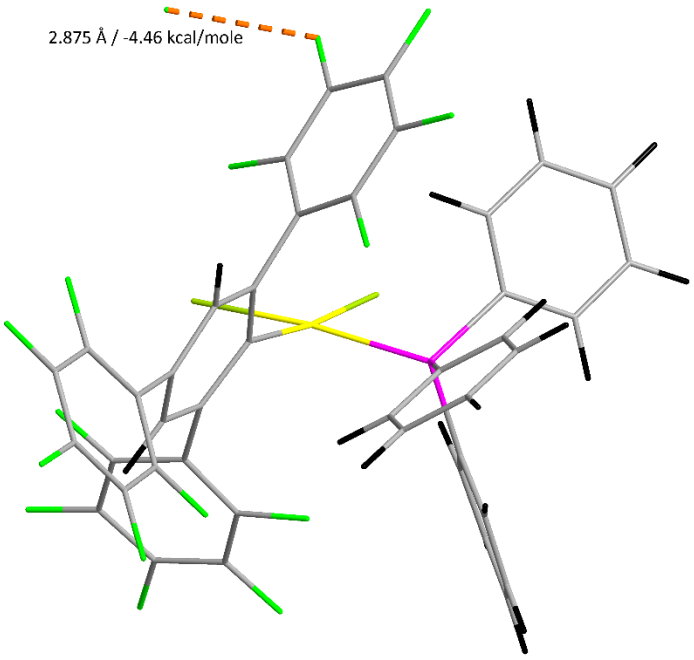


Figure S67. F···F contacts in **3c**. The complexation corrected energies are listed after the interatomic distances. These values correspond to the complexation energy between pairs of molecules, not only to the F···F interactions.

Table S8. BCP Properties (in a.u.) of F···F Interactions in Compounds **2a**-**2c**.[†]

Compound	Pair[‡]	ρ	$\nabla^2\rho$	BPL	V	G	K	L	|V(rb)|/G(rb)	H
2a	**8**	**0.005527**	**0.031760**	**5.647540**	**-0.005431**	**0.006686**	**-0.001254**	**-0.007940**	**0.81**	**0.001255**
	8	0.000459	0.005253	6.991956	-0.000392	0.000852	-0.000461	-0.001313	0.46	0.000460
	8	0.000459	0.005253	6.991971	-0.000392	0.000852	-0.000461	-0.001313	0.46	0.000460
2b1	**1**	**0.002419**	**0.016518**	**6.238122**	**-0.002014**	**0.003072**	**-0.001058**	**-0.004129**	**0.66**	**0.001058**
	4	**0.004404**	**0.028184**	**5.720995**	**-0.004382**	**0.005714**	**-0.001332**	**-0.007046**	**0.77**	**0.001332**
	5	**0.005531**	**0.031702**	**5.638692**	**-0.005478**	**0.006702**	**-0.001224**	**-0.007925**	**0.82**	**0.001224**
	5	**0.005769**	**0.034237**	**5.464605**	**-0.006101**	**0.007330**	**-0.001229**	**-0.008559**	**0.83**	**0.001229**
2b2	**6**	**0.005531**	**0.031702**	**5.638692**	**-0.005478**	**0.006702**	**-0.001224**	**-0.007925**	**0.82**	**0.001224**
	6	**0.005769**	**0.034237**	**5.464605**	**-0.006101**	**0.007330**	**-0.001229**	**-0.008559**	**0.83**	**0.001229**
	8	**0.006159**	**0.035287**	**5.449960**	**-0.006457**	**0.007639**	**-0.001182**	**-0.008822**	**0.85**	**0.001182**
	8	**0.006810**	**0.037989**	**5.316416**	**-0.007255**	**0.008376**	**-0.001121**	**-0.009497**	**0.87**	**0.001121**
	8	**0.006810**	**0.037989**	**5.316407**	**-0.007256**	**0.008376**	**-0.001121**	**-0.009497**	**0.87**	**0.001120**
	8	**0.006159**	**0.035287**	**5.449967**	**-0.006457**	**0.007639**	**-0.001182**	**-0.008822**	**0.85**	**0.001182**
2c	**2**	**0.009635**	**0.048242**	**5.082374**	**-0.010342**	**0.011201**	**-0.000859**	**-0.012060**	**0.92**	**0.000859**
	2	**0.002239**	**0.018480**	**6.022676**	**-0.002263**	**0.003442**	**-0.001178**	**-0.004620**	**0.66**	**0.001179**
	6	**0.004933**	**0.030634**	**5.513558**	**-0.005129**	**0.006394**	**-0.001265**	**-0.007658**	**0.80**	**0.001265**
	10	0.002668	0.020933	5.960644	-0.002721	0.003977	-0.001256	-0.005233	0.68	0.001256
	10	**0.004643**	**0.029841**	**5.538080**	**-0.004925**	**0.006193**	**-0.001268**	**-0.007460**	**0.80**	**0.001268**
	10	**0.002333**	**0.019166**	**5.945746**	**-0.002452**	**0.003622**	**-0.001170**	**-0.004792**	**0.68**	**0.001170**
	10	0.000174	0.002723	7.238932	-0.000178	0.000429	-0.000251	-0.000681	0.41	0.000251
	10	0.000174	0.002723	7.238940	-0.000178	0.000429	-0.000251	-0.000681	0.41	0.000251
	10	**0.004643**	**0.029842**	**5.538070**	**-0.004925**	**0.006193**	**-0.001268**	**-0.007460**	**0.80**	**0.001268**
	10	**0.002333**	**0.019167**	**5.945734**	**-0.002452**	**0.003622**	**-0.001170**	**-0.004792**	**0.68**	**0.001170**
	10	0.002668	0.020933	5.960638	-0.002721	0.003977	-0.001256	-0.005233	0.68	0.001256
	10	**0.000066**	**0.001201**	**7.730533**	**-0.000065**	**0.000183**	**-0.000118**	**-0.000300**	**0.36**	**0.000118**

[†] The BCP properties of bonds that have corresponding in the experimental data are marked in bold. The additional BCPs found by AIMALL are not bold. [‡] Pair of molecules from Table S7.

Table S9. BCP Properties (in a.u.) of F···F Interactions in Compounds **3a**-**3c**.[†]

Compound	Pair[‡]	ρ	$\nabla^2\rho$	BPL	V	G	K	L	|V(rb)|/G(rb)	H
3a	**7**	**0.006202**	**0.035157**	**5.493154**	**-0.006413**	**0.007601**	**-0.001188**	**-0.008789**	**0.84**	**0.001188**
	7	**0.006202**	**0.035157**	**5.493154**	**-0.006413**	**0.007601**	**-0.001188**	**-0.008789**	**0.84**	**0.001188**
3b	**6**	**0.006859**	**0.038401**	**5.330646**	**-0.007340**	**0.008470**	**-0.001130**	**-0.009600**	**0.87**	**0.001130**
	6	**0.006859**	**0.038402**	**5.330632**	**-0.007340**	**0.008470**	**-0.001130**	**-0.009600**	**0.87**	**0.001130**
	12	**0.004774**	**0.030452**	**5.408429**	**-0.005210**	**0.006411**	**-0.001202**	**-0.007613**	**0.81**	**0.001201**
	13	**0.004822**	**0.030739**	**5.485000**	**-0.005134**	**0.006409**	**-0.001275**	**-0.007685**	**0.80**	**0.001275**
	13	**0.004822**	**0.030739**	**5.485009**	**-0.005134**	**0.006409**	**-0.001275**	**-0.007685**	**0.80**	**0.001275**
	13	0.004772	0.030424	5.580564	-0.004989	0.006298	-0.001308	-0.007606	0.79	0.001309
3c	2	0.003727	0.023819	5.923903	-0.003445	0.004700	-0.001255	-0.005955	0.73	0.001255
	2	**0.007008**	**0.037643**	**5.433299**	**-0.007260**	**0.008335**	**-0.001076**	**-0.009411**	**0.87**	**0.001075**
	2	0.003727	0.023818	5.923932	-0.003444	0.004699	-0.001255	-0.005955	0.73	0.001255

[†] The BCP properties of bonds that have corresponding in the experimental data are marked in bold. The additional BCPs found by AIMALL are not bold. [‡] Pair of molecules from Table S7.

References

1. M. Olaru, J. Beckmann and C. I. Raț, *Organometallics*, 2014, **33**, 3012.
2. R. Uson, A. Laguna and M. Laguna, *Inorg. Synth.*, 1989, **26**, 85.
3. X.-F. Zhao and C. Zhang, *Synthesis*, 2007, 551.
4. S. Adimurthy, G. Ramachandraiah, P. K. Ghosh and A. V. Bedekar, *Tetrahedron Lett*., 2003, **44**, 5099.
5. L. Emmanuvel, R. K. Shukla, A. Sudalai, S. Gurunath and S. Sivaram, *Tetrahedron Lett*., 2006, **47**, 4793.
6. A. K. Al-Sa'ady, C. A. McAuliffe, R. V. Parish and J. A. Sandbank, *Inorg. Synth*., 1985, **23**, 191.
7. E. A. Krasnokutskaya, N. I. Semenischeva, V. D. Filimonov and P. Knochel, *Synthesis*, 2007, 81.
8. M. P. Doyle, B. Siegfried and J. F. Dellaria Jr., *J. Org. Chem.*, 1977, **42**, 2426.
9. *Qual Browser Thermo Xcalibur*, Thermo Fischer Scientific Inc., Waltham, MA, 02454, 2011.
10. G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg, *Organometallics*, 2010, **29**, 2176.
11. *MestReNova*, Mestrelab Research S.L. Feliciano Barrera 9B, Bajo, 15706 Santiago de Compostela, Spain., 2015.
12. G. M. Sheldrick, *Acta Crystallogr.*, *Sect. C: Struct. Chem.*, 2015, **71**, 3.
13. *DIAMOND-Visual Crystal Structure Information System*, Crystal Impact, Postfach 1251, D-53002 Bonn, Germany, 2015.
14. D. J. Gorin, B. D. Sherry and F. D. Toste, "*Triphenylphosphinegold(I) chloride*" in *Encyclopedia of Reagents for Organic Synthesis*, ed. L. A. Paquette, John Wiley & Sons, Hoboken NJ, 2001.
15. S. Kajigaeshi, T. Kakinami, H. Yamasaki, S. Fujisaki and T. Okamoto, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 600.
16. S. M. Walter, S. H. Jungbauer, F. Kniep, S. Schindler, E. Herdtweck and S. M. Huber, *J. Fluorine Chem.*, 2013, **150**, 14.
17. S. C. Cohen, A. J. Tomlinson, M. R. Wiles and A. G. Massey, *J. Organomet. Chem.*, 1968, **11**, 385.
18. (a) A. Mele, G. Salani, F. Viani and P. Bravo, *Magn. Reson. Chem.*, 1997, **35**, 168; (b) K. Matsubara, A. Oba and Y. Usui, *Magn. Reson. Chem.*, 1998, **36**, 761; (c) J. Chen, J. Reibenspies, A. Derecskei-Kovacs and K. Burgess, *Chem. Commun.*, 1999, 2501.
19. I. D. Rae, A. Staffa, A. C. Diz, C. G. Girbet, M. C. Ruiz de Azúa and R. H. Contreras, *Aust. J. Chem.*, 1987, **40**, 1923.
20. M. J. Turner, J. J. McKinnon, S. K. Wolff, D. J. Grimwood, P. R. Spackman, D. Jayatilaka and M. A. Spackman, *CrystalExplorer* version 17.5, revision: f4e298a, University of Western Australia, 35 Stirling Hwy, Crawley WA 6009, Australia.
21. (a) D. Jayatilaka and D. J. Grimwood, "*Tonto: A Fortran Based Object-Oriented System for Quantum Chemistry and Crystallography"* in *Computational Science*···ICCS 2003. *Lecture Notes in Computer Science*, eds P. M. A. Sloot, D. Abramson, A. V. Bogdanov, Y. E. Gorbachev, J. J. Dongarra, A. Y. Zomaya, vol 2660. Springer, Berlin, Heidelberg, 2003. (b) D. Jayatilaka, D. Grimwood and P. Spackman, *tonto_hpc* Python script, 2019, https://github.com/peterspackman/crystalexplorer-scripts.
22. Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
23. (a) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648; (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B* 1988, **37**, 785; (c) S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.* 1980, **58**, 1200; (d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623.
24. (a) R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Phys.* 1971, **54**, 724; (b) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.* 1972, **56**, 2257; (c) P. C. Hariharan and J. A. Pople, *Mol. Phys.*, 1974, **27**, 209; (d) M. S. Gordon, *Chem. Phys. Lett.*, 1980; **76**, 163; (e) P. C. Hariharan and J. A. Pople, *Theo. Chim. Acta*, 1973, **28**, 213.
25. (a) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270; (b) W. R. Wadt and P. J. Hay, *J. Chem. Phys.*, 1985, **82** 284; (c) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299.
26. S. Grimme, S. Ehrlich and L. Goerigk, *J. Comp. Chem*., 2011, **32**, 1456.

27. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215.
28. (a) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297; (b) F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057.
29. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, J. Chem. Phys., 2010, **132**, 154104.
30. Keith A. Todd, AIMAll Version 19.10.12, TK Gristmill Software, Overland Park KS, USA, 2019.

Single point calculations compact archive entries

Compound 2a

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,0,-6.774423,3.818301,-4.389553\C,0,-6.698264,5.567613,-2.796663\H,0,-
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72,7.772204,-7.245638\C,0,-3.458,8.870129,-6.110871\H,0,-4.363355,7.81
6258,-4.500729\F,0,-3.0668,2.585777,-11.301661\C,0,-1.519102,4.039894,
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3113\H,0,-0.403752,7.985486,-1.162178\H,0,-1.634957,4.198678,0.203376\
H,0,-7.326911,3.052268,-4.919558\C,0,-7.412362,4.588448,-3.473306\H,0,
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99201,8.830626,-7.103792\H,0,-4.08281,9.746492,-5.990495\F,0,-1.690156
,4.925964,-11.297828\H,0,-0.478412,6.310762,0.609554\H,0,-8.466589,4.4
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9,-22.3268922\PG=C01 [X(C74H40Au2F20P2)]\\@

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 10.8969\\0,1\F,
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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 10.8584\\0,1\F,
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11,4.912849\C,0,4.811507,8.821339,3.005598\F,0,1.868312,8.151542,0.300
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4679,8.02234\H,0,6.178256,-0.149595,5.990494\F,0,3.785602,4.670933,11.
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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = x, y, z, r = 8.861\\0,1\F,0,1.2
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912849\C,0,4.811507,8.821339,3.005598\F,0,1.868312,8.151542,0.300943\C
,0,4.126244,8.350523,0.795487\C,0,3.330222,8.109827,5.842515\C,0,2.705
016,10.42122,5.275131\F,0,5.806449,9.026751,3.854756\C,0,5.098701,8.57
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,0,3.619419,2.771929,2.549391\C,0,3.938395,2.90401,6.409897\C,0,5.7078
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9401\H,0,7.027888,6.238653,5.377873\C,0,8.869868,5.778597,4.389553\C,0
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1.334117\H,0,3.561776,2.017936,3.324751\H,0,3.276315,3.753978,6.519924
\C,0,3.803217,1.824693,7.245638\C,0,5.553445,0.726769,6.110871\H,0,6.4
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8.02234\H,0,6.178256,-0.149595,5.990494\F,0,3.785602,4.670933,11.29782
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98,4.670933,11.297828\F,0,-4.443887,8.088404,-0.49071\\Version=ES64L-G
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22249,-31.4169559\PG=C01 [X(C74H40Au2F20P2)]\\@

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = x, y, z, r = 11.7419\\0,1\F,0,1
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7828,1.801023,5.280881\F,0,4.803569,8.788987,9.346489\C,0,4.299752,6.7
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,0,8.793709,4.029285,2.796663\H,0,6.912505,3.070448,2.518914\H,0,4.824
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9,8.02234\H,0,6.178256,-0.149595,5.990494\F,0,3.785602,4.670933,11.297
828\H,0,10.562034,5.155231,3.273763\H,0,2.573857,3.286135,-0.609553\H,
0,4.485969,-0.075011,7.777176\C,0,-2.170909,10.363168,7.103792\C,0,-1.
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,9.521887,7.777176\H,0,-0.587299,9.447302,5.990494\C,0,-1.057727,11.39

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,0,-1.666854,18.169481,1.679148\F,0,-5.534312,18.316063,2.882921\C,0,-
3.939111,17.95392,1.190355\H,0,-4.061009,22.12896,7.665424\H,0,-5.7526
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608017,11.301662\C,0,-3.151008,15.153901,10.316408\F,0,-4.707916,13.71
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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = x, y, z, r = 9.823\\0,1\F,0,1.2
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912849\C,0,4.811507,8.821339,3.005598\F,0,1.868312,8.151542,0.300943\C
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8,6.188859,8.280729\H,0,1.012866,12.039183,7.512461\H,0,1.866064,12.71
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28,1.801023,5.280881\F,0,4.803569,8.788987,9.346489\C,0,4.299752,6.735
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8.02234\H,0,6.178256,-0.149595,5.990494\F,0,3.785602,4.670933,11.29782
8\H,0,10.562034,5.155231,3.273763\H,0,2.573857,3.286135,-0.609553\H,0,
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55436\C,0,2.215303,-4.725263,1.771156\C,0,1.523974,-6.824968,2.549391\
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90157,-4.925964,11.297828\F,0,2.321668,-1.508494,-0.49071\H,0,4.932443
,-3.358244,5.377873\C,0,6.774424,-3.8183,4.389553\C,0,6.698264,-5.5676
12,2.796663\H,0,4.81706,-6.526449,2.518914\H,0,2.728955,-3.784456,1.92
6036\C,0,1.603071,-4.954875,0.571217\C,0,0.919405,-7.048758,1.334117\H
,0,1.466331,-7.578962,3.324751\H,0,1.18087,-5.842919,6.519924\C,0,1.70
7772,-7.772204,7.245638\C,0,3.458,-8.870129,6.110871\H,0,4.363355,-7.8
16258,4.50073\H,0,7.326911,-3.052268,4.919558\C,0,7.412362,-4.588448,3
.473306\H,0,7.197404,-6.183012,2.05849\H,0,1.634957,-4.198677,-0.20337
6\C,0,0.957016,-6.120661,0.343114\H,0,0.403751,-7.985486,1.162177\H,0,
0.953243,-7.762218,8.02234\C,0,2.499201,-8.830626,7.103792\H,0,4.08281
,-9.746492,5.990494\H,0,8.466589,-4.441666,3.273763\H,0,0.478412,-6.31
0762,-0.609553\H,0,2.390524,-9.671907,7.777176\\Version=ES64L-G09RevE.
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597\Quadrupole=23.1421032,17.3063752,-40.4484785,-29.7059508,-1.359337
6,-23.3868529\PG=C01 [X(C74H40Au2F20P2)]\\@

1\1\GINC-COMPUTE021\SP\RB3LYP\Gen\C74H40Au2F20P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 13.3158\\0,1\F,

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11,4.912849\C,0,4.811507,8.821339,3.005598\F,0,1.868312,8.151542,0.300
943\C,0,4.126244,8.350523,0.795487\C,0,3.330222,8.109827,5.842515\C,0,
2.705016,10.42122,5.275131\F,0,5.806449,9.026751,3.854756\C,0,5.098701
,8.572584,1.679148\F,0,4.417113,8.088404,-0.49071\Au,0,4.107889,6.3102
17,5.224526\C,0,3.012221,8.428408,7.167048\C,0,2.408583,10.708395,6.59
3914\H,0,2.588373,11.187275,4.518556\F,0,6.397193,8.53266,1.301531\P,0
,5.041866,4.392788,4.387828\C,0,2.555685,9.690279,7.538914\C,0,3.21744
3,7.412128,8.246226\C,0,1.966301,12.098473,7.0022\C,0,6.806679,4.61921
2,4.008103\C,0,4.295743,3.943177,2.790912\C,0,4.903099,2.917195,5.4399
79\H,0,2.310526,9.884323,8.575729\C,0,4.103024,7.638809,9.287067\C,0,2
.55738,6.188859,8.280729\H,0,1.012866,12.039183,7.512461\H,0,1.866064,
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57,4.655993\C,0,7.460616,3.835062,3.055436\C,0,4.310748,4.871634,1.771
156\C,0,3.619419,2.771929,2.549391\C,0,3.938395,2.90401,6.409897\C,0,5
.707828,1.801023,5.280881\F,0,4.803569,8.788987,9.346489\C,0,4.299752,
6.73547,10.324076\F,0,1.638003,5.906563,7.343397\C,0,2.741114,5.284722
,9.279401\H,0,7.027888,6.238653,5.377873\C,0,8.869868,5.778597,4.38955
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5.557004,10.316408\F,0,2.057639,4.114397,9.275567\H,0,9.422357,6.54462
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H,0,3.730402,5.39822,-0.203376\C,0,3.052461,3.476237,0.343114\H,0,2.49
9197,1.611411,1.162177\C,0,4.594646,0.76627,7.103792\H,0,3.048688,1.83
4679,8.02234\H,0,6.178256,-0.149595,5.990494\F,0,3.785602,4.670933,11.
297828\H,0,10.562034,5.155231,3.273763\H,0,2.573857,3.286135,-0.609553
\H,0,4.485969,-0.075011,7.777176\H,0,1.756966,8.980567,11.502929\C,0,2
.49521,9.414157,12.166154\H,0,3.448645,9.473446,11.655893\H,0,2.595448
,8.794334,13.048665\C,0,2.052929,10.804235,12.574441\C,0,1.905826,11.8
2235,11.62944\C,0,1.756496,11.091409,13.893223\H,0,2.150986,11.628305,
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.162107,18.372868\F,0,2.5932,13.361087,18.867411\F,0,0.67591,16.841696
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.112919\C,0,0.150764,16.640995,17.397198\C,0,0.842093,18.7407,16.61896
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,0,0.044398,13.424226,19.659063\H,0,-2.566376,15.273975,13.790481\C,0,
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9,15.695047\H,0,-4.831338,18.098745,17.109865\H,0,0.73111,16.114408,19
.371731\C,0,1.40905,18.036392,18.825241\H,0,1.962315,19.901218,18.0061
76\H,0,1.412824,19.67795,11.146015\C,0,-0.133134,20.746359,12.064562\H
,0,-1.716743,21.662224,13.177859\H,0,-6.100522,16.357399,15.89459\H,0,
1.887655,18.226494,19.777908\H,0,-0.024458,21.587639,11.391177\\Versio
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1\1\GINC-COMPUTE021\SP\RB3LYP\Gen\C74H40Au2F20P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 12.9063\\0,1\F,
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11,4.912849\C,0,4.811507,8.821339,3.005598\F,0,1.868312,8.151542,0.300
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2.705016,10.42122,5.275131\F,0,5.806449,9.026751,3.854756\C,0,5.098701
,8.572584,1.679148\F,0,4.417113,8.088404,-0.49071\Au,0,4.107889,6.3102
17,5.224526\C,0,3.012221,8.428408,7.167048\C,0,2.408583,10.708395,6.59
3914\H,0,2.588373,11.187275,4.518556\F,0,6.397193,8.53266,1.301531\P,0
,5.041866,4.392788,4.387828\C,0,2.555685,9.690279,7.538914\C,0,3.21744
3,7.412128,8.246226\C,0,1.966301,12.098473,7.0022\C,0,6.806679,4.61921
2,4.008103\C,0,4.295743,3.943177,2.790912\C,0,4.903099,2.917195,5.4399
79\H,0,2.310526,9.884323,8.575729\C,0,4.103024,7.638809,9.287067\C,0,2
.55738,6.188859,8.280729\H,0,1.012866,12.039183,7.512461\H,0,1.866064,
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57,4.655993\C,0,7.460616,3.835062,3.055436\C,0,4.310748,4.871634,1.771
156\C,0,3.619419,2.771929,2.549391\C,0,3.938395,2.90401,6.409897\C,0,5
.707828,1.801023,5.280881\F,0,4.803569,8.788987,9.346489\C,0,4.299752,
6.73547,10.324076\F,0,1.638003,5.906563,7.343397\C,0,2.741114,5.284722
,9.279401\H,0,7.027888,6.238653,5.377873\C,0,8.869868,5.778597,4.38955
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9197,1.611411,1.162177\C,0,4.594646,0.76627,7.103792\H,0,3.048688,1.83
4679,8.02234\H,0,6.178256,-0.149595,5.990494\F,0,3.785602,4.670933,11.
297828\H,0,10.562034,5.155231,3.273763\H,0,2.573857,3.286135,-0.609553
\H,0,4.485969,-0.075011,7.777176\F,0,2.322579,11.042253,-0.300943\C,0,
1.364446,10.83677,-1.190355\C,0,0.064646,10.843271,-0.795486\C,0,1.663
33,10.528251,-2.511054\F,0,-0.226223,11.105391,0.49071\C,0,-0.907811,1
0.62121,-1.679148\F,0,2.959647,10.474627,-2.88292\C,0,0.705502,10.3127
,-3.459887\F,0,-2.206303,10.661133,-1.301531\C,0,-0.620617,10.372456,-
3.005597\C,0,1.038388,10.042884,-4.912848\F,0,-1.615559,10.167045,-3.8

54756\C,0,0.860669,11.083967,-5.842514\C,0,1.485875,8.772574,-5.275131
\Au,0,0.083001,12.883576,-5.224526\C,0,1.17867,10.765387,-7.167048\C,0
,1.782307,8.485399,-6.593914\H,0,1.602517,8.006519,-4.518556\P,0,-0.85
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067\C,0,1.63351,13.004935,-8.280728\H,0,1.486345,6.661732,-7.665425\H,
0,3.178024,7.154612,-7.512461\H,0,2.324826,6.4755,-6.119689\C,0,-3.331
624,13.593138,-4.655993\C,0,-3.269726,15.358732,-3.055435\C,0,-0.11985
8,14.32216,-1.771156\C,0,0.571471,16.421865,-2.549392\C,0,0.252495,16.
289783,-6.409897\C,0,-1.516937,17.392771,-5.280881\F,0,-0.612679,10.40
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77874\C,0,-4.678978,13.415198,-4.389553\C,0,-4.602818,15.16451,-2.7966
63\H,0,-2.721615,16.123346,-2.518914\H,0,-0.63351,13.381353,-1.926037\
C,0,0.492375,14.551772,-0.571217\C,0,1.176041,16.645655,-1.334117\H,0,
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,13.63679,-10.316408\F,0,2.133251,15.079397,-9.275567\H,0,-5.231466,12
.649165,-4.919558\C,0,-5.316917,14.185345,-3.473306\H,0,-5.101959,15.7
7991,-2.058489\H,0,0.460488,13.795574,0.203376\C,0,1.138429,15.717557,
-0.343113\H,0,1.691694,17.582382,-1.162178\H,0,1.142202,17.359116,-8.0
22339\C,0,-0.403756,18.427525,-7.103792\H,0,-1.987365,19.34339,-5.9904
95\F,0,0.405289,14.522861,-11.297828\H,0,-6.371144,14.038564,-3.273763
\H,0,1.617033,15.90766,0.609554\H,0,-0.295079,19.268805,-7.777176\\Ver
sion=ES64L-G09RevE.01\HF=-2897.2883983\RMSD=4.898e-09\Dipole=-0.000000
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.7261435,2.3701743,-7.8382378\PG=C01 [X(C74H40Au2F20P2)]\\@

1\1\GINC-COMPUTE008\SP\RB3LYP\Gen\C74H40Au2F20P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 13.6043\\0,1\F,
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8,8.881094,3.459888\C,0,2.826444,8.357024,1.190355\C,0,3.152502,9.1509
11,4.912849\C,0,4.811507,8.821339,3.005598\F,0,1.868312,8.151542,0.300
943\C,0,4.126244,8.350523,0.795487\C,0,3.330222,8.109827,5.842515\C,0,
2.705016,10.42122,5.275131\F,0,5.806449,9.026751,3.854756\C,0,5.098701
,8.572584,1.679148\F,0,4.417113,8.088404,-0.49071\Au,0,4.107889,6.3102
17,5.224526\C,0,3.012221,8.428408,7.167048\C,0,2.408583,10.708395,6.59
3914\H,0,2.588373,11.187275,4.518556\F,0,6.397193,8.53266,1.301531\P,0
,5.041866,4.392788,4.387828\C,0,2.555685,9.690279,7.538914\C,0,3.21744
3,7.412128,8.246226\C,0,1.966301,12.098473,7.0022\C,0,6.806679,4.61921
2,4.008103\C,0,4.295743,3.943177,2.790912\C,0,4.903099,2.917195,5.4399
79\H,0,2.310526,9.884323,8.575729\C,0,4.103024,7.638809,9.287067\C,0,2
.55738,6.188859,8.280729\H,0,1.012866,12.039183,7.512461\H,0,1.866064,
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57,4.655993\C,0,7.460616,3.835062,3.055436\C,0,4.310748,4.871634,1.771
156\C,0,3.619419,2.771929,2.549391\C,0,3.938395,2.90401,6.409897\C,0,5
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,9.279401\H,0,7.027888,6.238653,5.377873\C,0,8.869868,5.778597,4.38955

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9,4.919558\C,0,9.507808,5.00845,3.473306\H,0,9.29285,3.413885,2.05849\
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9197,1.611411,1.162177\C,0,4.594646,0.76627,7.103792\H,0,3.048688,1.83
4679,8.02234\H,0,6.178256,-0.149595,5.990494\F,0,3.785602,4.670933,11.
297828\H,0,10.562034,5.155231,3.273763\H,0,2.573857,3.286135,-0.609553
\H,0,4.485969,-0.075011,7.777176\F,0,5.34602,-2.352098,7.870526\C,0,5.
517075,-3.238169,8.851946\C,0,6.390507,-2.965888,9.888954\C,0,4.831869
,-4.416636,8.844278\F,0,7.073982,-1.795562,9.892787\C,0,6.574242,-3.87
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53,-3.459762,14.778802\C,0,0.337913,-1.71045,16.371691\H,0,2.219116,-0
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2868\F,0,7.26331,-5.832707,18.867411\C,0,4.536975,1.552565,12.064562\H
,0,2.953366,2.46843,13.177859\H,0,6.082933,0.484156,11.146015\H,0,-0.2
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.157402,18.825241\H,0,6.632425,0.707423,18.006176\F,0,4.714508,-5.7695
69,19.659063\H,0,4.645652,2.393846,11.391177\H,0,-1.430413,-2.836396,1
5.89459\H,0,6.557765,-0.9673,19.777908\\Version=ES64L-G09RevE.01\HF=-2
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drupole=5.8331407,-20.7342972,14.9011565,7.0836848,-25.5800404,27.4695
015\PG=C01 [X(C74H40Au2F20P2)]\\@

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 9.41464\\0,1\F,
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,9.279401\H,0,7.027888,6.238653,5.377873\C,0,8.869868,5.778597,4.38955
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4679,8.02234\H,0,6.178256,-0.149595,5.990494\F,0,3.785602,4.670933,11.
297828\H,0,10.562034,5.155231,3.273763\H,0,2.573857,3.286135,-0.609553
\H,0,4.485969,-0.075011,7.777176\Au,0,7.119178,5.605514,13.943828\P,0,
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,15.313599\C,0,6.128366,3.343148,17.489206\F,0,9.995824,3.196566,16.28

5435\C,0,8.400622,3.558708,17.977999\H,0,6.741097,11.990743,11.391177\
H,0,0.665033,6.760501,15.89459\H,0,8.65321,8.629598,19.777908\F,0,6.06
4822,4.904612,7.866693\C,0,7.61252,6.358728,8.851946\F,0,9.169428,7.80
1335,9.892787\H,0,8.522521,-0.61633,11.502929\H,0,10.2142,-0.123451,11
.655893\H,0,9.361003,-0.802563,13.048665\F,0,4.829873,3.383071,17.8668
23\C,0,7.100822,3.565209,18.372868\F,0,9.358755,3.76419,18.867411\F,0,
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93,-23.2719419,40.2166506\PG=C01 [X(C74H40Au2F20P2)]\\@

1\1\GINC-COMPUTE021\SP\RB3LYP\Gen\C74H40Au2F20P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 13.0247\\0,1\F,
0,1.231243,8.719167,2.882921\C,0,2.52756,8.665544,2.511054\C,0,3.48538
8,8.881094,3.459888\C,0,2.826444,8.357024,1.190355\C,0,3.152502,9.1509
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79\H,0,2.310526,9.884323,8.575729\C,0,4.103024,7.638809,9.287067\C,0,2
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8139,1.334117\H,0,3.561776,2.017936,3.324751\H,0,3.276315,3.753978,6.5
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9197,1.611411,1.162177\C,0,4.594646,0.76627,7.103792\H,0,3.048688,1.83
4679,8.02234\H,0,6.178256,-0.149595,5.990494\F,0,3.785602,4.670933,11.
297828\H,0,10.562034,5.155231,3.273763\H,0,2.573857,3.286135,-0.609553
\H,0,4.485969,-0.075011,7.777176\F,0,6.654696,10.661133,-1.301531\C,0,
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7,-3.459887\F,0,11.183578,11.042253,-0.300943\C,0,10.52433,10.528251,-
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,-5.439979\H,0,10.741364,9.309471,-8.57573\C,0,8.948867,11.554985,-9.2
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404806,-9.34649\C,0,8.752138,12.458323,-10.324076\F,0,11.413888,13.287
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63\H,0,6.139385,16.123346,-2.518914\H,0,8.22749,13.381353,-1.926037\C,
0,9.353374,14.551772,-0.571217\C,0,10.037041,16.645655,-1.334117\H,0,9
.490114,17.175859,-3.324751\H,0,9.775575,15.439816,-6.519924\C,0,9.248
673,17.369101,-7.245638\C,0,7.498445,18.467026,-6.110871\H,0,6.593091,
17.413157,-4.500729\F,0,7.889646,12.182674,-11.301661\C,0,9.437344,13.
63679,-10.316408\F,0,10.994251,15.079397,-9.275567\H,0,3.629534,12.649
165,-4.919558\C,0,3.544083,14.185345,-3.473306\H,0,3.759041,15.77991,-
2.058489\H,0,9.321488,13.795574,0.203376\C,0,9.999429,15.717557,-0.343
113\H,0,10.552693,17.582382,-1.162178\H,0,10.003202,17.359116,-8.02233
9\C,0,8.457244,18.427525,-7.103792\H,0,6.873635,19.34339,-5.990495\F,0
,9.266289,14.522861,-11.297828\H,0,2.489856,14.038564,-3.273763\H,0,10
.478033,15.90766,0.609554\H,0,8.565921,19.268805,-7.777176\\Version=ES
64L-G09RevE.01\HF=-2897.2884031\RMSD=4.898e-09\Dipole=0.0000023,0.0000
003,-0.0000025\Quadrupole=-20.3541062,71.5100165,-51.1559103,-11.70363
54,16.015442,-8.2142716\PG=C01 [X(C74H40Au2F20P2)]\\@

Compound 2b

1\1\GINC-COMPUTE008\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 7.21701\\0,1\C,
0,0.646857,0.690313,4.643787\C,0,-0.289448,-0.110887,5.29309\H,0,0.362
348,1.671908,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.2
56179,5.453665\C,0,0.05887,-1.354789,5.724367\C,0,2.27384,-1.023049,4.
896824\P,0,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095
\C,0,1.338807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4
.487348,0.199656,3.179673\Au,0,2.221456,2.414068,1.803565\C,0,3.724226
,2.46836,4.860221\H,0,1.616944,-2.800786,5.906744\C,0,4.370838,-0.5220
15,2.016339\C,0,5.59884,0.017405,3.999259\C,0,1.425201,3.420273,0.1877
89\C,0,4.044777,3.775149,4.483053\C,0,3.878666,2.089865,6.212935\H,0,3
.52822,-0.348835,1.358284\C,0,5.318672,-1.460937,1.680548\C,0,6.544506
,-0.933937,3.660285\H,0,5.720281,0.614896,4.894278\C,0,1.523154,2.8657
07,-1.107634\C,0,0.728777,4.638079,0.337383\H,0,3.945341,4.07722,3.447
829\C,0,4.490199,4.684927,5.42677\H,0,3.630856,1.085734,6.534245\C,0,4
.35471,3.027983,7.131189\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,
-1.691513,2.514457\H,0,7.406222,-1.08676,4.298129\C,0,0.99051,3.550285
,-2.194579\C,0,2.100222,1.523253,-1.32566\C,0,0.472935,5.217031,1.6853
22\C,0,0.227739,5.279076,-0.775025\H,0,4.721585,5.697423,5.119943\C,0,
4.642397,4.327659,6.741289\H,0,4.502676,2.737405,8.163867\H,0,7.124159
,-2.458232,2.269854\F,0,1.072627,3.028912,-3.437485\C,0,0.374494,4.764
704,-2.040211\C,0,1.290925,0.412258,-1.518222\C,0,3.475182,1.27802,-1.

298605\C,0,-0.812592,5.196018,2.227999\C,0,1.461431,5.763367,2.473079\
F,0,-0.438008,6.450929,-0.641346\H,0,4.984092,5.05336,7.469049\F,0,-0.
11192,5.430765,-3.117608\C,0,1.784695,-0.855341,-1.653494\F,0,-0.04595
3,0.58478,-1.542094\F,0,4.31998,2.308739,-1.131505\C,0,3.993993,0.0106
47,-1.42592\F,0,-1.813887,4.661423,1.502308\C,0,-1.097406,5.716374,3.4
6613\C,0,1.205181,6.288127,3.731899\F,0,2.718475,5.851897,2.013156\F,0
,0.981832,-1.901302,-1.850831\C,0,3.145651,-1.058009,-1.605751\F,0,5.3
21927,-0.183328,-1.371811\F,0,-2.345824,5.655281,3.951516\C,0,-0.08431
,6.239904,4.215693\F,0,2.179548,6.835141,4.460773\F,0,3.656967,-2.2908
33,-1.71556\F,0,-0.342828,6.745131,5.43791\Au,0,-2.221455,-2.414068,-1
.803566\C,0,-1.425201,-3.420273,-0.187788\P,0,-3.119179,-1.326103,-3.6
01402\C,0,-0.728777,-4.638079,-0.337383\C,0,-1.523154,-2.865707,1.1076
34\C,0,-1.940133,-0.237901,-4.455998\C,0,-3.724226,-2.46836,-4.860221\
C,0,-4.487348,-0.199656,-3.179674\C,0,-0.472935,-5.217031,-1.685322\C,
0,-0.227739,-5.279075,0.775025\C,0,-0.99051,-3.550285,2.194579\C,0,-2.
100222,-1.523254,1.32566\C,0,-0.646857,-0.690313,-4.643787\C,0,-2.2738
4,1.023049,-4.896824\C,0,-4.044777,-3.775149,-4.483053\C,0,-3.878666,-
2.089864,-6.212935\C,0,-4.370838,0.522015,-2.016339\C,0,-5.598839,-0.0
17405,-3.999259\C,0,0.812592,-5.196017,-2.227999\C,0,-1.46143,-5.76336
7,-2.473079\F,0,0.438008,-6.450929,0.641346\C,0,-0.374494,-4.764704,2.
040211\F,0,-1.072627,-3.028912,3.437485\C,0,-1.290925,-0.412258,1.5182
22\C,0,-3.475182,-1.27802,1.298605\H,0,-0.362348,-1.671908,-4.285556\C
,0,0.289448,0.110887,-5.29309\C,0,-1.338807,1.818717,-5.544536\H,0,-3.
276515,1.398855,-4.734499\H,0,-3.945341,-4.07722,-3.447829\C,0,-4.4901
99,-4.684927,-5.42677\C,0,-4.35471,-3.027983,-7.131189\H,0,-3.630855,-
1.085734,-6.534245\H,0,-3.52822,0.348834,-1.358284\C,0,-5.318672,1.460
937,-1.680548\C,0,-6.544506,0.933937,-3.660285\H,0,-5.720282,-0.614897
,-4.894278\F,0,1.813888,-4.661422,-1.502308\C,0,1.097406,-5.716375,-3.
466131\F,0,-2.718475,-5.851897,-2.013157\C,0,-1.205181,-6.288126,-3.73
1899\F,0,0.11192,-5.430765,3.117608\F,0,0.045953,-0.58478,1.542094\C,0
,-1.784695,0.85534,1.653494\C,0,-3.993993,-0.010647,1.42592\F,0,-4.319
98,-2.308739,1.131505\C,0,-0.05887,1.354788,-5.724367\H,0,1.295551,-0.
256179,-5.453665\H,0,-1.616944,2.800786,-5.906744\H,0,-4.721586,-5.697
423,-5.119943\C,0,-4.642398,-4.327659,-6.74129\H,0,-4.502676,-2.737405
,-8.163867\H,0,-5.217137,2.023348,-0.760703\C,0,-6.399437,1.691512,-2.
514456\H,0,-7.406221,1.08676,-4.298129\F,0,2.345824,-5.655281,-3.95151
6\C,0,0.08431,-6.239904,-4.215693\F,0,-2.179548,-6.835142,-4.460773\F,
0,-0.981832,1.901302,1.850831\C,0,-3.145652,1.058009,1.605751\F,0,-5.3
21927,0.183328,1.371811\H,0,0.676865,1.981443,-6.213095\H,0,-4.984092,
-5.05336,-7.469049\H,0,-7.124159,2.458232,-2.269854\F,0,0.342828,-6.74
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013153\PG=C01 [X(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE008\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 12.6477\\0,1\C,
0,0.646857,0.690313,4.643787\C,0,-0.289448,-0.110887,5.29309\H,0,0.362
348,1.671908,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.2
56179,5.453665\C,0,0.05887,-1.354789,5.724367\C,0,2.27384,-1.023049,4.
896824\P,0,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095
\C,0,1.338807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4

.487348,0.199656,3.179673\Au,0,2.221456,2.414068,1.803565\C,0,3.724226
,2.46836,4.860221\H,0,1.616944,-2.800786,5.906744\C,0,4.370838,-0.5220
15,2.016339\C,0,5.59884,0.017405,3.999259\C,0,1.425201,3.420273,0.1877
89\C,0,4.044777,3.775149,4.483053\C,0,3.878666,2.089865,6.212935\H,0,3
.52822,-0.348835,1.358284\C,0,5.318672,-1.460937,1.680548\C,0,6.544506
,-0.933937,3.660285\H,0,5.720281,0.614896,4.894278\C,0,1.523154,2.8657
07,-1.107634\C,0,0.728777,4.638079,0.337383\H,0,3.945341,4.07722,3.447
829\C,0,4.490199,4.684927,5.42677\H,0,3.630856,1.085734,6.534245\C,0,4
.35471,3.027983,7.131189\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,
-1.691513,2.514457\H,0,7.406222,-1.08676,4.298129\C,0,0.99051,3.550285
,-2.194579\C,0,2.100222,1.523253,-1.32566\C,0,0.472935,5.217031,1.6853
22\C,0,0.227739,5.279076,-0.775025\H,0,4.721585,5.697423,5.119943\C,0,
4.642397,4.327659,6.741289\H,0,4.502676,2.737405,8.163867\H,0,7.124159
,-2.458232,2.269854\F,0,1.072627,3.028912,-3.437485\C,0,0.374494,4.764
704,-2.040211\C,0,1.290925,0.412258,-1.518222\C,0,3.475182,1.27802,-1.
298605\C,0,-0.812592,5.196018,2.227999\C,0,1.461431,5.763367,2.473079\
F,0,-0.438008,6.450929,-0.641346\H,0,4.984092,5.05336,7.469049\F,0,-0.
11192,5.430765,-3.117608\C,0,1.784695,-0.855341,-1.653494\F,0,-0.04595
3,0.58478,-1.542094\F,0,4.31998,2.308739,-1.131505\C,0,3.993993,0.0106
47,-1.42592\F,0,-1.813887,4.661423,1.502308\C,0,-1.097406,5.716374,3.4
6613\C,0,1.205181,6.288127,3.731899\F,0,2.718475,5.851897,2.013156\F,0
,0.981832,-1.901302,-1.850831\C,0,3.145651,-1.058009,-1.605751\F,0,5.3
21927,-0.183328,-1.371811\F,0,-2.345824,5.655281,3.951516\C,0,-0.08431
,6.239904,4.215693\F,0,2.179548,6.835141,4.460773\F,0,3.656967,-2.2908
33,-1.71556\F,0,-0.342828,6.745131,5.43791\C,0,1.3434,-0.940842,9.1729
91\H,0,1.001706,-1.666543,8.445231\C,0,1.631088,0.358834,8.783092\C,0,
1.495599,-1.298109,10.487511\H,0,1.483121,0.649412,7.750414\C,0,2.1071
32,1.296953,9.701345\C,0,1.941021,-0.388332,11.431228\H,0,1.264212,-2.
310606,10.794338\H,0,2.354943,2.301083,9.380036\C,0,2.261572,0.918457,
11.054059\H,0,2.040457,-0.690404,12.466452\P,0,2.866619,2.060714,12.31
288\C,0,4.045664,3.148916,11.458282\Au,0,3.764343,0.972749,14.110715\C
,0,1.49845,3.187161,12.734608\C,0,3.711958,4.409866,11.017457\C,0,5.33
8941,2.696504,11.270494\C,0,4.560597,-0.033456,15.726493\C,0,1.61496,3
.908832,13.897942\C,0,0.386959,3.369412,11.915023\C,0,4.646991,5.20553
4,10.369745\H,0,2.709283,4.785672,11.179782\H,0,5.62345,1.714909,11.62
8725\C,0,6.275246,3.497704,10.621191\C,0,4.462644,0.52111,17.021915\C,
0,5.25702,-1.251262,15.576899\H,0,2.457577,3.735651,14.555998\C,0,0.66
7126,4.847754,14.233733\C,0,-0.558708,4.320754,12.253996\H,0,0.265516,
2.77192,11.020003\C,0,5.926928,4.741605,10.189914\H,0,4.368854,6.18760
3,10.007537\H,0,7.281349,3.130638,10.460616\C,0,4.995287,-0.163468,18.
10886\C,0,3.885576,1.863563,17.239941\C,0,5.758059,-1.892258,16.689306
\C,0,5.512863,-1.830214,14.228959\H,0,0.76866,5.410165,15.153578\C,0,-
0.413639,5.07833,13.399825\H,0,-1.420424,4.473577,11.616153\H,0,6.6626
63,5.368259,9.701186\F,0,4.913171,0.357905,19.351767\C,0,5.611304,-1.3
77887,17.954491\C,0,4.694873,2.974559,17.432503\C,0,2.510616,2.108797,
17.212887\F,0,6.423806,-3.064112,16.555626\C,0,6.79839,-1.8092,13.6862
82\C,0,4.524368,-2.37655,13.441202\H,0,-1.138361,5.845049,13.644427\F,
0,6.097718,-2.043947,19.031889\F,0,6.031751,2.802037,17.456375\C,0,4.2
01103,4.242157,17.567774\F,0,1.665818,1.078078,17.045786\C,0,1.991805,
3.37617,17.3402\F,0,7.799685,-1.274605,14.411973\C,0,7.083204,-2.32955
8,12.448151\F,0,3.267323,-2.46508,13.901124\C,0,4.780617,-2.90131,12.1
82383\F,0,5.003966,5.288119,17.765112\C,0,2.840146,4.444826,17.520031\
F,0,0.663871,3.570145,17.286093\F,0,8.331622,-2.268464,11.962765\C,0,6

.070107,-2.853087,11.698587\F,0,3.80625,-3.448325,11.453507\F,0,2.3288
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0.0000007\Quadrupole=35.1435079,43.0720121,-78.21552,11.3946966,-40.54
64485,36.8142499\PG=C01 [X(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE041\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 10.953\\0,1\C,0,0.646857
,0.690313,4.643787\C,0,-0.289448,-0.110887,5.29309\H,0,0.362348,1.6719
08,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.256179,5.45
3665\C,0,0.05887,-1.354789,5.724367\C,0,2.27384,-1.023049,4.896824\P,0
,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095\C,0,1.338
807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4.487348,0.
199656,3.179673\Au,0,2.221456,2.414068,1.803565\C,0,3.724226,2.46836,4
.860221\H,0,1.616944,-2.800786,5.906744\C,0,4.370838,-0.522015,2.01633
9\C,0,5.59884,0.017405,3.999259\C,0,1.425201,3.420273,0.187789\C,0,4.0
44777,3.775149,4.483053\C,0,3.878666,2.089865,6.212935\H,0,3.52822,-0.
348835,1.358284\C,0,5.318672,-1.460937,1.680548\C,0,6.544506,-0.933937
,3.660285\H,0,5.720281,0.614896,4.894278\C,0,1.523154,2.865707,-1.1076
34\C,0,0.728777,4.638079,0.337383\H,0,3.945341,4.07722,3.447829\C,0,4.
490199,4.684927,5.42677\H,0,3.630856,1.085734,6.534245\C,0,4.35471,3.0
27983,7.131189\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,-1.691513,
2.514457\H,0,7.406222,-1.08676,4.298129\C,0,0.99051,3.550285,-2.194579
\C,0,2.100222,1.523253,-1.32566\C,0,0.472935,5.217031,1.685322\C,0,0.2
27739,5.279076,-0.775025\H,0,4.721585,5.697423,5.119943\C,0,4.642397,4
.327659,6.741289\H,0,4.502676,2.737405,8.163867\H,0,7.124159,-2.458232
,2.269854\F,0,1.072627,3.028912,-3.437485\C,0,0.374494,4.764704,-2.040
211\C,0,1.290925,0.412258,-1.518222\C,0,3.475182,1.27802,-1.298605\C,0
,-0.812592,5.196018,2.227999\C,0,1.461431,5.763367,2.473079\F,0,-0.438
008,6.450929,-0.641346\H,0,4.984092,5.05336,7.469049\F,0,-0.11192,5.43
0765,-3.117608\C,0,1.784695,-0.855341,-1.653494\F,0,-0.045953,0.58478,
-1.542094\F,0,4.31998,2.308739,-1.131505\C,0,3.993993,0.010647,-1.4259
2\F,0,-1.813887,4.661423,1.502308\C,0,-1.097406,5.716374,3.46613\C,0,1
.205181,6.288127,3.731899\F,0,2.718475,5.851897,2.013156\F,0,0.981832,
-1.901302,-1.850831\C,0,3.145651,-1.058009,-1.605751\F,0,5.321927,-0.1
83328,-1.371811\F,0,-2.345824,5.655281,3.951516\C,0,-0.08431,6.239904,
4.215693\F,0,2.179548,6.835141,4.460773\F,0,3.656967,-2.290833,-1.7155
6\F,0,-0.342828,6.745131,5.43791\F,0,-1.550032,-0.027747,8.339083\C,0,
-2.763259,0.01345,8.891309\C,0,-3.699981,-0.921408,8.553926\C,0,-3.011
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311604\F,0,-5.91795,-1.660837,8.783092\C,0,-5.202398,0.199718,10.05623
4\F,0,-4.48635,2.014998,11.337334\C,0,-2.353197,-4.201649,7.196438\Au,
0,-2.115347,-3.317456,10.089018\F,0,-4.498177,-0.958941,5.853272\C,0,-
3.510799,-3.032573,5.441092\F,0,-6.41648,0.250287,10.638697\C,0,-2.786
026,-4.114792,5.880327\C,0,-1.595872,-5.407727,7.646812\P,0,-1.605227,
-3.571131,12.304127\F,0,-3.944279,-2.968411,4.163176\F,0,-2.522608,-5.
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,8.506184\C,0,-3.026299,-4.089452,13.296382\C,0,-0.347724,-4.863861,12
.602519\C,0,-1.020773,-2.047081,13.113367\F,0,0.315004,-4.781067,6.432
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0,-1.466802,-7.433188,8.964515\C,0,-3.751964,-5.210039,12.879428\C,0,-
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72,-2.046315,14.144613\F,0,1.706217,-6.89594,7.330118\C,0,-0.167279,-7
.608748,8.560291\F,0,-2.039382,-8.314556,9.788875\H,0,-3.453518,-5.739
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,15.131298\H,0,-2.911624,-2.534741,14.76145\H,0,0.513275,-4.620015,10.
641243\C,0,1.542717,-6.118572,11.803622\C,0,0.679517,-6.53412,13.98228
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,0,-1.187918,0.341227,13.286834\C,0,0.25955,-0.858667,14.752538\H,0,0.
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94,-6.526075,13.277285\C,0,-5.251994,-4.966431,14.741398\H,0,-4.898991
,-3.291007,16.000536\H,0,2.270873,-6.335932,11.031939\C,0,1.578027,-6.
790506,12.984462\H,0,0.722704,-7.083195,14.914865\H,0,-1.607175,1.2806
05,12.948176\C,0,-0.301491,0.324039,14.337175\H,0,0.982073,-0.860593,1
5.559392\H,0,-6.099929,-5.316884,15.316858\H,0,2.336353,-7.548068,13.1
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upole=-53.527976,-65.0676193,118.5955953,1.4387918,18.62166,-33.429801
2\PG=C01 [X(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE021\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 10.852\\0,1\C,0
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48,1.671908,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.25
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96824\P,0,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095\
C,0,1.338807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4.
487348,0.199656,3.179673\Au,0,2.221456,2.414068,1.803565\C,0,3.724226,
2.46836,4.860221\H,0,1.616944,-2.800786,5.906744\C,0,4.370838,-0.52201
5,2.016339\C,0,5.59884,0.017405,3.999259\C,0,1.425201,3.420273,0.18778
9\C,0,4.044777,3.775149,4.483053\C,0,3.878666,2.089865,6.212935\H,0,3.
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-0.933937,3.660285\H,0,5.720281,0.614896,4.894278\C,0,1.523154,2.86570
7,-1.107634\C,0,0.728777,4.638079,0.337383\H,0,3.945341,4.07722,3.4478
29\C,0,4.490199,4.684927,5.42677\H,0,3.630856,1.085734,6.534245\C,0,4.
35471,3.027983,7.131189\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,-
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2\C,0,0.227739,5.279076,-0.775025\H,0,4.721585,5.697423,5.119943\C,0,4
.642397,4.327659,6.741289\H,0,4.502676,2.737405,8.163867\H,0,7.124159,
-2.458232,2.269854\F,0,1.072627,3.028912,-3.437485\C,0,0.374494,4.7647
04,-2.040211\C,0,1.290925,0.412258,-1.518222\C,0,3.475182,1.27802,-1.2
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,0,-0.438008,6.450929,-0.641346\H,0,4.984092,5.05336,7.469049\F,0,-0.1
1192,5.430765,-3.117608\C,0,1.784695,-0.855341,-1.653494\F,0,-0.045953
,0.58478,-1.542094\F,0,4.31998,2.308739,-1.131505\C,0,3.993993,0.01064
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1927,-0.183328,-1.371811\F,0,-2.345824,5.655281,3.951516\C,0,-0.08431,
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3,-1.71556\F,0,-0.342828,6.745131,5.43791\F,0,-0.966361,7.842705,-4.46
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,0,1.297496,8.437943,-4.215693\F,0,-1.505288,8.825951,-2.013157\C,0,0.
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83,-2.227999\F,0,3.559011,9.022566,-3.951516\C,0,0.985448,9.398772,0.7
75025\C,0,-0.212014,11.257574,-0.187788\F,0,3.027074,10.016425,-1.5023
08\F,0,1.651195,8.226917,0.641346\C,0,0.838693,9.913143,2.040211\Au,0,
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8222\C,0,-2.261996,13.399827,1.298605\C,0,0.56633,13.987534,-4.643787\
C,0,-1.060654,15.700896,-4.896824\C,0,-2.83159,10.902699,-4.483053\C,0
,-2.665479,12.587982,-6.212935\C,0,-3.157651,15.199862,-2.016339\C,0,-
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4,-5.29309\C,0,-0.125621,16.496565,-5.544536\H,0,-2.063328,16.076702,-
4.734499\H,0,-2.732154,10.600626,-3.447829\C,0,-3.277013,9.992921,-5.4
2677\C,0,-3.141523,11.649863,-7.131189\H,0,-2.417669,13.592113,-6.5342
45\H,0,-2.315034,15.026681,-1.358284\C,0,-4.105485,16.138784,-1.680548
\C,0,-5.331319,15.611784,-3.660285\H,0,-4.507095,14.06295,-4.894278\F,
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,16.032635,-5.724367\H,0,-0.403757,17.478634,-5.906744\H,0,-3.508399,8
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,-2.514456\H,0,-6.193035,15.764606,-4.298129\F,0,-2.443781,16.968679,1
.715559\H,0,1.890052,16.65929,-6.213095\H,0,-3.770906,9.624487,-7.4690
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e=-25.5735674,20.7603797,4.8131877,-35.1251466,33.7465,-75.9368863\PG=
C01 [X(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE008\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 9.78419\\0,1\C,0,0.64685
7,0.690313,4.643787\C,0,-0.289448,-0.110887,5.29309\H,0,0.362348,1.671
908,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.256179,5.4
53665\C,0,0.05887,-1.354789,5.724367\C,0,2.27384,-1.023049,4.896824\P,
0,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095\C,0,1.33
8807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4.487348,0
.199656,3.179673\Au,0,2.221456,2.414068,1.803565\C,0,3.724226,2.46836,
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,-1.901302,-1.850831\C,0,3.145651,-1.058009,-1.605751\F,0,5.321927,-0.
183328,-1.371811\F,0,-2.345824,5.655281,3.951516\C,0,-0.08431,6.239904
,4.215693\F,0,2.179548,6.835141,4.460773\F,0,3.656967,-2.290833,-1.715
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,8.534614,4.328685\C,0,-7.581162,8.946888,2.127739\C,0,-6.324659,4.221
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6566\C,0,-5.516305,7.588465,8.717843\H,0,-8.382777,8.006832,5.273037\C
,0,-9.412219,9.505389,4.110659\C,0,-8.54902,9.920937,1.931994\H,0,-6.8
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1.440402\C,0,-4.169521,4.308225,7.360355\C,0,-4.074255,5.4063,9.602677
\C,0,-5.083476,7.501609,10.033955\C,0,-6.273629,8.794543,8.267469\H,0,
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\C,0,-5.702681,9.724236,7.408098\C,0,-7.568932,9.019219,8.633497\H,0,-
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F,0,-1.453022,3.13653,5.275584\C,0,-3.632731,2.296952,5.503159\F,0,-5.
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,10.995564,7.353989\F,0,-9.575719,10.282757,8.584163\F,0,-3.383152,1.3
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,-40.2423429\PG=C01 [X(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE041\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 13.0292\\0,1\C,0,0.64685

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908,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.256179,5.4
53665\C,0,0.05887,-1.354789,5.724367\C,0,2.27384,-1.023049,4.896824\P,
0,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095\C,0,1.33
8807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4.487348,0
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634\C,0,0.728777,4.638079,0.337383\H,0,3.945341,4.07722,3.447829\C,0,4
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027983,7.131189\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,-1.691513
,2.514457\H,0,7.406222,-1.08676,4.298129\C,0,0.99051,3.550285,-2.19457
9\C,0,2.100222,1.523253,-1.32566\C,0,0.472935,5.217031,1.685322\C,0,0.
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2,2.269854\F,0,1.072627,3.028912,-3.437485\C,0,0.374494,4.764704,-2.04
0211\C,0,1.290925,0.412258,-1.518222\C,0,3.475182,1.27802,-1.298605\C,
0,-0.812592,5.196018,2.227999\C,0,1.461431,5.763367,2.473079\F,0,-0.43
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30765,-3.117608\C,0,1.784695,-0.855341,-1.653494\F,0,-0.045953,0.58478
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,4.215693\F,0,2.179548,6.835141,4.460773\F,0,3.656967,-2.290833,-1.715
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.551221,-3.930986\C,0,-9.623628,5.641768,-2.312345\C,0,-9.340499,7.445
3,-0.782983\H,0,-7.684235,8.756289,-1.152831\H,0,-7.004815,10.471567,-
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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 12.5273\\0,1\C,0,0.64685
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908,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.256179,5.4
53665\C,0,0.05887,-1.354789,5.724367\C,0,2.27384,-1.023049,4.896824\P,
0,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095\C,0,1.33
8807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4.487348,0
.199656,3.179673\Au,0,2.221456,2.414068,1.803565\C,0,3.724226,2.46836,
4.860221\H,0,1.616944,-2.800786,5.906744\C,0,4.370838,-0.522015,2.0163
39\C,0,5.59884,0.017405,3.999259\C,0,1.425201,3.420273,0.187789\C,0,4.
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7,3.660285\H,0,5.720281,0.614896,4.894278\C,0,1.523154,2.865707,-1.107
634\C,0,0.728777,4.638079,0.337383\H,0,3.945341,4.07722,3.447829\C,0,4
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027983,7.131189\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,-1.691513
,2.514457\H,0,7.406222,-1.08676,4.298129\C,0,0.99051,3.550285,-2.19457
9\C,0,2.100222,1.523253,-1.32566\C,0,0.472935,5.217031,1.685322\C,0,0.
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2,2.269854\F,0,1.072627,3.028912,-3.437485\C,0,0.374494,4.764704,-2.04
0211\C,0,1.290925,0.412258,-1.518222\C,0,3.475182,1.27802,-1.298605\C,
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30765,-3.117608\C,0,1.784695,-0.855341,-1.653494\F,0,-0.045953,0.58478
,-1.542094\F,0,4.31998,2.308739,-1.131505\C,0,3.993993,0.010647,-1.425
92\F,0,-1.813887,4.661423,1.502308\C,0,-1.097406,5.716374,3.46613\C,0,
1.205181,6.288127,3.731899\F,0,2.718475,5.851897,2.013156\F,0,0.981832
,-1.901302,-1.850831\C,0,3.145651,-1.058009,-1.605751\F,0,5.321927,-0.
183328,-1.371811\F,0,-2.345824,5.655281,3.951516\C,0,-0.08431,6.239904
,4.215693\F,0,2.179548,6.835141,4.460773\F,0,3.656967,-2.290833,-1.715
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726462,10.057832,10.641243\C,0,2.755904,8.559275,11.803622\C,0,1.89270
4,8.143727,13.982287\H,0,0.210636,9.331479,14.572071\H,0,-1.019017,13.
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98\H,0,-3.685805,11.38684,16.000536\H,0,3.484059,8.341914,11.031939\C,
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9,13.817253,15.559392\F,0,-3.273163,16.692846,11.337334\H,0,-4.886743,
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6P2)]\\@

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 12.4681\\0,1\C,0,0.64685
7,0.690313,4.643787\C,0,-0.289448,-0.110887,5.29309\H,0,0.362348,1.671
908,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.256179,5.4
53665\C,0,0.05887,-1.354789,5.724367\C,0,2.27384,-1.023049,4.896824\P,
0,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095\C,0,1.33
8807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4.487348,0
.199656,3.179673\Au,0,2.221456,2.414068,1.803565\C,0,3.724226,2.46836,
4.860221\H,0,1.616944,-2.800786,5.906744\C,0,4.370838,-0.522015,2.0163
39\C,0,5.59884,0.017405,3.999259\C,0,1.425201,3.420273,0.187789\C,0,4.
044777,3.775149,4.483053\C,0,3.878666,2.089865,6.212935\H,0,3.52822,-0
.348835,1.358284\C,0,5.318672,-1.460937,1.680548\C,0,6.544506,-0.93393
7,3.660285\H,0,5.720281,0.614896,4.894278\C,0,1.523154,2.865707,-1.107
634\C,0,0.728777,4.638079,0.337383\H,0,3.945341,4.07722,3.447829\C,0,4
.490199,4.684927,5.42677\H,0,3.630856,1.085734,6.534245\C,0,4.35471,3.
027983,7.131189\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,-1.691513
,2.514457\H,0,7.406222,-1.08676,4.298129\C,0,0.99051,3.550285,-2.19457
9\C,0,2.100222,1.523253,-1.32566\C,0,0.472935,5.217031,1.685322\C,0,0.
227739,5.279076,-0.775025\H,0,4.721585,5.697423,5.119943\C,0,4.642397,
4.327659,6.741289\H,0,4.502676,2.737405,8.163867\H,0,7.124159,-2.45823
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0211\C,0,1.290925,0.412258,-1.518222\C,0,3.475182,1.27802,-1.298605\C,
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92\F,0,-1.813887,4.661423,1.502308\C,0,-1.097406,5.716374,3.46613\C,0,
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,-1.901302,-1.850831\C,0,3.145651,-1.058009,-1.605751\F,0,5.321927,-0.
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56\F,0,-0.342828,6.745131,5.43791\F,0,1.453022,-3.13653,-5.275584\C,0,
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67,-7.022972\C,0,4.501388,-5.44472,-8.286566\F,0,6.31947,-3.414564,-7.
575198\C,0,5.224297,-6.564312,-7.809138\C,0,4.074255,-5.4063,-9.602677
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9,-5.433898,-2.800913\C,0,4.843203,-7.476269,-2.617899\C,0,7.521779,-8
.250677,-3.311762\F,0,5.346894,-8.504876,-10.899691\C,0,5.702681,-9.72
4236,-7.408098\C,0,7.568932,-9.019218,-8.633497\C,0,6.324659,-4.221949
,-3.251287\C,0,7.77413,-5.433132,-1.769668\C,0,4.117538,-8.596856,-3.0
34853\C,0,4.417608,-6.798405,-1.487986\C,0,8.433332,-8.534614,-4.32868
5\C,0,7.581162,-8.946888,-2.12774\F,0,4.437137,-9.592145,-7.015015\C,0
,6.402699,-10.820004,-6.949766\F,0,8.184506,-8.167884,-9.481729\C,0,8.
302629,-10.106857,-8.199038\H,0,5.637299,-4.20628,-4.08806\C,0,6.68158
4,-3.04559,-2.627447\C,0,8.129052,-4.245483,-1.161743\H,0,8.217257,-6.
364822,-1.440402\H,0,4.415984,-9.126625,-3.930986\C,0,3.018486,-9.0360
79,-2.312345\C,0,3.301615,-7.232547,-0.782983\H,0,4.957879,-5.921558,-
1.152831\H,0,8.382777,-8.006832,-5.273038\C,0,9.41222,-9.505389,-4.110
659\C,0,8.549019,-9.920937,-1.931994\H,0,6.866952,-8.733185,-1.34221\F
,0,5.830121,-11.701373,-6.125406\C,0,7.702223,-10.995565,-7.35399\F,0,
9.57572,-10.282757,-8.584164\H,0,6.262328,-2.106211,-2.966104\C,0,7.56
8011,-3.062778,-1.577105\H,0,8.851575,-4.24741,-0.354889\H,0,2.472008,
-9.912892,-2.636997\C,0,2.617508,-8.353248,-1.172883\H,0,2.970511,-6.6
77824,0.086255\H,0,10.140375,-9.72275,-4.882342\C,0,9.44753,-10.177323
,-2.929819\H,0,8.592206,-10.470012,-0.999417\F,0,8.412341,-12.071688,-
6.906798\H,0,7.826214,-2.138661,-1.07501\H,0,1.769573,-8.703701,-0.597
422\H,0,10.205855,-10.934884,-2.774814\\Version=ES64L-G09RevE.01\HF=-3
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pole=33.7910573,4.1589054,-37.9499627,-7.2816909,51.9832655,-40.609425
3\PG=C01 [X(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE041\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 11.4335\\0,1\C,
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348,1.671908,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.2
56179,5.453665\C,0,0.05887,-1.354789,5.724367\C,0,2.27384,-1.023049,4.
896824\P,0,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095
\C,0,1.338807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4
.487348,0.199656,3.179673\Au,0,2.221456,2.414068,1.803565\C,0,3.724226
,2.46836,4.860221\H,0,1.616944,-2.800786,5.906744\C,0,4.370838,-0.5220
15,2.016339\C,0,5.59884,0.017405,3.999259\C,0,1.425201,3.420273,0.1877

89\C,0,4.044777,3.775149,4.483053\C,0,3.878666,2.089865,6.212935\H,0,3
.52822,-0.348835,1.358284\C,0,5.318672,-1.460937,1.680548\C,0,6.544506
,-0.933937,3.660285\H,0,5.720281,0.614896,4.894278\C,0,1.523154,2.8657
07,-1.107634\C,0,0.728777,4.638079,0.337383\H,0,3.945341,4.07722,3.447
829\C,0,4.490199,4.684927,5.42677\H,0,3.630856,1.085734,6.534245\C,0,4
.35471,3.027983,7.131189\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,
-1.691513,2.514457\H,0,7.406222,-1.08676,4.298129\C,0,0.99051,3.550285
,-2.194579\C,0,2.100222,1.523253,-1.32566\C,0,0.472935,5.217031,1.6853
22\C,0,0.227739,5.279076,-0.775025\H,0,4.721585,5.697423,5.119943\C,0,
4.642397,4.327659,6.741289\H,0,4.502676,2.737405,8.163867\H,0,7.124159
,-2.458232,2.269854\F,0,1.072627,3.028912,-3.437485\C,0,0.374494,4.764
704,-2.040211\C,0,1.290925,0.412258,-1.518222\C,0,3.475182,1.27802,-1.
298605\C,0,-0.812592,5.196018,2.227999\C,0,1.461431,5.763367,2.473079\
F,0,-0.438008,6.450929,-0.641346\H,0,4.984092,5.05336,7.469049\F,0,-0.
11192,5.430765,-3.117608\C,0,1.784695,-0.855341,-1.653494\F,0,-0.04595
3,0.58478,-1.542094\F,0,4.31998,2.308739,-1.131505\C,0,3.993993,0.0106
47,-1.42592\F,0,-1.813887,4.661423,1.502308\C,0,-1.097406,5.716374,3.4
6613\C,0,1.205181,6.288127,3.731899\F,0,2.718475,5.851897,2.013156\F,0
,0.981832,-1.901302,-1.850831\C,0,3.145651,-1.058009,-1.605751\F,0,5.3
21927,-0.183328,-1.371811\F,0,-2.345824,5.655281,3.951516\C,0,-0.08431
,6.239904,4.215693\F,0,2.179548,6.835141,4.460773\F,0,3.656967,-2.2908
33,-1.71556\F,0,-0.342828,6.745131,5.43791\F,0,8.533373,0.183328,1.371
811\C,0,9.861307,-0.010647,1.42592\C,0,10.380118,-1.27802,1.298605\C,0
,10.709648,1.058009,1.605751\F,0,9.53532,-2.308739,1.131505\C,0,11.755
077,-1.523254,1.32566\F,0,10.198332,2.290832,1.715559\C,0,12.070605,0.
85534,1.653494\C,0,12.332146,-2.865707,1.107634\C,0,12.564376,-0.41225
8,1.518222\F,0,12.873467,1.901302,1.850831\C,0,12.430099,-3.420273,-0.
187788\C,0,12.86479,-3.550285,2.194579\F,0,13.901253,-0.58478,1.542094
\Au,0,11.633844,-2.414068,-1.803566\C,0,13.126523,-4.638079,-0.337383\
F,0,12.782673,-3.028912,3.437485\C,0,13.480806,-4.764704,2.040211\P,0,
10.736121,-1.326103,-3.601402\C,0,13.627561,-5.279075,0.775025\C,0,13.
382364,-5.217031,-1.685322\F,0,13.967219,-5.430765,3.117608\C,0,9.3679
51,-0.199656,-3.179674\C,0,11.915167,-0.237901,-4.455998\C,0,10.131074
,-2.46836,-4.860221\F,0,14.293308,-6.450929,0.641346\C,0,14.667892,-5.
196017,-2.227999\C,0,12.393869,-5.763367,-2.473079\C,0,9.484463,0.5220
15,-2.016339\C,0,8.256461,-0.017405,-3.999259\C,0,13.208443,-0.690313,
-4.643787\C,0,11.58146,1.023049,-4.896824\C,0,9.810523,-3.775149,-4.48
3053\C,0,9.976634,-2.089864,-6.212935\F,0,15.669188,-4.661422,-1.50230
8\C,0,14.952706,-5.716375,-3.466131\F,0,11.136826,-5.851897,-2.013157\
C,0,12.65012,-6.288126,-3.731899\C,0,8.536629,1.460937,-1.680548\H,0,1
0.32708,0.348834,-1.358284\C,0,7.310794,0.933937,-3.660285\H,0,8.13501
8,-0.614897,-4.894278\H,0,13.492952,-1.671908,-4.285556\C,0,14.144749,
0.110887,-5.29309\C,0,12.516493,1.818717,-5.544536\H,0,10.578785,1.398
855,-4.734499\H,0,9.909959,-4.07722,-3.447829\C,0,9.365101,-4.684927,-
5.42677\C,0,9.50059,-3.027983,-7.131189\H,0,10.224444,-1.085734,-6.534
245\F,0,16.201124,-5.655281,-3.951516\C,0,13.93961,-6.239904,-4.215693
\F,0,11.675752,-6.835142,-4.460773\C,0,7.455863,1.691512,-2.514456\H,0
,8.638163,2.023348,-0.760703\H,0,6.449079,1.08676,-4.298129\H,0,15.150
851,-0.256179,-5.453665\C,0,13.79643,1.354788,-5.724367\H,0,12.238356,
2.800786,-5.906744\H,0,9.133715,-5.697423,-5.119943\C,0,9.212902,-4.32
7659,-6.74129\H,0,9.352624,-2.737405,-8.163867\F,0,14.198128,-6.745131
,-5.43791\H,0,6.731141,2.458232,-2.269854\H,0,14.532166,1.981443,-6.21
3095\H,0,8.871208,-5.05336,-7.469049\\Version=ES64L-G09RevE.01\HF=-315

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le=-46.7769884,-12.7394356,59.516424,48.1001092,-37.5172444,4.494488\P
G=C01 [X(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE021\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 12.1629\\0,1\C,0,0.64685
7,0.690313,4.643787\C,0,-0.289448,-0.110887,5.29309\H,0,0.362348,1.671
908,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.256179,5.4
53665\C,0,0.05887,-1.354789,5.724367\C,0,2.27384,-1.023049,4.896824\P,
0,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095\C,0,1.33
8807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4.487348,0
.199656,3.179673\Au,0,2.221456,2.414068,1.803565\C,0,3.724226,2.46836,
4.860221\H,0,1.616944,-2.800786,5.906744\C,0,4.370838,-0.522015,2.0163
39\C,0,5.59884,0.017405,3.999259\C,0,1.425201,3.420273,0.187789\C,0,4.
044777,3.775149,4.483053\C,0,3.878666,2.089865,6.212935\H,0,3.52822,-0
.348835,1.358284\C,0,5.318672,-1.460937,1.680548\C,0,6.544506,-0.93393
7,3.660285\H,0,5.720281,0.614896,4.894278\C,0,1.523154,2.865707,-1.107
634\C,0,0.728777,4.638079,0.337383\H,0,3.945341,4.07722,3.447829\C,0,4
.490199,4.684927,5.42677\H,0,3.630856,1.085734,6.534245\C,0,4.35471,3.
027983,7.131189\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,-1.691513
,2.514457\H,0,7.406222,-1.08676,4.298129\C,0,0.99051,3.550285,-2.19457
9\C,0,2.100222,1.523253,-1.32566\C,0,0.472935,5.217031,1.685322\C,0,0.
227739,5.279076,-0.775025\H,0,4.721585,5.697423,5.119943\C,0,4.642397,
4.327659,6.741289\H,0,4.502676,2.737405,8.163867\H,0,7.124159,-2.45823
2,2.269854\F,0,1.072627,3.028912,-3.437485\C,0,0.374494,4.764704,-2.04
0211\C,0,1.290925,0.412258,-1.518222\C,0,3.475182,1.27802,-1.298605\C,
0,-0.812592,5.196018,2.227999\C,0,1.461431,5.763367,2.473079\F,0,-0.43
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30765,-3.117608\C,0,1.784695,-0.855341,-1.653494\F,0,-0.045953,0.58478
,-1.542094\F,0,4.31998,2.308739,-1.131505\C,0,3.993993,0.010647,-1.425
92\F,0,-1.813887,4.661423,1.502308\C,0,-1.097406,5.716374,3.46613\C,0,
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,-1.901302,-1.850831\C,0,3.145651,-1.058009,-1.605751\F,0,5.321927,-0.
183328,-1.371811\F,0,-2.345824,5.655281,3.951516\C,0,-0.08431,6.239904
,4.215693\F,0,2.179548,6.835141,4.460773\F,0,3.656967,-2.290833,-1.715
56\F,0,-0.342828,6.745131,5.43791\F,0,6.811993,-2.976474,6.125407\C,0,
6.239414,-3.857842,6.949766\C,0,4.93989,-3.682282,7.353989\C,0,6.93943
2,-4.95361,7.408098\F,0,4.229773,-2.60616,6.906798\C,0,4.339484,-4.570
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267469\F,0,3.066394,-4.395091,8.584163\C,0,5.073182,-5.658628,8.633497
\C,0,7.125809,-7.089382,8.717843\F,0,4.457607,-6.509964,9.481729\C,0,7
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958,-7.973574,5.825263\C,0,8.140725,-9.233128,8.286566\F,0,7.295219,-6
.172971,10.899691\C,0,8.28341,-8.258457,10.473188\P,0,6.377839,-7.7198
99,3.610155\C,0,8.567859,-9.271546,9.602677\C,0,8.472592,-10.369622,7.
360355\F,0,8.71689,-8.322618,11.751104\C,0,7.79891,-7.201579,2.617899\
C,0,5.120335,-6.427169,3.311762\C,0,5.793384,-9.243949,2.800913\F,0,9.
270789,-10.332088,10.061008\C,0,9.728885,-10.501144,6.790624\C,0,7.535
871,-11.30448,7.022972\C,0,8.524575,-6.080991,3.034853\C,0,8.224505,-7
.879442,1.487985\C,0,4.208781,-6.143233,4.328685\C,0,5.060951,-5.73095
9,2.127739\C,0,6.317454,-10.455898,3.251288\C,0,4.867984,-9.244715,1.7
69668\F,0,10.690562,-9.630192,7.131189\C,0,9.97501,-11.490748,5.858047

\F,0,6.322643,-11.263283,7.575198\C,0,7.784147,-12.295665,6.096761\H,0
,8.22613,-5.551221,3.930986\C,0,9.623628,-5.641768,2.312345\C,0,9.3404
99,-7.4453,0.782983\H,0,7.684235,-8.756289,1.15283\C,0,3.229894,-5.172
458,4.110659\H,0,4.259336,-6.671015,5.273037\C,0,4.093094,-4.75691,1.9
31994\H,0,5.775161,-5.944662,1.34221\H,0,7.004815,-10.471567,4.08806\C
,0,5.96053,-11.632257,2.627448\C,0,4.513061,-10.432364,1.161742\H,0,4.
424857,-8.313025,1.440402\F,0,11.189091,-11.541317,5.275584\C,0,9.0093
82,-12.380895,5.503159\F,0,6.819795,-13.16052,5.743464\H,0,10.170105,-
4.764955,2.636997\C,0,10.024606,-6.324599,1.172883\H,0,9.671603,-8.000
023,-0.086256\H,0,2.501739,-4.955097,4.882342\C,0,3.194585,-4.500523,2
.929819\H,0,4.049907,-4.207835,0.999417\H,0,6.379786,-12.571635,2.9661
04\C,0,5.074103,-11.615069,1.577105\H,0,3.790539,-10.430436,0.354888\F
,0,9.258961,-13.306028,4.576947\H,0,10.87254,-5.974146,0.597422\H,0,2.
436258,-3.742962,2.774814\H,0,4.815899,-12.539186,1.07501\\Version=ES6
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-30.9960819,57.4344442\PG=C01 [X(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE008\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 13.9482\\0,1\C,0,0.64685
7,0.690313,4.643787\C,0,-0.289448,-0.110887,5.29309\H,0,0.362348,1.671
908,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.256179,5.4
53665\C,0,0.05887,-1.354789,5.724367\C,0,2.27384,-1.023049,4.896824\P,
0,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095\C,0,1.33
8807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4.487348,0
.199656,3.179673\Au,0,2.221456,2.414068,1.803565\C,0,3.724226,2.46836,
4.860221\H,0,1.616944,-2.800786,5.906744\C,0,4.370838,-0.522015,2.0163
39\C,0,5.59884,0.017405,3.999259\C,0,1.425201,3.420273,0.187789\C,0,4.
044777,3.775149,4.483053\C,0,3.878666,2.089865,6.212935\H,0,3.52822,-0
.348835,1.358284\C,0,5.318672,-1.460937,1.680548\C,0,6.544506,-0.93393
7,3.660285\H,0,5.720281,0.614896,4.894278\C,0,1.523154,2.865707,-1.107
634\C,0,0.728777,4.638079,0.337383\H,0,3.945341,4.07722,3.447829\C,0,4
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027983,7.131189\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,-1.691513
,2.514457\H,0,7.406222,-1.08676,4.298129\C,0,0.99051,3.550285,-2.19457
9\C,0,2.100222,1.523253,-1.32566\C,0,0.472935,5.217031,1.685322\C,0,0.
227739,5.279076,-0.775025\H,0,4.721585,5.697423,5.119943\C,0,4.642397,
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2,2.269854\F,0,1.072627,3.028912,-3.437485\C,0,0.374494,4.764704,-2.04
0211\C,0,1.290925,0.412258,-1.518222\C,0,3.475182,1.27802,-1.298605\C,
0,-0.812592,5.196018,2.227999\C,0,1.461431,5.763367,2.473079\F,0,-0.43
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92\F,0,-1.813887,4.661423,1.502308\C,0,-1.097406,5.716374,3.46613\C,0,
1.205181,6.288127,3.731899\F,0,2.718475,5.851897,2.013156\F,0,0.981832
,-1.901302,-1.850831\C,0,3.145651,-1.058009,-1.605751\F,0,5.321927,-0.
183328,-1.371811\F,0,-2.345824,5.655281,3.951516\C,0,-0.08431,6.239904
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56\F,0,-0.342828,6.745131,5.43791\F,0,9.357123,-0.958941,5.853272\C,0,
10.060053,-2.019483,6.311604\C,0,10.344501,-3.032573,5.441092\C,0,10.4
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.123657\C,0,11.092041,0.01345,8.891309\C,0,12.259428,-5.407727,7.64681
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-5.632402,7.280784\C,0,10.829001,-4.089452,13.296382\C,0,13.507576,-4.
863861,12.602519\C,0,12.834527,-2.047081,13.113367\F,0,7.43882,0.25028
7,10.638697\C,0,9.618529,1.089865,10.411123\F,0,11.808116,1.86949,10.1
70817\F,0,10.422935,-6.205328,8.899265\C,0,12.388497,-7.433188,8.96451
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,10.103336,-5.210039,12.879428\C,0,10.403406,-3.411588,14.426295\C,0,1
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9,11.983294\C,0,9.004283,-5.649262,13.601936\C,0,9.287413,-3.84573,15.
131298\H,0,10.943676,-2.534741,14.76145\H,0,14.368575,-4.620015,10.641
243\C,0,15.398018,-6.118572,11.803622\C,0,14.534817,-6.53412,13.982287
\H,0,12.85275,-5.346368,14.572071\H,0,11.623096,-0.819463,11.826221\C,
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.203054,-2.978005,14.473879\F,0,14.398139,-8.684871,9.007483\H,0,8.457
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.790506,12.984462\H,0,14.578004,-7.083195,14.914865\H,0,12.248125,1.28
0605,12.948176\C,0,13.553808,0.324039,14.337175\H,0,14.837373,-0.86059
3,15.559392\H,0,7.755371,-5.316884,15.316858\H,0,16.191654,-7.548068,1
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.5401913\PG=C01 [X(C72H30Au2F26P2)]\\@

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gfprint\\CrystalExplorer Job symop = -, r = 11.8152\\0,1\C,0,0.646857,
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8,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.256179,5.453
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3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095\C,0,1.3388
07,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4.487348,0.1
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\C,0,5.59884,0.017405,3.999259\C,0,1.425201,3.420273,0.187789\C,0,4.04
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3.660285\H,0,5.720281,0.614896,4.894278\C,0,1.523154,2.865707,-1.10763
4\C,0,0.728777,4.638079,0.337383\H,0,3.945341,4.07722,3.447829\C,0,4.4
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.514457\H,0,7.406222,-1.08676,4.298129\C,0,0.99051,3.550285,-2.194579\
C,0,2.100222,1.523253,-1.32566\C,0,0.472935,5.217031,1.685322\C,0,0.22
7739,5.279076,-0.775025\H,0,4.721585,5.697423,5.119943\C,0,4.642397,4.

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-0.812592,5.196018,2.227999\C,0,1.461431,5.763367,2.473079\F,0,-0.4380
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1.901302,-1.850831\C,0,3.145651,-1.058009,-1.605751\F,0,5.321927,-0.18
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.215693\F,0,2.179548,6.835141,4.460773\F,0,3.656967,-2.290833,-1.71556
\F,0,-0.342828,6.745131,5.43791\F,0,-0.315004,4.781066,-6.432553\C,0,0
.30057,5.632402,-7.280783\C,0,1.595873,5.407726,-7.646811\C,0,-0.43312
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742,-8.506184\F,0,-1.706217,6.895939,-7.330118\C,0,0.167279,7.608747,-
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,-0.542839,8.684871,-9.007483\F,0,2.522608,5.118059,-5.01459\C,0,3.510
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.317456,-10.089018\F,0,2.039382,8.314556,-9.788874\F,0,3.944279,2.9684
11,-4.163176\C,0,3.795247,2.019483,-6.311604\C,0,3.699981,0.921408,-8.
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623,2.534741,-14.761451\H,0,-0.513276,4.620015,-10.641243\C,0,-1.54271
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46368,-14.57207\H,0,2.232203,0.819463,-11.826221\C,0,1.187919,-0.34122
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\H,0,-0.722705,7.083195,-14.914865\H,0,1.607174,-1.280605,-12.948177\C
,0,0.301491,-0.324039,-14.337175\H,0,-0.982072,0.860593,-15.559392\H,0
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[X(C72H30Au2F26P2)]\\@

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 10.5873\\0,1\C,0,0.64685
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908,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.256179,5.4

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0,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095\C,0,1.33
8807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4.487348,0
.199656,3.179673\Au,0,2.221456,2.414068,1.803565\C,0,3.724226,2.46836,
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39\C,0,5.59884,0.017405,3.999259\C,0,1.425201,3.420273,0.187789\C,0,4.
044777,3.775149,4.483053\C,0,3.878666,2.089865,6.212935\H,0,3.52822,-0
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027983,7.131189\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,-1.691513
,2.514457\H,0,7.406222,-1.08676,4.298129\C,0,0.99051,3.550285,-2.19457
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0211\C,0,1.290925,0.412258,-1.518222\C,0,3.475182,1.27802,-1.298605\C,
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30765,-3.117608\C,0,1.784695,-0.855341,-1.653494\F,0,-0.045953,0.58478
,-1.542094\F,0,4.31998,2.308739,-1.131505\C,0,3.993993,0.010647,-1.425
92\F,0,-1.813887,4.661423,1.502308\C,0,-1.097406,5.716374,3.46613\C,0,
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,-1.901302,-1.850831\C,0,3.145651,-1.058009,-1.605751\F,0,5.321927,-0.
183328,-1.371811\F,0,-2.345824,5.655281,3.951516\C,0,-0.08431,6.239904
,4.215693\F,0,2.179548,6.835141,4.460773\F,0,3.656967,-2.290833,-1.715
56\F,0,-0.342828,6.745131,5.43791\C,0,4.231672,5.641768,-2.312345\H,0,
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,0,7.477462,7.7199,-3.610154\H,0,6.171065,8.756289,-1.152831\Au,0,6.96
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C,0,6.729492,7.089381,-8.717843\H,0,9.595964,6.671015,-5.273038\C,0,10
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,6.7103265\Quadrupole=43.1949542,-11.8016188,-31.3933354,5.3648879,63.
6991125,60.4498576\PG=C01 [X(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE021\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 8.58411\\0,1\C,0,0.64685
7,0.690313,4.643787\C,0,-0.289448,-0.110887,5.29309\H,0,0.362348,1.671
908,4.285557\C,0,1.940134,0.237901,4.455999\H,0,-1.295551,0.256179,5.4
53665\C,0,0.05887,-1.354789,5.724367\C,0,2.27384,-1.023049,4.896824\P,
0,3.119179,1.326103,3.601402\H,0,-0.676865,-1.981443,6.213095\C,0,1.33
8807,-1.818717,5.544536\H,0,3.276515,-1.398855,4.734499\C,0,4.487348,0
.199656,3.179673\Au,0,2.221456,2.414068,1.803565\C,0,3.724226,2.46836,
4.860221\H,0,1.616944,-2.800786,5.906744\C,0,4.370838,-0.522015,2.0163
39\C,0,5.59884,0.017405,3.999259\C,0,1.425201,3.420273,0.187789\C,0,4.
044777,3.775149,4.483053\C,0,3.878666,2.089865,6.212935\H,0,3.52822,-0
.348835,1.358284\C,0,5.318672,-1.460937,1.680548\C,0,6.544506,-0.93393
7,3.660285\H,0,5.720281,0.614896,4.894278\C,0,1.523154,2.865707,-1.107
634\C,0,0.728777,4.638079,0.337383\H,0,3.945341,4.07722,3.447829\C,0,4
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027983,7.131189\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,-1.691513
,2.514457\H,0,7.406222,-1.08676,4.298129\C,0,0.99051,3.550285,-2.19457
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227739,5.279076,-0.775025\H,0,4.721585,5.697423,5.119943\C,0,4.642397,
4.327659,6.741289\H,0,4.502676,2.737405,8.163867\H,0,7.124159,-2.45823
2,2.269854\F,0,1.072627,3.028912,-3.437485\C,0,0.374494,4.764704,-2.04
0211\C,0,1.290925,0.412258,-1.518222\C,0,3.475182,1.27802,-1.298605\C,
0,-0.812592,5.196018,2.227999\C,0,1.461431,5.763367,2.473079\F,0,-0.43
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30765,-3.117608\C,0,1.784695,-0.855341,-1.653494\F,0,-0.045953,0.58478
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183328,-1.371811\F,0,-2.345824,5.655281,3.951516\C,0,-0.08431,6.239904
,4.215693\F,0,2.179548,6.835141,4.460773\F,0,3.656967,-2.290833,-1.715
56\F,0,-0.342828,6.745131,5.43791\Au,0,8.101145,6.704273,5.825263\P,0,
7.591025,6.957948,3.610155\C,0,8.631003,6.564312,7.809138\C,0,6.333521
,8.250678,3.311762\C,0,7.006571,5.433898,2.800913\C,0,9.012096,7.47626
8,2.617899\C,0,9.353911,5.44472,8.286566\C,0,8.338995,7.588465,8.71784
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596856,3.034853\C,0,9.437692,6.798405,1.487985\C,0,9.685779,4.308225,7
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\C,0,5.726247,4.245483,1.161742\H,0,5.638043,6.364822,1.440402\H,0,9.4

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7.232547,0.782983\H,0,8.897421,5.921558,1.15283\C,0,8.749058,3.373367,
7.022972\C,0,10.942071,4.176702,6.790624\F,0,10.483975,4.345758,10.061
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,8.152618,9.724236,7.408098\F,0,8.508406,8.504876,10.899691\H,0,3.7149
25,9.72275,4.882342\C,0,4.407771,10.177323,2.929819\H,0,5.263093,10.47
0012,0.999417\H,0,7.592972,2.106212,2.966104\C,0,6.28729,3.062778,1.57
7105\H,0,5.003726,4.24741,0.354888\H,0,11.383292,9.912892,2.636997\C,0
,11.237792,8.353248,1.172883\H,0,10.884789,6.677824,-0.086256\F,0,7.53
583,3.414565,7.575198\C,0,8.997334,2.382182,6.096761\C,0,11.188196,3.1
87099,5.858047\F,0,11.903749,5.047655,7.131189\F,0,9.930077,6.355228,1
1.751104\F,0,5.670794,8.167883,9.481729\C,0,5.55267,10.106857,8.199038
\F,0,9.418163,9.592145,7.015015\C,0,7.4526,10.820004,6.949766\H,0,3.64
9445,10.934885,2.774814\H,0,6.029086,2.138661,1.07501\H,0,12.085727,8.
703701,0.597422\F,0,8.032982,1.517327,5.743464\C,0,10.222569,2.296952,
5.503159\F,0,12.402278,3.13653,5.275584\F,0,4.279581,10.282757,8.58416
3\C,0,6.153077,10.995564,7.353989\F,0,8.02518,11.701373,6.125407\F,0,1
0.472147,1.371818,4.576947\F,0,5.442959,12.071688,6.906798\\Version=ES
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5517,-0.6480546\Quadrupole=7.9289944,19.3443737,-27.2733681,0.9141769,
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1\1\GINC-COMPUTE008\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 12.5273\\0,1\H,0,10.8847
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353248,1.172883\C,0,9.437692,6.798405,1.487985\C,0,10.836815,9.036078,
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9\H,0,8.897421,5.921558,1.15283\C,0,9.737761,8.596856,3.034853\H,0,11.
383292,9.912892,2.636997\P,0,7.591025,6.957948,3.610155\H,0,9.439317,9
.126626,3.930986\Au,0,8.101145,6.704273,5.825263\C,0,6.333521,8.250678
,3.311762\C,0,7.006571,5.433898,2.800913\C,0,8.631003,6.564312,7.80913
8\C,0,5.421968,8.534614,4.328685\C,0,6.274137,8.946888,2.127739\C,0,7.
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,6.988348,8.733185,1.34221\H,0,8.218001,4.20628,4.08806\C,0,7.173717,3
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1.440402\C,0,9.781045,5.4063,9.602677\C,0,9.685779,4.308225,7.360355\C
,0,8.771824,7.501609,10.033955\C,0,7.581671,8.794543,8.267469\H,0,3.71
4925,9.72275,4.882342\C,0,4.407771,10.177323,2.929819\H,0,5.263093,10.
470012,0.999417\H,0,7.592972,2.106212,2.966104\C,0,6.28729,3.062778,1.
577105\H,0,5.003726,4.24741,0.354888\F,0,10.483975,4.345758,10.061008\
C,0,9.496596,6.419389,10.473188\C,0,10.942071,4.176702,6.790624\C,0,8.
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4\C,0,10.222569,2.296952,5.503159\F,0,8.032982,1.517327,5.743464\F,0,8
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4,14.644391,15.726493\C,0,6.971245,12.785589,16.689306\Au,0,4.977529,1
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\F,0,7.310904,12.6339,19.031889\C,0,3.474758,15.596304,11.054059\C,0,5
.258851,17.826763,11.458282\C,0,2.711636,17.865007,12.734608\F,0,6.126
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6.786644,17.212887\C,0,3.154207,14.289515,11.431228\C,0,3.320319,15.97
4799,9.701345\C,0,6.552127,17.374352,11.270494\C,0,4.925144,19.087713,
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15023\F,0,7.244937,17.479885,17.456375\C,0,5.414289,18.920004,17.56777
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1,10.369745\H,0,3.92247,19.463518,11.179782\H,0,3.670764,18.413498,14.
555998\C,0,1.880313,19.5256,14.233733\C,0,0.654479,18.9986,12.253996\H
,0,1.478703,17.449768,11.020003\F,0,6.217152,19.965965,17.765112\C,0,4
.053333,19.122673,17.520031\F,0,1.877058,18.247992,17.286093\H,0,2.477
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453,10.189914\H,0,5.58204,20.86545,10.007537\H,0,1.981847,20.088013,15
.153578\C,0,0.799547,19.756176,13.399825\H,0,-0.207237,19.151424,11.61
6153\F,0,3.542017,20.355495,17.629841\H,0,2.214892,13.011304,8.445231\
H,0,7.87585,20.046106,9.701186\H,0,0.074826,20.522896,13.644427\\Versi
on=ES64L-G09RevE.01\HF=-3155.6679215\RMSD=6.087e-09\Dipole=-2.2459677,
1.9089446,-6.4437221\Quadrupole=4.4832956,160.7861882,-165.2694838,-29
.0880351,-125.0281735,-92.9735409\PG=C01 [X(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE021\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 13.0292\\0,1\H,0,10.8847
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353248,1.172883\C,0,9.437692,6.798405,1.487985\C,0,10.836815,9.036078,
2.312345\H,0,12.085727,8.703701,0.597422\C,0,9.012096,7.476268,2.61789
9\H,0,8.897421,5.921558,1.15283\C,0,9.737761,8.596856,3.034853\H,0,11.
383292,9.912892,2.636997\P,0,7.591025,6.957948,3.610155\H,0,9.439317,9
.126626,3.930986\Au,0,8.101145,6.704273,5.825263\C,0,6.333521,8.250678
,3.311762\C,0,7.006571,5.433898,2.800913\C,0,8.631003,6.564312,7.80913
8\C,0,5.421968,8.534614,4.328685\C,0,6.274137,8.946888,2.127739\C,0,7.
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44472,8.286566\C,0,8.338995,7.588465,8.717843\H,0,5.472522,8.006832,5.
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,6.988348,8.733185,1.34221\H,0,8.218001,4.20628,4.08806\C,0,7.173717,3
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470012,0.999417\H,0,7.592972,2.106212,2.966104\C,0,6.28729,3.062778,1.
577105\H,0,5.003726,4.24741,0.354888\F,0,10.483975,4.345758,10.061008\
C,0,9.496596,6.419389,10.473188\C,0,10.942071,4.176702,6.790624\C,0,8.
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9.724236,7.408098\C,0,6.286368,9.019219,8.633497\H,0,3.649445,10.93488
5,2.774814\H,0,6.029086,2.138661,1.07501\F,0,9.930077,6.355228,11.7511
04\F,0,11.903749,5.047655,7.131189\C,0,11.188196,3.187099,5.858047\F,0
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,9.481729\C,0,5.55267,10.106857,8.199038\F,0,12.402278,3.13653,5.27558
4\C,0,10.222569,2.296952,5.503159\F,0,8.032982,1.517327,5.743464\F,0,8
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,10.282757,8.584163\F,0,10.472147,1.371818,4.576947\F,0,5.442959,12.07
1688,6.906798\F,0,0.14056,11.648934,3.437485\C,0,0.222676,11.127563,2.
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F,0,1.325106,9.247083,3.117608\C,0,0.985448,9.398772,0.775025\C,0,-0.2
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263779,-1.803566\C,0,-0.077738,14.265589,1.518222\C,0,-2.261996,13.399
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,14.47819,-3.179674\F,0,0.231354,16.579149,1.850831\C,0,-1.932465,15.7
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-1.502308\C,0,2.310592,8.961473,-3.466131\F,0,-1.505288,8.825951,-2.01
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34,-5.29309\C,0,-0.125621,16.496565,-5.544536\H,0,-2.063328,16.076702,
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,0,1.556014,7.932715,-5.43791\H,0,2.508738,14.421667,-5.453665\C,0,1.1
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36936,-2.514456\H,0,-6.193035,15.764606,-4.298129\H,0,1.890052,16.6592
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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym

m gfprint\\CrystalExplorer Job symop = -, r = 12.1629\\0,1\H,0,10.8847
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1688,6.906798\C,0,2.551994,12.85913,5.544536\H,0,2.830131,11.877061,5.
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,0,7.757692,13.74391,3.660285\H,0,6.933468,15.292744,4.894278\C,0,2.73
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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
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8,2.617899\H,0,8.897421,5.921558,1.15283\C,0,9.737761,8.596856,3.03485
3\H,0,11.383292,9.912892,2.636997\P,0,7.591025,6.957948,3.610155\H,0,9
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5.131298\H,0,-1.698437,12.143106,14.76145\H,0,-1.019017,13.858384,11.8
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\H,0,1.560941,11.699841,14.473879\F,0,-5.203293,14.928134,10.638697\C,
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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 12.4681\\0,1\H,0,10.8847
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383292,9.912892,2.636997\P,0,7.591025,6.957948,3.610155\H,0,9.439317,9
.126626,3.930986\Au,0,8.101145,6.704273,5.825263\C,0,6.333521,8.250678
,3.311762\C,0,7.006571,5.433898,2.800913\C,0,8.631003,6.564312,7.80913
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,-7.131189\H,0,10.224444,-1.085734,-6.534245\F,0,16.201124,-5.655281,-
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15,-5.697423,-5.119943\C,0,9.212902,-4.327659,-6.74129\H,0,9.352624,-2
.737405,-8.163867\F,0,14.198128,-6.745131,-5.43791\H,0,6.731141,2.4582
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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 9.78419\\0,1\H,0,10.8847
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4\C,0,10.222569,2.296952,5.503159\F,0,8.032982,1.517327,5.743464\F,0,8
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,10.282757,8.584163\F,0,10.472147,1.371818,4.576947\F,0,5.442959,12.07
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5,-3.117608\F,0,12.041412,4.661423,1.502308\C,0,12.757894,5.716374,3.4
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423325\PG=C01 [X(C72H30Au2F26P2)]\\@

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 8.58411\\0,1\H,0,10.8847
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.126626,3.930986\Au,0,8.101145,6.704273,5.825263\C,0,6.333521,8.250678
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4925,9.72275,4.882342\C,0,4.407771,10.177323,2.929819\H,0,5.263093,10.
470012,0.999417\H,0,7.592972,2.106212,2.966104\C,0,6.28729,3.062778,1.
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4\C,0,10.222569,2.296952,5.503159\F,0,8.032982,1.517327,5.743464\F,0,8
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,10.282757,8.584163\F,0,10.472147,1.371818,4.576947\F,0,5.442959,12.07
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455999\H,0,5.217138,-2.023348,0.760703\C,0,6.399437,-1.691513,2.514457
\H,0,7.406222,-1.08676,4.298129\C,0,1.425201,3.420273,0.187789\C,0,4.0
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\C,0,1.784695,-0.855341,-1.653494\F,0,-0.045953,0.58478,-1.542094\F,0,
-0.11192,5.430765,-3.117608\F,0,2.718475,5.851897,2.013156\C,0,1.20518
1,6.288127,3.731899\C,0,-1.097406,5.716374,3.46613\F,0,-1.813887,4.661
423,1.502308\F,0,5.321927,-0.183328,-1.371811\C,0,3.145651,-1.058009,-
1.605751\F,0,0.981832,-1.901302,-1.850831\F,0,2.179548,6.835141,4.4607
73\C,0,-0.08431,6.239904,4.215693\F,0,-2.345824,5.655281,3.951516\F,0,
3.656967,-2.290833,-1.71556\F,0,-0.342828,6.745131,5.43791\\Version=ES
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41.7258723,-41.2325775\PG=C01 [X(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE008\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 11.4892\\0,1\H,
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464\F,0,8.02518,11.701373,6.125407\C,0,6.153077,10.995564,7.353989\F,0
,4.279581,10.282757,8.584163\F,0,10.472147,1.371818,4.576947\F,0,5.442
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\H,0,14.368575,-4.620015,10.641243\C,0,15.398018,-6.118572,11.803622\C
,0,14.534817,-6.53412,13.982287\H,0,12.85275,-5.346368,14.572071\H,0,1
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1485,-0.858667,14.752538\H,0,14.203054,-2.978005,14.473879\F,0,11.8159
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6.89594,7.330118\H,0,8.457806,-6.526075,13.277285\C,0,8.603306,-4.9664
31,14.741398\H,0,8.956308,-3.291007,16.000536\H,0,16.126173,-6.335932,
11.031939\C,0,15.433328,-6.790506,12.984462\H,0,14.578004,-7.083195,14
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175\H,0,14.837373,-0.860593,15.559392\F,0,14.398139,-8.684871,9.007483
\H,0,7.755371,-5.316884,15.316858\H,0,16.191654,-7.548068,13.139467\H,
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C01 [X(C72H30Au2F26P2)]\\@

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 10.5873\\0,1\H,0,10.8847
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383292,9.912892,2.636997\P,0,7.591025,6.957948,3.610155\H,0,9.439317,9
.126626,3.930986\Au,0,8.101145,6.704273,5.825263\C,0,6.333521,8.250678
,3.311762\C,0,7.006571,5.433898,2.800913\C,0,8.631003,6.564312,7.80913
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.194579\C,0,12.968265,13.154593,1.32566\P,0,11.949307,13.351744,-3.601
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,0,11.593305,13.399827,1.298605\C,0,13.777562,14.265589,1.518222\C,0,1
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.212935\C,0,10.697649,15.199862,-2.016339\C,0,9.469647,14.660441,-3.99
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,13.592113,-6.534245\H,0,11.540266,15.026681,-1.358284\C,0,9.749815,16
.138784,-1.680548\C,0,8.523981,15.611784,-3.660285\H,0,9.348205,14.062
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-5.453665\C,0,15.009616,16.032635,-5.724367\H,0,13.451543,17.478634,-5
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129\H,0,10.56581,11.940442,-8.163867\H,0,9.851349,16.701195,-0.760703\
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(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE041\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 11.8967\\0,1\H,
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237792,8.353248,1.172883\C,0,9.437692,6.798405,1.487985\C,0,10.836815,
9.036078,2.312345\H,0,12.085727,8.703701,0.597422\C,0,9.012096,7.47626
8,2.617899\H,0,8.897421,5.921558,1.15283\C,0,9.737761,8.596856,3.03485
3\H,0,11.383292,9.912892,2.636997\P,0,7.591025,6.957948,3.610155\H,0,9

.439317,9.126626,3.930986\Au,0,8.101145,6.704273,5.825263\C,0,6.333521
,8.250678,3.311762\C,0,7.006571,5.433898,2.800913\C,0,8.631003,6.56431
2,7.809138\C,0,5.421968,8.534614,4.328685\C,0,6.274137,8.946888,2.1277
39\C,0,7.530641,4.221949,3.251288\C,0,6.08117,5.433132,1.769668\C,0,9.
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464\F,0,8.02518,11.701373,6.125407\C,0,6.153077,10.995564,7.353989\F,0
,4.279581,10.282757,8.584163\F,0,10.472147,1.371818,4.576947\F,0,5.442
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764955,-2.636997\C,0,3.830694,6.324599,-1.172883\C,0,5.330725,6.080991
,-3.034853\H,0,2.982759,5.974146,-0.597422\C,0,4.514801,7.4453,-0.7829
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9,-3.311762\C,0,8.061915,9.243949,-2.800913\Au,0,6.967342,7.973574,-5.
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.437483,8.113535,-7.809138\C,0,9.762206,4.75691,-1.931994\H,0,8.080138
,5.944662,-1.34221\C,0,10.625406,5.172458,-4.110659\H,0,9.595964,6.671
015,-5.273038\C,0,9.342239,10.432364,-1.161743\H,0,9.430443,8.313025,-
1.440402\C,0,7.894771,11.632257,-2.627447\H,0,6.850485,10.471567,-4.08
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.322618,-11.751105\F,0,3.164739,9.630193,-7.131189\C,0,3.880291,11.490
748,-5.858047\F,0,7.532657,11.263283,-7.575198\C,0,6.071153,12.295665,
-6.096761\F,0,5.650323,5.085702,-7.015015\C,0,7.615886,3.857842,-6.949
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9754053\PG=C01 [X(C72H30Au2F26P2)]\\@

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 11.8152\\0,1\H,0,10.8847
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353248,1.172883\C,0,9.437692,6.798405,1.487985\C,0,10.836815,9.036078,
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1688,6.906798\F,0,10.305778,5.695556,14.782776\C,0,9.46098,4.664836,14
.615675\C,0,8.08602,4.91007,14.588621\C,0,9.979791,3.397464,14.488361\
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\C,0,9.864464,5.476682,22.127216\C,0,10.356636,2.864802,17.93062\C,0,1
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67945\C,0,6.044668,2.032028,21.638647\H,0,7.602742,0.586031,21.821026\
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6P2)]\\@

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 10.953\\0,1\H,0,10.88478
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53248,1.172883\C,0,9.437692,6.798405,1.487985\C,0,10.836815,9.036078,2
.312345\H,0,12.085727,8.703701,0.597422\C,0,9.012096,7.476268,2.617899
\H,0,8.897421,5.921558,1.15283\C,0,9.737761,8.596856,3.034853\H,0,11.3
83292,9.912892,2.636997\P,0,7.591025,6.957948,3.610155\H,0,9.439317,9.
126626,3.930986\Au,0,8.101145,6.704273,5.825263\C,0,6.333521,8.250678,
3.311762\C,0,7.006571,5.433898,2.800913\C,0,8.631003,6.564312,7.809138
\C,0,5.421968,8.534614,4.328685\C,0,6.274137,8.946888,2.127739\C,0,7.5
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77105\H,0,5.003726,4.24741,0.354888\F,0,10.483975,4.345758,10.061008\C
,0,9.496596,6.419389,10.473188\C,0,10.942071,4.176702,6.790624\C,0,8.7
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\C,0,10.222569,2.296952,5.503159\F,0,8.032982,1.517327,5.743464\F,0,8.
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110715\C,0,2.261572,0.918457,11.054059\C,0,1.49845,3.187161,12.734608\
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,3.369412,11.915023\C,0,4.462644,0.52111,17.021915\C,0,5.25702,-1.2512
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\H,0,2.457577,3.735651,14.555998\C,0,0.667126,4.847754,14.233733\C,0,-
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,13.686282\C,0,4.524368,-2.37655,13.441202\H,0,1.001706,-1.666543,8.44
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\F,0,6.031751,2.802037,17.456375\C,0,4.201103,4.242157,17.567774\F,0,1
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.765112\C,0,2.840146,4.444826,17.520031\F,0,0.663871,3.570145,17.28609
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[X(C72H30Au2F26P2)]\\@

1\1\GINC-COMPUTE041\SP\RB3LYP\Gen\C72H30Au2F26P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -, r = 13.9481\\0,1\H,0,10.8847
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353248,1.172883\C,0,9.437692,6.798405,1.487985\C,0,10.836815,9.036078,
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72H30Au2F26P2)]\\@

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m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 7.74108\\0,1\H,
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2)]\\@

Compound 2c

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x+1/2, y+1/2, -z+1/2, r = 10.6
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34Au2F30P2)]\\@

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x+1/2, -y+1/2, -z, r = 8.63074
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4\C,0,1.541808,19.953541,-2.568658\H,0,2.561009,21.600897,-3.359776\H,
0,9.101624,18.43103,0.237583\H,0,7.213101,19.285921,-8.58979\H,0,0.687
844,20.548302,-2.268804\\Version=ES64L-G09RevE.01\HF=-3585.1434029\RMS
D=6.089e-09\Dipole=0.0000005,0.0000034,0.000002\Quadrupole=-6.4018065,
38.4825654,-32.0807589,-8.2054333,-17.2964529,-46.30693\PG=C01 [X(C84H
34Au2F30P2)]\\@

1\1\GINC-COMPUTE041\SP\RB3LYP\Gen\C84H34Au2F30P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 14.7861\\0,1\F,
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76914,12.892916,-0.401574\C,0,7.735065,14.296986,0.65101\F,0,9.71301,1
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820838\C,0,9.532567,13.509828,1.866346\C,0,7.919339,14.970646,3.069299
\F,0,10.242269,13.381686,2.977308\C,0,7.159447,14.254882,3.99451\C,0,8
.258155,16.303324,3.253279\Au,0,6.753403,12.270512,3.797262\C,0,6.7233
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5153,4.396085\P,0,6.272816,10.051458,3.686342\C,0,7.066087,16.29417,5.
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\C,0,5.033016,9.652754,2.421827\C,0,5.604558,9.409284,5.238152\C,0,7.6
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3.780456\C,0,8.647276,18.763649,5.912158\C,0,3.994187,10.527781,2.2696
89\C,0,5.077668,8.548902,1.615141\C,0,6.064059,9.931005,6.426952\C,0,4
.625498,8.459202,5.292992\C,0,8.769074,9.592343,2.706644\C,0,7.747105,
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,7.166414\F,0,7.765901,14.750975,7.700666\C,0,5.966749,13.553762,8.519

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0,8.928812,17.864824,6.862138\C,0,8.905136,20.096327,6.255354\H,0,3.93
8395,11.409946,2.895578\C,0,3.018513,10.295294,1.325017\C,0,4.088934,8
.307262,0.675776\H,0,5.901785,7.852908,1.712615\H,0,6.816466,10.709742
,6.409792\C,0,5.582373,9.473354,7.644057\C,0,4.144681,7.99606,6.492407
\H,0,4.222387,8.061779,4.369726\H,0,8.773628,10.660499,2.528324\C,0,9.
872934,8.81983,2.335144\C,0,8.84661,6.92516,3.175441\H,0,6.932061,7.18
6752,4.099238\F,0,2.993164,12.484691,6.996585\C,0,4.785675,13.002751,8
.369367\F,0,6.583515,13.493352,9.717381\F,0,8.044508,21.677965,3.18251
8\C,0,8.655381,21.05007,5.328373\F,0,9.333188,20.389221,7.479536\H,0,2
.196081,10.991838,1.218343\C,0,3.08036,9.191442,0.521869\H,0,4.122635,
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0,9.885691,7.50546,2.568658\H,0,8.866489,5.858103,3.359776\F,0,4.17630
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8804\F,0,11.769047,6.262483,-0.820839\C,0,12.894934,5.502783,-0.765997
\C,0,13.578085,5.413085,0.401574\C,0,13.322432,4.796172,-1.866345\F,0,
13.141989,6.086745,1.500153\C,0,14.716163,4.679014,0.468798\F,0,12.612
73,4.924314,-2.977308\C,0,14.453104,4.047457,-1.834503\F,0,15.391476,4
.605789,1.609834\C,0,15.119934,4.009014,-0.65101\C,0,14.93566,3.335353
,-3.069299\F,0,16.254421,3.282266,-0.55725\C,0,15.695553,4.051118,-3.9
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,-0.108006,-4.680901\C,0,15.158529,9.297618,-3.28866\C,0,17.821983,8.6
53246,-2.421827\C,0,17.250443,8.896716,-5.238152\H,0,16.137592,1.49267
2,-6.193084\C,0,18.065628,4.561855,-6.097908\C,0,16.281387,4.111528,-7
.490149\C,0,14.873229,-1.096529,-3.780456\C,0,14.207723,-0.457649,-5.9
12159\C,0,14.085925,8.713656,-2.706644\C,0,15.107893,10.641278,-3.5699
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0,16.790939,8.374995,-6.426952\C,0,18.229502,9.846797,-5.292992\F,0,18
.734198,4.477648,-4.912647\C,0,18.6936,5.237347,-7.166414\F,0,15.08909
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175,-6.862138\C,0,13.949862,-1.790327,-6.255354\C,0,12.982064,9.486169
,-2.335144\H,0,14.08137,7.645501,-2.528324\C,0,14.008389,11.38084,-3.1
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,0,16.953213,10.453093,-1.712615\H,0,16.038532,7.596258,-6.409792\C,0,
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632612,10.244221,-4.369726\F,0,19.861835,5.821308,-6.996585\C,0,18.069
323,5.303249,-8.369367\F,0,16.271482,4.812648,-9.717381\F,0,14.810491,
-3.371965,-3.182517\C,0,14.199617,-2.744069,-5.328372\F,0,13.521811,-2
.083222,-7.479536\C,0,12.969307,10.80054,-2.568658\H,0,12.133506,9.017
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,-1.218344\C,0,19.774639,9.114557,-0.521869\H,0,18.732363,10.895731,-0
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H,0,19.46242,11.088861,-6.51452\F,0,18.678692,5.942128,-9.3848\F,0,13.
966358,-4.030981,-5.632649\H,0,12.115344,11.395302,-2.268804\H,0,20.52
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1\1\GINC-COMPUTE008\SP\RB3LYP\Gen\C84H34Au2F30P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = x, -y, z+1/2, r = 12.6673\\0,1\
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99\F,0,10.242269,13.381686,2.977308\C,0,7.159447,14.254882,3.99451\C,0
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186752,4.099238\F,0,2.993164,12.484691,6.996585\C,0,4.785675,13.002751
,8.369367\F,0,6.583515,13.493352,9.717381\F,0,8.044508,21.677965,3.182
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\C,0,7.505644,5.303248,-0.475874\C,0,7.50934,4.561855,-2.747332\F,0,6.
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.492671,-2.652157\P,0,8.992785,8.254541,-5.158898\C,0,10.978125,2.0026
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-4.16434\C,0,8.324526,8.896716,-3.607089\C,0,10.416439,9.297618,-5.556
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7991\C,0,10.858806,4.679014,-9.314038\F,0,12.962238,4.924314,-5.867933
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,0,10.183492,4.60579,-10.455074\C,0,11.996882,5.413085,-9.246815\F,0,1
3.805921,6.262483,-8.024402\F,0,10.764479,-3.371965,-5.662723\C,0,11.3
75352,-2.74407,-3.516868\F,0,12.053158,-2.083222,-1.365705\H,0,8.69002
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8886,-2.330721\C,0,12.605659,10.80054,-6.276582\H,0,11.586458,12.44789
7,-5.485464\H,0,13.441463,9.017536,-6.993047\H,0,4.91605,7.314162,-7.6
26897\C,0,5.800329,9.114558,-8.323371\H,0,6.842604,10.895732,-8.77554\
F,0,12.432979,6.086746,-10.345393\F,0,11.608611,-4.030981,-3.212591\H,
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[X(C84H34Au2F30P2)]\\@

1\1\GINC-COMPUTE021\SP\RB3LYP\Gen\C84H34Au2F30P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, y, -z+1/2, r = 6.07284\\0,1
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023734,0.55725\C,0,8.401895,14.258544,1.834503\F,0,11.085952,12.043517
,0.820838\C,0,9.532567,13.509828,1.866346\C,0,7.919339,14.970646,3.069
299\F,0,10.242269,13.381686,2.977308\C,0,7.159447,14.254882,3.99451\C,
0,8.258155,16.303324,3.253279\Au,0,6.753403,12.270512,3.797262\C,0,6.7
23353,14.965155,5.130239\H,0,8.85154,16.818821,2.508333\C,0,7.83817,16
.975153,4.396085\P,0,6.272816,10.051458,3.686342\C,0,7.066087,16.29417
,5.308913\C,0,6.004399,14.296986,6.227049\C,0,8.184832,18.414005,4.680
902\C,0,5.033016,9.652754,2.421827\C,0,5.604558,9.409284,5.238152\C,0,
7.69647,9.008382,3.288661\H,0,6.717406,16.813328,6.193084\C,0,4.789371
,13.744144,6.097909\C,0,6.573611,14.194471,7.49015\C,0,7.98177,19.4025
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69689\C,0,5.077668,8.548902,1.615141\C,0,6.064059,9.931005,6.426952\C,
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C84H34Au2F30P2)]\\@

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym

m gfprint\\CrystalExplorer Job symop = x, -y, z+1/2, r = 13.3743\\0,1\
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u2F30P2)]\\@

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m gfprint\\CrystalExplorer Job symop = -x+1/2, -y+1/2, -z, r = 12.4998
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30P2)]\\@

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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = x, y, z, r = 18.306\\0,1\F,0,7.
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p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 13.9451\\0,1\F,
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689\C,0,11.832687,27.138643,10.046424\C,0,13.270379,28.615938,11.19807
5\H,0,13.192674,28.55022,13.320756\H,0,8.641432,25.9515,15.162157\C,0,
7.542126,27.792168,15.355337\C,0,8.568451,29.686838,14.51504\H,0,10.48
3,29.425247,13.591244\H,0,15.21898,25.620161,16.472137\C,0,14.334701,2
7.420557,17.168612\H,0,13.292425,29.201731,17.620781\H,0,11.445008,26.
742502,9.116081\C,0,12.799998,28.090555,10.044655\H,0,14.022481,29.394
859,11.175961\H,0,6.693567,27.323534,15.838287\C,0,7.529369,29.106539,
15.121823\H,0,8.548571,30.753895,14.330705\H,0,15.089186,27.584028,17.
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1\1\GINC-COMPUTE021\SP\RB3LYP\Gen\C84H34Au2F30P2\CRAT\17-Sep-2020\0\\#
p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj nosym
m gfprint\\CrystalExplorer Job symop = -x, y, -z+1/2, r = 19.287\\0,1\
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.276914,12.892916,-0.401574\C,0,7.735065,14.296986,0.65101\F,0,9.71301
,12.219255,-1.500153\C,0,9.960066,12.803216,0.765998\F,0,6.600577,15.0
23734,0.55725\C,0,8.401895,14.258544,1.834503\F,0,11.085952,12.043517,
0.820838\C,0,9.532567,13.509828,1.866346\C,0,7.919339,14.970646,3.0692
99\F,0,10.242269,13.381686,2.977308\C,0,7.159447,14.254882,3.99451\C,0
,8.258155,16.303324,3.253279\Au,0,6.753403,12.270512,3.797262\C,0,6.72
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9,3.780456\C,0,8.647276,18.763649,5.912158\C,0,3.994187,10.527781,2.26
9689\C,0,5.077668,8.548902,1.615141\C,0,6.064059,9.931005,6.426952\C,0
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19735\F,0,7.546317,19.135262,2.558044\C,0,8.198596,20.733376,4.093577\
F,0,8.928812,17.864824,6.862138\C,0,8.905136,20.096327,6.255354\H,0,3.
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07\H,0,4.222387,8.061779,4.369726\H,0,8.773628,10.660499,2.528324\C,0,
9.872934,8.81983,2.335144\C,0,8.84661,6.92516,3.175441\H,0,6.932061,7.
186752,4.099238\F,0,2.993164,12.484691,6.996585\C,0,4.785675,13.002751
,8.369367\F,0,6.583515,13.493352,9.717381\F,0,8.044508,21.677965,3.182
518\C,0,8.655381,21.05007,5.328373\F,0,9.333188,20.389221,7.479536\H,0
,2.196081,10.991838,1.218343\C,0,3.08036,9.191442,0.521869\H,0,4.12263
5,7.410269,0.069701\H,0,5.970052,9.869496,8.5744\C,0,4.615062,8.521442
,7.645826\H,0,3.39258,7.21714,6.51452\H,0,10.721494,9.288464,1.852193\
C,0,9.885691,7.50546,2.568658\H,0,8.866489,5.858103,3.359776\F,0,4.176
307,12.363872,9.3848\F,0,8.888641,22.336981,5.632649\H,0,2.325875,9.02
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268804\F,0,11.246388,4.030981,3.212591\C,0,11.479649,2.744069,3.516868
\C,0,11.936434,2.427375,4.751663\C,0,11.229894,1.790327,2.589886\F,0,1
2.090521,3.371965,5.662723\C,0,12.15326,1.096529,5.064785\F,0,10.80184
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261,6.287197\C,0,11.950197,0.108005,4.16434\F,0,11.206218,-0.441175,1.
983103\C,0,12.29686,-1.330847,4.449156\C,0,11.876875,-2.002676,5.59196
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,11.28349,-1.48718,6.336907\H,0,13.417624,-1.492671,2.652157\C,0,13.41
1676,-3.340845,3.715001\C,0,12.975584,-4.051118,4.85073\C,0,11.733136,
-4.047456,7.010737\C,0,14.130632,-4.009014,2.618191\Au,0,13.381627,-6.
035488,5.047979\C,0,12.399965,-4.009014,8.194231\C,0,10.602464,-4.7961
73,6.978895\C,0,15.34566,-4.561855,2.747332\C,0,13.561419,-4.111528,1.
355091\P,0,13.862214,-8.254541,5.158898\F,0,13.534452,-3.282266,8.2879
91\C,0,11.996194,-4.679014,9.314038\F,0,9.892761,-4.924314,5.867933\C,
0,10.174965,-5.502784,8.079243\F,0,16.014231,-4.477648,3.932594\C,0,15
.973632,-5.237346,1.678827\F,0,12.369128,-3.555025,1.144574\C,0,14.168
282,-4.752237,0.325505\C,0,15.102015,-8.653247,6.423414\C,0,14.530474,
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723,-5.942127,-0.53956\H,0,16.196636,-6.896053,5.949663\C,0,17.116518,
-8.010706,7.520224\C,0,16.046097,-9.998737,8.169464\H,0,14.233245,-10.
453093,7.132625\H,0,13.318564,-7.596258,2.435448\C,0,14.552657,-8.8326

45,1.201184\C,0,15.99035,-10.309939,2.352834\H,0,15.912643,-10.244221,
4.475515\H,0,11.361402,-7.645501,6.316917\C,0,10.262096,-9.48617,6.510
097\C,0,11.288422,-11.38084,5.669799\H,0,13.202971,-11.119247,4.746002
\H,0,17.93895,-7.314163,7.626897\C,0,17.05467,-9.114558,8.323371\H,0,1
6.012396,-10.895732,8.77554\H,0,14.164979,-8.436503,0.270841\C,0,15.51
9969,-9.784557,1.199415\H,0,16.742451,-11.08886,2.330721\H,0,9.413537,
-9.017536,6.993047\C,0,10.249339,-10.80054,6.276582\H,0,11.268541,-12.
447897,5.485464\H,0,17.809156,-9.27803,9.082824\H,0,15.920633,-10.1329
2,0.255451\H,0,9.395376,-11.395302,6.576437\\Version=ES64L-G09RevE.01\
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uadrupole=51.3967442,-51.1918634,-0.2048808,-155.3440261,4.1712874,-64
.0768584\PG=C01 [X(C84H34Au2F30P2)]\\@

Compound 3a

1\1\GINC-COMPUTE035\SP\RB3LYP\Gen\C74H40Au2Cl4F20P2\CRAT\18-Sep-2020\0
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symm gfprint\\CrystalExplorer Job symop = y, -x+y, -z, r = 10.4624\\0,
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l,0,3.732833,8.167566,12.804891\P,0,8.341955,8.522474,13.075194\C,0,6.
057256,6.61786,11.750736\C,0,9.44938,7.440873,12.075381\C,0,8.831812,8
.173018,14.78546\C,0,8.870785,10.177328,12.649391\C,0,6.408011,6.63343
7,10.36982\C,0,5.697508,5.387233,12.305926\C,0,9.233531,6.070049,12.06
1267\C,0,10.536118,8.004261,11.421387\C,0,8.02088,8.450817,15.844086\C
,0,10.102921,7.700499,15.004243\C,0,8.415104,10.795238,11.503724\C,0,9
.771653,10.880914,13.446889\C,0,6.397518,5.436563,9.628781\C,0,6.78874
3,7.890026,9.598199\C,0,5.737979,4.216321,11.522544\C,0,5.22384,5.2729
98,13.722131\H,0,8.37883,5.624531,12.555291\C,0,10.176371,5.283383,11.
374336\C,0,11.442983,7.181248,10.788565\H,0,10.670874,9.078852,11.4068
01\H,0,7.027976,8.845448,15.666708\C,0,8.451078,8.230135,17.1756\C,0,1
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\C,0,5.9943,5.433966,14.818396\C,0,3.943736,4.893945,13.980906\H,0,10.
064399,4.206715,11.336931\C,0,11.225636,5.880523,10.757981\H,0,12.3258
66,7.599764,10.321122\H,0,7.785995,8.445884,18.002504\C,0,9.67722,7.75
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.652027\C,0,6.004794,2.985696,9.367654\F,0,8.855796,6.942392,8.948909\
C,0,8.371634,9.047957,8.174936\F,0,4.696209,8.902567,9.925197\C,0,6.27
91,10.029343,8.657199\F,0,7.317873,5.711766,14.667836\C,0,5.520632,5.2
93768,16.121681\F,0,3.074346,4.675859,12.952864\C,0,3.414607,4.725188,
15.246552\H,0,11.925345,5.257421,10.214789\H,0,10.011636,7.588081,18.4
29247\H,0,10.14669,13.675527,11.56583\H,0,4.978013,2.7053,9.168398\H,0
,6.494051,2.19176,9.918139\H,0,6.525379,3.147962,8.43183\F,0,9.548311,
9.092093,7.560934\C,0,7.512737,10.089056,8.029082\F,0,5.378232,11.0340
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210149,-0.968405,9.544091\C,0,5.799437,-0.594543,8.278447\C,0,7.178472
,-1.887481,9.802867\F,0,4.823621,0.29078,8.099657\C,0,6.415506,-1.1838

94,7.203354\C,0,7.514236,-2.240571,11.219071\C,0,7.703104,-2.474235,8.
706601\F,0,6.019783,-0.82561,5.96594\C,0,7.344854,-2.134124,7.403317\C
,0,8.759864,-1.936809,11.774261\C,0,6.520432,-2.861076,12.002455\F,0,8
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-3.097337,13.338673\H,0,5.590934,-3.160426,11.534307\Cl,0,8.939737,0.8
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9616\C,0,11.493948,-3.562066,8.739536\C,0,13.249219,-2.593662,10.87560
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,0,10.727984,-0.667239,14.138524\H,0,4.831715,-2.958177,14.356601\H,0,
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64,-2.720878,7.680912\C,0,11.720291,-4.899139,8.520754\C,0,13.556503,-
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19815,14.576089\C,0,12.021579,-2.726072,15.35006\F,0,10.057954,0.38424
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4.839604,-1.682377,12.421199\C,0,15.614562,-2.79617,10.485091\H,0,14.1
14263,-3.527535,9.140403\F,0,12.64814,-3.723035,15.964064\C,0,12.49374
8,-1.461694,15.495915\F,0,12.244923,0.85936,15.004243\H,0,8.675173,-6.
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4372,13.203876\H,0,11.20735,-2.519929,5.522493\C,0,11.556904,-4.501911
,6.111794\H,0,11.915154,-6.435604,7.015154\H,0,15.035968,-1.167279,13.
353495\C,0,15.893367,-2.126336,11.651931\H,0,16.43119,-3.158607,9.8729
71\F,0,13.578987,-1.186491,16.208723\H,0,10.515734,-7.698944,13.310208
\H,0,11.577291,-4.876292,5.09575\H,0,16.9167,-1.94953,11.959168\\Versi
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1\1\GINC-COMPUTE035\SP\RB3LYP\Gen\C74H40Au2Cl4F20P2\CRAT\17-Sep-2020\0
\\#p b3lyp/gen pseudo=read scf=maxcycle=2024 counterpoise=2 empiricald
ispersion=gd3bj nosymm gfprint\\CrystalExplorer Job symop = -x, -y, -z
, r = 10.7472\\0,1\Au,0,6.040917,8.340476,12.833357\Cl,0,5.871086,10.3
93337,13.990787\Cl,0,3.732833,8.167566,12.804891\P,0,8.341955,8.522474
,13.075194\C,0,6.057256,6.61786,11.750736\C,0,9.44938,7.440873,12.0753
81\C,0,8.831812,8.173018,14.78546\C,0,8.870785,10.177328,12.649391\C,0
,6.408011,6.633437,10.36982\C,0,5.697508,5.387233,12.305926\C,0,9.2335
31,6.070049,12.061267\C,0,10.536118,8.004261,11.421387\C,0,8.02088,8.4
50817,15.844086\C,0,10.102921,7.700499,15.004243\C,0,8.415104,10.79523
8,11.503724\C,0,9.771653,10.880914,13.446889\C,0,6.397518,5.436563,9.6
28781\C,0,6.788743,7.890026,9.598199\C,0,5.737979,4.216321,11.522544\C
,0,5.22384,5.272998,13.722131\H,0,8.37883,5.624531,12.555291\C,0,10.17
6371,5.283383,11.374336\C,0,11.442983,7.181248,10.788565\H,0,10.670874
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X(C74H40Au2Cl4F20P2)]\\@

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+1/3, -z+1/3, r = 9.39732\\0,1\Au,0,6.040917,8.340476,12.833357\Cl,0,5
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\H,0,20.074236,14.176604,10.902895\C,0,20.95232,12.269913,11.103799\C,
0,20.375227,11.041883,13.039907\H,0,18.991695,11.975496,14.384594\C,0,
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,0,14.572791,19.269424,9.367654\F,0,16.573889,14.822035,8.948909\C,0,1
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1,18.534683,16.121681\F,0,17.50174,20.962183,12.952864\C,0,17.374329,2
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7.560934\C,0,19.97051,14.411826,8.029082\F,0,21.856188,15.787842,8.520
754\F,0,16.566395,17.71686,17.170897\C,0,17.171968,19.814636,16.321642
\F,0,17.653131,21.930586,15.425342\F,0,20.751461,13.609582,7.316274\F,
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gd3bj nosymm gfprint\\CrystalExplorer Job symop = x-y, x, -z, r = 10.4
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90787\Cl,0,3.732833,8.167566,12.804891\P,0,8.341955,8.522474,13.075194
\C,0,6.057256,6.61786,11.750736\C,0,9.44938,7.440873,12.075381\C,0,8.8
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,12.002455\C,0,-1.954632,7.160478,9.802867\H,0,-3.421354,10.965813,5.5
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Compound 3b

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symm gfprint\\CrystalExplorer Job symop = x, y, z, r = 10.384\\0,1\H,0
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63653\H,0,0.369066,5.742112,5.618678\C,0,1.954344,5.003757,8.500895\H,
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7769,7.590517\C,0,2.40037,7.22883,4.944126\Cl,0,3.273652,3.639745,5.13
4192\Cl,0,6.543721,3.741215,5.203681\C,0,6.323387,6.343048,6.716457\C,
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,5.939973\C,0,8.193188,7.818846,6.387172\C,0,7.012127,7.087772,4.36303
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,4.994972\F,0,-1.3907,8.512303,5.564926\C,0,-1.927091,7.846147,7.73336
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95231,-86.2509902,-80.0574979,87.4155613\PG=C01 [X(C72H30Au2Cl4F26P2)]
\\@

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symm gfprint\\CrystalExplorer Job symop = -x+1/2, y+1/2, -z+1/2, r = 9
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3702\C,0,-0.261154,4.110392,8.505737\C,0,0.531718,5.337443,6.609924\C,
0,0.94661,4.304536,9.135254\H,0,-1.051578,3.562845,9.004024\C,0,1.7479
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8281\H,0,2.915588,5.121306,8.985622\Au,0,4.852028,5.148152,5.961279\C,
0,3.287514,7.947769,7.590517\C,0,2.40037,7.22883,4.944126\Cl,0,3.27365
2,3.639745,5.134192\Cl,0,6.543721,3.741215,5.203681\C,0,6.323387,6.343
048,6.716457\C,0,4.33689,8.850236,7.355659\C,0,2.332058,8.243536,8.554
162\C,0,2.556391,6.596345,3.723832\C,0,1.68806,8.410378,4.994972\C,0,7
.147326,7.072605,5.852083\C,0,6.589951,6.344565,8.098973\H,0,5.087709,
8.634402,6.605566\C,0,4.398926,10.025717,8.098973\C,0,2.424787,9.42508
4,9.275684\H,0,1.516869,7.555083,8.739385\H,0,3.125113,5.67674,3.66257
6\C,0,1.994636,7.128725,2.590703\C,0,1.123485,8.936691,3.859421\H,0,1.
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.087772,4.363034\C,0,7.659499,7.105973,8.559004\C,0,5.832413,5.564955,
9.10862\H,0,5.209247,10.724635,7.932393\C,0,3.44746,10.304799,9.038404
\H,0,1.684252,9.652444,10.032557\H,0,2.115167,6.625315,1.639406\C,0,1.
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.512303,5.564926\C,0,8.456908,7.846147,7.733369\C,0,6.067505,7.864348,
3.704463\C,0,7.956422,6.452254,3.576138\F,0,7.949246,7.10749,9.870577\
C,0,5.114925,6.177722,10.113425\C,0,5.906926,4.171062,9.178836\H,0,3.5
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.527168,8.207443\F,0,5.183177,8.577221,4.408311\C,0,6.02985,7.965971,2
.343739\F,0,8.933347,5.742415,4.131566\C,0,7.936265,6.531125,2.20815\F
,0,5.070955,7.519742,10.158945\C,0,4.450375,5.480017,11.084334\F,0,6.6
79865,3.4999,8.31543\C,0,5.262105,3.46274,10.149744\F,0,5.118653,8.751
648,1.760225\C,0,6.970908,7.29405,1.600425\F,0,8.861542,5.910774,1.466

532\F,0,3.71672,6.112502,12.00028\C,0,4.512689,4.105842,11.101282\F,0,
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.743053\F,0,-1.40237,1.167897,10.345862\C,0,-3.254625,-0.2897,10.50566
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0,-3.240125,-0.17746,11.843386\C,0,-4.219983,-1.052625,9.897938\C,0,-2
.607104,-1.240701,5.38963\C,0,-4.476905,0.235096,5.718916\F,0,-5.21706
3,-1.841335,7.974522\F,0,-5.145258,-1.672976,10.639556\Au,0,-1.135744,
-2.435597,6.144808\C,0,-2.873667,-1.239185,4.007115\F,0,-5.277017,0.92
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.623278\Cl,0,0.442632,-3.944005,6.971896\Cl,0,-2.827438,-3.842535,6.90
2407\C,0,-3.943215,-0.477776,3.547084\C,0,-2.11613,-2.018794,2.997467\
F,0,-5.784579,0.943418,3.898644\C,0,1.315913,-0.35492,7.161962\C,0,0.4
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0.47626,2.23551\C,0,-1.398642,-1.406027,1.992662\C,0,-2.190642,-3.4126
88,2.927252\C,0,2.028223,0.826628,7.111116\C,0,1.159892,-0.987405,8.38
2255\C,0,-0.620607,1.266486,4.750429\C,0,1.384225,0.659786,3.551926\C,
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4672,-0.064007,1.947143\C,0,-0.734091,-2.103732,1.021754\F,0,-2.963582
,-4.083849,3.790658\C,0,-1.545821,-4.12101,1.956344\C,0,2.592798,1.352
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15385\H,0,0.59117,-1.90701,8.443512\H,0,-1.371427,1.050652,5.500522\C,
0,-0.682643,2.441967,4.007115\C,0,1.291496,1.841334,2.830403\H,0,2.199
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.279213,2.970834\C,0,4.179992,-2.971314,4.869069\H,0,3.347217,-1.84163
9,6.487411\F,0,-0.000437,-1.471248,0.105807\C,0,-0.796406,-3.477908,1.
004805\F,0,-1.66111,-5.467732,1.913972\C,0,2.434536,0.712872,9.442748\
H,0,3.162429,2.272394,8.192432\H,0,1.601116,-0.958435,10.466681\H,0,-1
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2.068695,2.073531\H,0,2.609023,-3.67554,1.975956\C,0,3.977437,-3.47335
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C72H30Au2Cl4F26P2)]\\@

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symm gfprint\\CrystalExplorer Job symop = -, r = 9.10485\\0,1\H,0,-1.4
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.110392,8.505737\C,0,0.531718,5.337443,6.609924\C,0,0.94661,4.304536,9
.135254\H,0,-1.051578,3.562845,9.004024\C,0,1.747952,5.546754,7.263653
\H,0,0.369066,5.742112,5.618678\C,0,1.954344,5.003757,8.500895\H,0,1.1
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121306,8.985622\Au,0,4.852028,5.148152,5.961279\C,0,3.287514,7.947769,
7.590517\C,0,2.40037,7.22883,4.944126\Cl,0,3.273652,3.639745,5.134192\
Cl,0,6.543721,3.741215,5.203681\C,0,6.323387,6.343048,6.716457\C,0,4.3
3689,8.850236,7.355659\C,0,2.332058,8.243536,8.554162\C,0,2.556391,6.5
96345,3.723832\C,0,1.68806,8.410378,4.994972\C,0,7.147326,7.072605,5.8
52083\C,0,6.589951,6.344565,8.098973\H,0,5.087709,8.634402,6.605566\C,
0,4.398926,10.025717,8.098973\C,0,2.424787,9.425084,9.275684\H,0,1.516

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725,2.590703\C,0,1.123485,8.936691,3.859421\H,0,1.573592,8.926831,5.93
9973\C,0,8.193188,7.818846,6.387172\C,0,7.012127,7.087772,4.363034\C,0
,7.659499,7.105973,8.559004\C,0,5.832413,5.564955,9.10862\H,0,5.209247
,10.724635,7.932393\C,0,3.44746,10.304799,9.038404\H,0,1.684252,9.6524
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3339\H,0,0.553853,9.856145,3.913656\F,0,8.993299,8.512303,5.564926\C,0
,8.456908,7.846147,7.733369\C,0,6.067505,7.864348,3.704463\C,0,7.95642
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,10.158945\C,0,4.450375,5.480017,11.084334\F,0,6.679865,3.4999,8.31543
\C,0,5.262105,3.46274,10.149744\F,0,5.118653,8.751648,1.760225\C,0,6.9
70908,7.29405,1.600425\F,0,8.861542,5.910774,1.466532\F,0,3.71672,6.11
2502,12.00028\C,0,4.512689,4.105842,11.101282\F,0,5.377394,2.116017,10
.192115\F,0,6.956409,7.40629,0.262702\F,0,3.869386,3.40662,12.034177\C
,0,-1.444203,10.731005,10.5783\H,0,-1.174394,10.489842,9.557514\Cl,0,-
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1\1\GINC-COMPUTE035\SP\RB3LYP\Gen\C72H30Au2Cl4F26P2\CRAT\18-Sep-2020\0
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symm gfprint\\CrystalExplorer Job symop = -x+1/2, y+1/2, -z+1/2, r = 8
.72648\\0,1\H,0,-1.405725,4.438617,6.731711\C,0,-0.463708,4.612436,7.2
3702\C,0,-0.261154,4.110392,8.505737\C,0,0.531718,5.337443,6.609924\C,
0,0.94661,4.304536,9.135254\H,0,-1.051578,3.562845,9.004024\C,0,1.7479
52,5.546754,7.263653\H,0,0.369066,5.742112,5.618678\C,0,1.954344,5.003
757,8.500895\H,0,1.107261,3.908209,10.130132\P,0,3.056298,6.529002,6.4
8281\H,0,2.915588,5.121306,8.985622\Au,0,4.852028,5.148152,5.961279\C,
0,3.287514,7.947769,7.590517\C,0,2.40037,7.22883,4.944126\Cl,0,3.27365
2,3.639745,5.134192\Cl,0,6.543721,3.741215,5.203681\C,0,6.323387,6.343
048,6.716457\C,0,4.33689,8.850236,7.355659\C,0,2.332058,8.243536,8.554
162\C,0,2.556391,6.596345,3.723832\C,0,1.68806,8.410378,4.994972\C,0,7
.147326,7.072605,5.852083\C,0,6.589951,6.344565,8.098973\H,0,5.087709,
8.634402,6.605566\C,0,4.398926,10.025717,8.098973\C,0,2.424787,9.42508
4,9.275684\H,0,1.516869,7.555083,8.739385\H,0,3.125113,5.67674,3.66257
6\C,0,1.994636,7.128725,2.590703\C,0,1.123485,8.936691,3.859421\H,0,1.
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9.10862\H,0,5.209247,10.724635,7.932393\C,0,3.44746,10.304799,9.038404
\H,0,1.684252,9.652444,10.032557\H,0,2.115167,6.625315,1.639406\C,0,1.
281747,8.296622,2.663339\H,0,0.553853,9.856145,3.913656\F,0,8.993299,8
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01013,11.229712,9.599159\H,0,0.841147,8.715852,1.767247\F,0,9.500862,8
.527168,8.207443\F,0,5.183177,8.577221,4.408311\C,0,6.02985,7.965971,2
.343739\F,0,8.933347,5.742415,4.131566\C,0,7.936265,6.531125,2.20815\F

,0,5.070955,7.519742,10.158945\C,0,4.450375,5.480017,11.084334\F,0,6.6
79865,3.4999,8.31543\C,0,5.262105,3.46274,10.149744\F,0,5.118653,8.751
648,1.760225\C,0,6.970908,7.29405,1.600425\F,0,8.861542,5.910774,1.466
532\F,0,3.71672,6.112502,12.00028\C,0,4.512689,4.105842,11.101282\F,0,
5.377394,2.116017,10.192115\F,0,6.956409,7.40629,0.262702\F,0,3.869386
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2349\C,0,6.143861,-1.131496,8.529949\F,0,5.238741,-1.672976,10.639556\
F,0,8.98163,1.167897,10.345862\C,0,8.032778,0.280598,8.401625\F,0,5.16
6937,-1.841335,7.974522\C,0,7.088156,-0.495978,7.743053\F,0,8.917106,0
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662\C,0,8.193357,-3.412688,2.927252\C,0,10.812769,0.36402,4.515571\C,0
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,4.750429\C,0,11.768225,0.659786,3.551926\C,0,12.14594,-2.579991,3.605
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1\C,0,12.818536,0.712872,9.442748\H,0,13.54643,2.272394,8.192432\H,0,1
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30Au2Cl4F26P2)]\\@

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.135254\H,0,-1.051578,3.562845,9.004024\C,0,1.747952,5.546754,7.263653
\H,0,0.369066,5.742112,5.618678\C,0,1.954344,5.003757,8.500895\H,0,1.1
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9973\C,0,8.193188,7.818846,6.387172\C,0,7.012127,7.087772,4.363034\C,0
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,8.456908,7.846147,7.733369\C,0,6.067505,7.864348,3.704463\C,0,7.95642
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,10.158945\C,0,4.450375,5.480017,11.084334\F,0,6.679865,3.4999,8.31543
\C,0,5.262105,3.46274,10.149744\F,0,5.118653,8.751648,1.760225\C,0,6.9
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(C37H16Au1Cl5F13P1)]\\@

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,7.263653\H,0,0.369066,5.742112,5.618678\C,0,1.954344,5.003757,8.50089
5\H,0,1.107261,3.908209,10.130132\P,0,3.056298,6.529002,6.48281\H,0,2.
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7.947769,7.590517\C,0,2.40037,7.22883,4.944126\Cl,0,3.273652,3.639745,
5.134192\Cl,0,6.543721,3.741215,5.203681\C,0,6.323387,6.343048,6.71645
7\C,0,4.33689,8.850236,7.355659\C,0,2.332058,8.243536,8.554162\C,0,2.5
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281\H,0,2.915588,5.121306,8.985622\Au,0,4.852028,5.148152,5.961279\C,0

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087772,4.363034\C,0,7.659499,7.105973,8.559004\C,0,5.832413,5.564955,9
.10862\H,0,5.209247,10.724635,7.932393\C,0,3.44746,10.304799,9.038404\
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808\C,0,3.431043,0.511145,-6.254005\F,0,4.232963,0.47626,-2.23551\C,0,
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4,-0.235096,-5.718915\C,0,3.295844,0.495978,-7.743054\F,0,5.784579,-0.
943418,-3.898644\C,0,-0.428769,-0.36402,-4.515571\C,0,-1.968331,2.0369
95,-4.842435\C,0,-1.315913,0.35492,-7.161961\F,0,5.277017,-0.928554,-6
.541162\C,0,2.351223,-0.280598,-8.401625\C,0,4.240139,1.131496,-8.5299
49\C,0,0.620607,-1.266486,-4.750429\C,0,-1.384225,-0.659786,-3.551927\
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,1.841335,-7.974522\C,0,4.219983,1.052625,-9.897938\H,0,1.371427,-1.05
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4,-2.830404\H,0,-2.199414,0.028667,-3.366703\H,0,-0.800696,2.462444,-3
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068\H,0,-3.347217,1.841638,-6.48741\H,0,-0.59117,1.90701,-8.443513\C,0
,-1.721647,0.455025,-9.515385\C,0,-2.592798,-1.352941,-8.246667\H,0,-2
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6681\C,0,-2.434536,-0.712872,-9.442748\H,0,-3.162429,-2.272395,-8.1924
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0,-4.767861,4.020905,-3.102064\H,0,-2.875136,-1.132101,-10.338841\\Ver
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\H,0,0.369066,5.742112,5.618678\C,0,1.954344,5.003757,8.500895\H,0,1.1
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Cl,0,6.543721,3.741215,5.203681\C,0,6.323387,6.343048,6.716457\C,0,4.3
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52083\C,0,6.589951,6.344565,8.098973\H,0,5.087709,8.634402,6.605566\C,
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9973\C,0,8.193188,7.818846,6.387172\C,0,7.012127,7.087772,4.363034\C,0
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2,10.113425\C,0,5.906926,4.171062,9.178836\H,0,3.501013,11.229712,9.59
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\C,0,5.262105,3.46274,10.149744\F,0,5.118653,8.751648,1.760225\C,0,6.9
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.135254\H,0,-1.051578,3.562845,9.004024\C,0,1.747952,5.546754,7.263653
\H,0,0.369066,5.742112,5.618678\C,0,1.954344,5.003757,8.500895\H,0,1.1

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7.590517\C,0,2.40037,7.22883,4.944126\Cl,0,3.273652,3.639745,5.134192\
Cl,0,6.543721,3.741215,5.203681\C,0,6.323387,6.343048,6.716457\C,0,4.3
3689,8.850236,7.355659\C,0,2.332058,8.243536,8.554162\C,0,2.556391,6.5
96345,3.723832\C,0,1.68806,8.410378,4.994972\C,0,7.147326,7.072605,5.8
52083\C,0,6.589951,6.344565,8.098973\H,0,5.087709,8.634402,6.605566\C,
0,4.398926,10.025717,8.098973\C,0,2.424787,9.425084,9.275684\H,0,1.516
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9973\C,0,8.193188,7.818846,6.387172\C,0,7.012127,7.087772,4.363034\C,0
,7.659499,7.105973,8.559004\C,0,5.832413,5.564955,9.10862\H,0,5.209247
,10.724635,7.932393\C,0,3.44746,10.304799,9.038404\H,0,1.684252,9.6524
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\C,0,5.262105,3.46274,10.149744\F,0,5.118653,8.751648,1.760225\C,0,6.9
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.135254\H,0,-1.051578,3.562845,9.004024\C,0,1.747952,5.546754,7.263653
\H,0,0.369066,5.742112,5.618678\C,0,1.954344,5.003757,8.500895\H,0,1.1
07261,3.908209,10.130132\P,0,3.056298,6.529002,6.48281\H,0,2.915588,5.
121306,8.985622\Au,0,4.852028,5.148152,5.961279\C,0,3.287514,7.947769,
7.590517\C,0,2.40037,7.22883,4.944126\Cl,0,3.273652,3.639745,5.134192\
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3689,8.850236,7.355659\C,0,2.332058,8.243536,8.554162\C,0,2.556391,6.5
96345,3.723832\C,0,1.68806,8.410378,4.994972\C,0,7.147326,7.072605,5.8
52083\C,0,6.589951,6.344565,8.098973\H,0,5.087709,8.634402,6.605566\C,
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2,6.452254,3.576138\F,0,7.949246,7.10749,9.870577\C,0,5.114925,6.17772
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,10.158945\C,0,4.450375,5.480017,11.084334\F,0,6.679865,3.4999,8.31543
\C,0,5.262105,3.46274,10.149744\F,0,5.118653,8.751648,1.760225\C,0,6.9
70908,7.29405,1.600425\F,0,8.861542,5.910774,1.466532\F,0,3.71672,6.11
2502,12.00028\C,0,4.512689,4.105842,11.101282\F,0,5.377394,2.116017,10
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5F13P1)]\\@

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.110392,8.505737\C,0,0.531718,5.337443,6.609924\C,0,0.94661,4.304536,9
.135254\H,0,-1.051578,3.562845,9.004024\C,0,1.747952,5.546754,7.263653
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07261,3.908209,10.130132\P,0,3.056298,6.529002,6.48281\H,0,2.915588,5.
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7.590517\C,0,2.40037,7.22883,4.944126\Cl,0,3.273652,3.639745,5.134192\
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3689,8.850236,7.355659\C,0,2.332058,8.243536,8.554162\C,0,2.556391,6.5
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52083\C,0,6.589951,6.344565,8.098973\H,0,5.087709,8.634402,6.605566\C,
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3339\H,0,0.553853,9.856145,3.913656\F,0,8.993299,8.512303,5.564926\C,0
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9159\H,0,0.841147,8.715852,1.767247\F,0,9.500862,8.527168,8.207443\F,0
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70908,7.29405,1.600425\F,0,8.861542,5.910774,1.466532\F,0,3.71672,6.11
2502,12.00028\C,0,4.512689,4.105842,11.101282\F,0,5.377394,2.116017,10
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62\C,0,2.556391,6.596345,3.723832\C,0,1.68806,8.410378,4.994972\C,0,7.
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.634402,6.605566\C,0,4.398926,10.025717,8.098973\C,0,2.424787,9.425084
,9.275684\H,0,1.516869,7.555083,8.739385\H,0,3.125113,5.67674,3.662576
\C,0,1.994636,7.128725,2.590703\C,0,1.123485,8.936691,3.859421\H,0,1.5
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087772,4.363034\C,0,7.659499,7.105973,8.559004\C,0,5.832413,5.564955,9
.10862\H,0,5.209247,10.724635,7.932393\C,0,3.44746,10.304799,9.038404\
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.704463\C,0,7.956422,6.452254,3.576138\F,0,7.949246,7.10749,9.870577\C
,0,5.114925,6.177722,10.113425\C,0,5.906926,4.171062,9.178836\H,0,3.50
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527168,8.207443\F,0,5.183177,8.577221,4.408311\C,0,6.02985,7.965971,2.
343739\F,0,8.933347,5.742415,4.131566\C,0,7.936265,6.531125,2.20815\F,
0,5.070955,7.519742,10.158945\C,0,4.450375,5.480017,11.084334\F,0,6.67
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48,1.760225\C,0,6.970908,7.29405,1.600425\F,0,8.861542,5.910774,1.4665
32\F,0,3.71672,6.112502,12.00028\C,0,4.512689,4.105842,11.101282\F,0,5
.377394,2.116017,10.192115\F,0,6.956409,7.40629,0.262702\F,0,3.869386,
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,14.314238\C,0,0.303192,0.289699,13.706512\C,0,1.288706,1.131495,15.68
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\C,0,0.991782,0.477775,20.665092\C,0,-0.835303,2.018793,21.214708\F,0,
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87,20.660248\C,0,-4.713373,2.579991,20.606983\C,0,-6.135999,2.246306,1
8.716011\C,0,-4.111325,0.987403,15.829921\C,0,-4.979656,-0.826629,17.1
01061\F,0,-1.59676,0.064006,22.265032\C,0,-2.217342,2.103731,23.19042\
F,0,0.012149,4.083848,20.421516\C,0,-1.405612,4.121008,22.255831\H,0,-
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2Cl4F26P2)]\\@

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.304536,9.135254\H,0,-1.051578,3.562845,9.004024\C,0,1.747952,5.546754
,7.263653\H,0,0.369066,5.742112,5.618678\C,0,1.954344,5.003757,8.50089
5\H,0,1.107261,3.908209,10.130132\P,0,3.056298,6.529002,6.48281\H,0,2.
915588,5.121306,8.985622\Au,0,4.852028,5.148152,5.961279\C,0,3.287514,
7.947769,7.590517\C,0,2.40037,7.22883,4.944126\Cl,0,3.273652,3.639745,
5.134192\Cl,0,6.543721,3.741215,5.203681\C,0,6.323387,6.343048,6.71645
7\C,0,4.33689,8.850236,7.355659\C,0,2.332058,8.243536,8.554162\C,0,2.5
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61\C,0,-0.503699,8.636374,22.004025\C,0,5.007779,5.742414,14.936492\H,
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857,6.533096,17.606609\H,0,4.516979,10.046192,15.226553\C,0,6.485956,1
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1473\C,0,6.309081,6.230808,20.352755\H,0,5.858974,6.240667,18.272203\F
,0,2.313914,6.415851,22.45195\C,0,0.461658,7.873448,22.61175\F,0,-1.42
8975,9.256724,22.745644\C,0,3.985106,4.8627,15.17377\H,0,5.748314,5.51
5054,14.179619\H,0,2.22332,4.442863,16.279781\H,0,6.325305,11.25929,14
.082044\C,0,7.69372,11.057106,15.706438\H,0,8.838291,10.728882,17.4804
65\H,0,5.317399,8.542183,22.572769\C,0,6.15082,6.870876,21.548836\H,0,
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2Cl4F26P2)]\\@

Compound 3c

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symm gfprint\\CrystalExplorer Job symop = -, r = 8.47953\\0,1\F,0,-1.1
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.272045,7.294133\C,0,-3.289746,7.72075,5.395464\C,0,-1.947517,5.696214
,8.291173\C,0,-4.225567,5.962825,7.275051\F,0,-2.829366,8.558322,4.465
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0,-1.180818,6.547177,9.080694\F,0,-4.723805,5.110645,8.185744\C,0,-5.1
07273,6.517959,6.349569\F,0,-5.470142,7.944752,4.539155\H,0,-2.401281,
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51,9.920306\H,0,-1.359815,7.61435,9.035135\F,0,-6.391539,6.183174,6.36

9128\C,0,0.051839,4.684555,9.985902\C,0,-0.679418,2.316712,9.366925\C,
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\F,0,-0.966629,2.257059,11.712593\C,0,-0.629347,0.226436,10.6335\F,0,2
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\F,0,-0.676029,-0.400525,11.812058\F,0,3.813807,8.611887,10.99439\C,0,
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6\H,0,4.911926,4.463718,11.260109\C,0,6.217889,5.791171,10.242317\C,0,
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.799148\H,0,2.90582,-1.213018,10.586272\C,0,4.835547,-0.603831,9.98470
9\H,0,6.650148,0.204036,9.297515\H,0,6.842899,5.952842,11.111745\C,0,6
.49363,6.437611,9.075924\H,0,5.950183,6.728326,7.034855\H,0,1.181705,3
.51719,3.930674\H,0,5.270361,-1.576412,10.179585\H,0,7.319936,7.136154
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23\PG=C01 [X(C43H18Au1Cl5F15P1)]\\@

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\\#p b3lyp/gen pseudo=read counterpoise=2 empiricaldispersion=gd3bj no
symm gfprint\\CrystalExplorer Job symop = -x, -y, -z, r = 11.7368\\0,1
\F,0,-1.154257,7.48701,6.256066\C,0,-2.444196,7.169269,6.325716\C,0,-2
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\C,0,-5.107273,6.517959,6.349569\F,0,-5.470142,7.944752,4.539155\H,0,-
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765,4.543336,7.117624\C,0,2.588604,2.399495,6.776531\C,0,2.962443,0.82
2962,10.003791\C,0,5.058256,1.645924,9.297753\C,0,5.151002,4.937774,10
.31626\C,0,4.693041,5.329777,8.014482\F,0,-0.325143,-1.824883,9.541288
\F,0,2.558406,9.789112,13.105587\H,0,1.339665,5.372507,7.770947\C,0,1.
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10.186979\C,0,5.604357,0.385915,9.512426\H,0,5.682237,2.452452,8.93304
6\H,0,4.911926,4.463718,11.260109\C,0,6.217889,5.791171,10.242317\C,0,
5.728672,6.209957,7.959621\H,0,4.108508,5.139254,7.12287\H,0,0.635316,
5.425951,5.408821\C,0,1.490647,3.501242,4.968502\H,0,2.4011,1.600394,4
.799148\H,0,2.90582,-1.213018,10.586272\C,0,4.835547,-0.603831,9.98470
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.49363,6.437611,9.075924\H,0,5.950183,6.728326,7.034855\H,0,1.181705,3
.51719,3.930674\H,0,5.270361,-1.576412,10.179585\H,0,7.319936,7.136154
,9.029411\Cl,0,-4.063099,5.711188,2.421995\C,0,-4.222633,4.14403,3.141
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.272045,7.294133\C,0,-3.289746,7.72075,5.395464\C,0,-1.947517,5.696214
,8.291173\C,0,-4.225567,5.962825,7.275051\F,0,-2.829366,8.558322,4.465
211\C,0,-4.604365,7.396922,5.428857\C,0,-1.766835,4.331509,8.439058\C,
0,-1.180818,6.547177,9.080694\F,0,-4.723805,5.110645,8.185744\C,0,-5.1
07273,6.517959,6.349569\F,0,-5.470142,7.944752,4.539155\H,0,-2.401281,
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9128\C,0,0.051839,4.684555,9.985902\C,0,-0.679418,2.316712,9.366925\C,
0,0.529038,7.053615,10.755148\Au,0,1.615334,3.994045,11.1127\C,0,-0.57
1375,1.532706,8.233926\C,0,-0.747661,1.615489,10.559557\C,0,1.836008,7
.429791,10.509467\C,0,-0.078645,7.698836,11.814205\Cl,0,3.260511,3.081
604,12.52382\Cl,0,0.443065,4.678102,13.002542\P,0,2.994464,3.494911,9.
291313\F,0,-0.558617,2.102449,7.021497\C,0,-0.444371,0.164349,8.274475
\F,0,-0.966629,2.257059,11.712593\C,0,-0.629347,0.226436,10.6335\F,0,2
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\F,0,-0.676029,-0.400525,11.812058\F,0,3.813807,8.611887,10.99439\C,0,
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2962,10.003791\C,0,5.058256,1.645924,9.297753\C,0,5.151002,4.937774,10
.31626\C,0,4.693041,5.329777,8.014482\F,0,-0.325143,-1.824883,9.541288

\F,0,2.558406,9.789112,13.105587\H,0,1.339665,5.372507,7.770947\C,0,1.
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10.186979\C,0,5.604357,0.385915,9.512426\H,0,5.682237,2.452452,8.93304
6\H,0,4.911926,4.463718,11.260109\C,0,6.217889,5.791171,10.242317\C,0,
5.728672,6.209957,7.959621\H,0,4.108508,5.139254,7.12287\H,0,0.635316,
5.425951,5.408821\C,0,1.490647,3.501242,4.968502\H,0,2.4011,1.600394,4
.799148\H,0,2.90582,-1.213018,10.586272\C,0,4.835547,-0.603831,9.98470
9\H,0,6.650148,0.204036,9.297515\H,0,6.842899,5.952842,11.111745\C,0,6
.49363,6.437611,9.075924\H,0,5.950183,6.728326,7.034855\H,0,1.181705,3
.51719,3.930674\H,0,5.270361,-1.576412,10.179585\H,0,7.319936,7.136154
,9.029411\Cl,0,-3.609945,10.039775,8.069819\C,0,-5.19054,10.231029,8.7
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,-1.947517,5.696214,8.291173\C,0,-4.225567,5.962825,7.275051\F,0,-2.82
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.331509,8.439058\C,0,-1.180818,6.547177,9.080694\F,0,-4.723805,5.11064
5,8.185744\C,0,-5.107273,6.517959,6.349569\F,0,-5.470142,7.944752,4.53
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,0,-0.194529,6.062651,9.920306\H,0,-1.359815,7.61435,9.035135\F,0,-6.3
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.316712,9.366925\C,0,0.529038,7.053615,10.755148\Au,0,1.615334,3.99404
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Cl,0,3.260511,3.081604,12.52382\Cl,0,0.443065,4.678102,13.002542\P,0,2
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26436,10.6335\F,0,2.472983,6.895353,9.43419\C,0,2.536792,8.319711,11.2
79906\F,0,-1.337059,7.417618,12.111408\C,0,0.600126,8.610669,12.601341
\C,0,2.288103,3.461068,7.616143\C,0,3.744577,1.863839,9.548205\C,0,4.3
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,-0.489395,9.483804\F,0,-0.676029,-0.400525,11.812058\F,0,3.813807,8.6
11887,10.99439\C,0,1.914796,8.915019,12.336577\F,0,-0.040857,9.231544,
13.605776\C,0,1.581765,4.543336,7.117624\C,0,2.588604,2.399495,6.77653
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.151002,4.937774,10.31626\C,0,4.693041,5.329777,8.014482\F,0,-0.325143
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271\H,0,3.140984,1.547924,7.154118\C,0,3.519912,-0.399308,10.22085\H,0
,1.906356,0.978424,10.186979\C,0,5.604357,0.385915,9.512426\H,0,5.6822
37,2.452452,8.933046\H,0,4.911926,4.463718,11.260109\C,0,6.217889,5.79
1171,10.242317\C,0,5.728672,6.209957,7.959621\H,0,4.108508,5.139254,7.
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41289,-0.646407\F,0,-5.350684,9.029455,1.679463\C,0,-5.388472,10.56216
2,-0.112107\F,0,-1.49602,9.649112,-0.931922\C,0,-3.473819,10.831207,-1
.416846\F,0,-6.646886,10.843381,0.185096\C,0,-4.780789,11.207384,-1.17
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\Au,0,-3.694493,14.266953,-0.813613\C,0,-6.107801,14.466364,-2.640486\
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37,13.686011,-6.130126\C,0,-3.135411,15.827417,-6.473602\H,0,-2.168844
,16.713076,-4.772195\H,0,-3.403472,17.282576,-1.739334\C,0,-1.789916,1
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,-1.683995\C,0,0.418844,12.051043,-3.966691\H,0,-1.20132,13.121746,-4.
803442\F,0,-5.593199,18.810047,-4.776011\C,0,-5.769368,18.750395,-2.44
2509\F,0,-5.985857,18.661524,-0.114254\F,0,-8.139194,9.702678,-7.46110
1\C,0,-9.914193,10.864079,-6.497456\F,0,-11.701365,12.077826,-5.557185
\H,0,-4.674511,12.835049,-6.51749\C,0,-3.81918,14.759758,-6.957811\H,0
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.532674,-4.891458\F,0,-5.634971,20.085882,-2.385024\F,0,-10.779969,10.
316248,-7.387158\H,0,-4.128123,14.74381,-7.995639\H,0,-0.039467,19.837
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,-144.6522364\PG=C01 [X(C84H34Au2Cl4F30P2)]\\@

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0,-1.947517,5.696214,8.291173\C,0,-4.225567,5.962825,7.275051\F,0,-2.8
29366,8.558322,4.465211\C,0,-4.604365,7.396922,5.428857\C,0,-1.766835,
4.331509,8.439058\C,0,-1.180818,6.547177,9.080694\F,0,-4.723805,5.1106

45,8.185744\C,0,-5.107273,6.517959,6.349569\F,0,-5.470142,7.944752,4.5
39155\H,0,-2.401281,3.656704,7.877806\C,0,-0.797973,3.794635,9.285827\
C,0,-0.194529,6.062651,9.920306\H,0,-1.359815,7.61435,9.035135\F,0,-6.
391539,6.183174,6.369128\C,0,0.051839,4.684555,9.985902\C,0,-0.679418,
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59557\C,0,1.836008,7.429791,10.509467\C,0,-0.078645,7.698836,11.814205
\Cl,0,3.260511,3.081604,12.52382\Cl,0,0.443065,4.678102,13.002542\P,0,
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279906\F,0,-1.337059,7.417618,12.111408\C,0,0.600126,8.610669,12.60134
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611887,10.99439\C,0,1.914796,8.915019,12.336577\F,0,-0.040857,9.231544
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5.151002,4.937774,10.31626\C,0,4.693041,5.329777,8.014482\F,0,-0.32514
3,-1.824883,9.541288\F,0,2.558406,9.789112,13.105587\H,0,1.339665,5.37
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.452452,8.933046\C,0,-15.903817,6.547177,9.080694\C,0,-14.193961,7.053
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,9.366925\H,0,-14.087684,5.425951,5.408821\C,0,-13.232352,3.501242,4.9
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\C,0,-9.887452,-0.603831,9.984709\H,0,-8.072851,0.204036,9.297515\H,0,
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.615489,10.559557\H,0,-13.541294,3.51719,3.930674\H,0,-9.452639,-1.576
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111408\C,0,-14.122873,8.610669,12.601341\F,0,-15.281617,2.102449,7.021
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\C,0,-15.352346,0.226436,10.6335\C,0,-17.167196,7.169269,6.325716\C,0,
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7.72075,5.395464\F,0,-19.446806,5.110645,8.185744\C,0,-19.830273,6.517
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,5.696214,8.291173\C,0,-4.225567,5.962825,7.275051\F,0,-2.829366,8.558
322,4.465211\C,0,-4.604365,7.396922,5.428857\C,0,-1.766835,4.331509,8.
439058\C,0,-1.180818,6.547177,9.080694\F,0,-4.723805,5.110645,8.185744
\C,0,-5.107273,6.517959,6.349569\F,0,-5.470142,7.944752,4.539155\H,0,-
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C,0,-0.571375,1.532706,8.233926\C,0,-0.747661,1.615489,10.559557\C,0,1
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,8.274475\F,0,-0.966629,2.257059,11.712593\C,0,-0.629347,0.226436,10.6
335\F,0,2.472983,6.895353,9.43419\C,0,2.536792,8.319711,11.279906\F,0,
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,9.483804\F,0,-0.676029,-0.400525,11.812058\F,0,3.813807,8.611887,10.9
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0.978424,10.186979\C,0,5.604357,0.385915,9.512426\H,0,5.682237,2.45245
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.600394,4.799148\H,0,2.90582,-1.213018,10.586272\C,0,4.835547,-0.60383
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,0,9.037889,-4.543337,16.735003\C,0,8.031051,-2.399496,17.076094\C,0,7
.657212,-0.822963,13.848835\C,0,5.561399,-1.645926,14.554872\C,0,11.80
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9958,15.893003\H,0,6.511147,-5.139255,16.729753\H,0,9.279989,-5.372509
,16.081678\C,0,9.437763,-4.57499,18.056438\C,0,8.445238,-2.433583,18.3
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\H,0,8.713299,-0.978425,13.665647\C,0,5.015297,-0.385917,14.340198\H,0
,4.937417,-2.452453,14.919579\H,0,11.97947,-7.614351,14.817489\C,0,12.
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952843,12.74088\C,0,4.126025,-6.437612,14.776701\H,0,4.669471,-6.72832
7,16.81777\H,0,9.984339,-5.425952,18.443804\C,0,9.129007,-3.501243,18.
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\H,0,7.713835,1.213017,13.266353\H,0,3.969507,-0.204037,14.55511\C,0,1
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7,-8.610671,11.251284\F,0,11.178272,-2.10245,16.831127\C,0,11.064025,-
0.164349,15.57815\F,0,11.586284,-2.25706,12.140032\C,0,11.249002,-0.22
6437,13.219125\H,0,3.299719,-7.136156,14.823214\H,0,9.437949,-3.517191
,19.921951\H,0,5.349293,1.576411,13.67304\C,0,13.06385,-7.16927,17.526
909\C,0,14.845222,-5.962826,16.577574\F,0,6.805848,-8.611888,12.858234
\C,0,8.704858,-8.915021,11.516047\F,0,10.660512,-9.231544,10.246849\F,
0,10.903026,0.549047,16.702324\C,0,11.079194,0.489394,14.368821\F,0,11
.295684,0.400524,12.040566\F,0,11.773912,-7.487011,17.59656\C,0,13.909
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30P2)]\\@

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8.291173\C,0,-4.225567,5.962825,7.275051\F,0,-2.829366,8.558322,4.4652
11\C,0,-4.604365,7.396922,5.428857\C,0,-1.766835,4.331509,8.439058\C,0
,-1.180818,6.547177,9.080694\F,0,-4.723805,5.110645,8.185744\C,0,-5.10
7273,6.517959,6.349569\F,0,-5.470142,7.944752,4.539155\H,0,-2.401281,3

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1,9.920306\H,0,-1.359815,7.61435,9.035135\F,0,-6.391539,6.183174,6.369
128\C,0,0.051839,4.684555,9.985902\C,0,-0.679418,2.316712,9.366925\C,0
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429791,10.509467\C,0,-0.078645,7.698836,11.814205\Cl,0,3.260511,3.0816
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91313\F,0,-0.558617,2.102449,7.021497\C,0,-0.444371,0.164349,8.274475\
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7.417618,12.111408\C,0,0.600126,8.610669,12.601341\C,0,2.288103,3.4610
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F,0,-0.676029,-0.400525,11.812058\F,0,3.813807,8.611887,10.99439\C,0,1
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962,10.003791\C,0,5.058256,1.645924,9.297753\C,0,5.151002,4.937774,10.
31626\C,0,4.693041,5.329777,8.014482\F,0,-0.325143,-1.824883,9.541288\
F,0,2.558406,9.789112,13.105587\H,0,1.339665,5.372507,7.770947\C,0,1.1
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47924,7.154118\C,0,3.519912,-0.399308,10.22085\H,0,1.906356,0.978424,1
0.186979\C,0,5.604357,0.385915,9.512426\H,0,5.682237,2.452452,8.933046
\H,0,4.911926,4.463718,11.260109\C,0,6.217889,5.791171,10.242317\C,0,5
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.425951,5.408821\C,0,1.490647,3.501242,4.968502\H,0,2.4011,1.600394,4.
799148\H,0,2.90582,-1.213018,10.586272\C,0,4.835547,-0.603831,9.984709
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49363,6.437611,9.075924\H,0,5.950183,6.728326,7.034855\H,0,1.181705,3.
51719,3.930674\H,0,5.270361,-1.576412,10.179585\H,0,7.319936,7.136154,
9.029411\Cl,0,9.372926,-0.375812,9.504317\C,0,9.53246,-1.942971,8.7849
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symm gfprint\\CrystalExplorer Job symop = x, y, z, r = 12.174\\0,1\F,0
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4.465211\C,0,-4.604365,7.396922,5.428857\C,0,-1.766835,4.331509,8.4390
58\C,0,-1.180818,6.547177,9.080694\F,0,-4.723805,5.110645,8.185744\C,0
,-5.107273,6.517959,6.349569\F,0,-5.470142,7.944752,4.539155\H,0,-2.40
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,6.369128\C,0,0.051839,4.684555,9.985902\C,0,-0.679418,2.316712,9.3669
25\C,0,0.529038,7.053615,10.755148\Au,0,1.615334,3.994045,11.1127\C,0,
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008,7.429791,10.509467\C,0,-0.078645,7.698836,11.814205\Cl,0,3.260511,
3.081604,12.52382\Cl,0,0.443065,4.678102,13.002542\P,0,2.994464,3.4949
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74475\F,0,-0.966629,2.257059,11.712593\C,0,-0.629347,0.226436,10.6335\
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37059,7.417618,12.111408\C,0,0.600126,8.610669,12.601341\C,0,2.288103,
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,9.197572\F,0,-0.283371,-0.549047,7.150301\C,0,-0.459539,-0.489395,9.4
83804\F,0,-0.676029,-0.400525,11.812058\F,0,3.813807,8.611887,10.99439
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1 [X(C43H18Au1Cl5F15P1)]\\@

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.272045,7.294133\C,0,-3.289746,7.72075,5.395464\C,0,-1.947517,5.696214
,8.291173\C,0,-4.225567,5.962825,7.275051\F,0,-2.829366,8.558322,4.465
211\C,0,-4.604365,7.396922,5.428857\C,0,-1.766835,4.331509,8.439058\C,
0,-1.180818,6.547177,9.080694\F,0,-4.723805,5.110645,8.185744\C,0,-5.1
07273,6.517959,6.349569\F,0,-5.470142,7.944752,4.539155\H,0,-2.401281,
3.656704,7.877806\C,0,-0.797973,3.794635,9.285827\C,0,-0.194529,6.0626
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9128\C,0,0.051839,4.684555,9.985902\C,0,-0.679418,2.316712,9.366925\C,
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1375,1.532706,8.233926\C,0,-0.747661,1.615489,10.559557\C,0,1.836008,7
.429791,10.509467\C,0,-0.078645,7.698836,11.814205\Cl,0,3.260511,3.081
604,12.52382\Cl,0,0.443065,4.678102,13.002542\P,0,2.994464,3.494911,9.
291313\F,0,-0.558617,2.102449,7.021497\C,0,-0.444371,0.164349,8.274475
\F,0,-0.966629,2.257059,11.712593\C,0,-0.629347,0.226436,10.6335\F,0,2
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,7.417618,12.111408\C,0,0.600126,8.610669,12.601341\C,0,2.288103,3.461
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\F,0,-0.676029,-0.400525,11.812058\F,0,3.813807,8.611887,10.99439\C,0,
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\F,0,2.558406,9.789112,13.105587\H,0,1.339665,5.372507,7.770947\C,0,1.
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6\H,0,4.911926,4.463718,11.260109\C,0,6.217889,5.791171,10.242317\C,0,
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.799148\H,0,2.90582,-1.213018,10.586272\C,0,4.835547,-0.603831,9.98470
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,9.029411\Cl,0,8.294206,9.980488,7.582749\C,0,9.53246,10.231029,8.7849
22\H,0,9.414454,9.483788,9.559894\Cl,0,9.372926,11.798187,9.504317\Cl,
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symm gfprint\\CrystalExplorer Job symop = -, r = 11.0881\\0,1\F,0,-1.1
54257,7.48701,6.256066\C,0,-2.444196,7.169269,6.325716\C,0,-2.893473,6
.272045,7.294133\C,0,-3.289746,7.72075,5.395464\C,0,-1.947517,5.696214
,8.291173\C,0,-4.225567,5.962825,7.275051\F,0,-2.829366,8.558322,4.465
211\C,0,-4.604365,7.396922,5.428857\C,0,-1.766835,4.331509,8.439058\C,
0,-1.180818,6.547177,9.080694\F,0,-4.723805,5.110645,8.185744\C,0,-5.1
07273,6.517959,6.349569\F,0,-5.470142,7.944752,4.539155\H,0,-2.401281,
3.656704,7.877806\C,0,-0.797973,3.794635,9.285827\C,0,-0.194529,6.0626
51,9.920306\H,0,-1.359815,7.61435,9.035135\F,0,-6.391539,6.183174,6.36
9128\C,0,0.051839,4.684555,9.985902\C,0,-0.679418,2.316712,9.366925\C,
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.429791,10.509467\C,0,-0.078645,7.698836,11.814205\Cl,0,3.260511,3.081
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\F,0,-0.966629,2.257059,11.712593\C,0,-0.629347,0.226436,10.6335\F,0,2
.472983,6.895353,9.43419\C,0,2.536792,8.319711,11.279906\F,0,-1.337059
,7.417618,12.111408\C,0,0.600126,8.610669,12.601341\C,0,2.288103,3.461
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7572\F,0,-0.283371,-0.549047,7.150301\C,0,-0.459539,-0.489395,9.483804
\F,0,-0.676029,-0.400525,11.812058\F,0,3.813807,8.611887,10.99439\C,0,
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765,4.543336,7.117624\C,0,2.588604,2.399495,6.776531\C,0,2.962443,0.82
2962,10.003791\C,0,5.058256,1.645924,9.297753\C,0,5.151002,4.937774,10
.31626\C,0,4.693041,5.329777,8.014482\F,0,-0.325143,-1.824883,9.541288
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547924,7.154118\C,0,3.519912,-0.399308,10.22085\H,0,1.906356,0.978424,
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.799148\H,0,2.90582,-1.213018,10.586272\C,0,4.835547,-0.603831,9.98470
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.51719,3.930674\H,0,5.270361,-1.576412,10.179585\H,0,7.319936,7.136154
,9.029411\Cl,0,1.246728,12.54981,14.348309\C,0,1.087194,14.116969,15.0
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