Perhalophenyl-phosphide: a couple needed to stabilize phosphide gold complexes

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Supplementary Material

Characterization of the complexes

IR Spectra

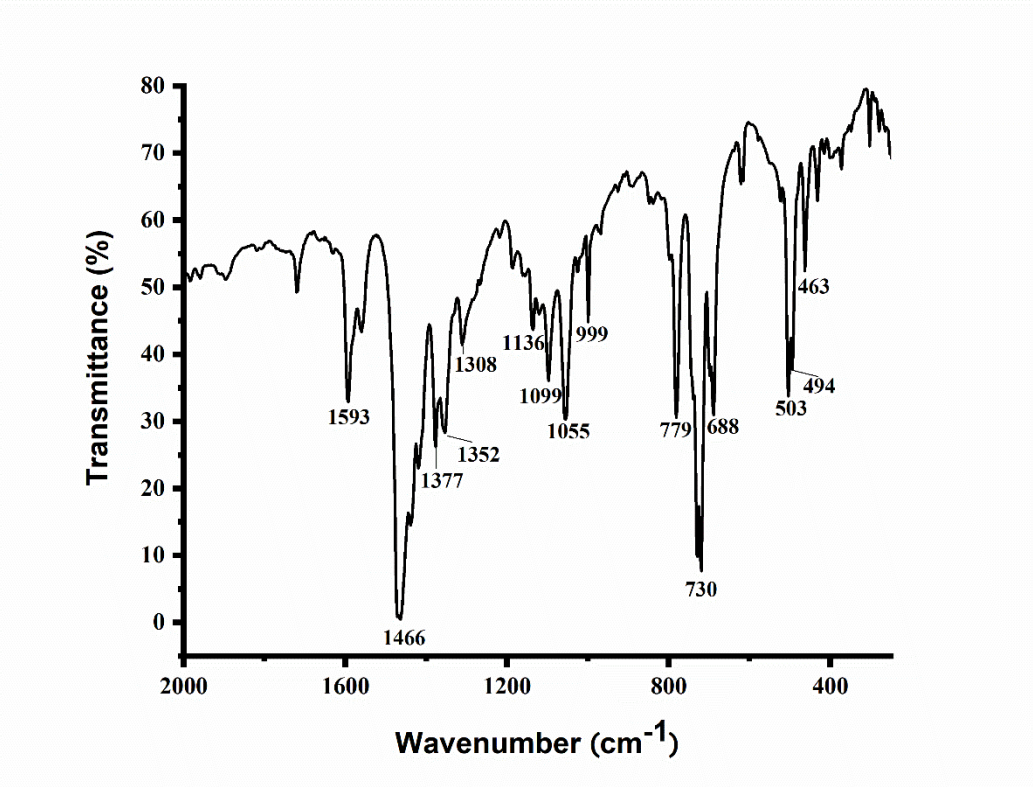

Figure S1. FT-IR spectrum of complex [{Au($C_6Cl_2F_3$)$_2$}$_2$(μ-PPh_2)$_2$] (**1**)

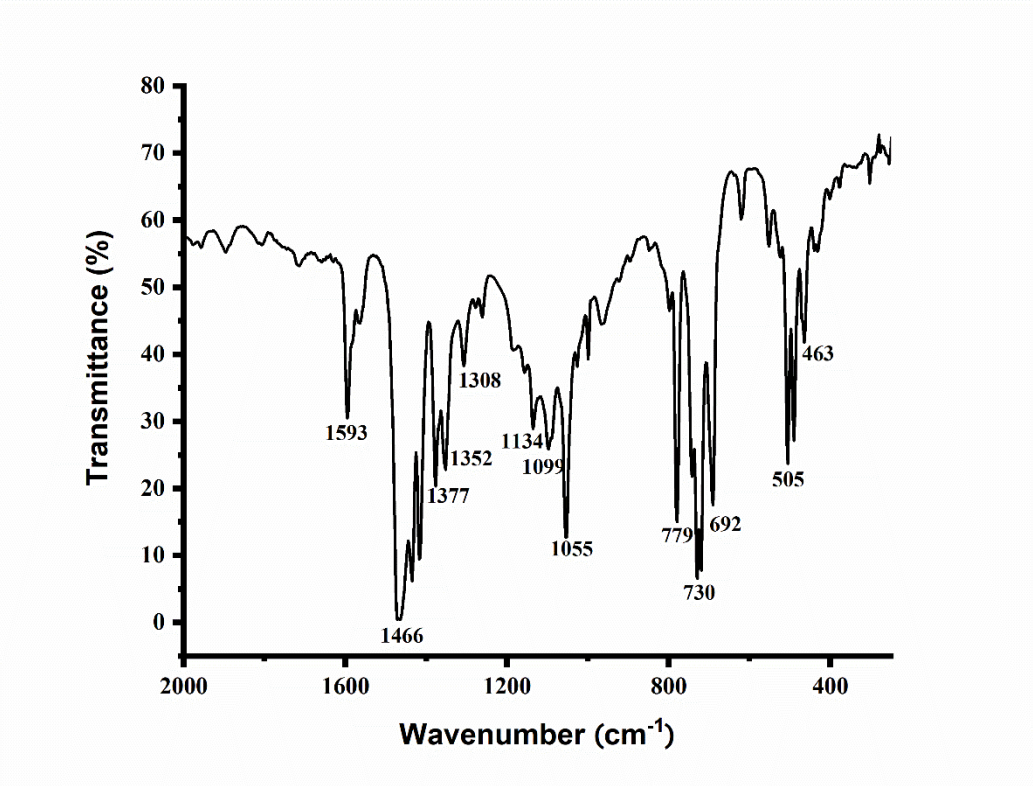

Figure S2. FT-IR spectrum of complex [{Au($C_6Cl_2F_3$)$_2$(μ-PPh_2)$_2$Au}$_2$] (**2**)

^{1}H NMR spectra (298K, $CDCl_3$)

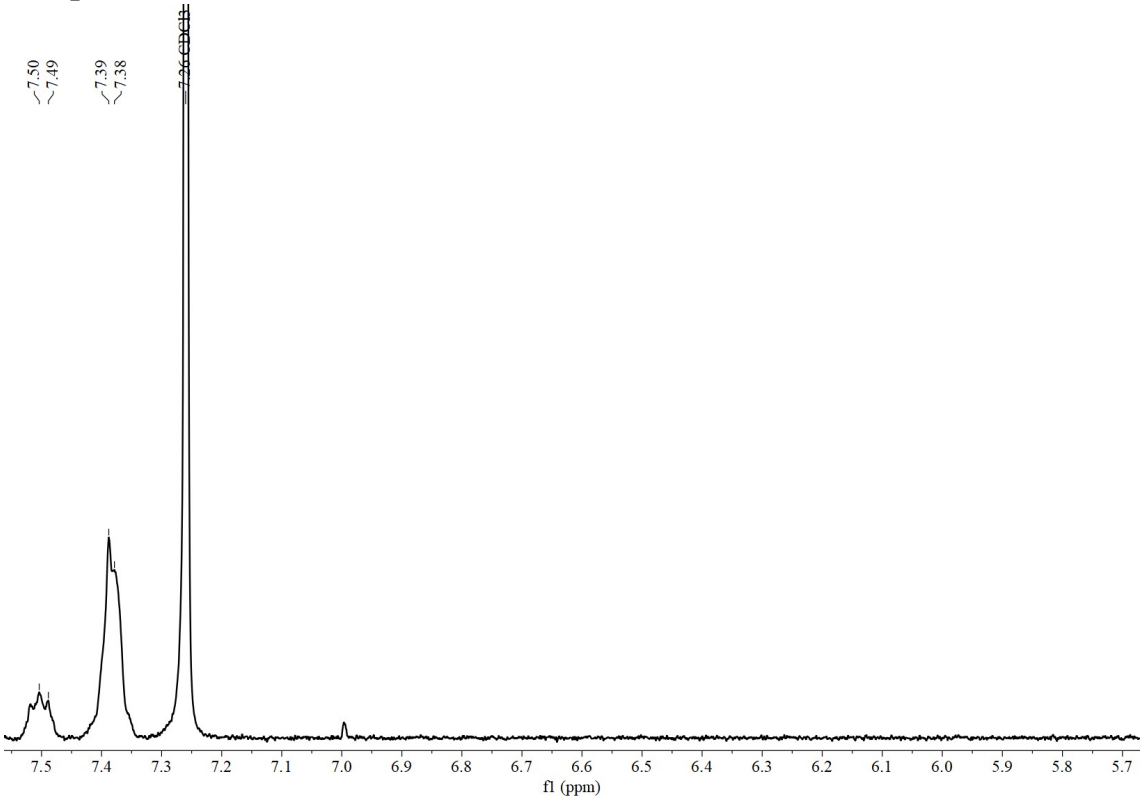

Figure S3. ^{1}H NMR spectrum of complex [{Au($C_6Cl_2F_3$)$_2$}$_2$(μ-PPh_2)$_2$] (**1**)

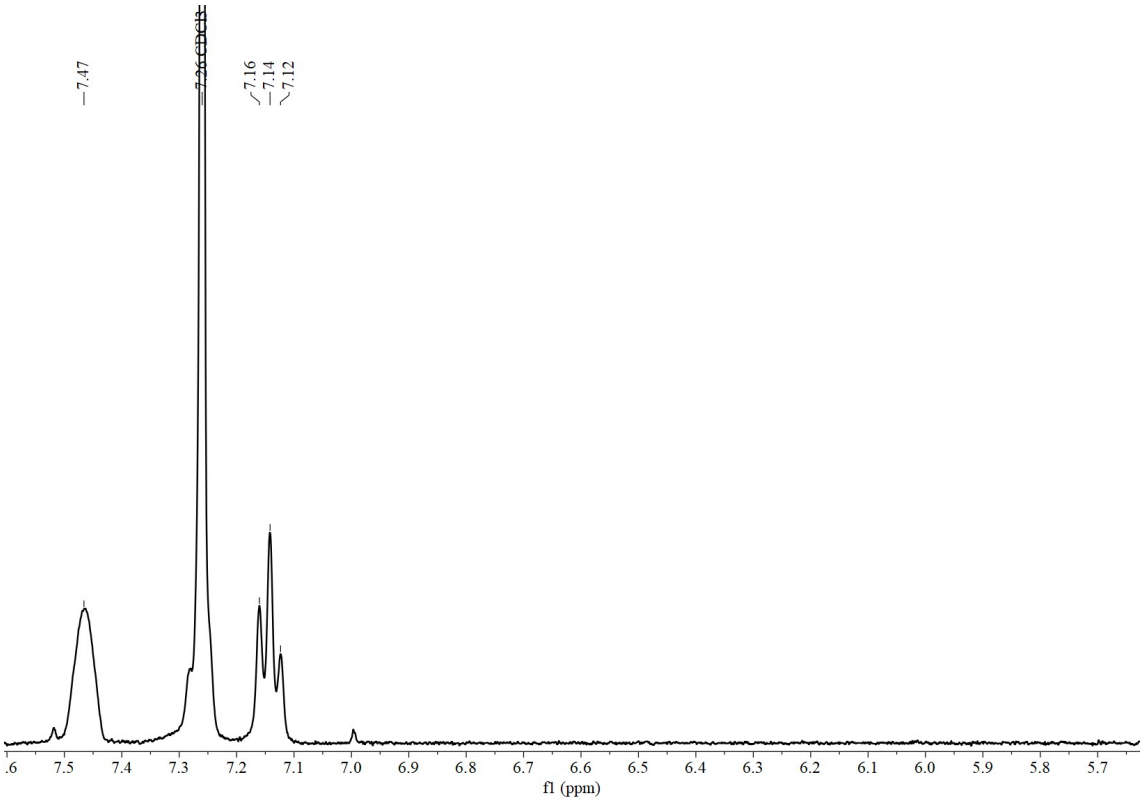

Figure S4. ^{1}H NMR spectrum of complex [{Au($C_6Cl_2F_3$)$_2$(μ-PPh_2)$_2$Au}$_2$] (**2**)

^{19}F NMR spectra (298K, $CDCl_3$)

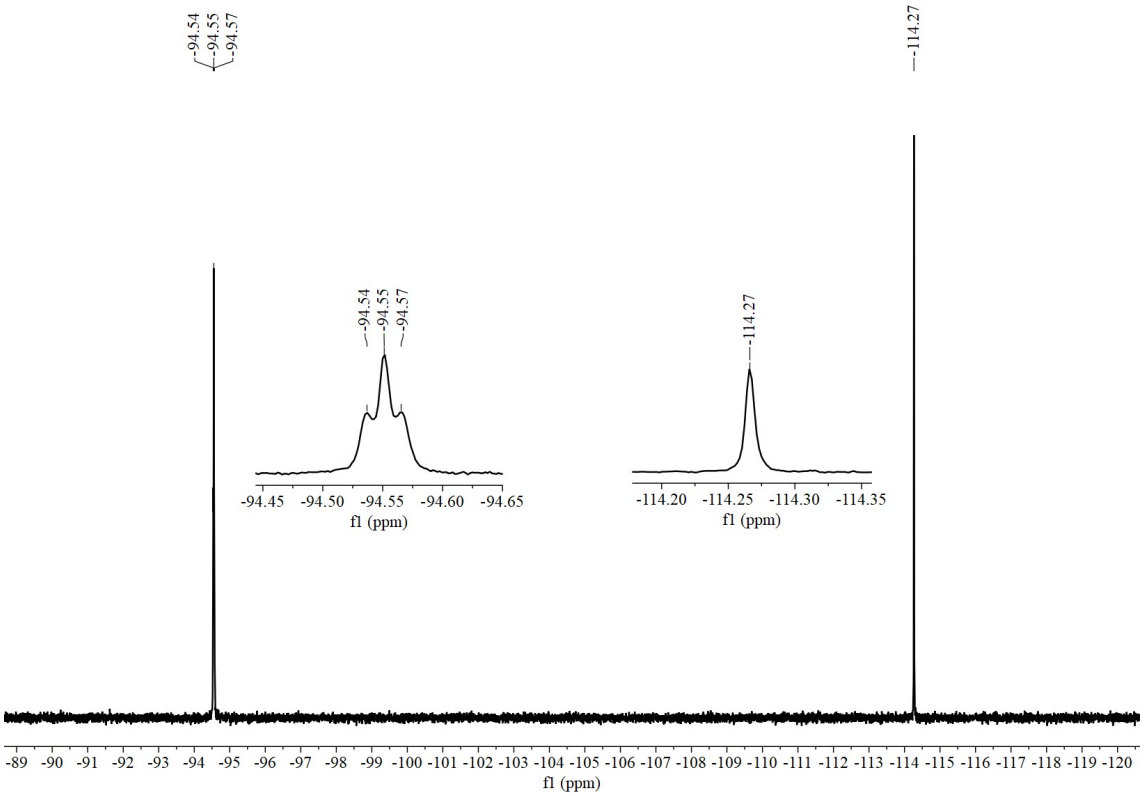

Figure S5. ^{19}F NMR spectrum of complex [{Au($C_6Cl_2F_3$)$_2$}$_2$(μ-PPh_2)$_2$] (**1**)

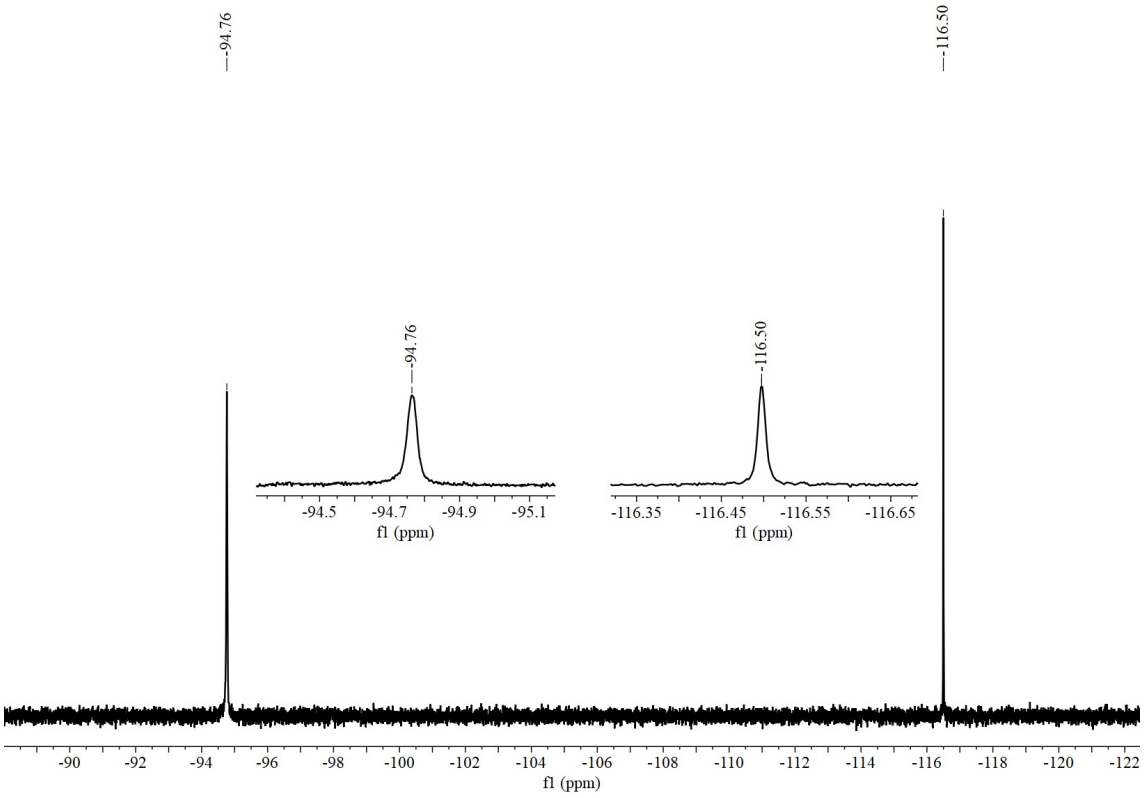

Figure S6. ^{19}F NMR spectrum of complex [{Au($C_6Cl_2F_3$)$_2$(μ-PPh_2)$_2$Au}$_2$] (**2**)

$^{31}P\{^{1}H\}$ NMR spectra (298K, $CDCl_3$)

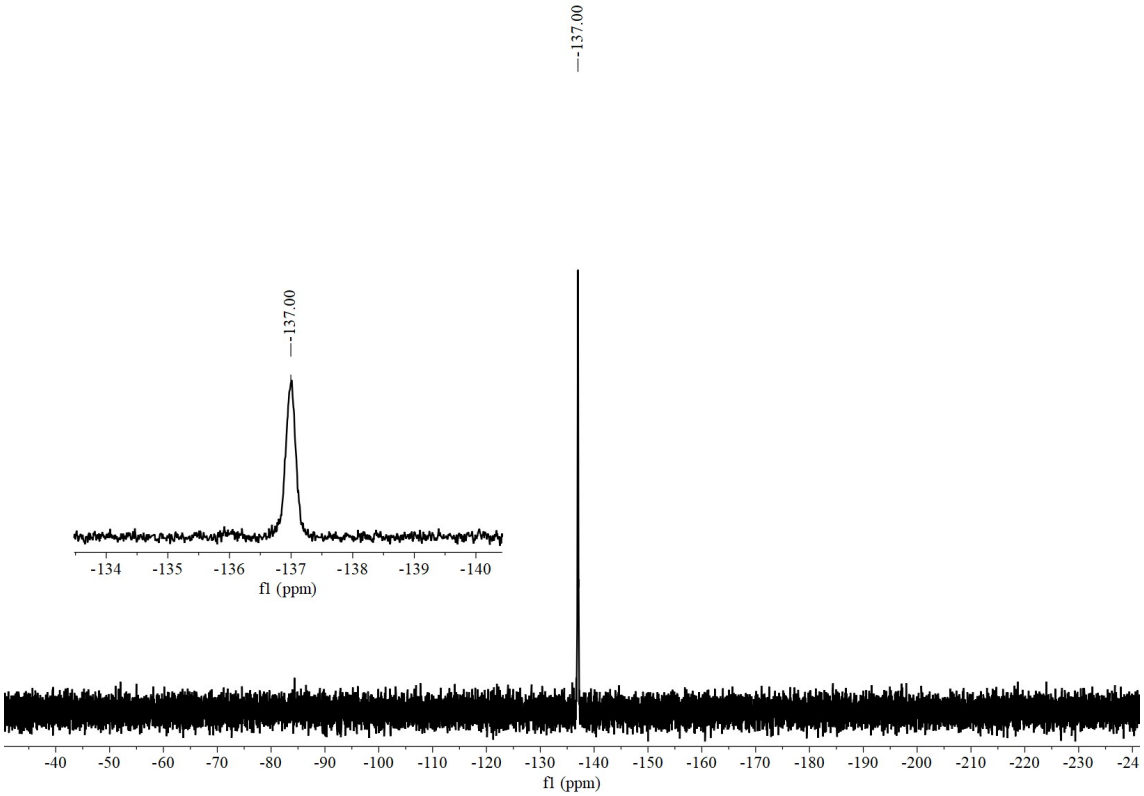

Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum of complex [{Au($C_6Cl_2F_3$)$_2$}$_2$(μ-PPh_2)$_2$] (**1**)

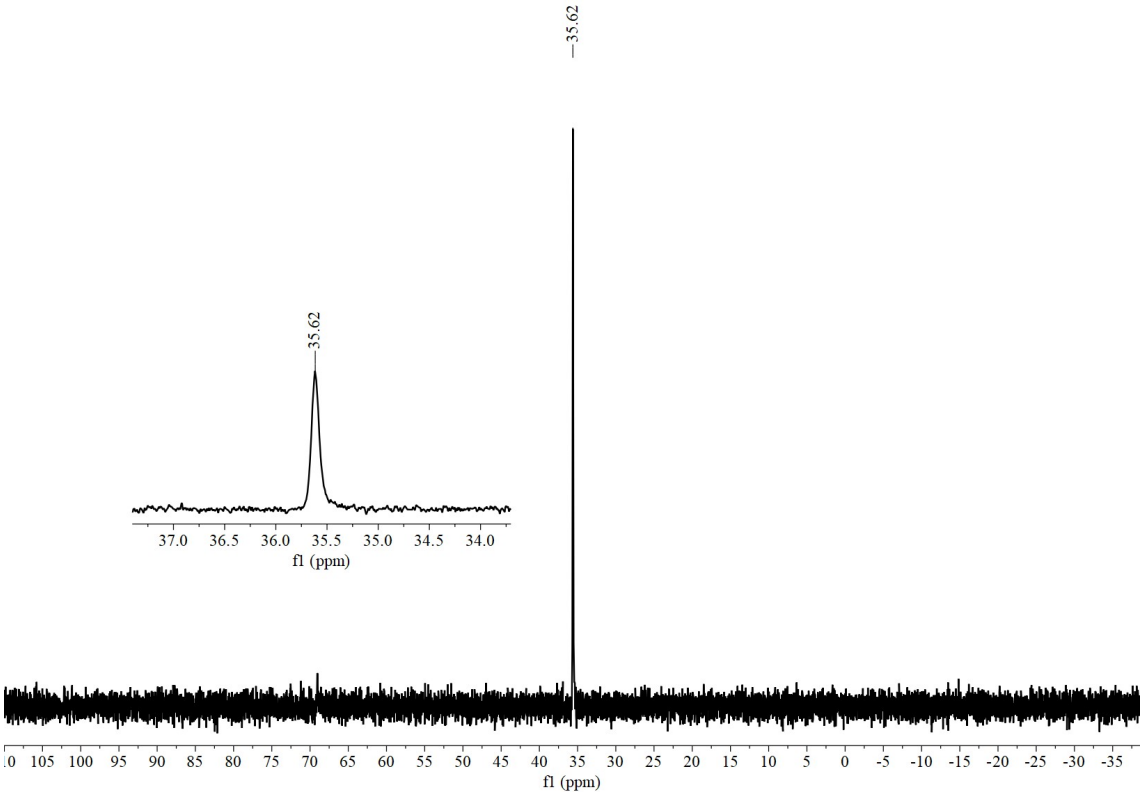

Figure S8. $^{31}P\{^{1}H\}$ NMR spectrum of complex [{Au($C_6Cl_2F_3$)$_2$(μ-PPh_2)$_2$Au}$_2$] (**2**)

High resolution mass spectra (HRMS)

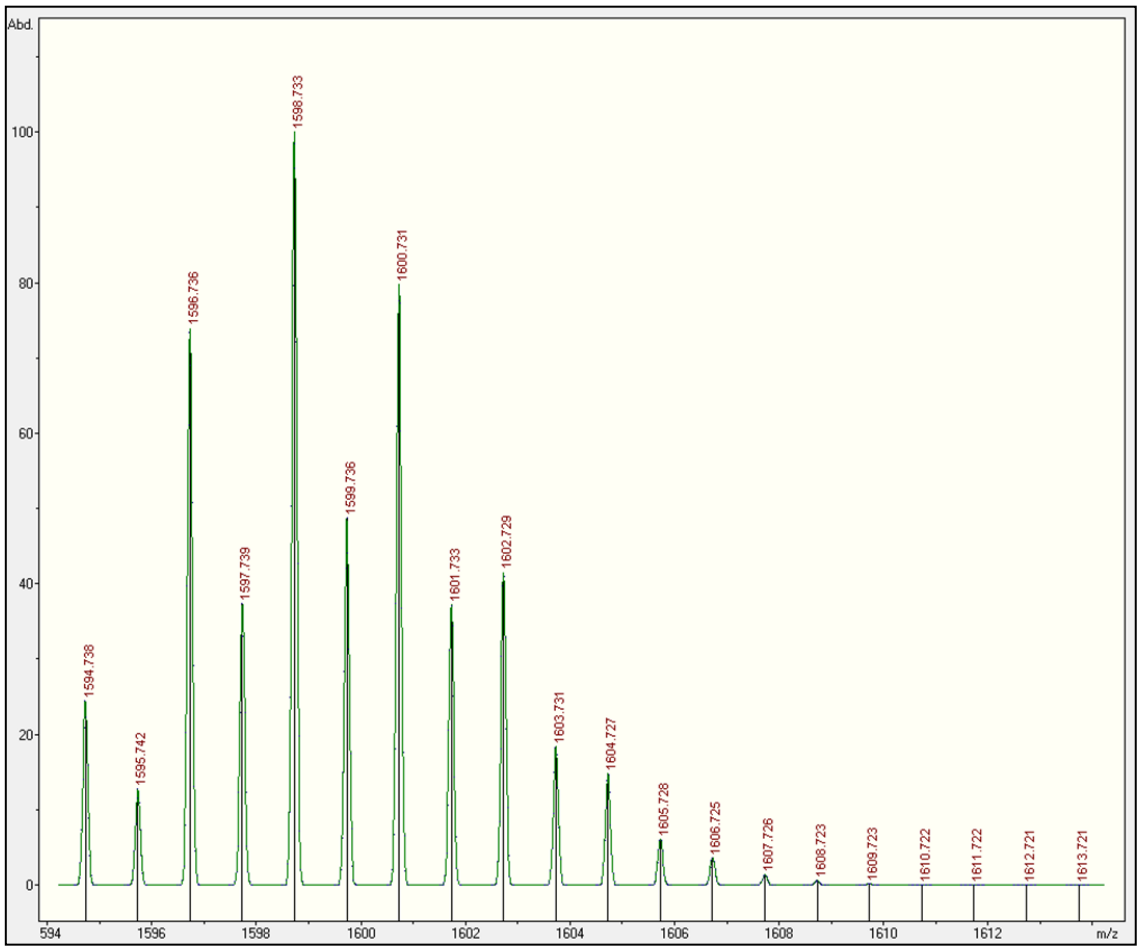

Figure S9. Simulated isotope pattern of $(M+Cl)^-$ for compound **1**. Ion formula: $C_{48}H_{20}Au_2Cl_9F_{12}P_2$.

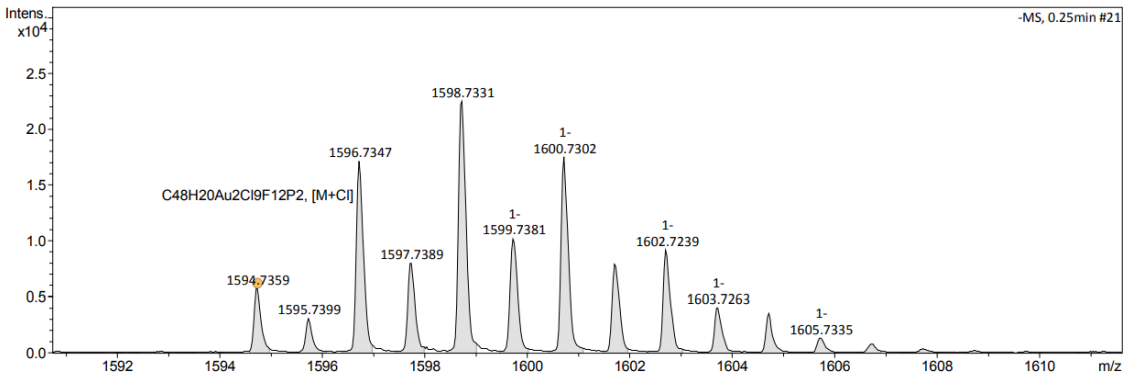

Figure S10. HR-MS (ESI-) for compound **1**. Ion formula: $C_{48}H_{20}Au_2Cl_9F_{12}P_2$. $[\{Au(C_6Cl_2F_3)_2\}_2(\mu\text{-}PPh_2)_2Cl]^-$: 1594.738223 Da. Measured m/z= 1594.7359 $(M+Cl)^-$.

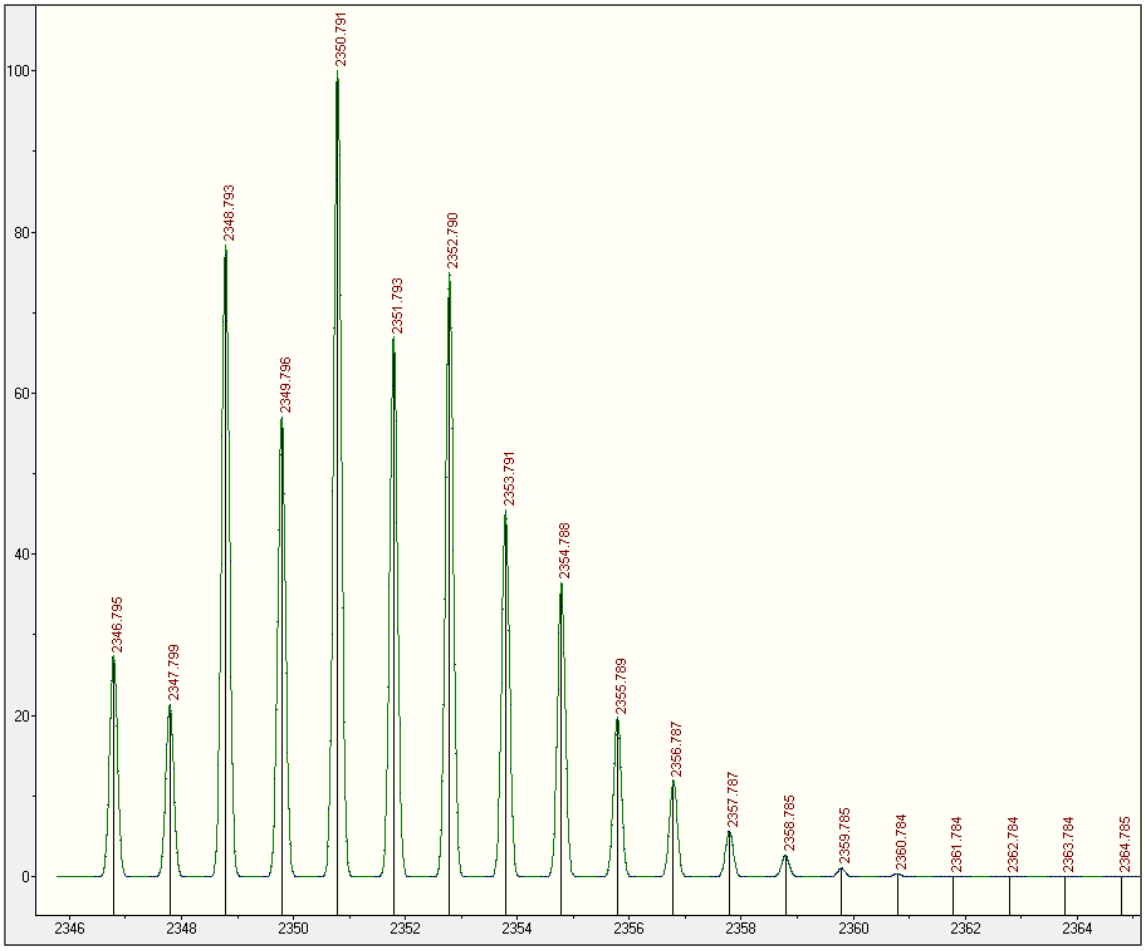

Figure S11. Simulated isotope pattern of $(M+Na)^+$ for compound **2**. Ion formula: $C_{72}H_{40}Au_4Cl_8F_{12}P_4Na_1$

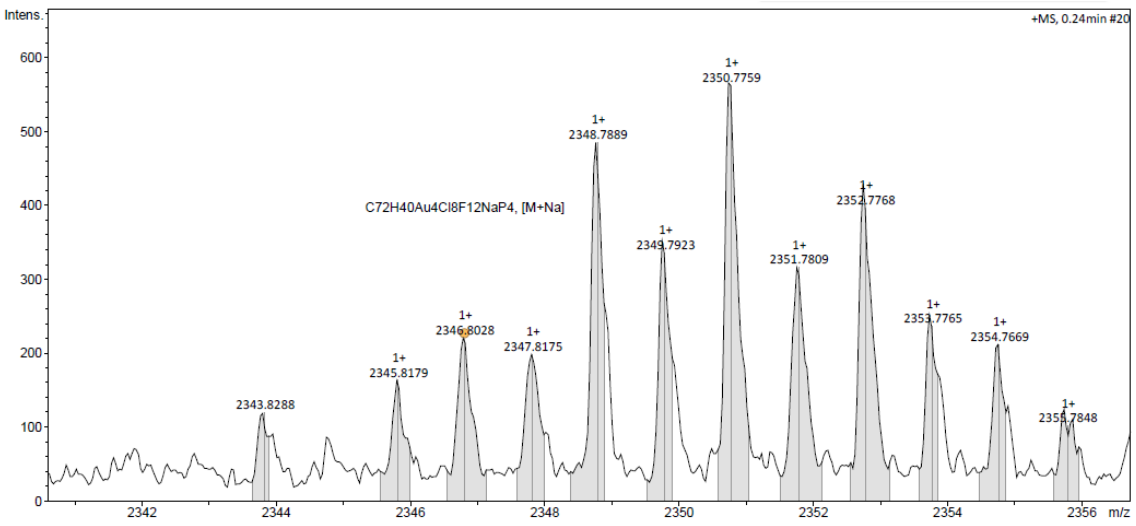

Figure S12. HR-MS (ESI+) for compound **2**. Ion formula: $C_{72}H_{40}Au_4Cl_8F_{12}P_4Na_1$. $[[\{Au(C_6Cl_2F_3)_2(\mu\text{-}PPh_2)_2Au\}_2]Na]^+$: 2346.795203 Da. Measured m/z= 2346.8028 $(M+Na)^+$.

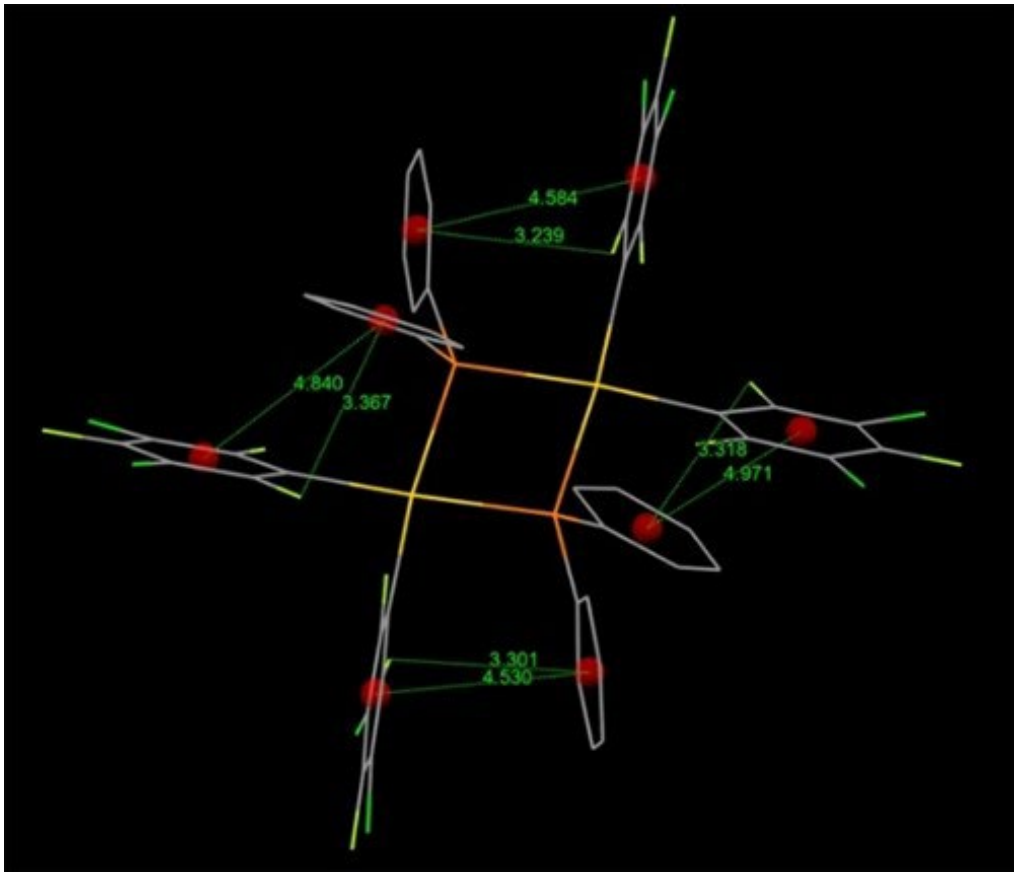

Figure S13. Shortest F···centroid distances found for π-π interactions in **1**. Distances are indicated in Å.

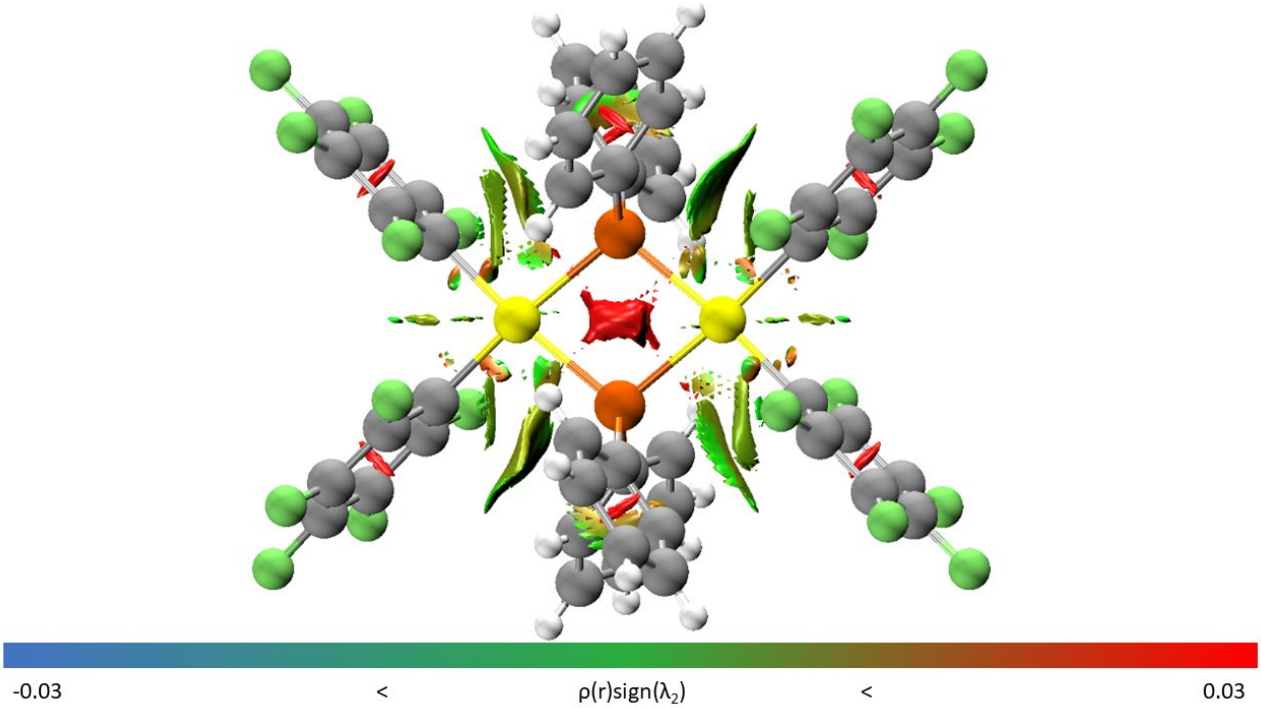

Figure S14. NCI-index isosurfaces from X-Ray for [{Au(C_6F_5)$_2$}$_2$(μ-PPh_2)$_2$] complex. The isosurface value of s equals 0.5 a.u. and the electron density is such that ϱ ≤ 0.015 a.u. The scale for the relative magnitude of the interactions is presented at the bottom of the figure.

Table S1. Crystallographic data and structure refinement details for compounds **1** and **2**.

Compound	1	2
Empirical formula	$C_{48}H_{20}Au_2Cl_8F_{12}P_2$	$C_{72}H_{40}Au_4Cl_8F_{12}P_4$
Formula weight	1564.11	2328.381
Temperature/K	100(2)	100(2)
Crystal system	Monoclinic	Orthorhombic
Space group	$P2_1/n$	Pbca
a/Å	13.1373(18)	23.750(2)
b/Å	18.0771(16)	22.049(2)
c/Å	22.9937(19)	27.057(3)
α/º	90	90
β/º	94.556(3)	90
γ/º	90	90
Volume/Å^3	5443.4(8)	14169(2)
Z	4	8
ρ_{calcd}/g·cm^{-3}	1.909	2.183
μ/mm^{-1}	5.910	8.725
F(000)	2960	8736
Crystal size/mm^3	0.255x0.211x0.079	0.139 x 0.138 x 0.074
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/º	5.788 to 55.876	5.67 to 55.85
Index rages	-17<=h<=17 -23<=k<=23 -30<=l<=30	-31<=h<=31 -29<=k<=29 -35<=l<35
Reflections collected	137218	709062
Independent reflections	12985 [R(int) = 0.0525]	16899 [R(int) = 0.0271]
Completeness to theta = 25.242°	99.4 %	99.8 %
Data/restraints/parameters	12985 / 0 / 649	16899 / 0 / 901
Goodness-of-fit in F^2	1.095	1.054
Final R indexes [I>2sigma(I)]	R1 = 0.0332 wR2 = 0.0683	R1 = 0.0511 wR2 = 0.1545
R indices (all data)	R1 = 0.0399 wR2 = 0.0710	R1 = 0.0637 wR2 = 0.1617
Largest peak and hole/e·Å^{-3}	2.27 and -1.57	4.467 and -8.373