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Triphenylene Chromophore Enhances Emission in Au/Cu Heterometallic Complexes

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Supporting Information

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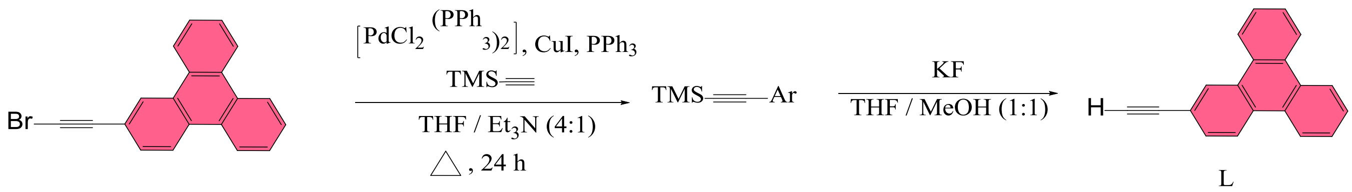
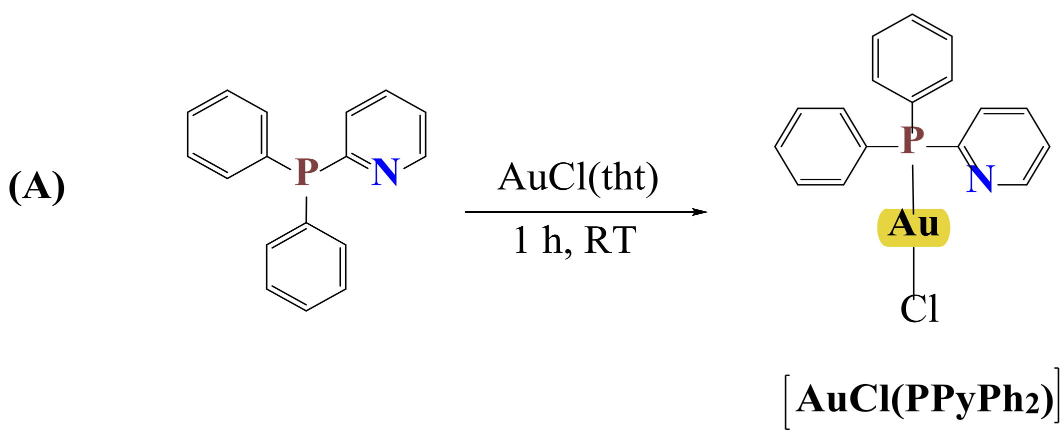


Scheme S1. Synthesis of 2-ethynyltriphenylene ligand (L).



Scheme S2. Synthesis of gold (I) precursor.

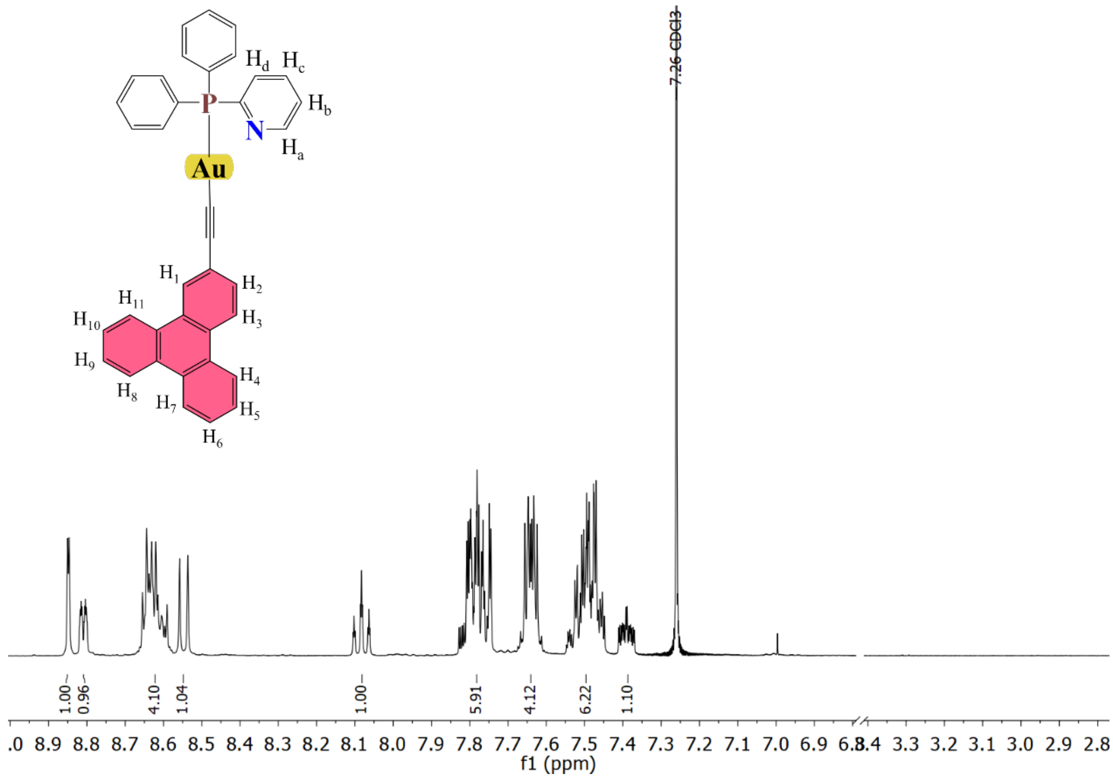


Figure S1. [1]H-NMR spectra of **[Au(L)(PPyPh$_2$)]** in CDCl$_3$.

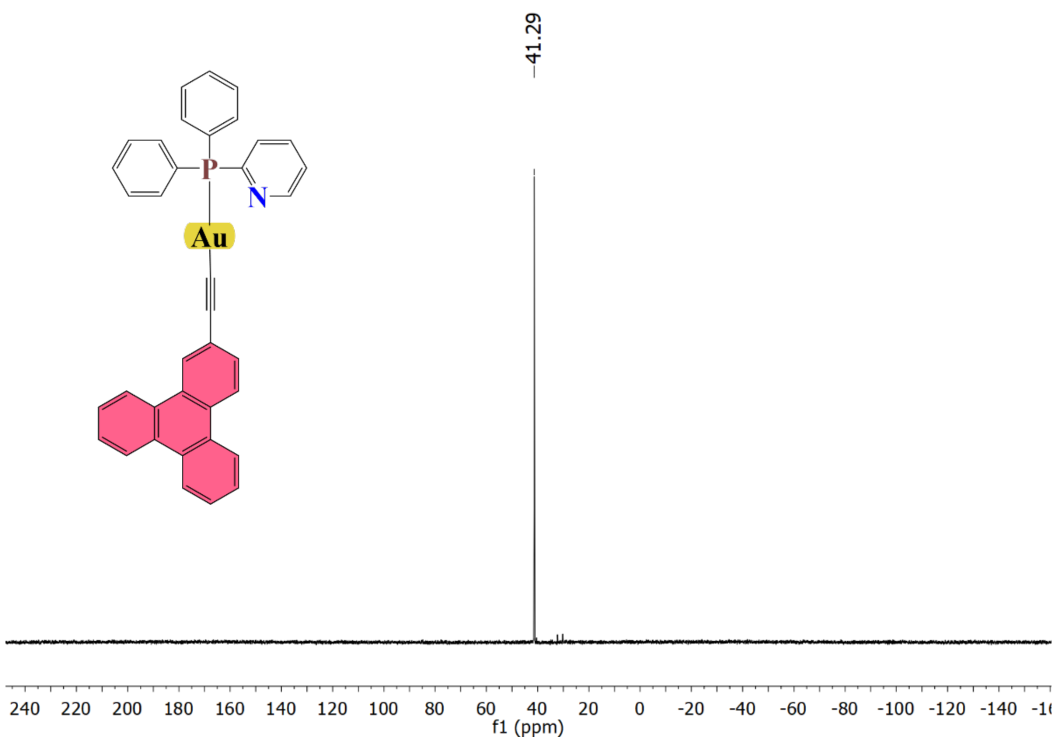


Figure S2. [31]P-NMR spectra of **[Au(L)(PPyPh$_2$)]** in CDCl$_3$.

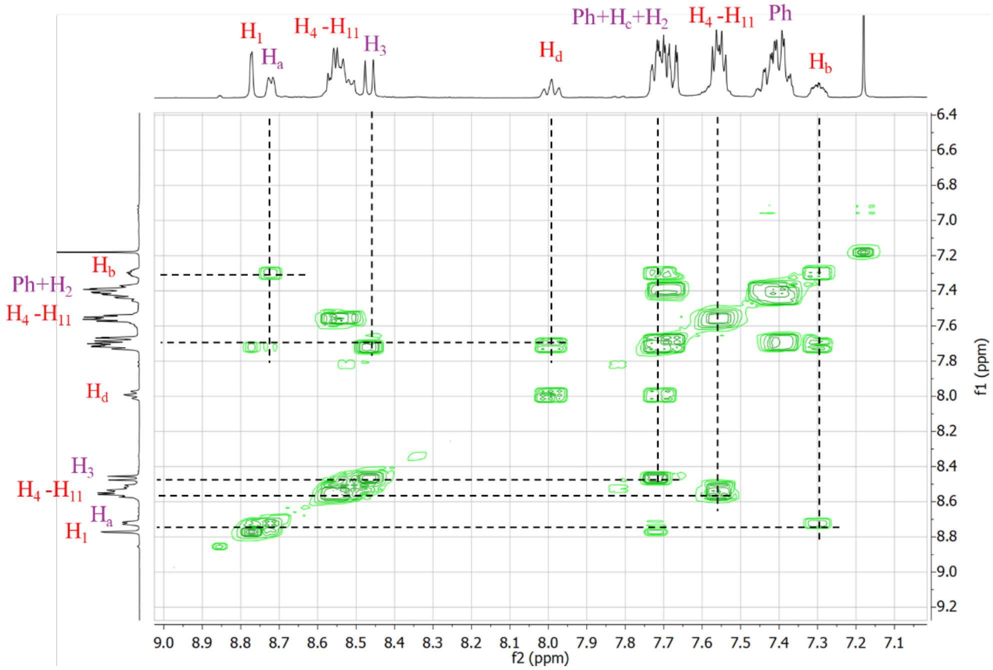


Figure S3. ^{1}H–^{1}H COSY NMR of the complex **[Au(L)(PPyPh$_2$)]** in $CDCl_3$.

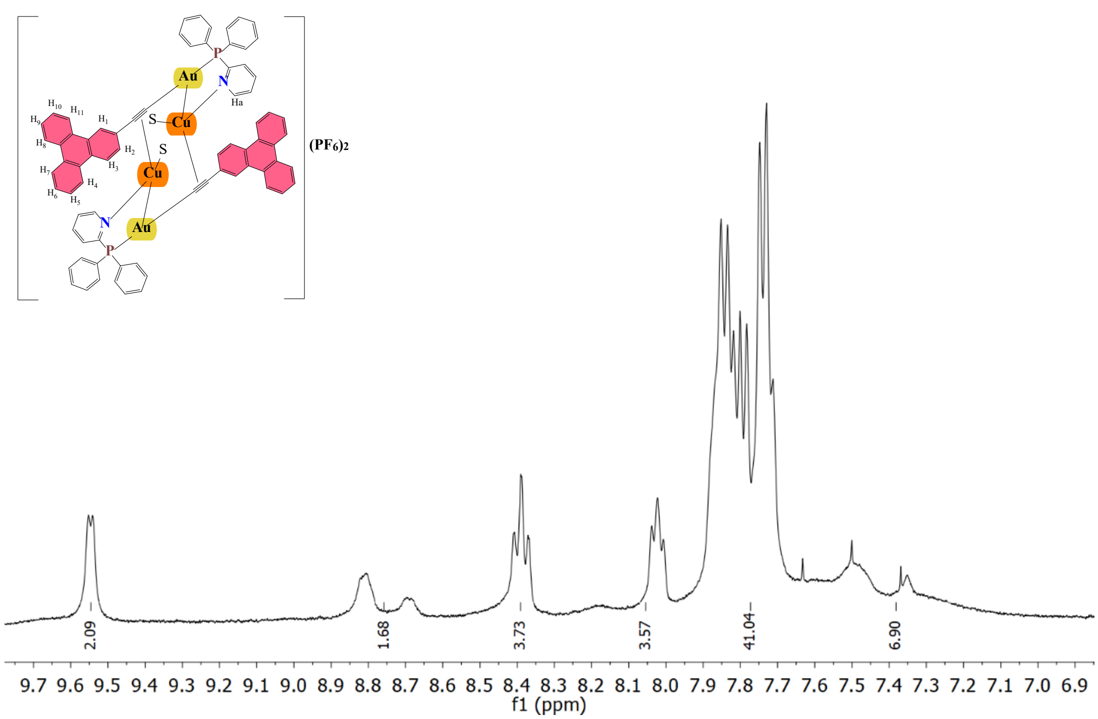


Figure S4. ^{1}H-NMR spectra of **Cu1a** in CD_3COCD_3.

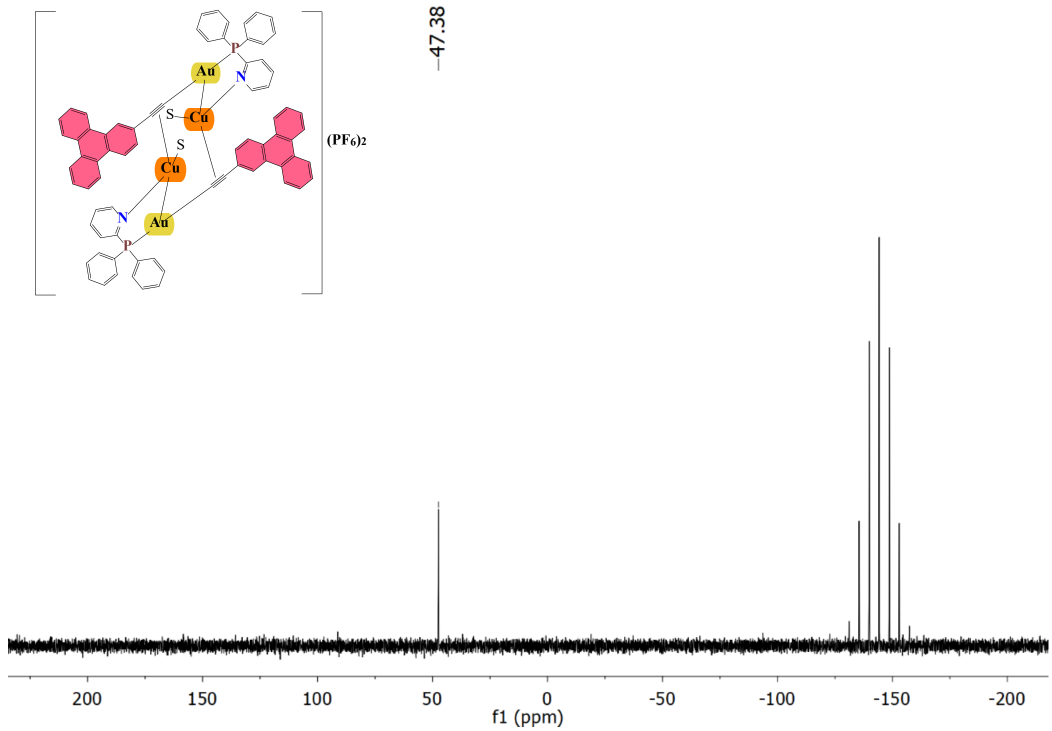


Figure S5. ^{31}P-NMR spectra of **Cu1a** in CD_3COCD_3.

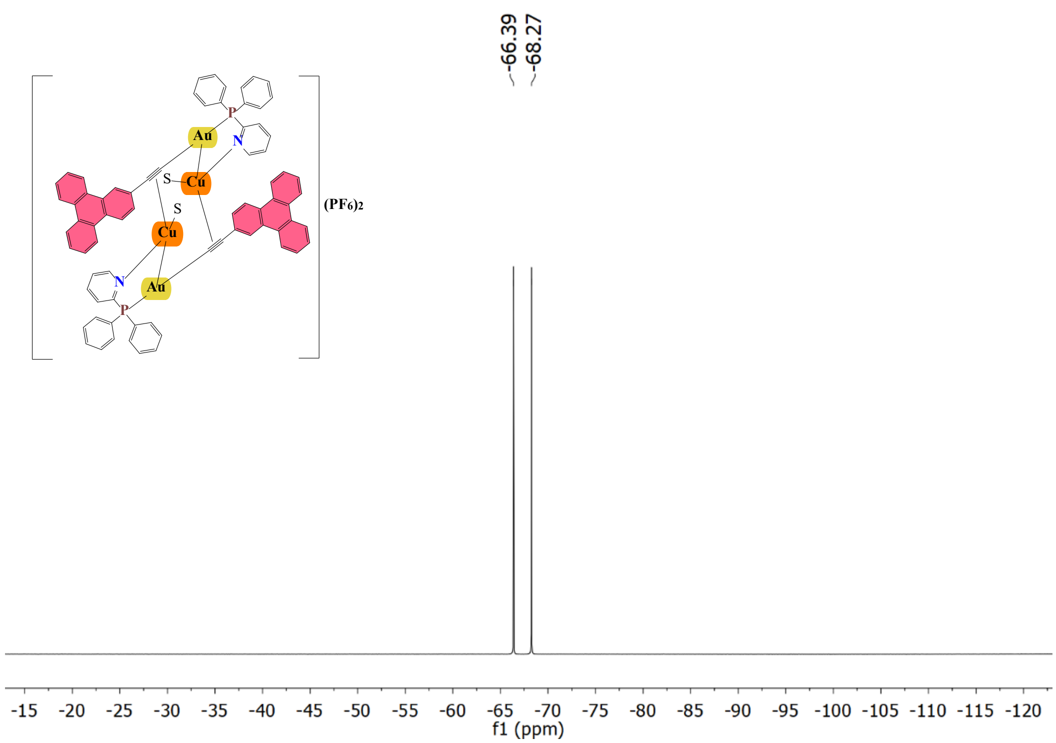


Figure S6. ^{19}F-NMR spectra of **Cu1a** in CD_3COCD_3.

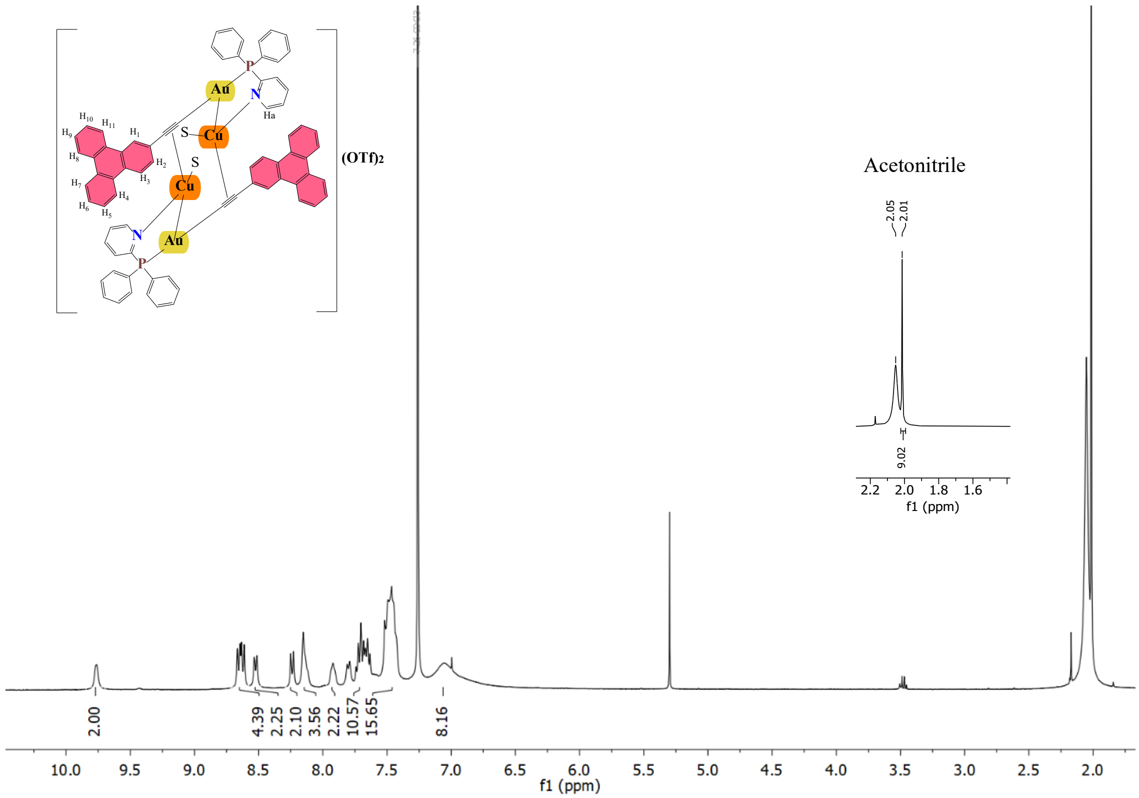


Figure S7. ^{1}H-NMR spectra of **Cu1b** in $CDCl_3$.

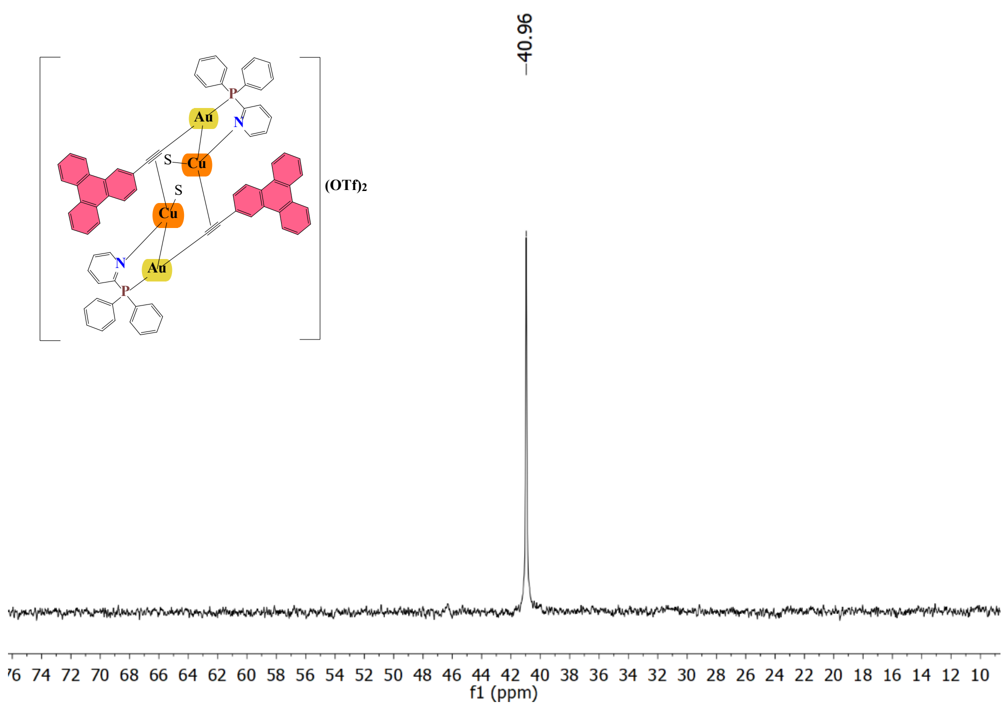


Figure S8. ^{31}P-NMR spectra of **Cu1b** in $CDCl_3$.

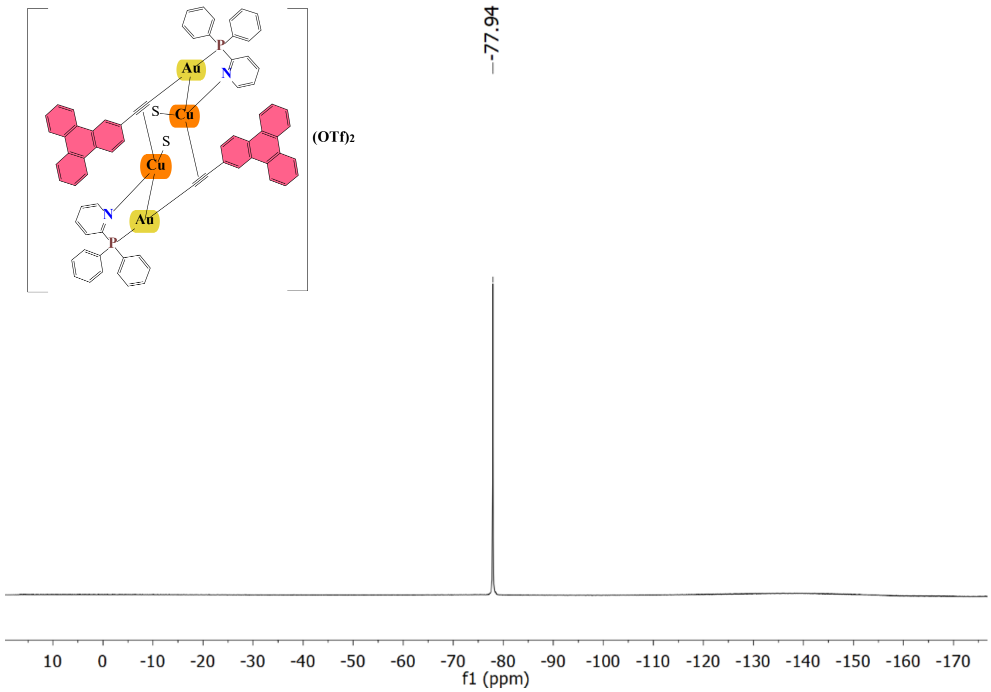


Figure S9. [19]F-NMR spectra of **Cu1b** in $CDCl_3$.

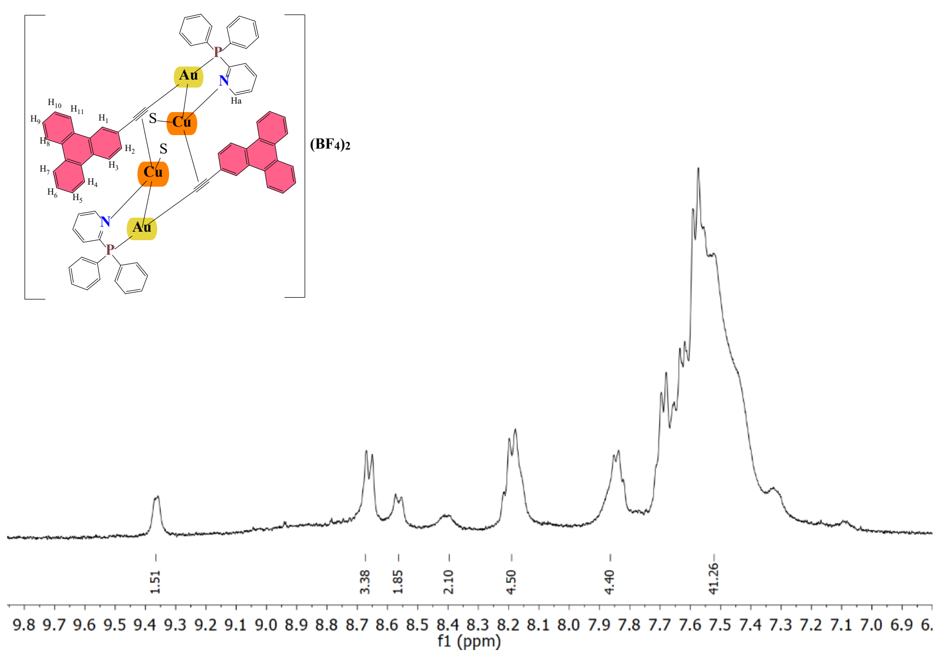


Figure S10. [1]H-NMR spectra of **Cu1c** in CD_3COCD_3.

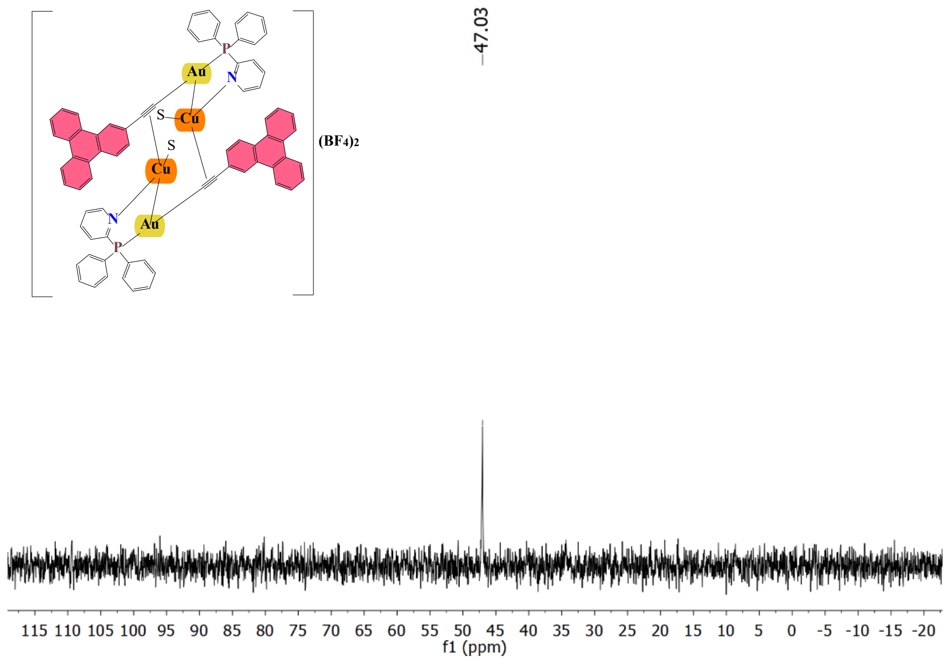


Figure S11. ^{31}P-NMR spectra of **Cu1c** in CD_3COCD_3.

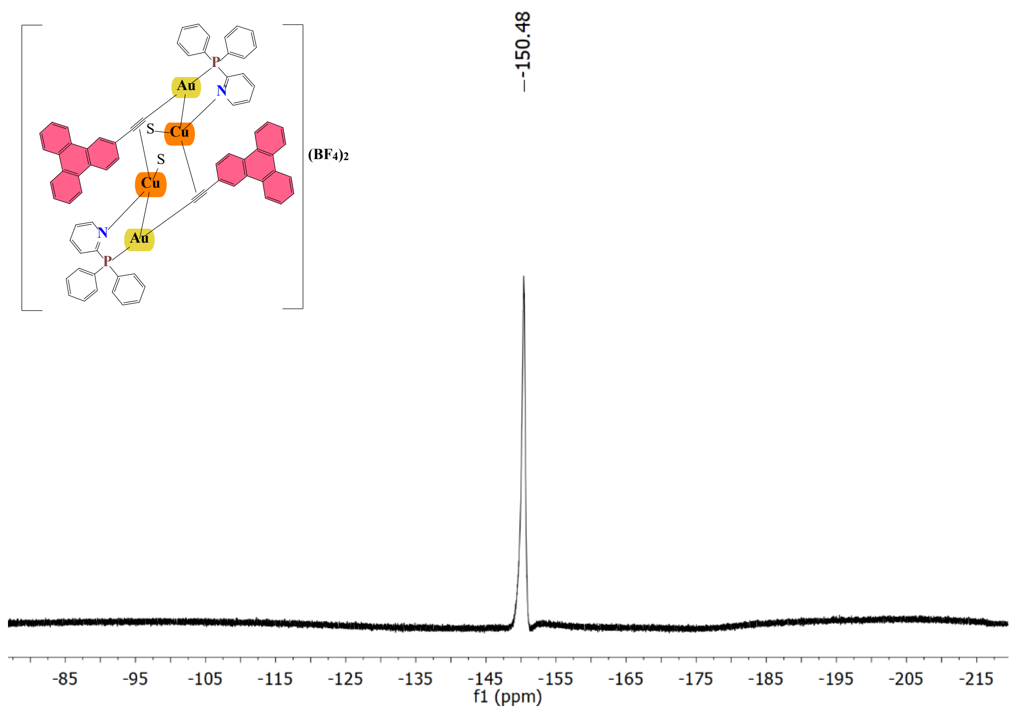


Figure S12. ^{19}F-NMR spectra of **Cu1c** in CD_3COCD_3.

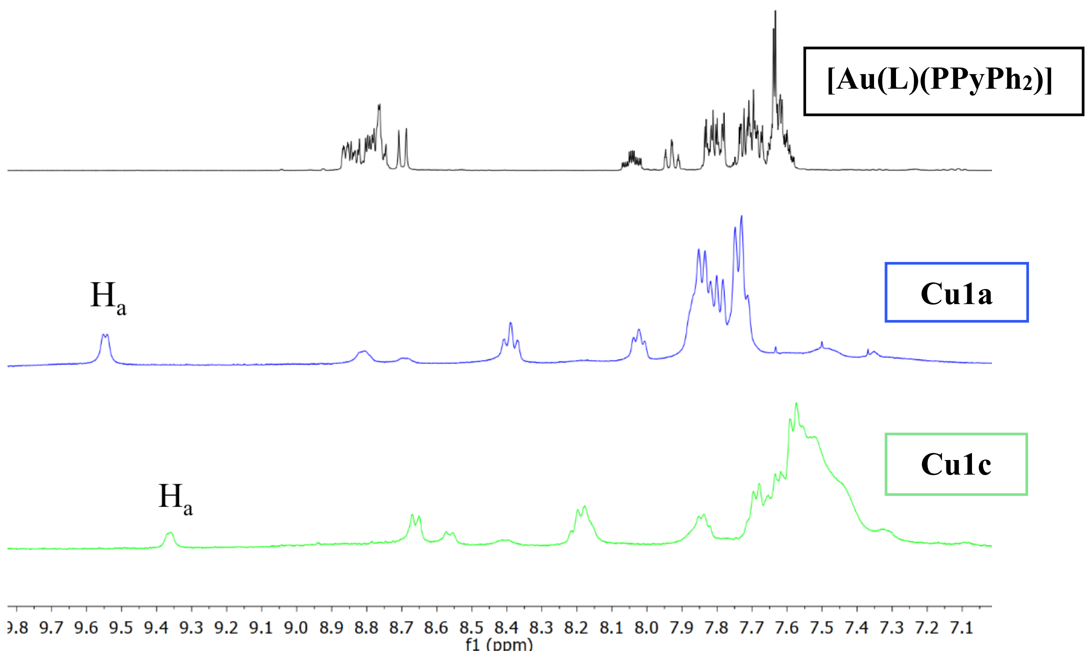


Figure S13. [1]H NMR spectra comparison between **[Au(L)(PPyPh$_2$)]** and **Cu1a, Cu1c** dimers in CD_3COCD_3.

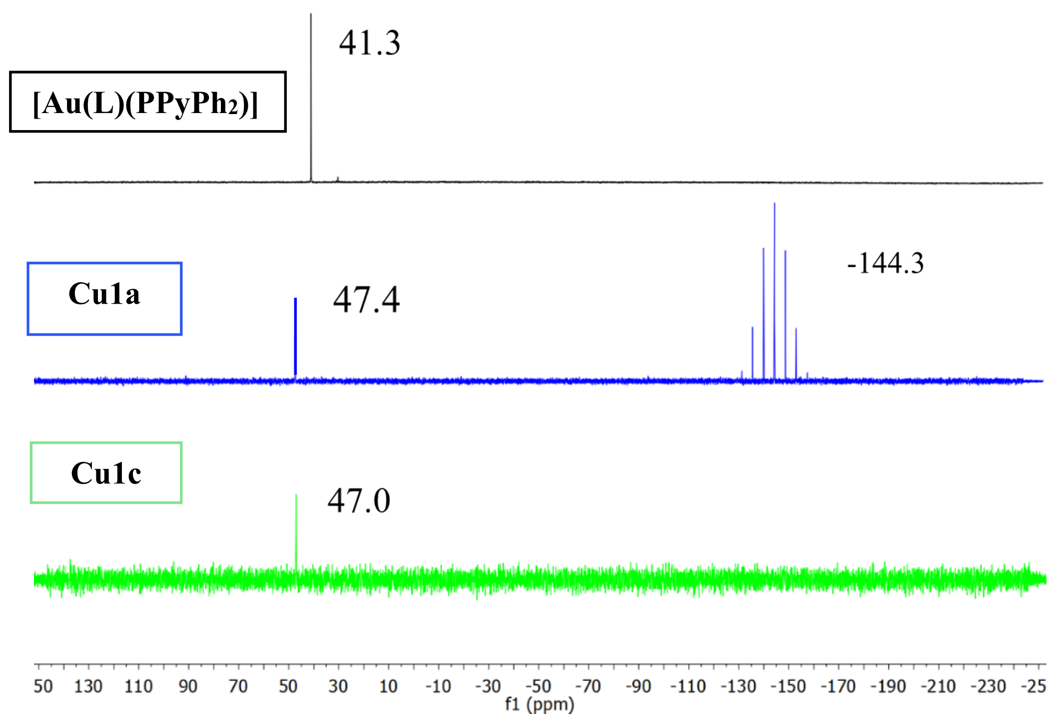


Figure S14. [31]P{[1]H} NMR comparison spectra between the precursor **[Au(L)(PPyPh$_2$)]** and the heterometallics **Cu1a** and **Cu1c** in CD_3COCD_3.

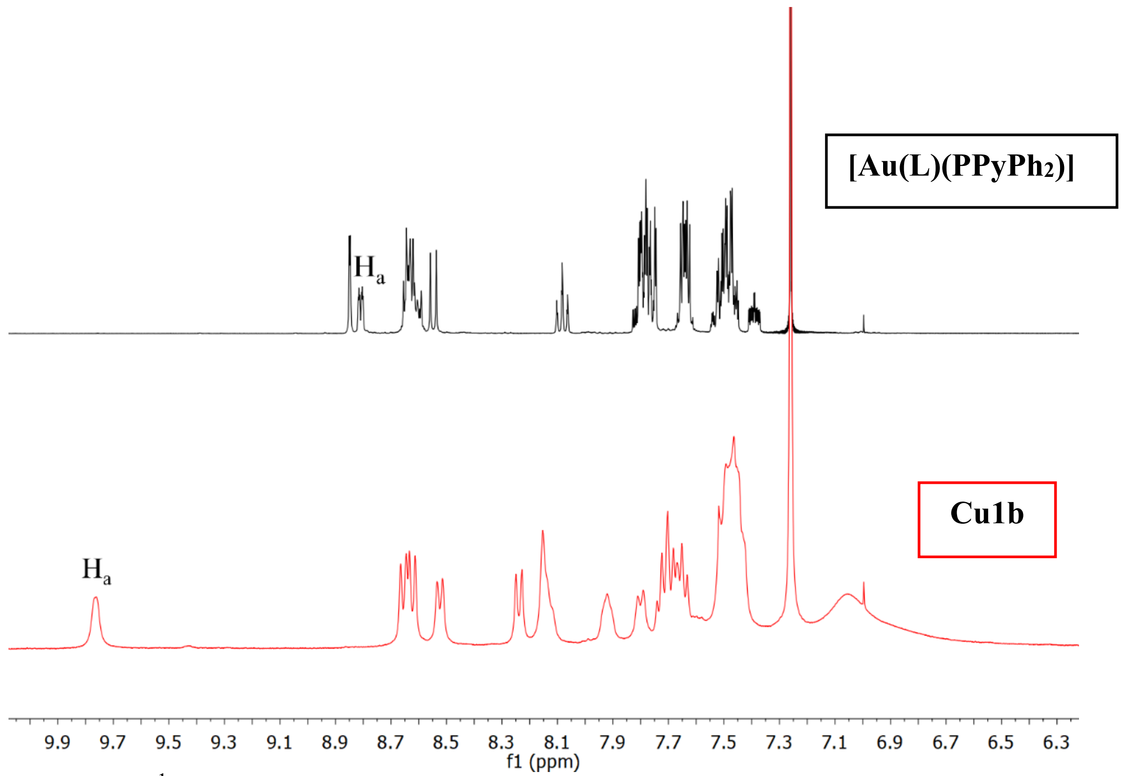


Figure S15. ^{1}H NMR spectra comparison between **[Au(L)(PPyPh$_2$)]** and **Cu1b** dimers in $CDCl_3$.

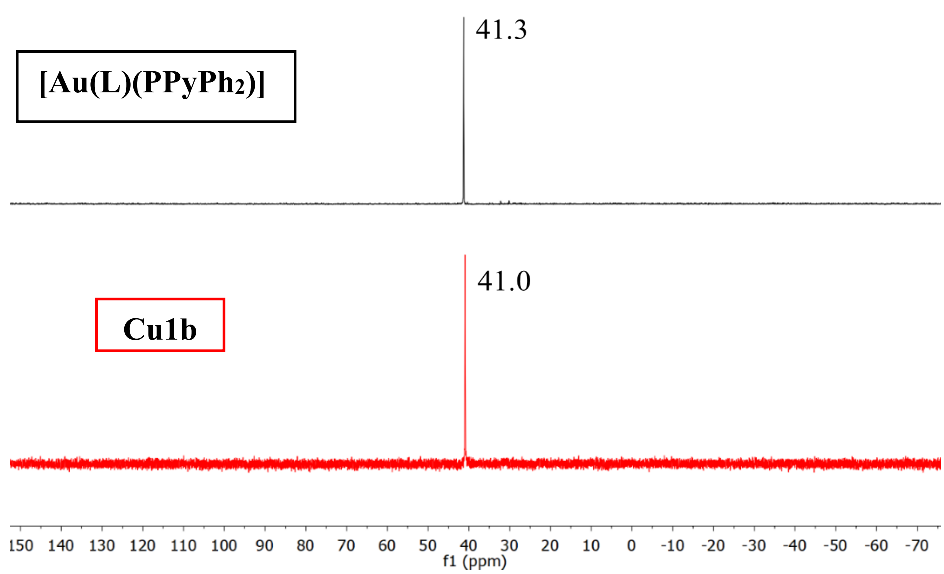


Figure S16. ^{31}P{^{1}H} NMR comparison spectra between the precursor **[Au(L)(PPyPh$_2$)]** and the heterometallic **Cu1b** in $CDCl_3$.

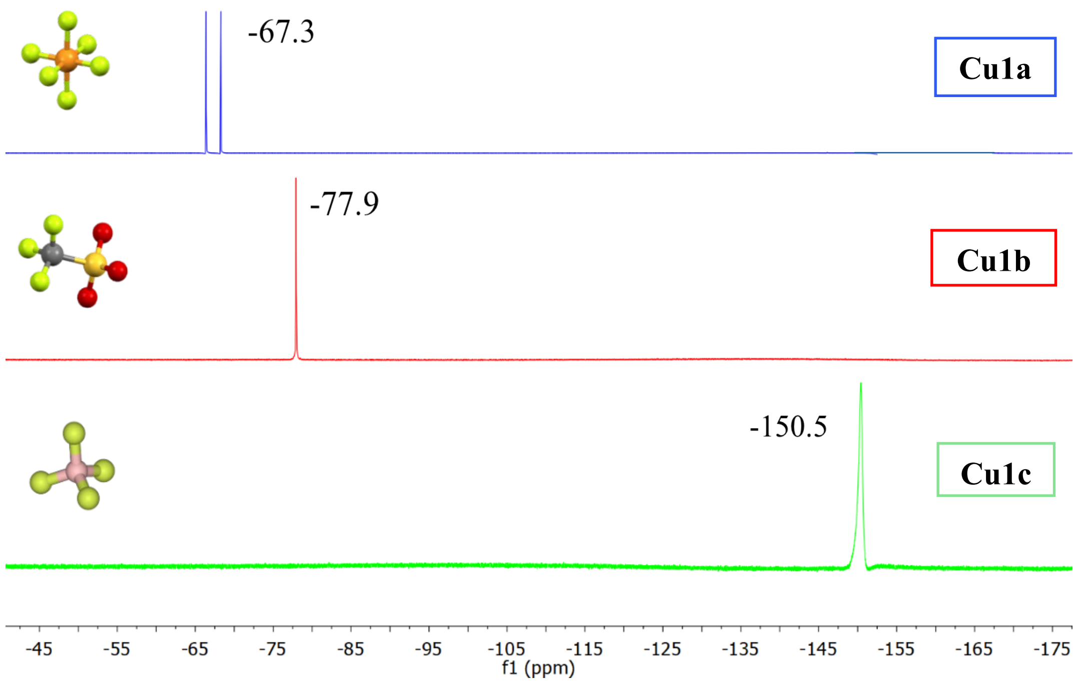


Figure S17. [19]F NMR spectra of **3.1b** in $CDCl_3$ and **3.1a-3.1c** in CD_3COCD_3.

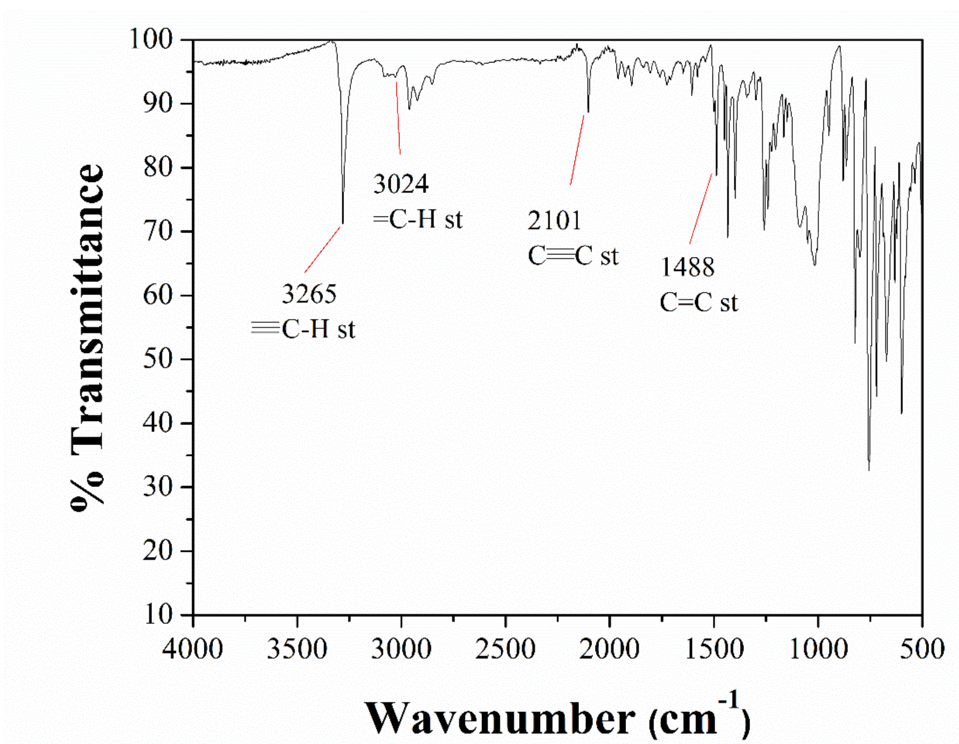


Figure S18. FT-IR Spectra of **L**.

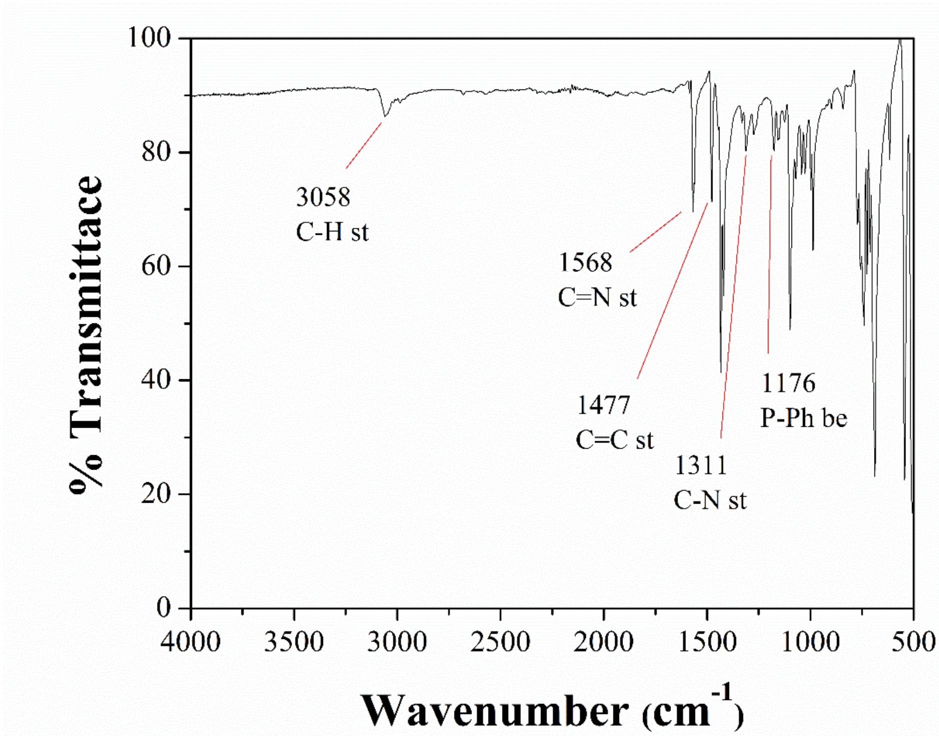


Figure S19. FT-IR Spectra of **[Au(L)(PPyPh$_2$)]**.

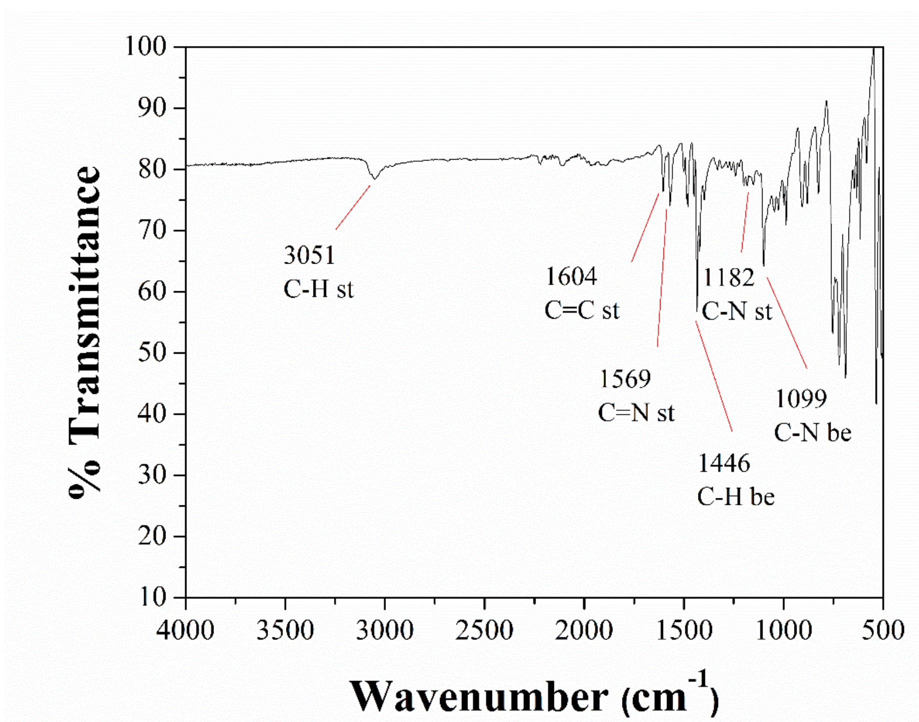


Figure S20. FT-IR Spectra of **[Au(L)(PPyPh$_2$)]**.

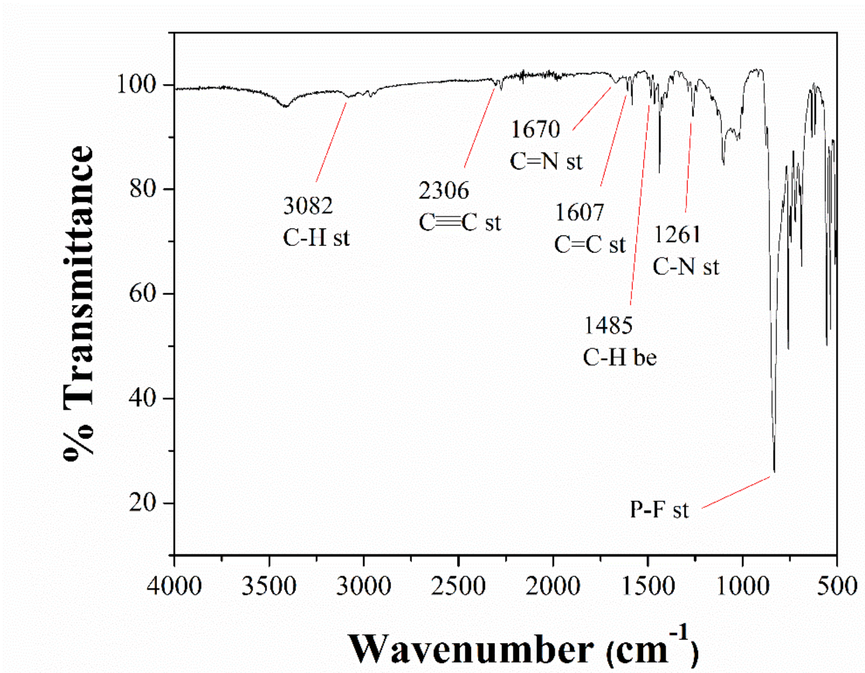


Figure S21. FT-IR Spectra of **Cu1a**.

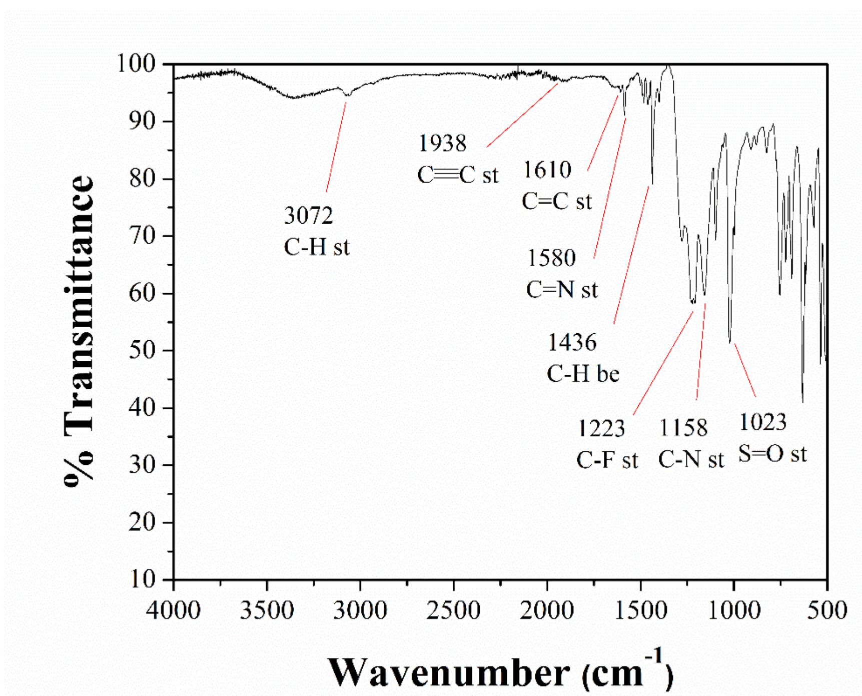


Figure S22. FT-IR Spectra of **Cu1b**.

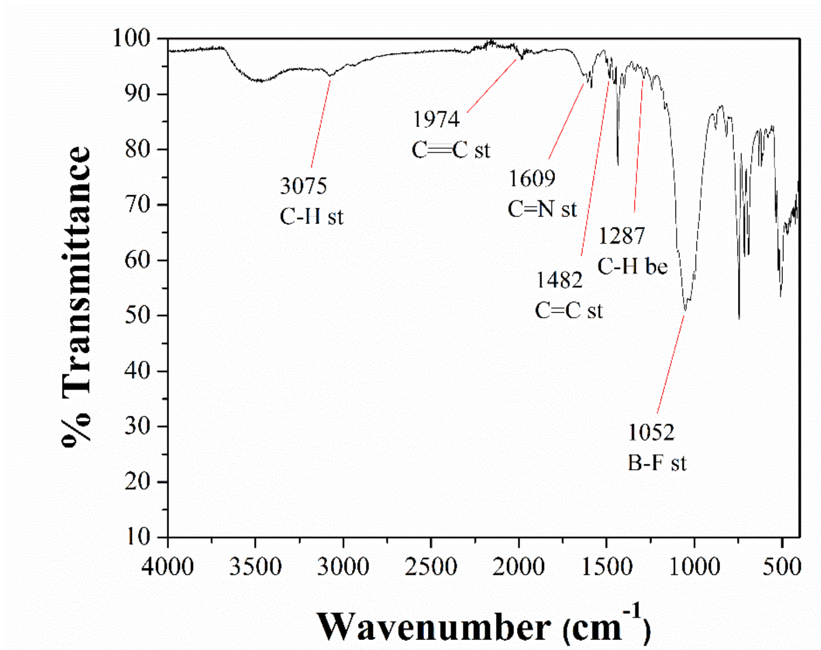


Figure S23. FT-IR Spectra of **Cu1c**.

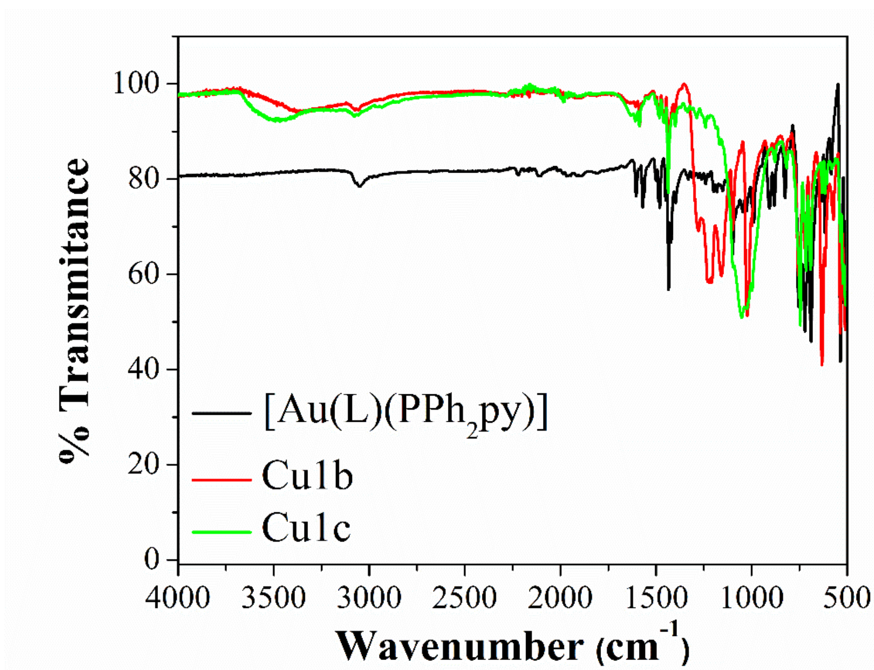


Figure S24. FT-IR comparison spectra between the precursor **[Au(L)(PPyPh$_2$)]** and the heterometallic complexes **Cu1b** and **Cu1c**.

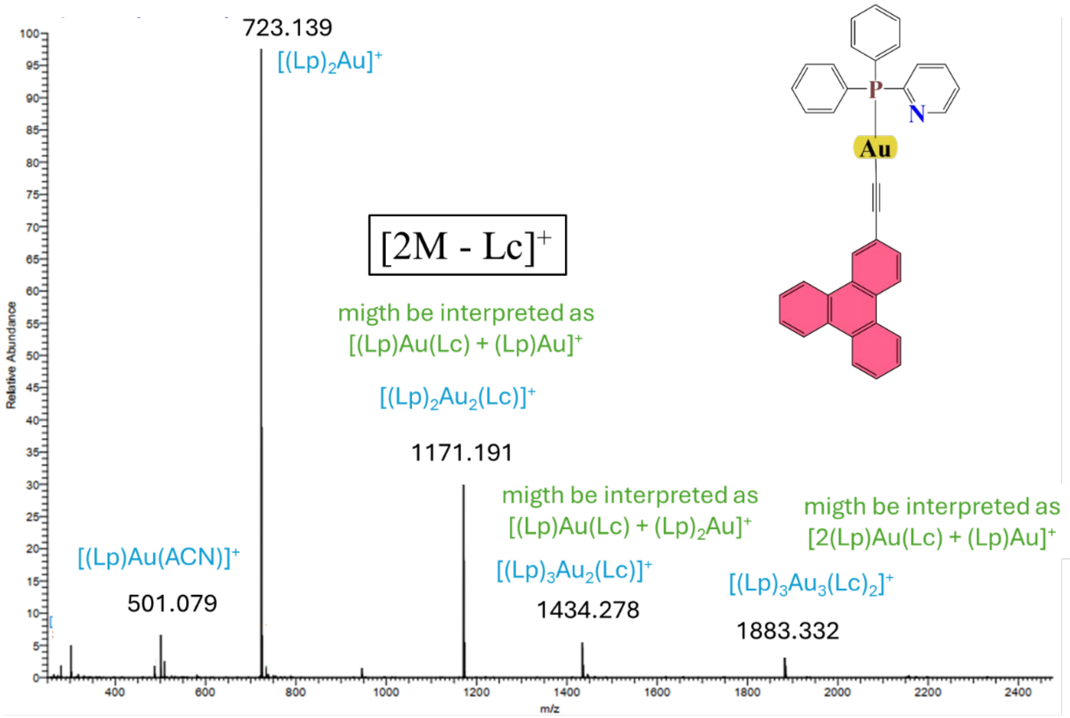


Figure S25. ESI(+) mass spectra of **[Au(L)(PPyPh2)]**, Lp = PPyPh2, L= chromophore ligand $C_{20}H_{11}$.

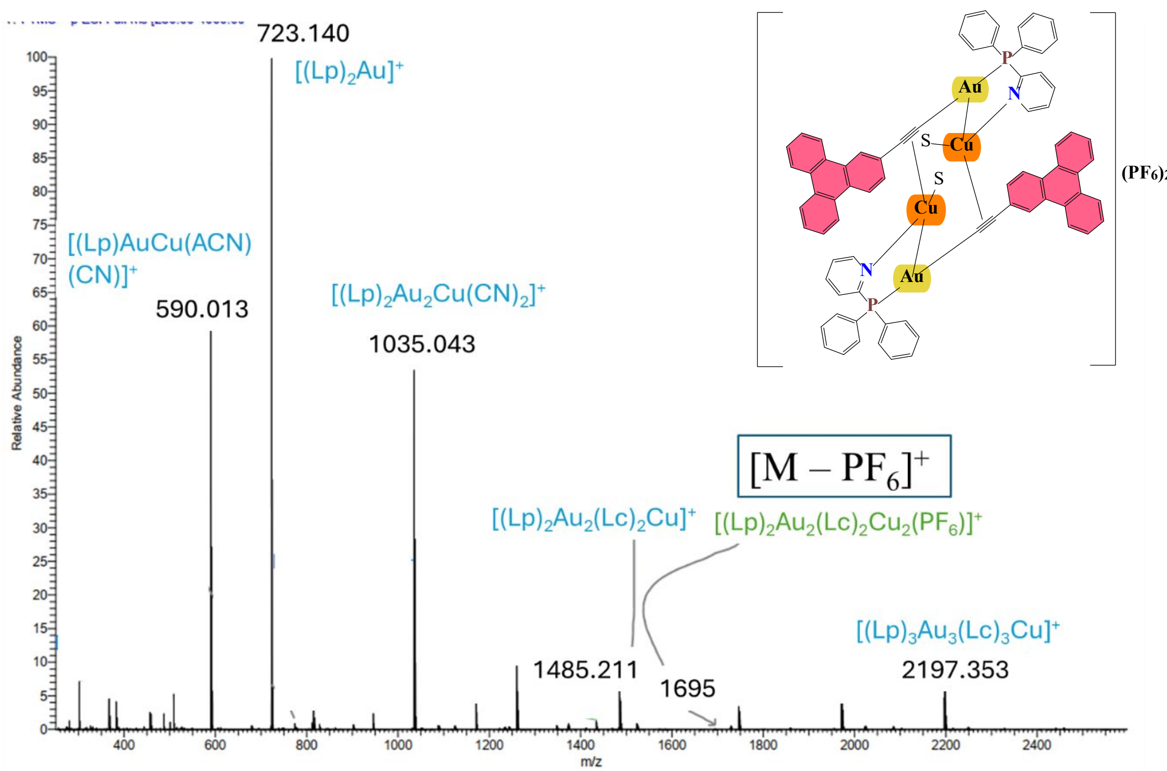


Figure S26. ESI(+) mass spectra of **Cu1a**, Lp = PPyPh2, L= chromophore ligand $C_{20}H_{11}$.

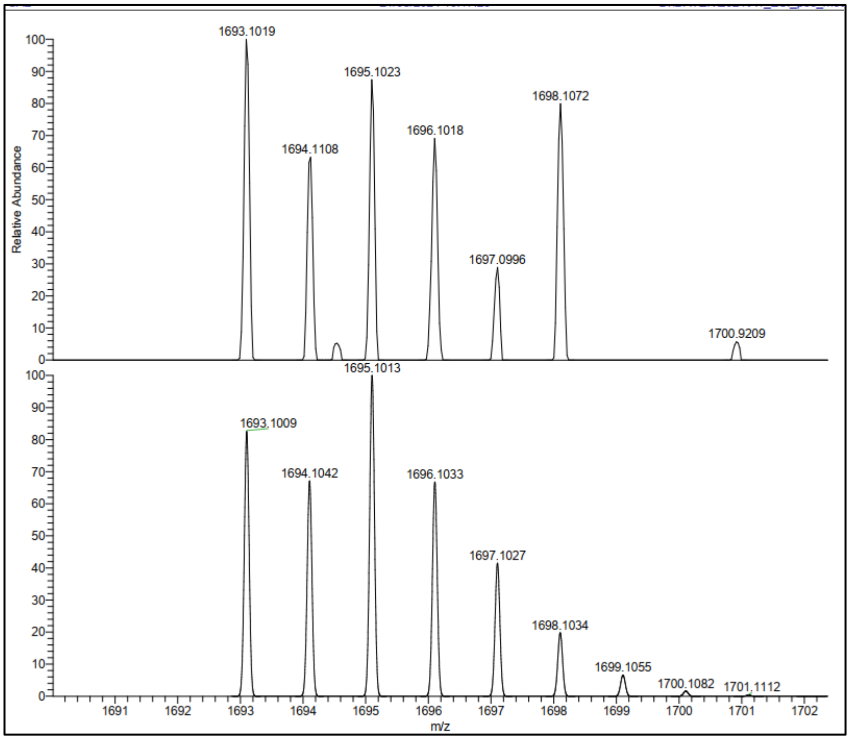


Figure S27. Above: Experimental isotopic distribution for the signal assigned to [**Cu1a** – PF_6]$^+$. below: Calculated isotopic mass distribution for [**Cu1a** – PF_6]$^+$ according to its elemental composition $C_{74}H_{50}N_2P_3Cu_2Au_2F_6$.

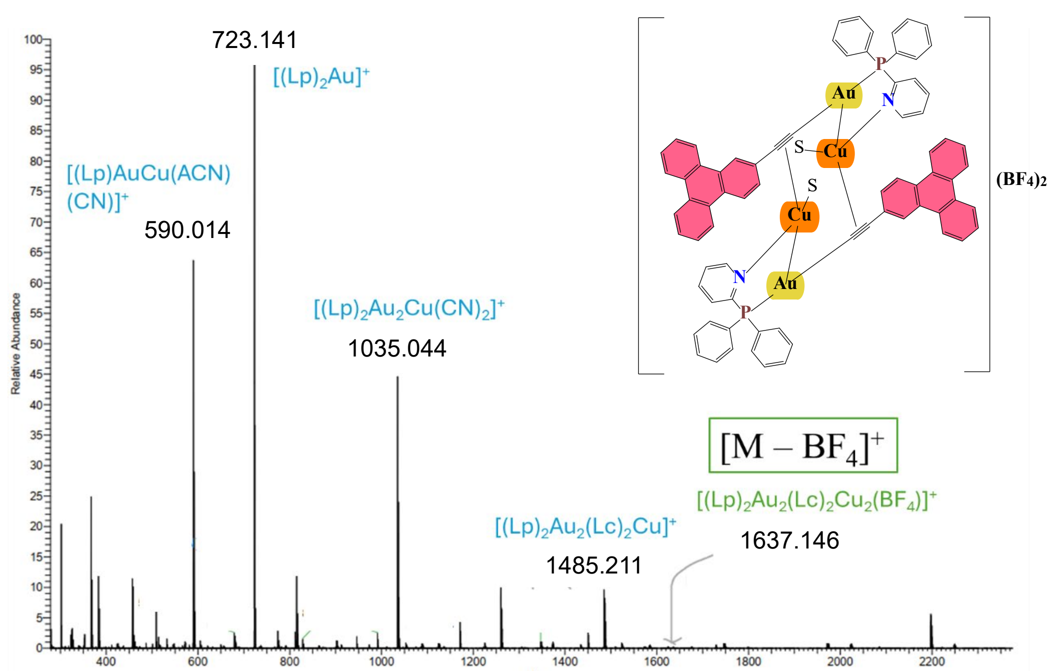


Figure S28. ESI(+) mass spectra of **Cu1c**, Lp = $PPyPh_2$, L= chromophore ligand $C_{20}H_{11}$.

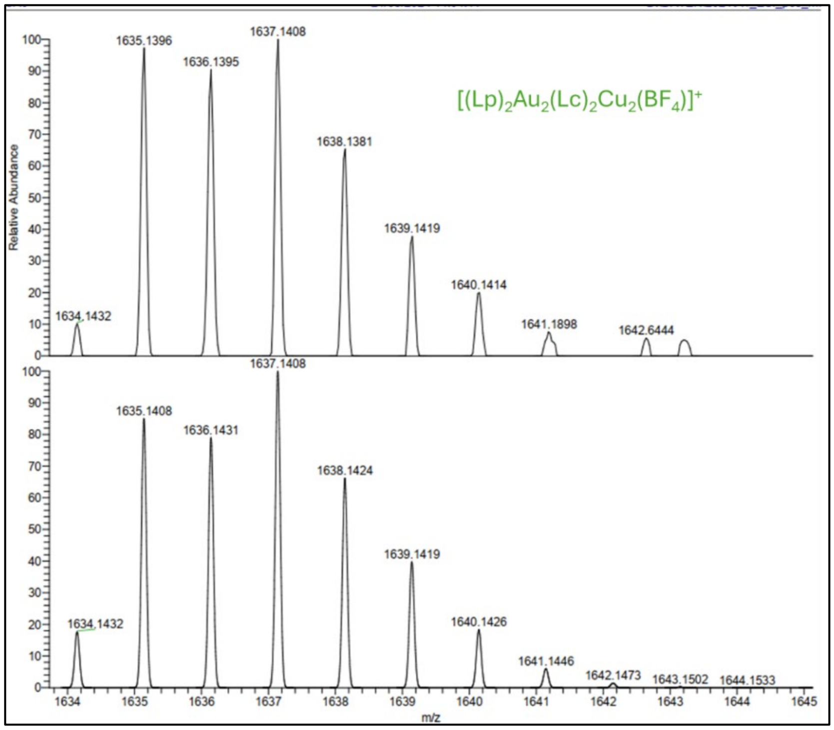


Figure S29. Above: Experimental isotopic distribution for the signal assigned to [**Cu1c** – BF_4]$^+$. below: Calculated isotopic mass distribution for [**Cu1c** – BF_4]$^+$ according to its elemental composition $C_{74}H_{50}N_2P_2Cu_2Au_2BF_4$.

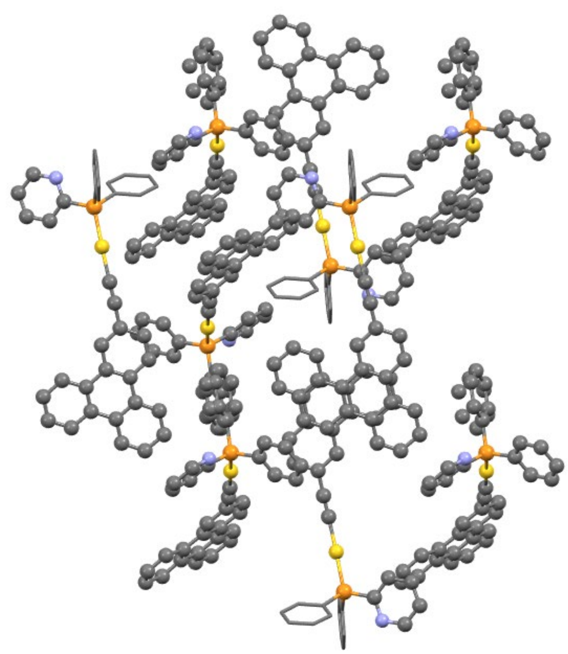


Figure S30. View of the molecular packing of **[Au(L)(PPyPh$_2$)]** along the crystallographic *a*- axis.

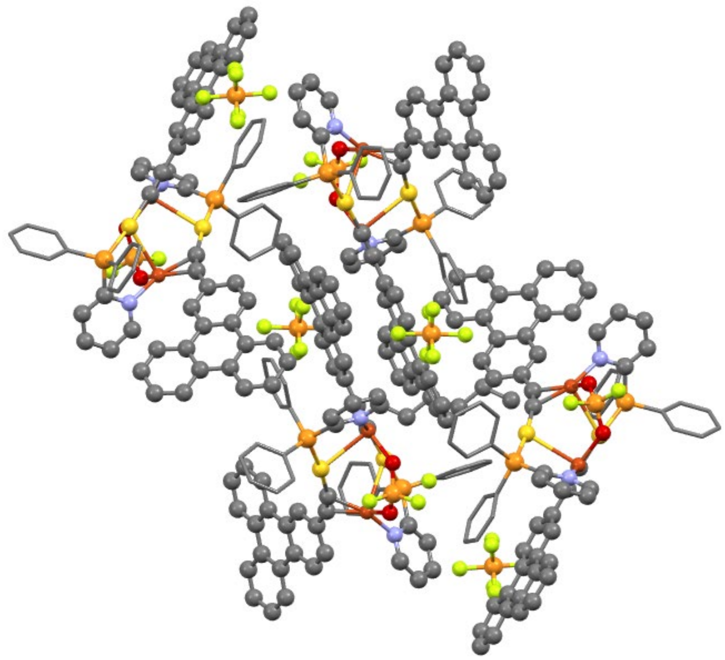


Figure S31. View of the molecular packing of cluster **Cu1a** along the crystallographic *a**-axis.

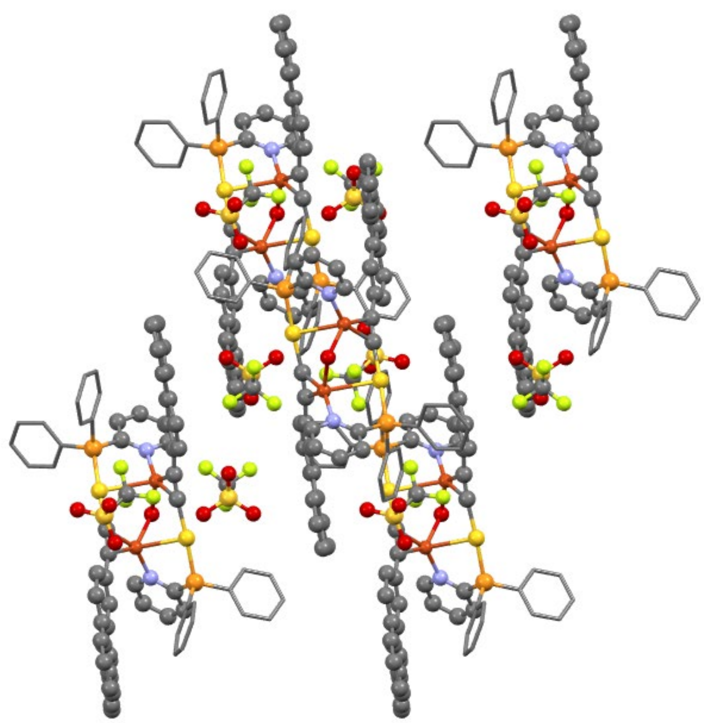


Figure S32. View of the molecular packing of cluster **Cu1b** along the crystallographic *c*-axis.

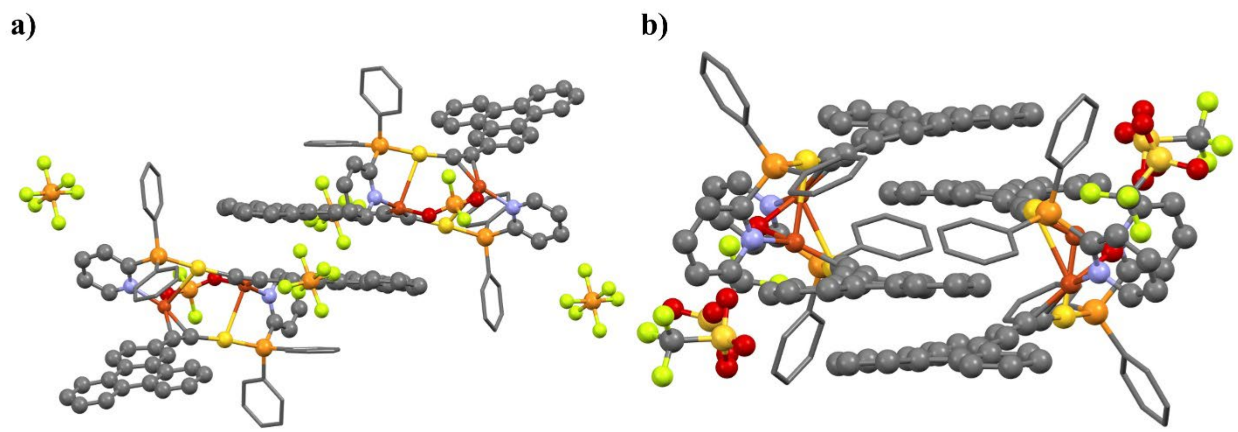


Figure S33. 3D crystal packing of complex **Cu1a** (a) **Cu1b** (b). Yellow: gold; bronze: copper; orange: phosphorus; blue: nitrogen; light green: fluorine. Hydrogen atoms have been omitted for clarity.

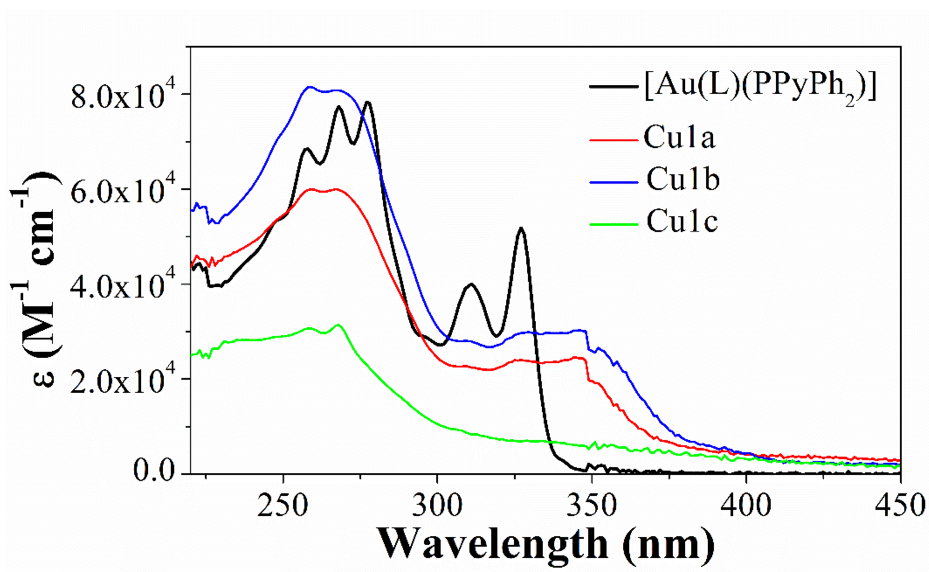


Figure S34. Absorption spectra of 1.0 x10^{-5} M dichloromethane complexes solutions at 298 K.

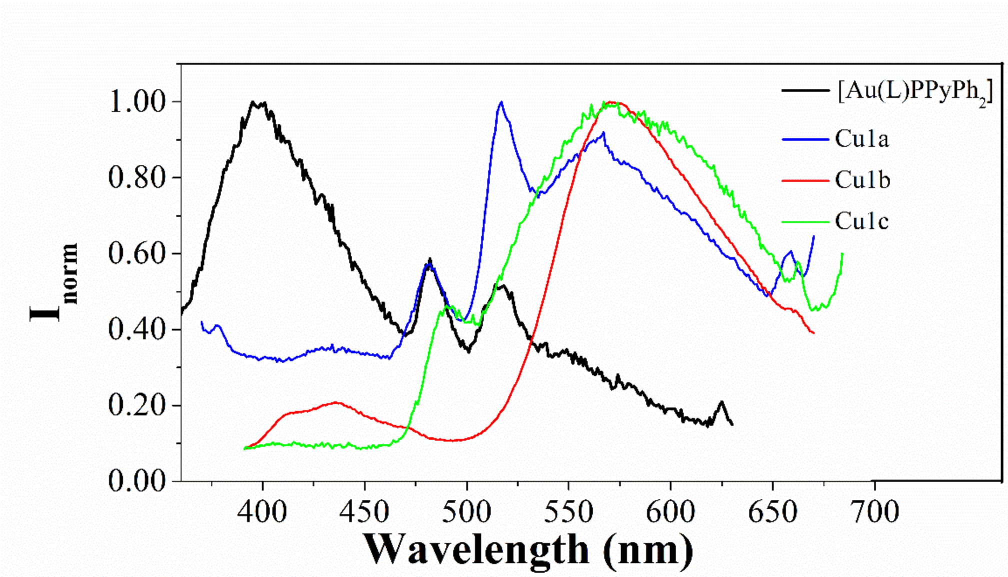


Figure S35. Normalized emission spectra of the complexes in the solid state at 298 K. λ_{exc}= 345 nm.

Table S1. Selected bond lengths (Å) and angles (°) for **[Au(L)(PPyPh$_2$)]**, **Cu1a**, and **Cu1b**.

Complex	[Au(L)(PPyPh$_2$)]	Cu1a	Cu1b
Au-P (Å)	2.2688(6) 2.2784(7)	2.2846(11) 2.2661(11) 2.2738(14) 2.2667(13)	2.2689(10) 2.2742(9)
Au-C (Å)	1.998(3) 2.001(3)	2.024(4) 2.008(4) 2.009(6) 2.014(6)	2.010(4) 2.007(4)
C≡C (Å)	1.203(4) 1.198(4)	1.221(7) 1.238(6) 1.240(8) 1.219(8)	1.229(6) 1.239(6)
Au-Cu (Å)	-	2.8889(7) 2.8465(7) 2.8808(8) 2.8389(7)	2.8153(6) 2.7789(6)
Cu-N (Å)	-	2.000(4) 2.008(4) 2.001(5) 2.026(4)	2.014(3) 1.984(3)
Au···Au (Å)	5.2142(3) 8.2093(5)	4.2122(6) 4.2955(6)	4.8628(4)
Cu···centroid(C≡C) (Å)	-	1.91 1.92 1.92 1.93	1.95 1.94
(C≡)C-Au-P (°)	176.50(8) 178.77(8)	173.43(13) 170.08(13) 173.92(15) 174.83(16)	174.89(12) 175.23(11)
(C≡)C-Cu-Au (°)	-	87.20(13) 89.93(14) 85.88(17) 93.13(15)	108.20(11) 108.22(12)
Au-Cu-N (°)	-	95.97(12) 95.09(12) 94.33(12) 94.89(11)	90.32(9) 91.97(10)

Table S2. Crystal data and structure refinement for all structures reported herein.

Complex	[Au(L)(PPyPh2)]	Cu1a	Cu1b
Formula	$C_{37}H_{25}AuNP$	$C_{315}H_{244}Au_8Cl_2Cu_8F_{32}N_8O_8P_{16}$	$C_{76}H_{52}Au_2Cu_2F_6N_2O_7P_2S_2$
Formula Weight (gmol^{-1})	711.51	7527.64	1866.27
Colour & Habit	Colourless needle	Colourless plate	Colourless block
Crystal Dimensions (mm)	0.06 × 0.07 × 0.22	0.01 × 0.07 × 0.14	0.04 × 0.12 × 0.18
Crystal System	Triclinic	Triclinic	Triclinic
Space Group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a (Å)	11.38880(10)	18.8859(4)	14.0784(3)
b (Å)	14.11400(10)	19.3043(3)	15.9050(3)
c (Å)	18.04900(10)	22.4193(4)	16.6057(2)
α (°)	87.6190(10)	89.9310(10)	95.5170(10)
β (°)	88.5930(10)	69.060(2)	91.2950(10)
γ (°)	88.9210(10)	66.344(2)	112.378(2)
V (Å)	2897.39(4)	6895.1(3)	3415.26(12)
Z	4	1	2
ρ_{calc} (gcm^{-3})	1.631	1.813	1.815
F(000)	1392	3680	1820
μ (mm^{-1})	10.26	10.18	10.24
Temperature (K)	120.0(1)	120.0(1)	120.0(1)
θ_{max} [°]	74.5	74.5	74.5
Total Reflections	59996	142176	81902
Independent Reflections	11833	28119	13937
Reflections ($I_o > 2\sigma[I_o]$)	11091	24698	12360
R_{int}	0.037	0.045	0.062
Parameters	764	1817	898
Restraints	72	92	9
GooF (F^2)	1.04	1.06	1.09
R_1 ($I_o > 2\sigma[I_o]$)	0.0232	0.0391	0.0317
R_1 (all reflections)	0.0249	0.0468	0.0366
wR_2 ($I_o > 2\sigma[I_o]$)	0.0604	0.0926	0.0821
wR_2 (all reflections)	0.0614	0.0960	0.0850
Largest Peak (eÅ^{-3})	0.856	1.523	1.135
Largest Hole (eÅ^{-3})	-1.703	-1.500	-1.897
CCDC Number	2481587	2520370	2520371

Table S3. Luminescence quantum yields (%) recorded for all the compounds in dichloromethane solution.

Complex	Air-equilibrated samples		N_2-saturated samples	
	Φ_{Fl}	Φ_{Phos}	Φ_{Fl}	Φ_{Phos}
[Au(L)(PPyPh$_2$)]	0.05	-	0.01	0.01
Cu1a	0.01	< 0.01	0.01	< 0.01
Cu1b	< 0.01	< 0.01	0.01	0.02

Table S4. Luminescence lifetimes in dichloromethane solution.

Complex	**Air-equilibrated samples**		**N_2-saturated samples**	
	τ_{Fl} (ns)	τ_{Phos} (μs)	τ_{Fl} (ns)	τ_{Phos} (μs)
[Au(L)(PPyPh$_2$]	7	-	14	84
Cu1a	10	0.3	20	45
Cu1b	7	0.5	10	39

Table S5. Emission data of the complexes in solid state at 298 K.

Complex	**Fluorescence emission air-equilibrated λ_{max} (nm)**	**Phosphorescence emission air-equilibrated λ_{max} (nm)**
[Au(L)(PPyPh$_2$)]	399	518
Cu1a	431	565
Cu1b	436	572
Cu1c	426	573

Table S6. Luminescence quantum yields recorded for all the compounds in solid state at 298 K.

Complex	Air-equilibrated samples	
	Φ_{Fl}	Φ_{Phos}
[Au(L)(PPyPh$_2$)]	0.01	-
Cu1a	-	< 0.01
Cu1b	-	< 0.01
Cu1c	-	0.01

Table S7. Emission data of the complexes in organic matrixes.

	PMMA		
Complex	**Air-equilibrated samples**		**N$_2$-saturated samples**
	Fluorescence emission λ_{max} (nm)	Phosphorescence emission λ_{max} (nm)	Phosphorescence emission λ_{max} (nm)
[Au(L)(PPyPh$_2$]	-	498	498
Cu1a	-	501	501
Cu1b	-	500	500
Cu1c	389	500	500
	PS		
Complex	**Air-equilibrated samples**		**N$_2$-saturated samples**
	Fluorescence emission λ_{max} (nm)	Phosphorescence emission λ_{max} (nm)	Phosphorescence emission λ_{max} (nm)
[Au(L)(PPyPh$_2$]	387	500	501
Cu1a	396	506	506
Cu1b	392	504	505
Cu1c	394	506	505

Table S8. Luminescence quantum yields recorded for all the compounds in organic matrixes.

Complex	PMMA		
	Air-equilibrated samples		N_2-saturated samples
	Φ_{Fl}	Φ_{Phos}	Φ_{Phos}
[Au(L)(PPyPh$_2$)]	-	0.04	0.28
Cu1a	-	0.13	0.38
Cu1b	-	0.08	0.30
Cu1c	<0.01	0.11	0.38
	PS		
Complex	Air-equilibrated samples		N_2-saturated samples
	Φ_{Fl}	Φ_{Phos}	Φ_{Phos}
[Au(L)(PPyPh$_2$)]	<0.01	0.02	0.12
Cu1a	<0.01	0.05	0.19
Cu1b	<0.01	0.05	0.17
Cu1c	<0.01	0.05	0.23

Table S9. Luminescence lifetimes for all the compounds in organic matrixes.

Complex	PMMA		
	Air-equilibrated samples		N_2-saturated samples
	τ_{Fl} (ns)	τ_{Phos} (μs)	τ_{Phos} (μs)
[Au(L)(PPyPh$_2$)]	-	88	635
Cu1a	-	38	135
Cu1b	-	86	194
Cu1c	16	53	308
	PS		
Complex	Air-equilibrated samples		N_2-saturated samples
	τ_{Fl} (ns)	τ_{Phos} (μs)	τ_{Phos} (μs)
[Au(L)(PPyPh$_2$)]	21	124	991
Cu1a	27	31	198
Cu1b	23	40	170
Cu1c	15	40	224