Copper(I)-assisted red-shifted phosphorescence in Au(I)···Cu(I) heteropolynuclear complexes.

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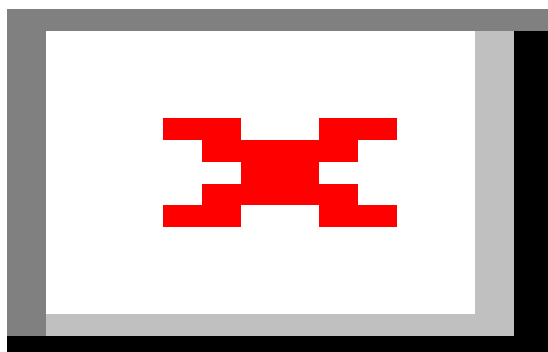# ELECTRONIC SUPPLEMENTARY INFORMATION

Figure S1. Thermal ellipsoid plot (50%) of Au(C$_6$Cl$_2$F$_3$)(PPh$_2$py), **1**. Two molecules crystallize in the asymmetric unit.

Table S1. Xray crystallographic information for $Au(C_6Cl_2F_3)(PPh_2py)$, **1.**

Identification code	cat3
Empirical formula	$C_{46}H_{28}Au_2Cl_4F_6N_2P_2$
Formula weight	1320.38
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 12.1417(4) Å α= 112.3340(10)°.
	b = 14.0807(4) Å β= 106.4260(10)°.
	c = 14.7208(4) Å γ = 93.7410(10)°.
Volume	2190.20(11) Å^3
Z	2
Density (calculated)	2.002 Mg/m^3
Absorption coefficient	7.070 mm^{-1}
F(000)	1256
Crystal size	0.340 x 0.230 x 0.230 mm^3
Theta range for data collection	1.586 to 27.499°.
Index ranges	-15<=h<=15, -18<=k<=18, -19<=l<=19
Reflections collected	46019
Independent reflections	10052 [R(int) = 0.0592]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10052 / 0 / 560
Goodness-of-fit on F^2	1.003
Final R indices [I>2sigma(I)]	R1 = 0.0286, wR2 = 0.0513
R indices (all data)	R1 = 0.0416, wR2 = 0.0540
Extinction coefficient	0.00009(4)
Largest diff. peak and hole	0.746 and -0.660 e.Å^{-3}

Table S2. Bond distance (Å) and angles (°) for Au(C$_6$Cl$_2$F$_3$)(PPh$_2$py), **1.**

Au(1)-C(1)	2.052(4)	N(2)-C(34)	1.402(6)
Au(1)-P(1)	2.2803(10)	C(46)-C(41)	1.382(5)
P(1)-C(18)	1.810(4)	C(46)-C(45)	1.393(6)
P(1)-C(12)	1.821(4)	C(46)-H(46A)	0.9500
P(1)-C(7)	1.822(4)	Cl(3)-C(26)	1.721(4)
N(1)-C(7)	1.374(5)	Cl(4)-C(28)	1.723(4)
N(1)-C(11)	1.374(5)	F(4)-C(25)	1.352(4)
Cl(1)-C(3)	1.724(4)	F(5)-C(27)	1.346(4)
Cl(2)-C(5)	1.727(4)	F(6)-C(29)	1.364(4)
F(1)-C(2)	1.363(4)	C(24)-C(29)	1.375(5)
F(2)-C(4)	1.353(4)	C(24)-C(25)	1.381(5)
F(3)-C(6)	1.350(4)	C(25)-C(26)	1.388(5)
C(1)-C(2)	1.373(5)	C(26)-C(27)	1.378(5)
C(1)-C(6)	1.386(5)	C(27)-C(28)	1.387(5)
C(2)-C(3)	1.376(5)	C(28)-C(29)	1.385(6)
C(3)-C(4)	1.380(5)	C(30)-C(31)	1.377(6)
C(4)-C(5)	1.387(5)	C(31)-C(32)	1.380(6)
C(5)-C(6)	1.377(5)	C(31)-H(31A)	0.9500
C(7)-C(8)	1.372(5)	C(32)-C(33)	1.355(8)
C(8)-C(9)	1.387(6)	C(32)-H(32A)	0.9500
C(8)-H(8A)	0.9500	C(33)-C(34)	1.381(8)
C(9)-C(10)	1.382(6)	C(33)-H(33A)	0.9500
C(9)-H(9A)	0.9500	C(34)-H(34A)	0.9500
C(10)-C(11)	1.384(6)	C(35)-C(40)	1.377(5)
C(10)-H(10A)	0.9500	C(35)-C(36)	1.381(5)
C(11)-H(11A)	0.9500	C(36)-C(37)	1.386(6)
C(12)-C(13)	1.386(5)	C(36)-H(36A)	0.9500
C(12)-C(17)	1.389(5)	C(37)-C(38)	1.384(6)
C(13)-C(14)	1.369(5)	C(37)-H(37A)	0.9500
C(13)-H(13A)	0.9500	C(38)-C(39)	1.393(6)
C(14)-C(15)	1.387(6)	C(38)-H(38A)	0.9500
C(14)-H(14A)	0.9500	C(39)-C(40)	1.369(6)
C(15)-C(16)	1.395(6)	C(39)-H(39A)	0.9500
C(15)-H(15A)	0.9500	C(40)-H(40A)	0.9500
C(16)-C(17)	1.381(5)	C(41)-C(42)	1.379(5)
C(16)-H(16A)	0.9500	C(42)-C(43)	1.384(6)
C(17)-H(17A)	0.9500	C(42)-H(42A)	0.9500
C(18)-C(23)	1.366(5)	C(43)-C(44)	1.374(6)
C(18)-C(19)	1.391(5)	C(43)-H(43A)	0.9500
C(19)-C(20)	1.381(6)	C(44)-C(45)	1.375(6)
C(19)-H(19A)	0.9500	C(44)-H(44A)	0.9500
C(20)-C(21)	1.379(6)	C(45)-H(45A)	0.9500
C(20)-H(20A)	0.9500		
C(21)-C(22)	1.372(6)	C(1)-Au(1)-P(1)	174.55(11)
C(21)-H(21A)	0.9500	C(18)-P(1)-C(12)	104.34(18)
C(22)-C(23)	1.379(6)	C(18)-P(1)-C(7)	106.29(18)
C(22)-H(22A)	0.9500	C(12)-P(1)-C(7)	104.99(17)
C(23)-H(23A)	0.9500	C(18)-P(1)-Au(1)	115.51(13)
Au(2)-C(24)	2.053(4)	C(12)-P(1)-Au(1)	114.00(12)
Au(2)-P(2)	2.2775(10)	C(7)-P(1)-Au(1)	110.85(13)
P(2)-C(35)	1.812(4)	C(7)-N(1)-C(11)	117.5(4)
P(2)-C(41)	1.820(4)	C(2)-C(1)-C(6)	113.9(3)
P(2)-C(30)	1.820(4)	C(2)-C(1)-Au(1)	121.2(3)
N(2)-C(30)	1.379(5)	C(6)-C(1)-Au(1)	124.9(3)

F(1)-C(2)-C(1)	118.6(3)	C(19)-C(20)-H(20A)	120.1
F(1)-C(2)-C(3)	115.9(3)	C(22)-C(21)-C(20)	119.1(4)
C(1)-C(2)-C(3)	125.5(4)	C(22)-C(21)-H(21A)	120.5
C(2)-C(3)-C(4)	117.4(4)	C(20)-C(21)-H(21A)	120.5
C(2)-C(3)-Cl(1)	122.7(3)	C(21)-C(22)-C(23)	121.6(4)
C(4)-C(3)-Cl(1)	119.9(3)	C(21)-C(22)-H(22A)	119.2
F(2)-C(4)-C(3)	120.1(4)	C(23)-C(22)-H(22A)	119.2
F(2)-C(4)-C(5)	119.0(3)	C(18)-C(23)-C(22)	119.3(4)
C(3)-C(4)-C(5)	120.9(4)	C(18)-C(23)-H(23A)	120.3
C(6)-C(5)-C(4)	117.7(3)	C(22)-C(23)-H(23A)	120.3
C(6)-C(5)-Cl(2)	122.2(3)	C(24)-Au(2)-P(2)	173.35(11)
C(4)-C(5)-Cl(2)	120.0(3)	C(35)-P(2)-C(41)	106.09(17)
F(3)-C(6)-C(5)	116.5(3)	C(35)-P(2)-C(30)	105.37(18)
F(3)-C(6)-C(1)	118.9(3)	C(41)-P(2)-C(30)	104.16(17)
C(5)-C(6)-C(1)	124.6(4)	C(35)-P(2)-Au(2)	114.92(13)
N(1)-C(7)-C(8)	121.8(4)	C(41)-P(2)-Au(2)	115.18(13)
N(1)-C(7)-P(1)	118.5(3)	C(30)-P(2)-Au(2)	110.15(14)
C(8)-C(7)-P(1)	119.7(3)	C(30)-N(2)-C(34)	114.8(4)
C(7)-C(8)-C(9)	120.3(4)	C(41)-C(46)-C(45)	120.2(4)
C(7)-C(8)-H(8A)	119.8	C(41)-C(46)-H(46A)	119.9
C(9)-C(8)-H(8A)	119.8	C(45)-C(46)-H(46A)	119.9
C(10)-C(9)-C(8)	118.7(4)	C(29)-C(24)-C(25)	114.2(4)
C(10)-C(9)-H(9A)	120.7	C(29)-C(24)-Au(2)	119.5(3)
C(8)-C(9)-H(9A)	120.7	C(25)-C(24)-Au(2)	126.2(3)
C(9)-C(10)-C(11)	119.6(4)	F(4)-C(25)-C(24)	119.0(3)
C(9)-C(10)-H(10A)	120.2	F(4)-C(25)-C(26)	116.4(3)
C(11)-C(10)-H(10A)	120.2	C(24)-C(25)-C(26)	124.6(4)
N(1)-C(11)-C(10)	122.0(4)	C(27)-C(26)-C(25)	117.5(4)
N(1)-C(11)-H(11A)	119.0	C(27)-C(26)-Cl(3)	119.9(3)
C(10)-C(11)-H(11A)	119.0	C(25)-C(26)-Cl(3)	122.6(3)
C(13)-C(12)-C(17)	120.2(4)	F(5)-C(27)-C(26)	119.1(3)
C(13)-C(12)-P(1)	117.1(3)	F(5)-C(27)-C(28)	119.4(3)
C(17)-C(12)-P(1)	122.6(3)	C(26)-C(27)-C(28)	121.5(4)
C(14)-C(13)-C(12)	119.9(4)	C(29)-C(28)-C(27)	117.0(4)
C(14)-C(13)-H(13A)	120.0	C(29)-C(28)-Cl(4)	122.3(3)
C(12)-C(13)-H(13A)	120.0	C(27)-C(28)-Cl(4)	120.7(3)
C(13)-C(14)-C(15)	120.6(4)	F(6)-C(29)-C(24)	119.0(4)
C(13)-C(14)-H(14A)	119.7	F(6)-C(29)-C(28)	115.7(3)
C(15)-C(14)-H(14A)	119.7	C(24)-C(29)-C(28)	125.2(4)
C(14)-C(15)-C(16)	119.4(4)	C(31)-C(30)-N(2)	123.3(4)
C(14)-C(15)-H(15A)	120.3	C(31)-C(30)-P(2)	119.9(3)
C(16)-C(15)-H(15A)	120.3	N(2)-C(30)-P(2)	116.6(3)
C(17)-C(16)-C(15)	120.1(4)	C(30)-C(31)-C(32)	119.2(5)
C(17)-C(16)-H(16A)	120.0	C(30)-C(31)-H(31A)	120.4
C(15)-C(16)-H(16A)	120.0	C(32)-C(31)-H(31A)	120.4
C(16)-C(17)-C(12)	119.7(4)	C(33)-C(32)-C(31)	120.2(5)
C(16)-C(17)-H(17A)	120.1	C(33)-C(32)-H(32A)	119.9
C(12)-C(17)-H(17A)	120.1	C(31)-C(32)-H(32A)	119.9
C(23)-C(18)-C(19)	119.9(4)	C(32)-C(33)-C(34)	119.4(5)
C(23)-C(18)-P(1)	121.0(3)	C(32)-C(33)-H(33A)	120.3
C(19)-C(18)-P(1)	119.1(3)	C(34)-C(33)-H(33A)	120.3
C(20)-C(19)-C(18)	120.2(4)	C(33)-C(34)-N(2)	122.9(5)
C(20)-C(19)-H(19A)	119.9	C(33)-C(34)-H(34A)	118.5
C(18)-C(19)-H(19A)	119.9	N(2)-C(34)-H(34A)	118.5
C(21)-C(20)-C(19)	119.9(4)	C(40)-C(35)-C(36)	120.1(4)
C(21)-C(20)-H(20A)	120.1	C(40)-C(35)-P(2)	118.5(3)

C(36)-C(35)-P(2)	121.1(3)	C(42)-C(41)-C(46)	119.8(4)
C(35)-C(36)-C(37)	120.3(4)	C(42)-C(41)-P(2)	121.4(3)
C(35)-C(36)-H(36A)	119.8	C(46)-C(41)-P(2)	118.6(3)
C(37)-C(36)-H(36A)	119.8	C(41)-C(42)-C(43)	119.5(4)
C(38)-C(37)-C(36)	119.5(4)	C(41)-C(42)-H(42A)	120.3
C(38)-C(37)-H(37A)	120.2	C(43)-C(42)-H(42A)	120.3
C(36)-C(37)-H(37A)	120.2	C(44)-C(43)-C(42)	121.0(4)
C(37)-C(38)-C(39)	119.5(4)	C(44)-C(43)-H(43A)	119.5
C(37)-C(38)-H(38A)	120.2	C(42)-C(43)-H(43A)	119.5
C(39)-C(38)-H(38A)	120.2	C(45)-C(44)-C(43)	119.7(4)
C(40)-C(39)-C(38)	120.6(4)	C(45)-C(44)-H(44A)	120.1
C(40)-C(39)-H(39A)	119.7	C(43)-C(44)-H(44A)	120.1
C(38)-C(39)-H(39A)	119.7	C(44)-C(45)-C(46)	119.8(4)
C(39)-C(40)-C(35)	120.0(4)	C(44)-C(45)-H(45A)	120.1
C(39)-C(40)-H(40A)	120.0	C(46)-C(45)-H(45A)	120.1
C(35)-C(40)-H(40A)	120.0		

Table S3. Torsion angles (°) for Au(C$_6$Cl$_2$F$_3$)(PPh$_2$py), **1.**

C(6)-C(1)-C(2)-F(1)	179.0(3)	C(7)-C(8)-C(9)-C(10)	-0.7(7)
Au(1)-C(1)-C(2)-F(1)	-0.3(5)	C(8)-C(9)-C(10)-C(11)	0.4(7)
C(6)-C(1)-C(2)-C(3)	-1.0(6)	C(7)-N(1)-C(11)-C(10)	-1.3(6)
Au(1)-C(1)-C(2)-C(3)	179.7(3)	C(9)-C(10)-C(11)-N(1)	0.6(7)
F(1)-C(2)-C(3)-C(4)	-178.3(4)	C(18)-P(1)-C(12)-C(13)	47.9(3)
C(1)-C(2)-C(3)-C(4)	1.8(7)	C(7)-P(1)-C(12)-C(13)	159.5(3)
F(1)-C(2)-C(3)-Cl(1)	2.3(5)	Au(1)-P(1)-C(12)-C(13)	-79.0(3)
C(1)-C(2)-C(3)-Cl(1)	-177.6(3)	C(18)-P(1)-C(12)-C(17)	-136.1(3)
C(2)-C(3)-C(4)-F(2)	179.7(4)	C(7)-P(1)-C(12)-C(17)	-24.5(4)
Cl(1)-C(3)-C(4)-F(2)	-0.9(6)	Au(1)-P(1)-C(12)-C(17)	97.0(3)
C(2)-C(3)-C(4)-C(5)	-1.3(6)	C(17)-C(12)-C(13)-C(14)	0.6(5)
Cl(1)-C(3)-C(4)-C(5)	178.2(3)	P(1)-C(12)-C(13)-C(14)	176.7(3)
F(2)-C(4)-C(5)-C(6)	179.2(4)	C(12)-C(13)-C(14)-C(15)	0.7(6)
C(3)-C(4)-C(5)-C(6)	0.1(6)	C(13)-C(14)-C(15)-C(16)	-1.4(6)
F(2)-C(4)-C(5)-Cl(2)	-1.4(5)	C(14)-C(15)-C(16)-C(17)	0.8(6)
C(3)-C(4)-C(5)-Cl(2)	179.5(3)	C(15)-C(16)-C(17)-C(12)	0.5(6)
C(4)-C(5)-C(6)-F(3)	-179.0(4)	C(13)-C(12)-C(17)-C(16)	-1.2(5)
Cl(2)-C(5)-C(6)-F(3)	1.6(5)	P(1)-C(12)-C(17)-C(16)	-177.1(3)
C(4)-C(5)-C(6)-C(1)	0.7(6)	C(12)-P(1)-C(18)-C(23)	45.4(4)
Cl(2)-C(5)-C(6)-C(1)	-178.7(3)	C(7)-P(1)-C(18)-C(23)	-65.3(4)
C(2)-C(1)-C(6)-F(3)	179.4(3)	Au(1)-P(1)-C(18)-C(23)	171.3(3)
Au(1)-C(1)-C(6)-F(3)	-1.3(5)	C(12)-P(1)-C(18)-C(19)	-135.3(3)
C(2)-C(1)-C(6)-C(5)	-0.3(6)	C(7)-P(1)-C(18)-C(19)	114.0(3)
Au(1)-C(1)-C(6)-C(5)	179.0(3)	Au(1)-P(1)-C(18)-C(19)	-9.4(4)
C(11)-N(1)-C(7)-C(8)	1.0(6)	C(23)-C(18)-C(19)-C(20)	1.9(6)
C(11)-N(1)-C(7)-P(1)	179.9(3)	P(1)-C(18)-C(19)-C(20)	-177.4(3)
C(18)-P(1)-C(7)-N(1)	50.7(4)	C(18)-C(19)-C(20)-C(21)	-1.2(6)
C(12)-P(1)-C(7)-N(1)	-59.5(4)	C(19)-C(20)-C(21)-C(22)	-0.8(7)
Au(1)-P(1)-C(7)-N(1)	176.9(3)	C(20)-C(21)-C(22)-C(23)	2.0(7)
C(18)-P(1)-C(7)-C(8)	-130.3(3)	C(19)-C(18)-C(23)-C(22)	-0.7(6)
C(12)-P(1)-C(7)-C(8)	119.5(3)	P(1)-C(18)-C(23)-C(22)	178.5(3)
Au(1)-P(1)-C(7)-C(8)	-4.1(4)	C(21)-C(22)-C(23)-C(18)	-1.2(7)
N(1)-C(7)-C(8)-C(9)	0.0(7)	C(29)-C(24)-C(25)-F(4)	-179.6(3)
P(1)-C(7)-C(8)-C(9)	-178.9(3)	Au(2)-C(24)-C(25)-F(4)	4.8(6)

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C(29)-C(24)-C(25)-C(26)	1.8(6)	C(30)-C(31)-C(32)-C(33)	1.3(8)
Au(2)-C(24)-C(25)-C(26)	-173.8(3)	C(31)-C(32)-C(33)-C(34)	-1.0(8)
F(4)-C(25)-C(26)-C(27)	179.6(4)	C(32)-C(33)-C(34)-N(2)	0.3(8)
C(24)-C(25)-C(26)-C(27)	-1.8(6)	C(30)-N(2)-C(34)-C(33)	0.1(7)
F(4)-C(25)-C(26)-Cl(3)	-0.3(5)	C(41)-P(2)-C(35)-C(40)	-42.0(4)
C(24)-C(25)-C(26)-Cl(3)	178.3(3)	C(30)-P(2)-C(35)-C(40)	-152.0(3)
C(25)-C(26)-C(27)-F(5)	-179.6(4)	Au(2)-P(2)-C(35)-C(40)	86.5(3)
Cl(3)-C(26)-C(27)-F(5)	0.3(6)	C(41)-P(2)-C(35)-C(36)	144.4(3)
C(25)-C(26)-C(27)-C(28)	0.4(6)	C(30)-P(2)-C(35)-C(36)	34.3(4)
Cl(3)-C(26)-C(27)-C(28)	-179.7(3)	Au(2)-P(2)-C(35)-C(36)	-87.1(3)
F(5)-C(27)-C(28)-C(29)	-179.2(4)	C(40)-C(35)-C(36)-C(37)	-0.7(6)
C(26)-C(27)-C(28)-C(29)	0.8(6)	P(2)-C(35)-C(36)-C(37)	172.8(3)
F(5)-C(27)-C(28)-Cl(4)	0.3(6)	C(35)-C(36)-C(37)-C(38)	0.2(7)
C(26)-C(27)-C(28)-Cl(4)	-179.7(3)	C(36)-C(37)-C(38)-C(39)	0.7(7)
C(25)-C(24)-C(29)-F(6)	179.8(3)	C(37)-C(38)-C(39)-C(40)	-1.1(7)
Au(2)-C(24)-C(29)-F(6)	-4.3(5)	C(38)-C(39)-C(40)-C(35)	0.5(6)
C(25)-C(24)-C(29)-C(28)	-0.4(6)	C(36)-C(35)-C(40)-C(39)	0.4(6)
Au(2)-C(24)-C(29)-C(28)	175.5(3)	P(2)-C(35)-C(40)-C(39)	-173.3(3)
C(27)-C(28)-C(29)-F(6)	179.0(3)	C(45)-C(46)-C(41)-C(42)	-1.6(6)
Cl(4)-C(28)-C(29)-F(6)	-0.5(5)	C(45)-C(46)-C(41)-P(2)	173.6(3)
C(27)-C(28)-C(29)-C(24)	-0.8(6)	C(35)-P(2)-C(41)-C(42)	-41.3(3)
Cl(4)-C(28)-C(29)-C(24)	179.7(3)	C(30)-P(2)-C(41)-C(42)	69.7(3)
C(34)-N(2)-C(30)-C(31)	0.1(6)	Au(2)-P(2)-C(41)-C(42)	-169.6(3)
C(34)-N(2)-C(30)-P(2)	176.5(3)	C(35)-P(2)-C(41)-C(46)	143.6(3)
C(35)-P(2)-C(30)-C(31)	-132.3(4)	C(30)-P(2)-C(41)-C(46)	-105.5(3)
C(41)-P(2)-C(30)-C(31)	116.2(4)	Au(2)-P(2)-C(41)-C(46)	15.3(3)
Au(2)-P(2)-C(30)-C(31)	-7.8(4)	C(46)-C(41)-C(42)-C(43)	0.3(6)
C(35)-P(2)-C(30)-N(2)	51.1(4)	P(2)-C(41)-C(42)-C(43)	-174.8(3)
C(41)-P(2)-C(30)-N(2)	-60.3(3)	C(41)-C(42)-C(43)-C(44)	1.1(7)
Au(2)-P(2)-C(30)-N(2)	175.6(3)	C(42)-C(43)-C(44)-C(45)	-1.1(7)
N(2)-C(30)-C(31)-C(32)	-0.8(7)	C(43)-C(44)-C(45)-C(46)	-0.2(6)
P(2)-C(30)-C(31)-C(32)	-177.1(4)	C(41)-C(46)-C(45)-C(44)	1.6(6)
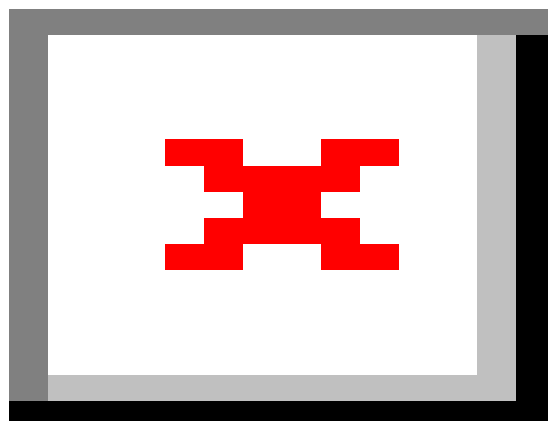
Figure S2. Thermal ellipsoid plot (50%) of $Au_2(C_6Cl_2F_3)_2(P_2phen)$, **2**. Only one-half of the molecules crystallizes in the asymmetric unit.

Table S4. X-ray crystallographic information for $Au_2(C_6Cl_2F_3)_2(P_2phen)$, **2**.

Identification code	cat12
Empirical formula	$C_{48}H_{26}Au_2Cl_4F_6N_2P_2$
Formula weight	1342.38
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 24.6243(7) Å $\quad$ α= 90°.
	b = 12.2228(4) Å $\quad$ β= 123.7960(6)°.
	c = 17.6926(9) Å $\quad$ γ = 90°.
Volume	4425.3(3) Å³
Z	4
Density (calculated)	2.015 Mg/m³
Absorption coefficient	7.001 mm⁻¹
F(000)	2552
Crystal size	0.400 x 0.080 x 0.050 mm³
Theta range for data collection	1.941 to 29.997°.
Index ranges	-33<=h<=34, -17<=k<=16, -24<=l<=24
Reflections collected	40972
Independent reflections	6470 [R(int) = 0.0664]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6470 / 0 / 289
Goodness-of-fit on F^2	1.007
Final R indices [I>2sigma(I)]	R1 = 0.0279, wR2 = 0.0470
R indices (all data)	R1 = 0.0457, wR2 = 0.0500
Extinction coefficient	n/a
Largest diff. peak and hole	0.909 and -0.701 e.Å⁻³

Table S5. Selected bond distances (Å) and angles (°) for $Au_2(C_6Cl_2F_3)_2(P_2phen)$, **2**.

Au(1)-C(1)	2.054(3)		
Au(1)-P(1)	2.2750(8)	C(8)-H(8A)	0.9500
P(1)-C(19)	1.807(3)	C(9)-C(10)	1.403(4)
P(1)-C(13)	1.814(3)	C(9)-H(9A)	0.9500
P(1)-C(7)	1.839(3)	C(10)-C(11)	1.417(4)
Cl(1)-C(3)	1.718(3)	C(10)-C(12)	1.436(4)
Cl(2)-C(5)	1.725(3)	C(11)-C(11)#1	1.471(6)
F(1)-C(2)	1.358(3)	C(12)-C(12)#1	1.342(6)
F(2)-C(4)	1.348(3)	C(12)-H(12A)	0.9500
F(3)-C(6)	1.352(4)	C(13)-C(14)	1.393(4)
N(1)-C(7)	1.330(4)	C(13)-C(18)	1.401(4)
N(1)-C(11)	1.351(4)	C(14)-C(15)	1.385(5)
C(1)-C(2)	1.371(4)	C(14)-H(14A)	0.9500
C(1)-C(6)	1.388(4)	C(15)-C(16)	1.389(5)
C(2)-C(3)	1.383(4)	C(15)-H(15A)	0.9500
C(3)-C(4)	1.388(5)	C(16)-C(17)	1.383(5)
C(4)-C(5)	1.371(5)	C(16)-H(16A)	0.9500
C(5)-C(6)	1.388(4)	C(17)-C(18)	1.385(4)
C(7)-C(8)	1.406(4)	C(17)-H(17A)	0.9500
C(8)-C(9)	1.367(4)	C(18)-H(18A)	0.9500

C(19)-C(24)	1.392(4)	C(10)-C(9)-H(9A)	120.3
C(19)-C(20)	1.394(4)	C(9)-C(10)-C(11)	117.6(3)
C(20)-C(21)	1.387(4)	C(9)-C(10)-C(12)	121.5(3)
C(20)-H(20A)	0.9500	C(11)-C(10)-C(12)	120.9(3)
C(21)-C(22)	1.382(5)	N(1)-C(11)-C(10)	122.8(3)
C(21)-H(21A)	0.9500	N(1)-C(11)-C(11)#1	118.94(16)
C(22)-C(23)	1.384(5)	C(10)-C(11)-C(11)#1	118.24(17)
C(22)-H(22A)	0.9500	C(12)#1-C(12)-C(10)	120.80(18)
C(23)-C(24)	1.387(4)	C(12)#1-C(12)-H(12A)	119.6
C(23)-H(23A)	0.9500	C(10)-C(12)-H(12A)	119.6
C(24)-H(24A)	0.9500	C(14)-C(13)-C(18)	119.1(3)
		C(14)-C(13)-P(1)	124.2(2)
C(1)-Au(1)-P(1)	174.87(9)	C(18)-C(13)-P(1)	116.7(2)
C(19)-P(1)-C(13)	105.48(14)	C(15)-C(14)-C(13)	120.3(3)
C(19)-P(1)-C(7)	106.58(14)	C(15)-C(14)-H(14A)	119.9
C(13)-P(1)-C(7)	106.44(14)	C(13)-C(14)-H(14A)	119.9
C(19)-P(1)-Au(1)	115.29(10)	C(14)-C(15)-C(16)	120.3(3)
C(13)-P(1)-Au(1)	112.54(10)	C(14)-C(15)-H(15A)	119.9
C(7)-P(1)-Au(1)	109.95(10)	C(16)-C(15)-H(15A)	119.9
C(7)-N(1)-C(11)	117.8(3)	C(17)-C(16)-C(15)	119.9(3)
C(2)-C(1)-C(6)	114.6(3)	C(17)-C(16)-H(16A)	120.1
C(2)-C(1)-Au(1)	121.2(2)	C(15)-C(16)-H(16A)	120.1
C(6)-C(1)-Au(1)	124.1(2)	C(16)-C(17)-C(18)	120.2(3)
F(1)-C(2)-C(1)	118.4(3)	C(16)-C(17)-H(17A)	119.9
F(1)-C(2)-C(3)	116.4(3)	C(18)-C(17)-H(17A)	119.9
C(1)-C(2)-C(3)	125.3(3)	C(17)-C(18)-C(13)	120.2(3)
C(2)-C(3)-C(4)	116.8(3)	C(17)-C(18)-H(18A)	119.9
C(2)-C(3)-Cl(1)	122.1(3)	C(13)-C(18)-H(18A)	119.9
C(4)-C(3)-Cl(1)	121.1(2)	C(24)-C(19)-C(20)	119.6(3)
F(2)-C(4)-C(5)	119.3(3)	C(24)-C(19)-P(1)	121.5(2)
F(2)-C(4)-C(3)	119.2(3)	C(20)-C(19)-P(1)	118.9(2)
C(5)-C(4)-C(3)	121.6(3)	C(21)-C(20)-C(19)	120.3(3)
C(4)-C(5)-C(6)	118.1(3)	C(21)-C(20)-H(20A)	119.9
C(4)-C(5)-Cl(2)	120.7(2)	C(19)-C(20)-H(20A)	119.9
C(6)-C(5)-Cl(2)	121.2(3)	C(22)-C(21)-C(20)	119.5(3)
F(3)-C(6)-C(1)	118.9(3)	C(22)-C(21)-H(21A)	120.3
F(3)-C(6)-C(5)	117.4(3)	C(20)-C(21)-H(21A)	120.3
C(1)-C(6)-C(5)	123.7(3)	C(21)-C(22)-C(23)	120.8(3)
N(1)-C(7)-C(8)	123.2(3)	C(21)-C(22)-H(22A)	119.6
N(1)-C(7)-P(1)	118.3(2)	C(23)-C(22)-H(22A)	119.6
C(8)-C(7)-P(1)	118.5(2)	C(22)-C(23)-C(24)	119.9(3)
C(9)-C(8)-C(7)	119.1(3)	C(22)-C(23)-H(23A)	120.0
C(9)-C(8)-H(8A)	120.4	C(24)-C(23)-H(23A)	120.0
C(7)-C(8)-H(8A)	120.4	C(23)-C(24)-C(19)	119.9(3)
C(8)-C(9)-C(10)	119.4(3)	C(23)-C(24)-H(24A)	120.0
C(8)-C(9)-H(9A)	120.3	C(19)-C(24)-H(24A)	120.0

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table S6. Torsion angles (°) for Au$_2$(C$_6$Cl$_2$F$_3$)$_2$(P$_2$phen), **2**.

C(6)-C(1)-C(2)-F(1)	-179.7(3)	C(7)-N(1)-C(11)-C(10)	0.7(4)
Au(1)-C(1)-C(2)-F(1)	-3.0(4)	C(7)-N(1)-C(11)-C(11)#1	-178.8(3)
C(6)-C(1)-C(2)-C(3)	0.0(5)	C(9)-C(10)-C(11)-N(1)	1.4(4)
Au(1)-C(1)-C(2)-C(3)	176.6(2)	C(12)-C(10)-C(11)-N(1)	-177.4(3)
F(1)-C(2)-C(3)-C(4)	179.8(3)	C(9)-C(10)-C(11)-C(11)#1	-179.0(3)
C(1)-C(2)-C(3)-C(4)	0.1(5)	C(12)-C(10)-C(11)-C(11)#1	2.1(5)
F(1)-C(2)-C(3)-Cl(1)	0.9(4)	C(9)-C(10)-C(12)-C(12)#1	-178.3(4)
C(1)-C(2)-C(3)-Cl(1)	-178.7(3)	C(11)-C(10)-C(12)-C(12)#1	0.5(5)
C(2)-C(3)-C(4)-F(2)	-178.6(3)	C(19)-P(1)-C(13)-C(14)	-92.8(3)
Cl(1)-C(3)-C(4)-F(2)	0.3(4)	C(7)-P(1)-C(13)-C(14)	20.2(3)
C(2)-C(3)-C(4)-C(5)	-0.8(5)	Au(1)-P(1)-C(13)-C(14)	140.7(3)
Cl(1)-C(3)-C(4)-C(5)	178.1(2)	C(19)-P(1)-C(13)-C(18)	87.4(3)
F(2)-C(4)-C(5)-C(6)	179.0(3)	C(7)-P(1)-C(13)-C(18)	-159.6(2)
C(3)-C(4)-C(5)-C(6)	1.2(5)	Au(1)-P(1)-C(13)-C(18)	-39.1(3)
F(2)-C(4)-C(5)-Cl(2)	1.6(4)	C(18)-C(13)-C(14)-C(15)	0.6(5)
C(3)-C(4)-C(5)-Cl(2)	-176.3(3)	P(1)-C(13)-C(14)-C(15)	-179.2(3)
C(2)-C(1)-C(6)-F(3)	178.5(3)	C(13)-C(14)-C(15)-C(16)	-0.9(5)
Au(1)-C(1)-C(6)-F(3)	2.0(4)	C(14)-C(15)-C(16)-C(17)	0.5(5)
C(2)-C(1)-C(6)-C(5)	0.5(5)	C(15)-C(16)-C(17)-C(18)	0.2(5)
Au(1)-C(1)-C(6)-C(5)	-176.0(2)	C(16)-C(17)-C(18)-C(13)	-0.5(5)
C(4)-C(5)-C(6)-F(3)	-179.1(3)	C(14)-C(13)-C(18)-C(17)	0.1(5)
Cl(2)-C(5)-C(6)-F(3)	-1.6(4)	P(1)-C(13)-C(18)-C(17)	179.9(2)
C(4)-C(5)-C(6)-C(1)	-1.1(5)	C(13)-P(1)-C(19)-C(24)	41.7(3)
Cl(2)-C(5)-C(6)-C(1)	176.3(3)	C(7)-P(1)-C(19)-C(24)	-71.1(3)
C(11)-N(1)-C(7)-C(8)	-2.4(4)	Au(1)-P(1)-C(19)-C(24)	166.5(2)
C(11)-N(1)-C(7)-P(1)	177.8(2)	C(13)-P(1)-C(19)-C(20)	-138.8(3)
C(19)-P(1)-C(7)-N(1)	50.6(3)	C(7)-P(1)-C(19)-C(20)	108.3(3)
C(13)-P(1)-C(7)-N(1)	-61.7(3)	Au(1)-P(1)-C(19)-C(20)	-14.0(3)
Au(1)-P(1)-C(7)-N(1)	176.2(2)	C(24)-C(19)-C(20)-C(21)	1.2(5)
C(19)-P(1)-C(7)-C(8)	-129.3(2)	P(1)-C(19)-C(20)-C(21)	-178.3(3)
C(13)-P(1)-C(7)-C(8)	118.5(3)	C(19)-C(20)-C(21)-C(22)	-0.6(5)
Au(1)-P(1)-C(7)-C(8)	-3.7(3)	C(20)-C(21)-C(22)-C(23)	-0.6(5)
N(1)-C(7)-C(8)-C(9)	1.8(5)	C(21)-C(22)-C(23)-C(24)	1.2(5)
P(1)-C(7)-C(8)-C(9)	-178.3(2)	C(22)-C(23)-C(24)-C(19)	-0.5(5)
C(7)-C(8)-C(9)-C(10)	0.5(5)	C(20)-C(19)-C(24)-C(23)	-0.6(5)
C(8)-C(9)-C(10)-C(11)	-2.0(4)	P(1)-C(19)-C(24)-C(23)	178.8(3)
C(8)-C(9)-C(10)-C(12)	176.9(3)		

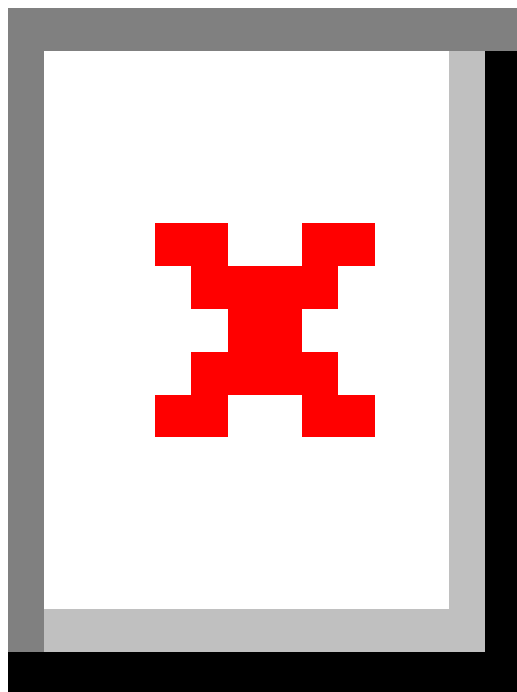Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Figure S3. Thermal ellipsoid plot (50%) of $[Au_2Cu(C_6Cl_2F_3)_2(PPh_2py)_2](BF_4)$ **3**.

Table S7. X-ray crystallographic data for [Au$_2$Cu(C$_6$Cl$_2$F$_3$)$_2$(PPh$_2$py)$_2$](BF$_4$), **3**.

Identification code	cat8_0m
Empirical formula	C$_{46}$H$_{28}$Au$_2$BCl$_4$CuF$_{10}$N$_2$P$_2$
Formula weight	1470.73
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 10.3133(3) Å α= 90.0760(10)°.
	b = 13.8966(5) Å β= 95.0190(10)°.
	c = 16.5360(6) Å γ = 104.8460(10)°.
Volume	2281.35(13) Å^3
Z	2
Density (calculated)	2.141 Mg/m^3
Absorption coefficient	7.261 mm^{-1}
F(000)	1396
Crystal size	0.340 x 0.330 x 0.220 mm^3
Theta range for data collection	1.516 to 31.500°.
Index ranges	-14<=h<=15, -20<=k<=20, -24<=l<=24
Reflections collected	49768
Independent reflections	15057 [R(int) = 0.0423]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15057 / 0 / 613
Goodness-of-fit on F^2	1.081
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0808
R indices (all data)	R1 = 0.0547, wR2 = 0.0850
Extinction coefficient	n/a
Largest diff. peak and hole	6.583 and -2.710 e.Å^{-3}

Table S8. Bond distances (Å) and angles (°) for [Au$_2$Cu(C$_6$Cl$_2$F$_3$)$_2$(PPh$_2$py)$_2$](BF$_4$), **3**.

Au(1)-C(1)	2.056(4)	C(15)-C(16)	1.384(7)
Au(1)-P(1)	2.2916(11)	C(15)-H(15A)	0.9500
Au(1)-Cu(1)	2.9647(6)	C(16)-C(17)	1.382(6)
Au(1)-Au(2)	3.0689(2)	C(16)-H(16A)	0.9500
Au(2)-C(24)	2.068(4)	C(17)-H(17A)	0.9500
Au(2)-P(2)	2.2988(10)	C(18)-C(23)	1.388(6)
Au(2)-Cu(1)	2.8403(5)	C(18)-C(19)	1.401(6)
Cu(1)-N(2)	1.907(4)	C(19)-C(20)	1.392(7)
Cu(1)-N(1)	1.908(3)	C(19)-H(19A)	0.9500
Cl(1)-C(3)	1.710(5)	C(20)-C(21)	1.368(7)
Cl(2)-C(5)	1.729(5)	C(20)-H(20A)	0.9500
Cl(3)-C(26)	1.725(5)	C(21)-C(22)	1.383(7)
Cl(4)-C(28)	1.726(5)	C(21)-H(21A)	0.9500
F(1)-C(2)	1.359(5)	C(22)-C(23)	1.386(6)
F(2)-C(4)	1.344(5)	C(22)-H(22A)	0.9500
F(3)-C(6)	1.352(5)	C(23)-H(23A)	0.9500
F(4)-C(25)	1.344(5)	C(24)-C(25)	1.376(6)
F(5)-C(27)	1.342(5)	C(24)-C(29)	1.392(6)
F(6)-C(29)	1.353(5)	C(25)-C(26)	1.397(6)
B(1)-F(7)	1.356(7)	C(26)-C(27)	1.381(7)
B(1)-F(10)	1.374(7)	C(27)-C(28)	1.368(7)
B(1)-F(8)	1.377(7)	C(28)-C(29)	1.392(6)
B(1)-F(9)	1.432(8)	C(30)-C(31)	1.379(6)
P(1)-C(18)	1.812(4)	C(31)-C(32)	1.397(7)
P(1)-C(12)	1.817(5)	C(31)-H(31A)	0.9500
P(1)-C(7)	1.841(4)	C(32)-C(33)	1.383(7)
P(2)-C(41)	1.815(4)	C(32)-H(32A)	0.9500
P(2)-C(35)	1.816(4)	C(33)-C(34)	1.383(7)
P(2)-C(30)	1.835(4)	C(33)-H(33A)	0.9500
N(1)-C(11)	1.342(6)	C(34)-H(34A)	0.9500
N(1)-C(7)	1.357(5)	C(35)-C(40)	1.397(6)
N(2)-C(34)	1.346(6)	C(35)-C(36)	1.408(6)
N(2)-C(30)	1.358(5)	C(36)-C(37)	1.394(6)
C(1)-C(2)	1.349(6)	C(36)-H(36A)	0.9500
C(1)-C(6)	1.418(6)	C(37)-C(38)	1.388(6)
C(2)-C(3)	1.401(6)	C(37)-H(37A)	0.9500
C(3)-C(4)	1.381(7)	C(38)-C(39)	1.388(6)
C(4)-C(5)	1.367(7)	C(38)-H(38A)	0.9500
C(5)-C(6)	1.386(6)	C(39)-C(40)	1.390(6)
C(7)-C(8)	1.379(6)	C(39)-H(39A)	0.9500
C(8)-C(9)	1.386(7)	C(40)-H(40A)	0.9500
C(8)-H(8A)	0.9500	C(41)-C(42)	1.399(6)
C(9)-C(10)	1.373(7)	C(41)-C(46)	1.400(6)
C(9)-H(9A)	0.9500	C(42)-C(43)	1.383(6)
C(10)-C(11)	1.389(7)	C(42)-H(42A)	0.9500
C(10)-H(10A)	0.9500	C(43)-C(44)	1.399(6)
C(11)-H(11A)	0.9500	C(43)-H(43A)	0.9500
C(12)-C(13)	1.394(6)	C(44)-C(45)	1.381(6)
C(12)-C(17)	1.402(6)	C(44)-H(44A)	0.9500
C(13)-C(14)	1.380(7)	C(45)-C(46)	1.385(6)
C(13)-H(13A)	0.9500	C(45)-H(45A)	0.9500
C(14)-C(15)	1.392(7)	C(46)-H(46A)	0.9500
C(14)-H(14A)	0.9500		

C(1)-Au(1)-P(1)	167.99(12)	C(6)-C(5)-Cl(2)	122.1(4)
C(1)-Au(1)-Cu(1)	115.32(12)	F(3)-C(6)-C(5)	116.3(4)
P(1)-Au(1)-Cu(1)	71.00(3)	F(3)-C(6)-C(1)	119.4(4)
C(1)-Au(1)-Au(2)	89.07(11)	C(5)-C(6)-C(1)	124.2(4)
P(1)-Au(1)-Au(2)	102.78(3)	N(1)-C(7)-C(8)	122.3(4)
Cu(1)-Au(1)-Au(2)	56.134(11)	N(1)-C(7)-P(1)	114.0(3)
C(24)-Au(2)-P(2)	172.24(12)	C(8)-C(7)-P(1)	123.5(3)
C(24)-Au(2)-Cu(1)	105.48(11)	C(7)-C(8)-C(9)	119.2(5)
P(2)-Au(2)-Cu(1)	76.38(3)	C(7)-C(8)-H(8A)	120.4
C(24)-Au(2)-Au(1)	89.02(11)	C(9)-C(8)-H(8A)	120.4
P(2)-Au(2)-Au(1)	98.34(3)	C(10)-C(9)-C(8)	118.7(4)
Cu(1)-Au(2)-Au(1)	60.079(12)	C(10)-C(9)-H(9A)	120.6
N(2)-Cu(1)-N(1)	166.92(16)	C(8)-C(9)-H(9A)	120.6
N(2)-Cu(1)-Au(2)	97.80(11)	C(9)-C(10)-C(11)	119.5(5)
N(1)-Cu(1)-Au(2)	95.06(11)	C(9)-C(10)-H(10A)	120.3
N(2)-Cu(1)-Au(1)	89.95(11)	C(11)-C(10)-H(10A)	120.3
N(1)-Cu(1)-Au(1)	97.91(11)	N(1)-C(11)-C(10)	122.3(5)
Au(2)-Cu(1)-Au(1)	63.788(12)	N(1)-C(11)-H(11A)	118.8
F(7)-B(1)-F(10)	113.4(5)	C(10)-C(11)-H(11A)	118.8
F(7)-B(1)-F(8)	113.8(5)	C(13)-C(12)-C(17)	118.9(4)
F(10)-B(1)-F(8)	112.1(5)	C(13)-C(12)-P(1)	118.9(3)
F(7)-B(1)-F(9)	104.3(5)	C(17)-C(12)-P(1)	122.1(3)
F(10)-B(1)-F(9)	105.5(5)	C(14)-C(13)-C(12)	120.8(5)
F(8)-B(1)-F(9)	106.8(5)	C(14)-C(13)-H(13A)	119.6
C(18)-P(1)-C(12)	110.4(2)	C(12)-C(13)-H(13A)	119.6
C(18)-P(1)-C(7)	105.0(2)	C(13)-C(14)-C(15)	119.8(5)
C(12)-P(1)-C(7)	100.34(19)	C(13)-C(14)-H(14A)	120.1
C(18)-P(1)-Au(1)	111.95(14)	C(15)-C(14)-H(14A)	120.1
C(12)-P(1)-Au(1)	110.98(15)	C(16)-C(15)-C(14)	119.8(4)
C(7)-P(1)-Au(1)	117.44(13)	C(16)-C(15)-H(15A)	120.1
C(41)-P(2)-C(35)	104.33(18)	C(14)-C(15)-H(15A)	120.1
C(41)-P(2)-C(30)	106.92(19)	C(17)-C(16)-C(15)	120.6(5)
C(35)-P(2)-C(30)	103.96(19)	C(17)-C(16)-H(16A)	119.7
C(41)-P(2)-Au(2)	114.25(14)	C(15)-C(16)-H(16A)	119.7
C(35)-P(2)-Au(2)	110.56(13)	C(16)-C(17)-C(12)	120.0(4)
C(30)-P(2)-Au(2)	115.72(14)	C(16)-C(17)-H(17A)	120.0
C(11)-N(1)-C(7)	117.9(4)	C(12)-C(17)-H(17A)	120.0
C(11)-N(1)-Cu(1)	121.1(3)	C(23)-C(18)-C(19)	119.0(4)
C(7)-N(1)-Cu(1)	120.9(3)	C(23)-C(18)-P(1)	117.9(3)
C(34)-N(2)-C(30)	118.4(4)	C(19)-C(18)-P(1)	123.1(3)
C(34)-N(2)-Cu(1)	117.3(3)	C(20)-C(19)-C(18)	119.6(4)
C(30)-N(2)-Cu(1)	124.1(3)	C(20)-C(19)-H(19A)	120.2
C(2)-C(1)-C(6)	113.1(4)	C(18)-C(19)-H(19A)	120.2
C(2)-C(1)-Au(1)	120.9(3)	C(21)-C(20)-C(19)	120.6(5)
C(6)-C(1)-Au(1)	125.5(3)	C(21)-C(20)-H(20A)	119.7
C(1)-C(2)-F(1)	118.4(4)	C(19)-C(20)-H(20A)	119.7
C(1)-C(2)-C(3)	125.8(4)	C(20)-C(21)-C(22)	120.5(4)
F(1)-C(2)-C(3)	115.8(4)	C(20)-C(21)-H(21A)	119.8
C(4)-C(3)-C(2)	117.7(4)	C(22)-C(21)-H(21A)	119.8
C(4)-C(3)-Cl(1)	120.3(4)	C(21)-C(22)-C(23)	119.6(4)
C(2)-C(3)-Cl(1)	122.0(4)	C(21)-C(22)-H(22A)	120.2
F(2)-C(4)-C(5)	120.0(4)	C(23)-C(22)-H(22A)	120.2
F(2)-C(4)-C(3)	119.4(4)	C(22)-C(23)-C(18)	120.8(4)
C(5)-C(4)-C(3)	120.6(4)	C(22)-C(23)-H(23A)	119.6
C(4)-C(5)-C(6)	118.5(4)	C(18)-C(23)-H(23A)	119.6
C(4)-C(5)-Cl(2)	119.4(4)	C(25)-C(24)-C(29)	114.0(4)

C(25)-C(24)-Au(2)	126.6(3)	C(36)-C(35)-P(2)	122.0(3)
C(29)-C(24)-Au(2)	119.5(3)	C(37)-C(36)-C(35)	119.5(4)
F(4)-C(25)-C(24)	119.0(4)	C(37)-C(36)-H(36A)	120.3
F(4)-C(25)-C(26)	116.5(4)	C(35)-C(36)-H(36A)	120.3
C(24)-C(25)-C(26)	124.5(4)	C(38)-C(37)-C(36)	120.3(4)
C(27)-C(26)-C(25)	117.7(4)	C(38)-C(37)-H(37A)	119.9
C(27)-C(26)-Cl(3)	120.7(4)	C(36)-C(37)-H(37A)	119.9
C(25)-C(26)-Cl(3)	121.6(4)	C(37)-C(38)-C(39)	120.4(4)
F(5)-C(27)-C(28)	119.9(5)	C(37)-C(38)-H(38A)	119.8
F(5)-C(27)-C(26)	118.8(5)	C(39)-C(38)-H(38A)	119.8
C(28)-C(27)-C(26)	121.3(4)	C(38)-C(39)-C(40)	119.9(4)
C(27)-C(28)-C(29)	117.9(4)	C(38)-C(39)-H(39A)	120.0
C(27)-C(28)-Cl(4)	120.0(4)	C(40)-C(39)-H(39A)	120.0
C(29)-C(28)-Cl(4)	122.2(4)	C(39)-C(40)-C(35)	120.3(4)
F(6)-C(29)-C(28)	116.3(4)	C(39)-C(40)-H(40A)	119.9
F(6)-C(29)-C(24)	119.2(4)	C(35)-C(40)-H(40A)	119.9
C(28)-C(29)-C(24)	124.5(4)	C(42)-C(41)-C(46)	119.2(4)
N(2)-C(30)-C(31)	121.7(4)	C(42)-C(41)-P(2)	122.9(3)
N(2)-C(30)-P(2)	114.5(3)	C(46)-C(41)-P(2)	117.7(3)
C(31)-C(30)-P(2)	123.8(3)	C(43)-C(42)-C(41)	120.2(4)
C(30)-C(31)-C(32)	119.3(4)	C(43)-C(42)-H(42A)	119.9
C(30)-C(31)-H(31A)	120.4	C(41)-C(42)-H(42A)	119.9
C(32)-C(31)-H(31A)	120.4	C(42)-C(43)-C(44)	120.1(4)
C(33)-C(32)-C(31)	119.2(4)	C(42)-C(43)-H(43A)	119.9
C(33)-C(32)-H(32A)	120.4	C(44)-C(43)-H(43A)	119.9
C(31)-C(32)-H(32A)	120.4	C(45)-C(44)-C(43)	119.9(4)
C(34)-C(33)-C(32)	118.5(4)	C(45)-C(44)-H(44A)	120.0
C(34)-C(33)-H(33A)	120.8	C(43)-C(44)-H(44A)	120.0
C(32)-C(33)-H(33A)	120.8	C(44)-C(45)-C(46)	120.2(4)
N(2)-C(34)-C(33)	123.0(4)	C(44)-C(45)-H(45A)	119.9
N(2)-C(34)-H(34A)	118.5	C(46)-C(45)-H(45A)	119.9
C(33)-C(34)-H(34A)	118.5	C(45)-C(46)-C(41)	120.3(4)
C(40)-C(35)-C(36)	119.6(4)	C(45)-C(46)-H(46A)	119.8
C(40)-C(35)-P(2)	118.2(3)	C(41)-C(46)-H(46A)	119.8

Table S9. Torsion angles (°) for [Au$_2$Cu(C$_6$Cl$_2$F$_3$)$_2$(PPh$_2$py)$_2$](BF$_4$), **3**.

C(6)-C(1)-C(2)-F(1)	-177.9(4)	P(1)-C(12)-C(17)-C(16)	-176.4(3)
Au(1)-C(1)-C(2)-F(1)	-5.4(6)	C(12)-P(1)-C(18)-C(23)	-145.5(3)
C(6)-C(1)-C(2)-C(3)	2.7(7)	C(7)-P(1)-C(18)-C(23)	107.1(4)
Au(1)-C(1)-C(2)-C(3)	175.2(4)	Au(1)-P(1)-C(18)-C(23)	-21.3(4)
C(1)-C(2)-C(3)-C(4)	-2.2(8)	C(12)-P(1)-C(18)-C(19)	35.6(5)
F(1)-C(2)-C(3)-C(4)	178.4(4)	C(7)-P(1)-C(18)-C(19)	-71.7(4)
C(1)-C(2)-C(3)-Cl(1)	178.0(4)	Au(1)-P(1)-C(18)-C(19)	159.8(4)
F(1)-C(2)-C(3)-Cl(1)	-1.4(6)	C(23)-C(18)-C(19)-C(20)	-0.9(7)
C(2)-C(3)-C(4)-F(2)	-180.0(4)	P(1)-C(18)-C(19)-C(20)	177.9(4)
Cl(1)-C(3)-C(4)-F(2)	-0.2(7)	C(18)-C(19)-C(20)-C(21)	1.8(8)
C(2)-C(3)-C(4)-C(5)	1.0(7)	C(19)-C(20)-C(21)-C(22)	-1.6(8)
Cl(1)-C(3)-C(4)-C(5)	-179.2(4)	C(20)-C(21)-C(22)-C(23)	0.5(7)
F(2)-C(4)-C(5)-C(6)	-179.7(4)	C(21)-C(22)-C(23)-C(18)	0.3(7)
C(3)-C(4)-C(5)-C(6)	-0.6(7)	C(19)-C(18)-C(23)-C(22)	-0.1(7)
F(2)-C(4)-C(5)-Cl(2)	-1.1(6)	P(1)-C(18)-C(23)-C(22)	-179.0(3)
C(3)-C(4)-C(5)-Cl(2)	178.0(4)	C(29)-C(24)-C(25)-F(4)	177.9(4)
C(4)-C(5)-C(6)-F(3)	180.0(4)	Au(2)-C(24)-C(25)-F(4)	-3.2(6)
Cl(2)-C(5)-C(6)-F(3)	1.4(6)	C(29)-C(24)-C(25)-C(26)	-3.1(6)
C(4)-C(5)-C(6)-C(1)	1.4(7)	Au(2)-C(24)-C(25)-C(26)	175.9(3)
Cl(2)-C(5)-C(6)-C(1)	-177.2(4)	F(4)-C(25)-C(26)-C(27)	179.2(4)
C(2)-C(1)-C(6)-F(3)	179.1(4)	C(24)-C(25)-C(26)-C(27)	0.1(7)
Au(1)-C(1)-C(6)-F(3)	7.1(6)	F(4)-C(25)-C(26)-Cl(3)	-1.5(6)
C(2)-C(1)-C(6)-C(5)	-2.3(7)	C(24)-C(25)-C(26)-Cl(3)	179.5(3)
Au(1)-C(1)-C(6)-C(5)	-174.3(4)	C(25)-C(26)-C(27)-F(5)	-178.4(4)
C(11)-N(1)-C(7)-C(8)	2.1(6)	Cl(3)-C(26)-C(27)-F(5)	2.3(6)
Cu(1)-N(1)-C(7)-C(8)	-174.6(3)	C(25)-C(26)-C(27)-C(28)	2.4(7)
C(11)-N(1)-C(7)-P(1)	-173.6(3)	Cl(3)-C(26)-C(27)-C(28)	-176.9(4)
Cu(1)-N(1)-C(7)-P(1)	9.7(4)	F(5)-C(27)-C(28)-C(29)	179.1(4)
C(18)-P(1)-C(7)-N(1)	-169.7(3)	C(26)-C(27)-C(28)-C(29)	-1.7(7)
C(12)-P(1)-C(7)-N(1)	75.7(3)	F(5)-C(27)-C(28)-Cl(4)	-0.3(6)
Au(1)-P(1)-C(7)-N(1)	-44.6(3)	C(26)-C(27)-C(28)-Cl(4)	178.9(4)
C(18)-P(1)-C(7)-C(8)	14.6(4)	C(27)-C(28)-C(29)-F(6)	178.4(4)
C(12)-P(1)-C(7)-C(8)	-100.0(4)	Cl(4)-C(28)-C(29)-F(6)	-2.2(6)
Au(1)-P(1)-C(7)-C(8)	139.7(3)	C(27)-C(28)-C(29)-C(24)	-1.7(7)
N(1)-C(7)-C(8)-C(9)	-2.0(7)	Cl(4)-C(28)-C(29)-C(24)	177.7(3)
P(1)-C(7)-C(8)-C(9)	173.3(3)	C(25)-C(24)-C(29)-F(6)	-176.1(4)
C(7)-C(8)-C(9)-C(10)	0.7(7)	Au(2)-C(24)-C(29)-F(6)	4.8(5)
C(8)-C(9)-C(10)-C(11)	0.5(7)	C(25)-C(24)-C(29)-C(28)	3.9(6)
C(7)-N(1)-C(11)-C(10)	-0.8(6)	Au(2)-C(24)-C(29)-C(28)	-175.1(3)
Cu(1)-N(1)-C(11)-C(10)	175.8(4)	C(34)-N(2)-C(30)-C(31)	3.0(6)
C(9)-C(10)-C(11)-N(1)	-0.4(7)	Cu(1)-N(2)-C(30)-C(31)	-172.0(3)
C(18)-P(1)-C(12)-C(13)	117.3(4)	C(34)-N(2)-C(30)-P(2)	-174.1(3)
C(7)-P(1)-C(12)-C(13)	-132.3(4)	Cu(1)-N(2)-C(30)-P(2)	10.9(5)
Au(1)-P(1)-C(12)-C(13)	-7.5(4)	C(41)-P(2)-C(30)-N(2)	-163.9(3)
C(18)-P(1)-C(12)-C(17)	-66.3(4)	C(35)-P(2)-C(30)-N(2)	86.1(3)
C(7)-P(1)-C(12)-C(17)	44.1(4)	Au(2)-P(2)-C(30)-N(2)	-35.3(4)
Au(1)-P(1)-C(12)-C(17)	169.0(3)	C(41)-P(2)-C(30)-C(31)	19.0(4)
C(17)-C(12)-C(13)-C(14)	-1.2(7)	C(35)-P(2)-C(30)-C(31)	-91.0(4)
P(1)-C(12)-C(13)-C(14)	175.3(4)	Au(2)-P(2)-C(30)-C(31)	147.6(3)
C(12)-C(13)-C(14)-C(15)	1.7(7)	N(2)-C(30)-C(31)-C(32)	-2.1(7)
C(13)-C(14)-C(15)-C(16)	-1.0(7)	P(2)-C(30)-C(31)-C(32)	174.8(4)
C(14)-C(15)-C(16)-C(17)	-0.1(7)	C(30)-C(31)-C(32)-C(33)	0.0(7)
C(15)-C(16)-C(17)-C(12)	0.6(7)	C(31)-C(32)-C(33)-C(34)	1.0(8)
C(13)-C(12)-C(17)-C(16)	0.0(6)	C(30)-N(2)-C(34)-C(33)	-2.0(7)

Cu(1)-N(2)-C(34)-C(33)	173.4(4)	P(2)-C(35)-C(40)-C(39)	-172.8(3)
C(32)-C(33)-C(34)-N(2)	0.0(8)	C(35)-P(2)-C(41)-C(42)	42.7(4)
C(41)-P(2)-C(35)-C(40)	100.1(3)	C(30)-P(2)-C(41)-C(42)	-67.0(4)
C(30)-P(2)-C(35)-C(40)	-147.9(3)	Au(2)-P(2)-C(41)-C(42)	163.6(3)
Au(2)-P(2)-C(35)-C(40)	-23.1(3)	C(35)-P(2)-C(41)-C(46)	-132.2(3)
C(41)-P(2)-C(35)-C(36)	-73.9(4)	C(30)-P(2)-C(41)-C(46)	118.0(4)
C(30)-P(2)-C(35)-C(36)	38.0(4)	Au(2)-P(2)-C(41)-C(46)	-11.4(4)
Au(2)-P(2)-C(35)-C(36)	162.8(3)	C(46)-C(41)-C(42)-C(43)	-0.8(6)
C(40)-C(35)-C(36)-C(37)	-1.7(6)	P(2)-C(41)-C(42)-C(43)	-175.7(3)
P(2)-C(35)-C(36)-C(37)	172.2(3)	C(41)-C(42)-C(43)-C(44)	0.2(7)
C(35)-C(36)-C(37)-C(38)	0.2(6)	C(42)-C(43)-C(44)-C(45)	0.3(8)
C(36)-C(37)-C(38)-C(39)	1.7(6)	C(43)-C(44)-C(45)-C(46)	-0.2(8)
C(37)-C(38)-C(39)-C(40)	-2.0(6)	C(44)-C(45)-C(46)-C(41)	-0.4(8)
C(38)-C(39)-C(40)-C(35)	0.4(6)	C(42)-C(41)-C(46)-C(45)	0.9(7)
C(36)-C(35)-C(40)-C(39)	1.4(6)	P(2)-C(41)-C(46)-C(45)	176.0(4)
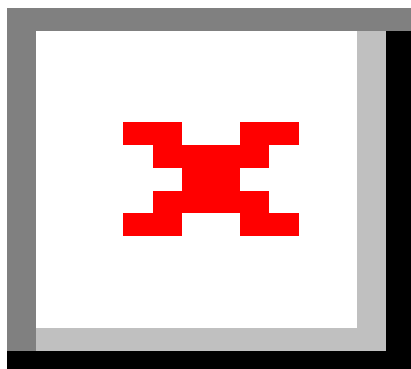
Figure S4. Thermal ellipsoid plot (50%) of [Au$_2$Cu(C$_6$Cl$_2$F$_3$)$_2${(PPh$_2$)$_2$phen)}](BF$_4$), **4**.
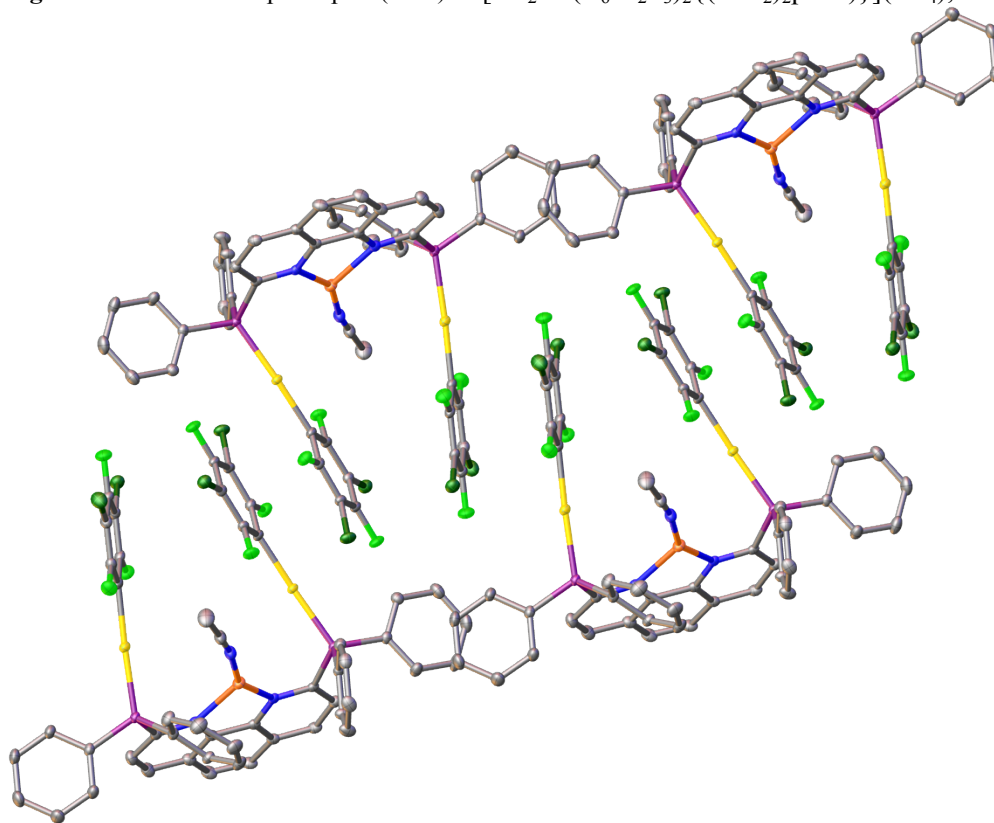
Figure S5. Thermal ellipsoid plot (50%) of [Au$_2$Cu(C$_6$Cl$_2$F$_3$)$_2${(PPh$_2$)$_2$phen)}](BF$_4$), **4** showing extended lattice packing. Hyrdogen atoms omitted (yellow = gold, orange = copper, fuscia = phosphorus, light green = fluorine, dark green = chlorine, blue = nitrogen, gray = carbon).

Table S10. Crystallographic information for [Au$_2$Cu(C$_6$Cl$_2$F$_3$)$_2${(PPh$_2$)$_2$phen)}](BF$_4$) •0.5CH$_2$Cl$_2$, **4•CH$_2$Cl$_2$**.

Identification code	cat16_0m
Empirical formula	C$_{50.5}$H$_{29}$Au$_2$BCl$_5$CuF$_{10}$N$_3$P$_2$
Formula weight	1575.24
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 8.6930(3) Å α= 80.5590(10)°.
	b = 14.8328(5) Å β= 86.5160(10)°.
	c = 20.3022(6) Å γ = 88.4640(10)°.
Volume	2577.19(15) Å^3
Z	2
Density (calculated)	2.030 Mg/m^3
Absorption coefficient	6.485 mm^{-1}
F(000)	1500
Crystal size	0.300 x 0.200 x 0.090 mm^3
Theta range for data collection	1.392 to 30.508°.
Index ranges	-12<=h<=12, -21<=k<=21, -28<=l<=28
Reflections collected	65604
Independent reflections	15695 [R(int) = 0.0214]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15695 / 0 / 687
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0159, wR2 = 0.0362
R indices (all data)	R1 = 0.0190, wR2 = 0.0369
Extinction coefficient	0.00002(3)
Largest diff. peak and hole	0.699 and -0.809 e.Å^{-3}

Table S11. Bond distances (Å) and angles (°) for [Au$_2$Cu(C$_6$Cl$_2$F$_3$)$_2${(PPh$_2$)$_2$phen)}](BF$_4$) •0.5CH$_2$Cl$_2$, **4•CH$_2$Cl$_2$**.

Au(1)-C(1)	2.0528(17)	C(17)-H(17A)	0.9500
Au(1)-P(1)	2.2772(4)	C(18)-H(18A)	0.9500
Au(2)-C(19)	2.0551(16)	C(19)-C(24)	1.385(2)
Au(2)-P(2)	2.2835(4)	C(19)-C(20)	1.386(2)
Cu(1)-N(3)	1.8586(15)	C(20)-C(21)	1.392(2)
Cu(1)-N(2)	1.9823(13)	C(21)-C(22)	1.388(2)
Cu(1)-N(1)	2.1330(14)	C(22)-C(23)	1.388(2)
P(1)-C(25)	1.8108(18)	C(23)-C(24)	1.394(2)
P(1)-C(31)	1.8176(17)	C(25)-C(26)	1.396(2)
P(1)-C(7)	1.8369(17)	C(25)-C(30)	1.399(2)
P(2)-C(43)	1.8090(16)	C(26)-C(27)	1.392(3)
P(2)-C(37)	1.8123(17)	C(26)-H(26A)	0.9500
P(2)-C(16)	1.8405(16)	C(27)-C(28)	1.387(3)
N(1)-C(7)	1.337(2)	C(27)-H(27A)	0.9500
N(1)-C(11)	1.358(2)	C(28)-C(29)	1.391(3)
N(2)-C(16)	1.337(2)	C(28)-H(28A)	0.9500
N(2)-C(12)	1.361(2)	C(29)-C(30)	1.387(3)
N(3)-C(49)	1.140(2)	C(29)-H(29A)	0.9500
Cl(1)-C(3)	1.7229(17)	C(30)-H(30A)	0.9500
Cl(2)-C(5)	1.7241(17)	C(31)-C(36)	1.394(2)
Cl(3)-C(21)	1.7221(17)	C(31)-C(32)	1.401(2)
Cl(4)-C(23)	1.7228(17)	C(32)-C(33)	1.391(3)
F(1)-C(2)	1.354(2)	C(32)-H(32A)	0.9500
F(2)-C(4)	1.3400(19)	C(33)-C(34)	1.386(3)
F(3)-C(6)	1.3598(19)	C(33)-H(33A)	0.9500
F(4)-C(20)	1.3547(19)	C(34)-C(35)	1.387(3)
F(5)-C(22)	1.3390(18)	C(34)-H(34A)	0.9500
F(6)-C(24)	1.3540(19)	C(35)-C(36)	1.394(2)
B(1)-F(8)	1.381(2)	C(35)-H(35A)	0.9500
B(1)-F(7)	1.383(2)	C(36)-H(36A)	0.9500
B(1)-F(10)	1.383(2)	C(37)-C(38)	1.393(2)
B(1)-F(9)	1.388(2)	C(37)-C(42)	1.398(2)
C(1)-C(6)	1.385(2)	C(38)-C(39)	1.394(3)
C(1)-C(2)	1.389(2)	C(38)-H(38A)	0.9500
C(2)-C(3)	1.390(2)	C(39)-C(40)	1.382(3)
C(3)-C(4)	1.382(2)	C(39)-H(39A)	0.9500
C(4)-C(5)	1.389(2)	C(40)-C(41)	1.393(3)
C(5)-C(6)	1.388(2)	C(40)-H(40A)	0.9500
C(7)-C(8)	1.409(2)	C(41)-C(42)	1.385(3)
C(8)-C(9)	1.375(3)	C(41)-H(41A)	0.9500
C(8)-H(8A)	0.9500	C(42)-H(42A)	0.9500
C(9)-C(10)	1.403(3)	C(43)-C(48)	1.395(2)
C(9)-H(9A)	0.9500	C(43)-C(44)	1.400(2)
C(10)-C(11)	1.414(2)	C(44)-C(45)	1.390(2)
C(10)-C(17)	1.438(2)	C(44)-H(44A)	0.9500
C(11)-C(12)	1.443(2)	C(45)-C(46)	1.388(3)
C(12)-C(13)	1.409(2)	C(45)-H(45A)	0.9500
C(13)-C(14)	1.402(2)	C(46)-C(47)	1.387(3)
C(13)-C(18)	1.437(2)	C(46)-H(46A)	0.9500
C(14)-C(15)	1.380(2)	C(47)-C(48)	1.393(2)
C(14)-H(14A)	0.9500	C(47)-H(47A)	0.9500
C(15)-C(16)	1.403(2)	C(48)-H(48A)	0.9500
C(15)-H(15A)	0.9500	C(49)-C(50)	1.457(3)
C(17)-C(18)	1.354(3)	C(50)-H(50A)	0.9800

C(50)-H(50B)	0.9800	C(1)-C(6)-C(5)	124.71(16)
C(50)-H(50C)	0.9800	N(1)-C(7)-C(8)	122.20(16)
C(1S)-Cl(1S)	1.316(6)	N(1)-C(7)-P(1)	117.19(12)
C(1S)-C(1S)#1	1.510(11)	C(8)-C(7)-P(1)	120.59(13)
C(1S)-Cl(2S)	1.756(5)	C(9)-C(8)-C(7)	119.48(17)
C(1S)-Cl(1S)#1	1.808(7)	C(9)-C(8)-H(8A)	120.3
Cl(1S)-Cl(2S)	0.622(3)	C(7)-C(8)-H(8A)	120.3
Cl(1S)-C(1S)#1	1.808(7)	C(8)-C(9)-C(10)	119.67(16)
		C(8)-C(9)-H(9A)	120.2
C(1)-Au(1)-P(1)	176.56(5)	C(10)-C(9)-H(9A)	120.2
C(19)-Au(2)-P(2)	173.39(5)	C(9)-C(10)-C(11)	117.22(16)
N(3)-Cu(1)-N(2)	151.12(6)	C(9)-C(10)-C(17)	123.02(16)
N(3)-Cu(1)-N(1)	126.54(6)	C(11)-C(10)-C(17)	119.75(16)
N(2)-Cu(1)-N(1)	82.27(6)	N(1)-C(11)-C(10)	123.05(16)
C(25)-P(1)-C(31)	107.17(8)	N(1)-C(11)-C(12)	117.78(14)
C(25)-P(1)-C(7)	103.71(8)	C(10)-C(11)-C(12)	119.17(15)
C(31)-P(1)-C(7)	105.24(8)	N(2)-C(12)-C(13)	122.71(15)
C(25)-P(1)-Au(1)	116.33(6)	N(2)-C(12)-C(11)	117.67(14)
C(31)-P(1)-Au(1)	112.05(6)	C(13)-C(12)-C(11)	119.57(15)
C(7)-P(1)-Au(1)	111.47(6)	C(14)-C(13)-C(12)	117.41(15)
C(43)-P(2)-C(37)	105.89(7)	C(14)-C(13)-C(18)	122.79(15)
C(43)-P(2)-C(16)	105.63(7)	C(12)-C(13)-C(18)	119.76(16)
C(37)-P(2)-C(16)	104.91(8)	C(15)-C(14)-C(13)	119.72(15)
C(43)-P(2)-Au(2)	111.20(5)	C(15)-C(14)-H(14A)	120.1
C(37)-P(2)-Au(2)	115.34(6)	C(13)-C(14)-H(14A)	120.1
C(16)-P(2)-Au(2)	113.11(5)	C(14)-C(15)-C(16)	119.31(16)
C(7)-N(1)-C(11)	118.26(14)	C(14)-C(15)-H(15A)	120.3
C(7)-N(1)-Cu(1)	133.10(12)	C(16)-C(15)-H(15A)	120.3
C(11)-N(1)-Cu(1)	108.62(11)	N(2)-C(16)-C(15)	122.19(15)
C(16)-N(2)-C(12)	118.56(14)	N(2)-C(16)-P(2)	114.68(11)
C(16)-N(2)-Cu(1)	128.01(11)	C(15)-C(16)-P(2)	122.82(13)
C(12)-N(2)-Cu(1)	113.44(11)	C(18)-C(17)-C(10)	120.82(16)
C(49)-N(3)-Cu(1)	170.84(15)	C(18)-C(17)-H(17A)	119.6
F(8)-B(1)-F(7)	109.56(17)	C(10)-C(17)-H(17A)	119.6
F(8)-B(1)-F(10)	110.12(17)	C(17)-C(18)-C(13)	120.85(16)
F(7)-B(1)-F(10)	106.95(17)	C(17)-C(18)-H(18A)	119.6
F(8)-B(1)-F(9)	109.55(16)	C(13)-C(18)-H(18A)	119.6
F(7)-B(1)-F(9)	110.16(17)	C(24)-C(19)-C(20)	114.17(15)
F(10)-B(1)-F(9)	110.47(16)	C(24)-C(19)-Au(2)	125.65(13)
C(6)-C(1)-C(2)	114.23(15)	C(20)-C(19)-Au(2)	120.00(12)
C(6)-C(1)-Au(1)	124.57(13)	F(4)-C(20)-C(19)	118.79(15)
C(2)-C(1)-Au(1)	121.20(13)	F(4)-C(20)-C(21)	116.34(15)
F(1)-C(2)-C(1)	118.91(16)	C(19)-C(20)-C(21)	124.86(16)
F(1)-C(2)-C(3)	116.57(15)	C(22)-C(21)-C(20)	117.66(15)
C(1)-C(2)-C(3)	124.51(16)	C(22)-C(21)-Cl(3)	120.97(13)
C(4)-C(3)-C(2)	117.83(15)	C(20)-C(21)-Cl(3)	121.35(13)
C(4)-C(3)-Cl(1)	120.72(13)	F(5)-C(22)-C(23)	119.71(15)
C(2)-C(3)-Cl(1)	121.44(14)	F(5)-C(22)-C(21)	119.44(15)
F(2)-C(4)-C(3)	119.45(15)	C(23)-C(22)-C(21)	120.84(15)
F(2)-C(4)-C(5)	119.45(15)	C(22)-C(23)-C(24)	117.91(15)
C(3)-C(4)-C(5)	121.09(16)	C(22)-C(23)-Cl(4)	119.99(13)
C(6)-C(5)-C(4)	117.63(15)	C(24)-C(23)-Cl(4)	122.10(13)
C(6)-C(5)-Cl(2)	121.56(13)	F(6)-C(24)-C(19)	118.98(15)
C(4)-C(5)-Cl(2)	120.81(13)	F(6)-C(24)-C(23)	116.49(15)
F(3)-C(6)-C(1)	118.76(15)	C(19)-C(24)-C(23)	124.53(16)
F(3)-C(6)-C(5)	116.53(15)	C(26)-C(25)-C(30)	120.13(16)

C(26)-C(25)-P(1)	118.88(14)	C(37)-C(38)-H(38A)	119.9
C(30)-C(25)-P(1)	120.88(13)	C(39)-C(38)-H(38A)	119.9
C(27)-C(26)-C(25)	119.76(17)	C(40)-C(39)-C(38)	119.84(18)
C(27)-C(26)-H(26A)	120.1	C(40)-C(39)-H(39A)	120.1
C(25)-C(26)-H(26A)	120.1	C(38)-C(39)-H(39A)	120.1
C(28)-C(27)-C(26)	119.92(17)	C(39)-C(40)-C(41)	120.39(18)
C(28)-C(27)-H(27A)	120.0	C(39)-C(40)-H(40A)	119.8
C(26)-C(27)-H(27A)	120.0	C(41)-C(40)-H(40A)	119.8
C(27)-C(28)-C(29)	120.39(18)	C(42)-C(41)-C(40)	119.85(18)
C(27)-C(28)-H(28A)	119.8	C(42)-C(41)-H(41A)	120.1
C(29)-C(28)-H(28A)	119.8	C(40)-C(41)-H(41A)	120.1
C(30)-C(29)-C(28)	120.14(18)	C(41)-C(42)-C(37)	120.17(18)
C(30)-C(29)-H(29A)	119.9	C(41)-C(42)-H(42A)	119.9
C(28)-C(29)-H(29A)	119.9	C(37)-C(42)-H(42A)	119.9
C(29)-C(30)-C(25)	119.64(17)	C(48)-C(43)-C(44)	120.24(15)
C(29)-C(30)-H(30A)	120.2	C(48)-C(43)-P(2)	122.83(12)
C(25)-C(30)-H(30A)	120.2	C(44)-C(43)-P(2)	116.87(12)
C(36)-C(31)-C(32)	119.64(16)	C(45)-C(44)-C(43)	119.94(16)
C(36)-C(31)-P(1)	123.49(13)	C(45)-C(44)-H(44A)	120.0
C(32)-C(31)-P(1)	116.61(13)	C(43)-C(44)-H(44A)	120.0
C(33)-C(32)-C(31)	119.94(17)	C(46)-C(45)-C(44)	119.61(16)
C(33)-C(32)-H(32A)	120.0	C(46)-C(45)-H(45A)	120.2
C(31)-C(32)-H(32A)	120.0	C(44)-C(45)-H(45A)	120.2
C(34)-C(33)-C(32)	120.00(17)	C(47)-C(46)-C(45)	120.66(16)
C(34)-C(33)-H(33A)	120.0	C(47)-C(46)-H(46A)	119.7
C(32)-C(33)-H(33A)	120.0	C(45)-C(46)-H(46A)	119.7
C(33)-C(34)-C(35)	120.26(18)	C(46)-C(47)-C(48)	120.23(17)
C(33)-C(34)-H(34A)	119.9	C(46)-C(47)-H(47A)	119.9
C(35)-C(34)-H(34A)	119.9	C(48)-C(47)-H(47A)	119.9
C(34)-C(35)-C(36)	120.18(17)	C(47)-C(48)-C(43)	119.32(16)
C(34)-C(35)-H(35A)	119.9	C(47)-C(48)-H(48A)	120.3
C(36)-C(35)-H(35A)	119.9	C(43)-C(48)-H(48A)	120.3
C(35)-C(36)-C(31)	119.79(16)	N(3)-C(49)-C(50)	178.1(2)
C(35)-C(36)-H(36A)	120.1	C(49)-C(50)-H(50A)	109.5
C(31)-C(36)-H(36A)	120.1	C(49)-C(50)-H(50B)	109.5
C(38)-C(37)-C(42)	119.47(16)	H(50A)-C(50)-H(50B)	109.5
C(38)-C(37)-P(2)	118.86(13)	C(49)-C(50)-H(50C)	109.5
C(42)-C(37)-P(2)	121.67(13)	H(50A)-C(50)-H(50C)	109.5
C(37)-C(38)-C(39)	120.20(17)	H(50B)-C(50)-H(50C)	109.5

Table S12. Torsion angles (°) for [Au$_2$Cu(C$_6$Cl$_2$F$_3$)$_2${(PPh$_2$)$_2$phen}](BF$_4$) •0.5CH$_2$Cl$_2$, **4•CH$_2$Cl$_2$**.

C(6)-C(1)-C(2)-F(1)	179.62(15)	C(10)-C(11)-C(12)-C(13)	2.6(2)
Au(1)-C(1)-C(2)-F(1)	-0.4(2)	N(2)-C(12)-C(13)-C(14)	-3.4(2)
C(6)-C(1)-C(2)-C(3)	0.0(3)	C(11)-C(12)-C(13)-C(14)	179.33(15)
Au(1)-C(1)-C(2)-C(3)	179.92(13)	N(2)-C(12)-C(13)-C(18)	174.24(15)
F(1)-C(2)-C(3)-C(4)	180.00(15)	C(11)-C(12)-C(13)-C(18)	-3.1(2)
C(1)-C(2)-C(3)-C(4)	-0.4(3)	C(12)-C(13)-C(14)-C(15)	2.9(2)
F(1)-C(2)-C(3)-Cl(1)	-1.5(2)	C(18)-C(13)-C(14)-C(15)	-174.66(16)
C(1)-C(2)-C(3)-Cl(1)	178.20(14)	C(13)-C(14)-C(15)-C(16)	-0.3(2)
C(2)-C(3)-C(4)-F(2)	179.87(15)	C(12)-N(2)-C(16)-C(15)	1.8(2)
Cl(1)-C(3)-C(4)-F(2)	1.3(2)	Cu(1)-N(2)-C(16)-C(15)	-177.63(12)
C(2)-C(3)-C(4)-C(5)	0.7(3)	C(12)-N(2)-C(16)-P(2)	-171.95(11)
Cl(1)-C(3)-C(4)-C(5)	-177.89(13)	Cu(1)-N(2)-C(16)-P(2)	8.63(18)
F(2)-C(4)-C(5)-C(6)	-179.80(15)	C(14)-C(15)-C(16)-N(2)	-2.2(2)
C(3)-C(4)-C(5)-C(6)	-0.6(2)	C(14)-C(15)-C(16)-P(2)	171.04(13)
F(2)-C(4)-C(5)-Cl(2)	1.3(2)	C(43)-P(2)-C(16)-N(2)	-67.87(13)
C(3)-C(4)-C(5)-Cl(2)	-179.52(13)	C(37)-P(2)-C(16)-N(2)	-179.50(12)
C(2)-C(1)-C(6)-F(3)	179.47(14)	Au(2)-P(2)-C(16)-N(2)	53.97(13)
Au(1)-C(1)-C(6)-F(3)	-0.5(2)	C(43)-P(2)-C(16)-C(15)	118.43(14)
C(2)-C(1)-C(6)-C(5)	0.1(2)	C(37)-P(2)-C(16)-C(15)	6.80(15)
Au(1)-C(1)-C(6)-C(5)	-179.85(13)	Au(2)-P(2)-C(16)-C(15)	-119.72(13)
C(4)-C(5)-C(6)-F(3)	-179.18(14)	C(9)-C(10)-C(17)-C(18)	177.25(18)
Cl(2)-C(5)-C(6)-F(3)	-0.3(2)	C(11)-C(10)-C(17)-C(18)	-2.0(3)
C(4)-C(5)-C(6)-C(1)	0.2(3)	C(10)-C(17)-C(18)-C(13)	1.5(3)
Cl(2)-C(5)-C(6)-C(1)	179.12(14)	C(14)-C(13)-C(18)-C(17)	178.51(17)
C(11)-N(1)-C(7)-C(8)	3.8(2)	C(12)-C(13)-C(18)-C(17)	1.0(3)
Cu(1)-N(1)-C(7)-C(8)	-173.87(13)	C(24)-C(19)-C(20)-F(4)	176.96(14)
C(11)-N(1)-C(7)-P(1)	-177.95(12)	Au(2)-C(19)-C(20)-F(4)	1.5(2)
Cu(1)-N(1)-C(7)-P(1)	4.4(2)	C(24)-C(19)-C(20)-C(21)	-2.0(2)
C(25)-P(1)-C(7)-N(1)	166.13(13)	Au(2)-C(19)-C(20)-C(21)	-177.42(13)
C(31)-P(1)-C(7)-N(1)	53.72(15)	F(4)-C(20)-C(21)-C(22)	-177.79(14)
Au(1)-P(1)-C(7)-N(1)	-67.96(14)	C(19)-C(20)-C(21)-C(22)	1.2(3)
C(25)-P(1)-C(7)-C(8)	-15.61(16)	F(4)-C(20)-C(21)-Cl(3)	0.6(2)
C(31)-P(1)-C(7)-C(8)	-128.02(15)	C(19)-C(20)-C(21)-Cl(3)	179.57(14)
Au(1)-P(1)-C(7)-C(8)	110.30(14)	C(20)-C(21)-C(22)-F(5)	179.70(14)
N(1)-C(7)-C(8)-C(9)	-1.5(3)	Cl(3)-C(21)-C(22)-F(5)	1.3(2)
P(1)-C(7)-C(8)-C(9)	-179.65(14)	C(20)-C(21)-C(22)-C(23)	0.7(2)
C(7)-C(8)-C(9)-C(10)	-1.5(3)	Cl(3)-C(21)-C(22)-C(23)	-177.65(13)
C(8)-C(9)-C(10)-C(11)	1.9(3)	F(5)-C(22)-C(23)-C(24)	179.42(14)
C(8)-C(9)-C(10)-C(17)	-177.35(18)	C(21)-C(22)-C(23)-C(24)	-1.6(2)
C(7)-N(1)-C(11)-C(10)	-3.4(2)	F(5)-C(22)-C(23)-Cl(4)	-1.7(2)
Cu(1)-N(1)-C(11)-C(10)	174.87(13)	C(21)-C(22)-C(23)-Cl(4)	177.28(13)
C(7)-N(1)-C(11)-C(12)	176.53(15)	C(20)-C(19)-C(24)-F(6)	-178.21(14)
Cu(1)-N(1)-C(11)-C(12)	-5.25(17)	Au(2)-C(19)-C(24)-F(6)	-3.1(2)
C(9)-C(10)-C(11)-N(1)	0.5(3)	C(20)-C(19)-C(24)-C(23)	1.0(2)
C(17)-C(10)-C(11)-N(1)	179.79(16)	Au(2)-C(19)-C(24)-C(23)	176.13(13)
C(9)-C(10)-C(11)-C(12)	-179.36(16)	C(22)-C(23)-C(24)-F(6)	179.95(14)
C(17)-C(10)-C(11)-C(12)	-0.1(2)	Cl(4)-C(23)-C(24)-F(6)	1.1(2)
C(16)-N(2)-C(12)-C(13)	1.1(2)	C(22)-C(23)-C(24)-C(19)	0.7(3)
Cu(1)-N(2)-C(12)-C(13)	-179.45(12)	Cl(4)-C(23)-C(24)-C(19)	-178.16(14)
C(16)-N(2)-C(12)-C(11)	178.41(14)	C(31)-P(1)-C(25)-C(26)	-144.80(14)
Cu(1)-N(2)-C(12)-C(11)	-2.10(18)	C(7)-P(1)-C(25)-C(26)	104.19(15)
N(1)-C(11)-C(12)-N(2)	5.2(2)	Au(1)-P(1)-C(25)-C(26)	-18.57(16)
C(10)-C(11)-C(12)-N(2)	-174.86(15)	C(31)-P(1)-C(25)-C(30)	39.04(17)
N(1)-C(11)-C(12)-C(13)	-177.32(15)	C(7)-P(1)-C(25)-C(30)	-71.96(16)

Au(1)-P(1)-C(25)-C(30)	165.28(13)
C(30)-C(25)-C(26)-C(27)	0.6(3)
P(1)-C(25)-C(26)-C(27)	-175.63(15)
C(25)-C(26)-C(27)-C(28)	0.2(3)
C(26)-C(27)-C(28)-C(29)	-0.5(3)
C(27)-C(28)-C(29)-C(30)	0.0(3)
C(28)-C(29)-C(30)-C(25)	0.8(3)
C(26)-C(25)-C(30)-C(29)	-1.0(3)
P(1)-C(25)-C(30)-C(29)	175.06(15)
C(25)-P(1)-C(31)-C(36)	-105.48(16)
C(7)-P(1)-C(31)-C(36)	4.47(17)
Au(1)-P(1)-C(31)-C(36)	125.77(14)
C(25)-P(1)-C(31)-C(32)	80.37(15)
C(7)-P(1)-C(31)-C(32)	-169.68(14)
Au(1)-P(1)-C(31)-C(32)	-48.38(15)
C(36)-C(31)-C(32)-C(33)	-2.6(3)
P(1)-C(31)-C(32)-C(33)	171.82(16)
C(31)-C(32)-C(33)-C(34)	-1.4(3)
C(32)-C(33)-C(34)-C(35)	3.6(3)
C(33)-C(34)-C(35)-C(36)	-1.8(3)
C(34)-C(35)-C(36)-C(31)	-2.2(3)
C(32)-C(31)-C(36)-C(35)	4.3(3)
P(1)-C(31)-C(36)-C(35)	-169.63(14)
C(43)-P(2)-C(37)-C(38)	130.47(13)
C(16)-P(2)-C(37)-C(38)	-118.08(13)
Au(2)-P(2)-C(37)-C(38)	7.05(15)
C(43)-P(2)-C(37)-C(42)	-50.28(16)
C(16)-P(2)-C(37)-C(42)	61.17(16)
Au(2)-P(2)-C(37)-C(42)	-173.69(12)
C(42)-C(37)-C(38)-C(39)	-1.4(3)
P(2)-C(37)-C(38)-C(39)	177.91(14)
C(37)-C(38)-C(39)-C(40)	-1.2(3)
C(38)-C(39)-C(40)-C(41)	2.1(3)
C(39)-C(40)-C(41)-C(42)	-0.5(3)
C(40)-C(41)-C(42)-C(37)	-2.1(3)
C(38)-C(37)-C(42)-C(41)	3.0(3)
P(2)-C(37)-C(42)-C(41)	-176.21(15)
C(37)-P(2)-C(43)-C(48)	87.20(15)
C(16)-P(2)-C(43)-C(48)	-23.75(16)
Au(2)-P(2)-C(43)-C(48)	-146.82(13)
C(37)-P(2)-C(43)-C(44)	-90.05(14)
C(16)-P(2)-C(43)-C(44)	159.01(13)
Au(2)-P(2)-C(43)-C(44)	35.94(14)
C(48)-C(43)-C(44)-C(45)	-0.1(3)
P(2)-C(43)-C(44)-C(45)	177.23(13)
C(43)-C(44)-C(45)-C(46)	0.3(3)
C(44)-C(45)-C(46)-C(47)	-0.3(3)
C(45)-C(46)-C(47)-C(48)	0.0(3)
C(46)-C(47)-C(48)-C(43)	0.3(3)
C(44)-C(43)-C(48)-C(47)	-0.2(3)
P(2)-C(43)-C(48)-C(47)	-177.38(14)
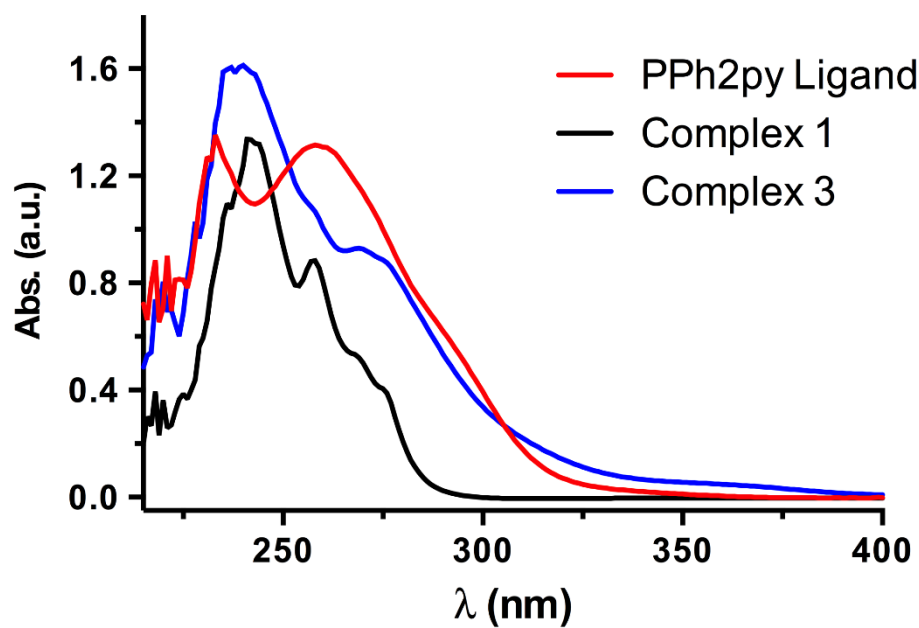
Figure S6. UV-Vis absorption spectra of PPh$_2$py ligand and complexes **1** and **3** in dichloromethane.
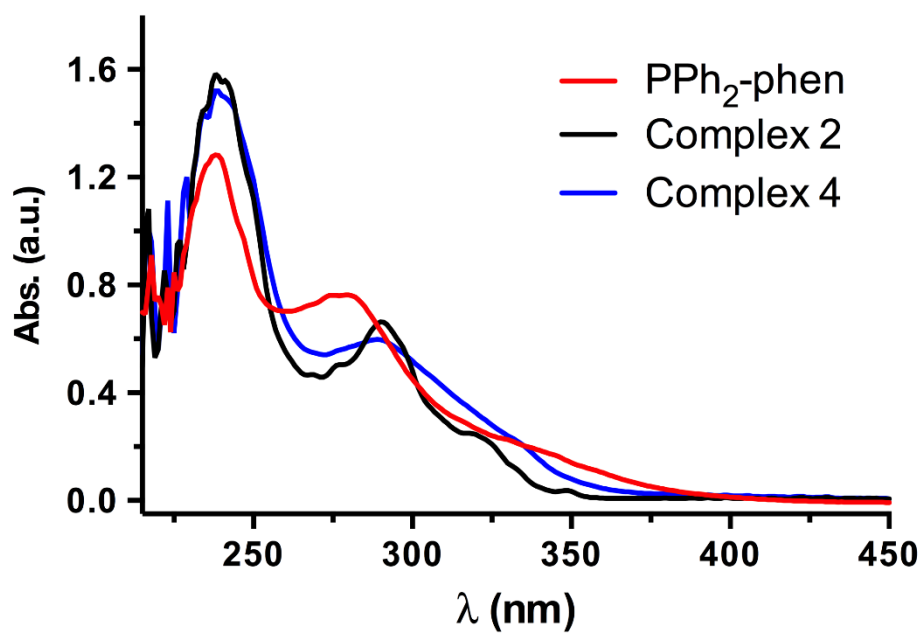
Figure S7. UV-Vis absorption spectra of PPh$_2$-phen ligand and complexes **2** and **4** in tetrahydrofuran.

Figure S8. Excitation and emission spectra for PPh$_2$py ligand in solid state at room temperature.
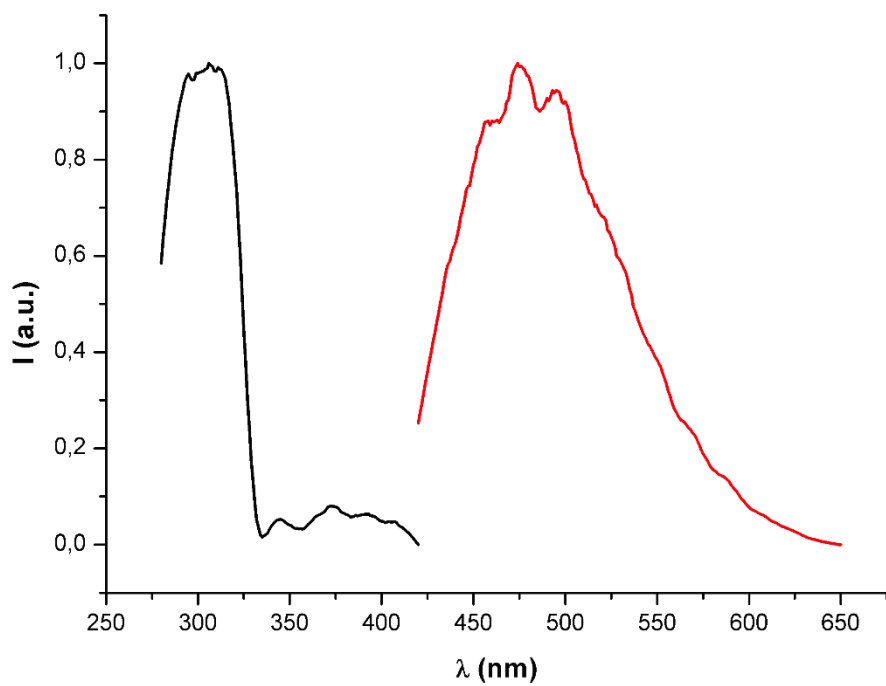
Figure S9. Excitation and emission spectra for PPh$_2$py ligand in solid state at 77 K.

Figure S10. Excitation and emission spectra for PPh$_2$phen ligand in solid state at room temperature.
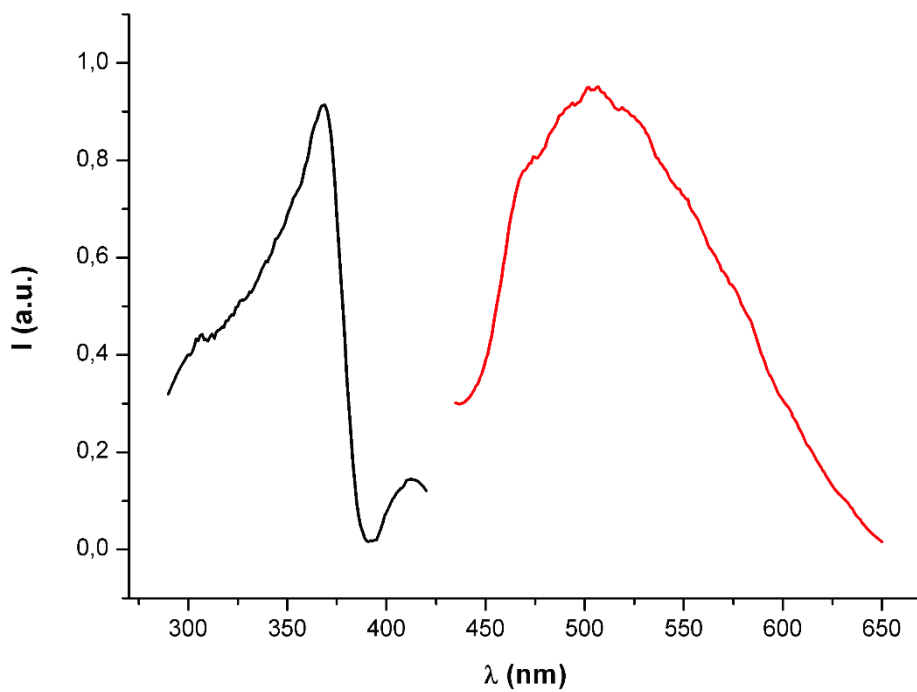
Figure S11. Excitation and emission spectra for PPh$_2$phen ligand in solid state at 77 K.
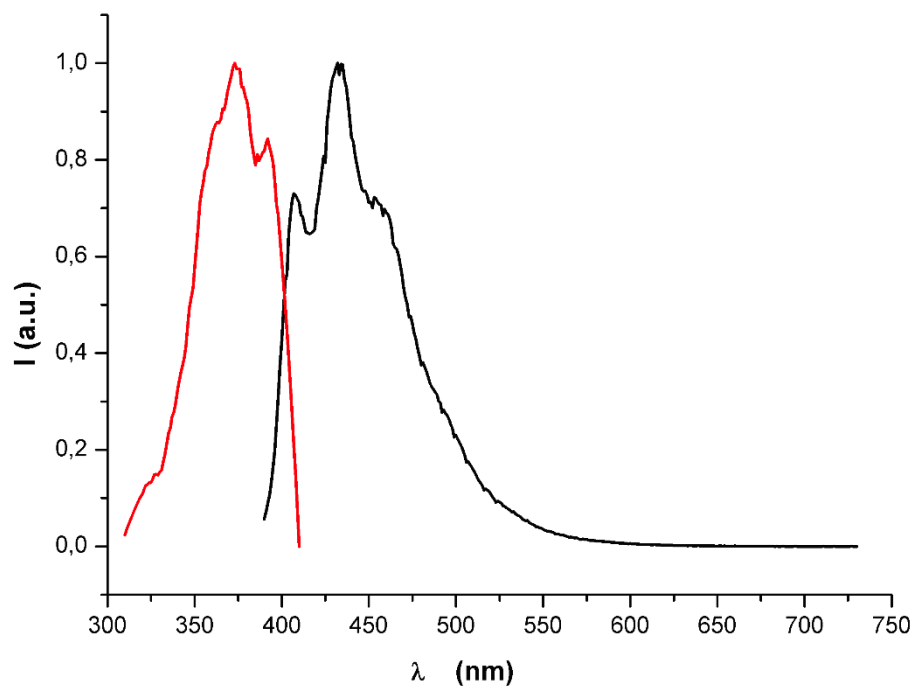
Figure S12. Excitation and emission spectra for PPh$_2$-phen ligand in tetrahydrofuran solutions.

Figure S13. Excitation and emission spectra for complex **1** in solid state at room temperature.

Figure S14. Excitation and emission spectra for complex **1** in solid state at 77 K.

Figure S15. Excitation and emission spectra for complex **2** in solid state at room temperature.

Figure S16. Excitation and emission spectra for complex **2** in solid state at 77 K.

Figure S17. Excitation and emission spectra for complex **2** in tetrahydrofuran solutions.
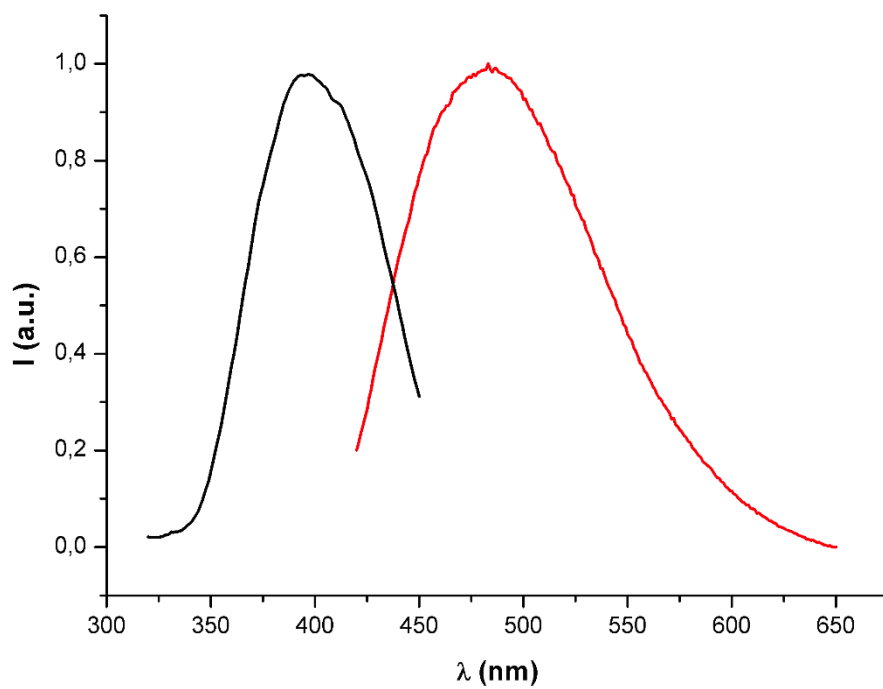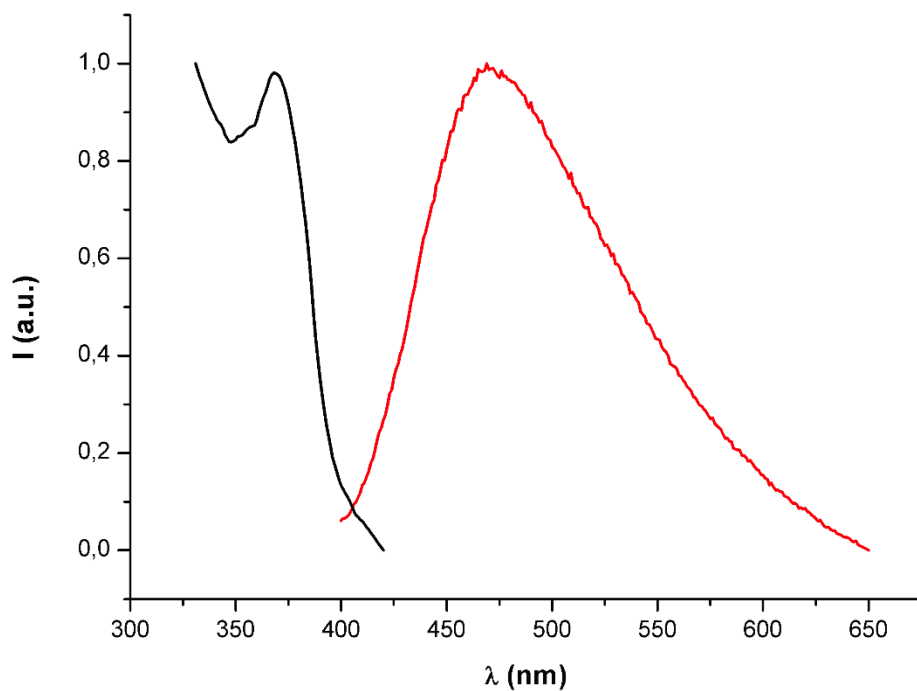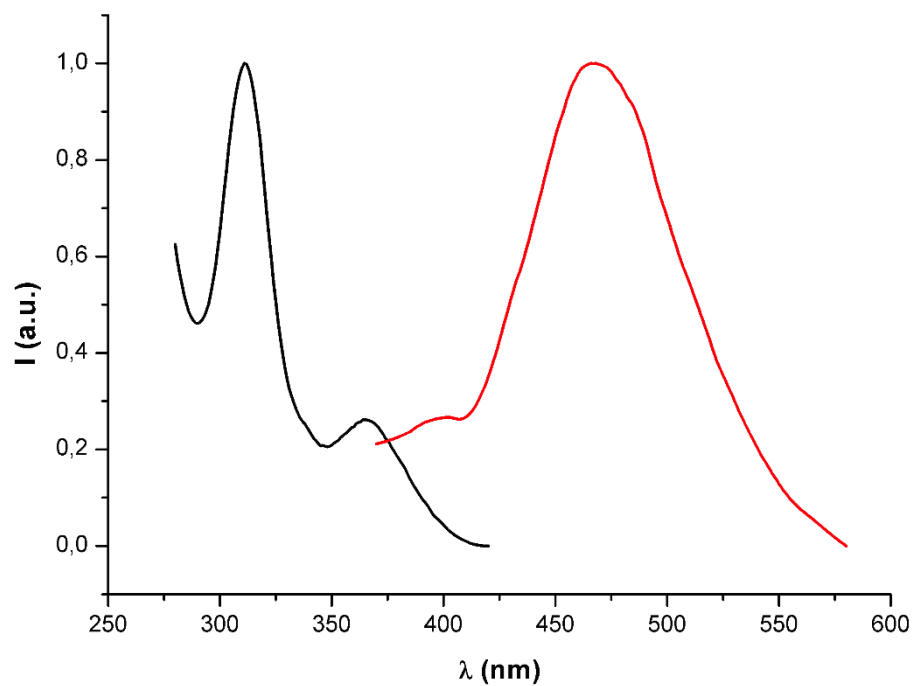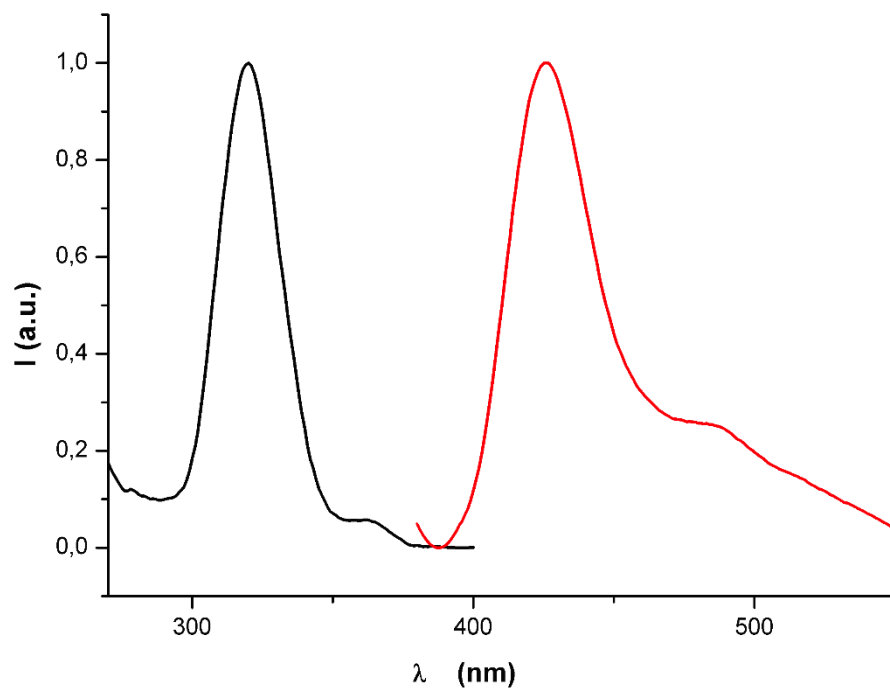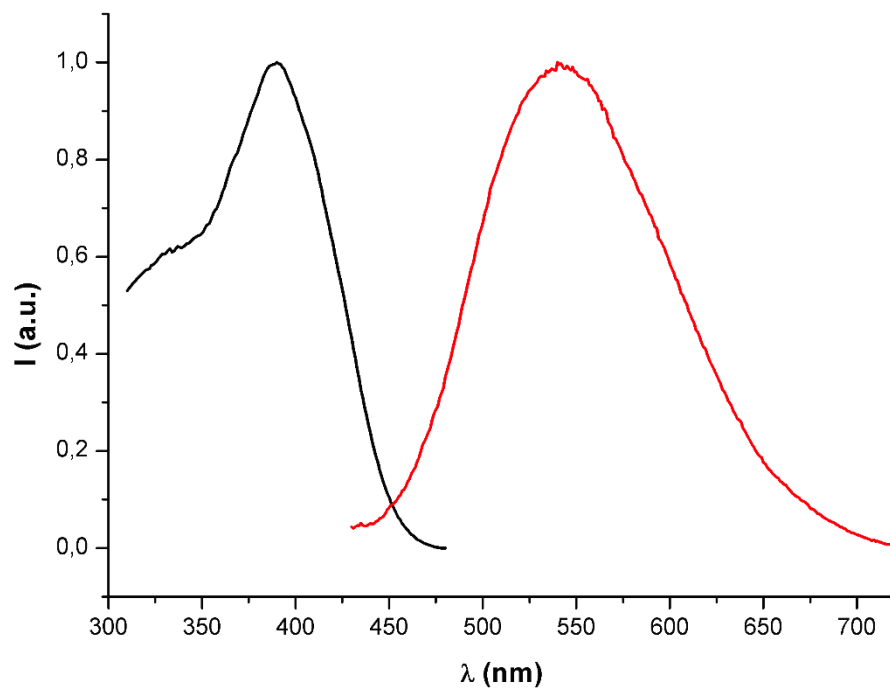
Figure S18. Excitation and emission spectra for complex **3** in solid state at room temperature.

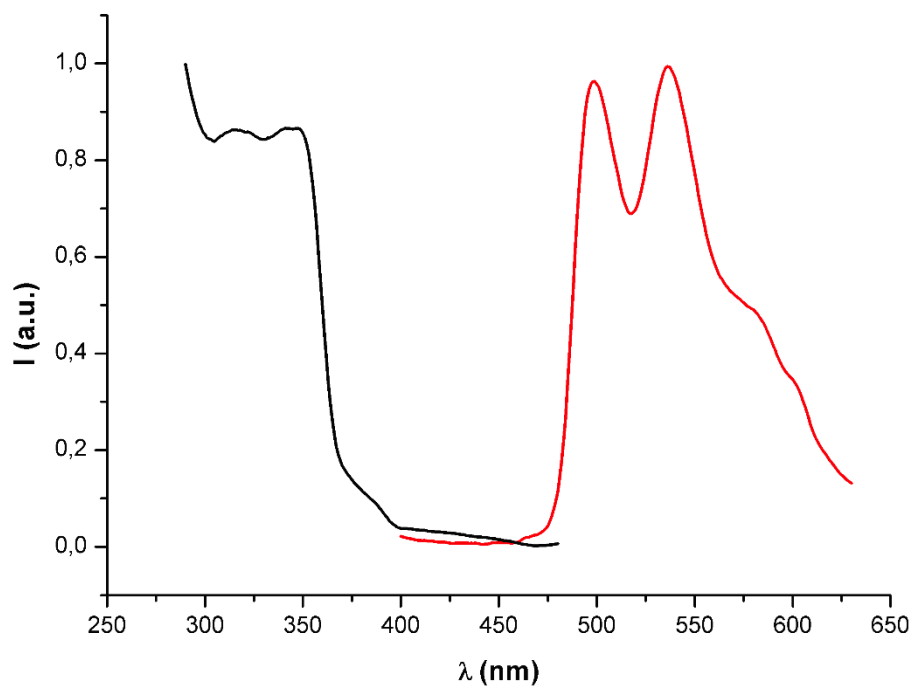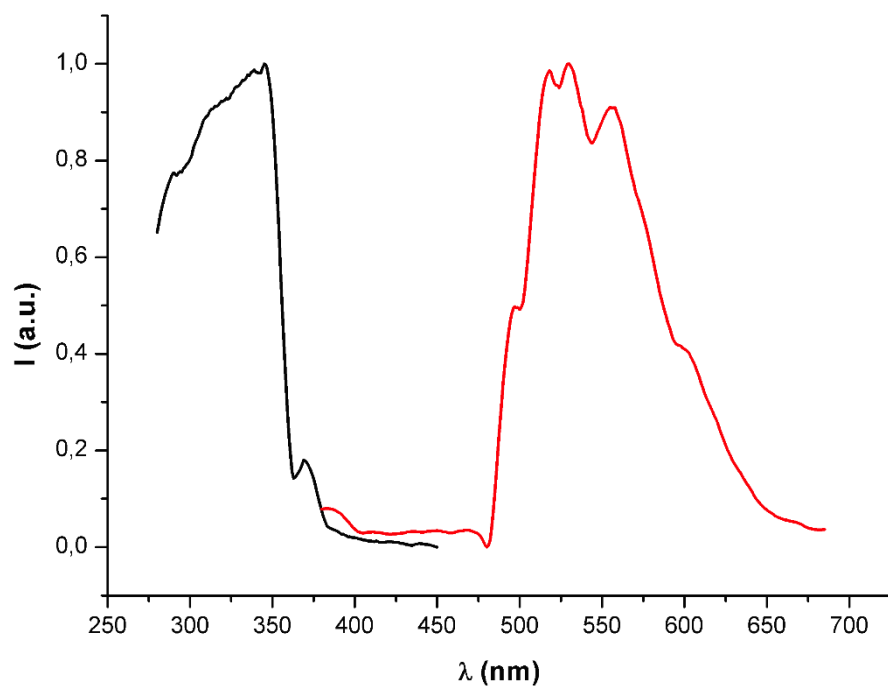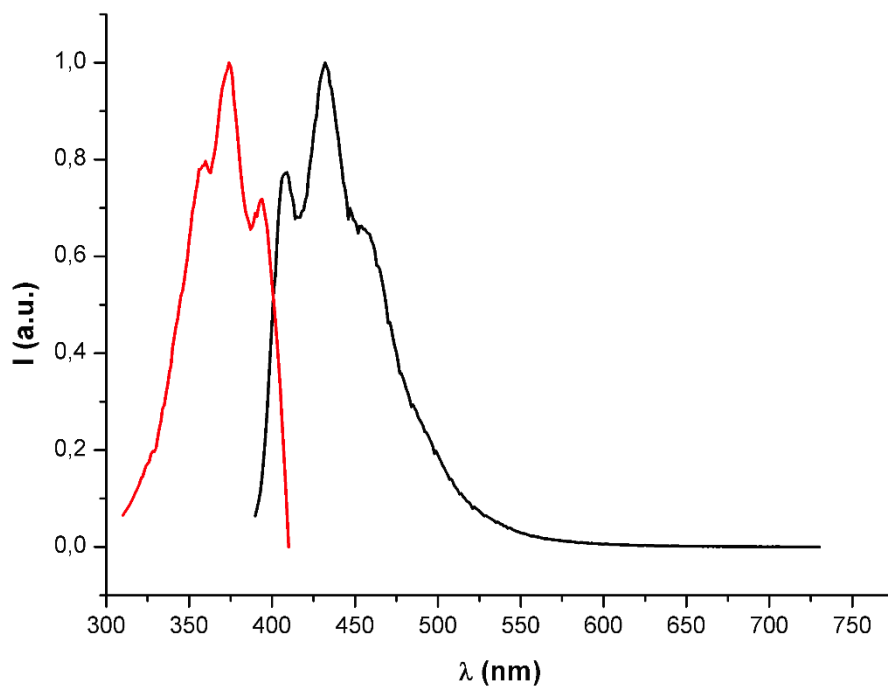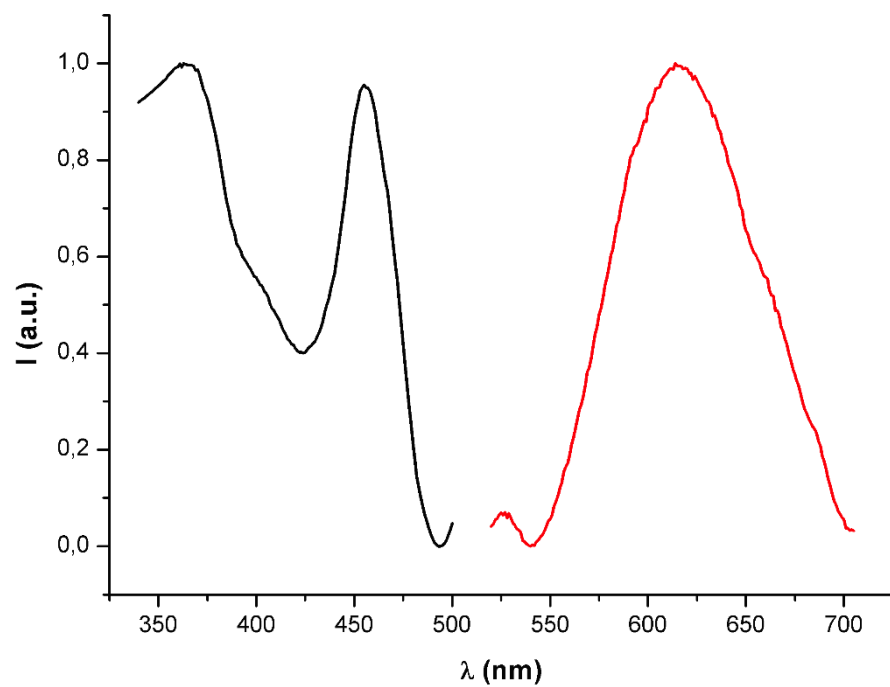**Figure S19.** Excitation and emission spectra for complex **4** in solid state at room temperature.

GEOMETRIES IN XYZ FORMAT FOR FULLY OPTIMIZED THEORETICAL MODELS

Model **3a S$_0$.**

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Au           0.17187900    1.72758000   -0.36512100
Au          -0.16145100   -1.72238200   -0.32614600
Cu          -0.03419900    0.03779600    1.90417200
P            2.21470700    1.88800900    0.75706700
N            1.83562900   -0.41347500    2.13858800
C            3.62903100    2.50478200   -0.22952500
N           -1.91454800    0.48075900    2.06801700
C            1.17875600    4.10165700    2.08545000
H            0.60254400    4.24541800    1.16660300
C            1.04691100    5.00359200    3.13656400
H            0.37424200    5.85860400    3.03275600
C           -2.84822300   -0.28657100    1.47247000
C            2.79970200    0.30697900    1.53276400
C            2.04630800    3.00988200    2.20635400
C            4.66478500    3.24654800    0.34794800
H            4.63935700    3.50286600    1.41010300
C            5.75042200    3.37922300   -1.80294500
H            6.58221300    3.72632600   -2.42097600
C            2.62413900    3.72542300    4.43998900
H            3.18950900    3.57550100    5.36313200
C            2.76790500    2.82357600    3.38944400
H            3.44504800    1.97285100    3.50093000
C            4.12175900   -0.11197900    1.50884300
H            4.87187600    0.48802800    0.99035100
C            2.17031200   -1.54880900    2.76385000
H            1.35527200   -2.10343700    3.23301600
C            1.76728200    4.81561100    4.31365500
H            1.66014100    5.52371300    5.13917500
C           -4.17527300    0.10737200    1.38641700
H           -4.90024000   -0.53232000    0.87958800
C           -2.28486300    1.64203800    2.62085500
H           -1.49344200    2.23373300    3.08499700
C            3.47371900   -2.02597300    2.79444200
H            3.69179700   -2.96808300    3.29927500
C            4.46356200   -1.30428800    2.14435100
H            5.49548000   -1.66320800    2.12639200
C            5.72400800    3.67942200   -0.44271400
H            6.53086200    4.26384600    0.00629100
C            4.71435000    2.65019400   -2.37969500
H            4.72694600    2.42115900   -3.44749000
C           -3.59539400    2.09925100    2.58450700
H           -3.84300600    3.06416100    3.02910500
C           -4.55372300    1.32682400    1.94531600
H           -5.58979100    1.66740600    1.87732200
C            3.64877300    2.21562400   -1.59772100
H            2.82607200    1.66071700   -2.05802900
P           -2.20642400   -1.88780800    0.79072300
F           -2.12837200    3.71338900    0.26232900
C           -3.58710900   -2.60134100   -0.17738300
C           -1.68240300    1.94852400   -1.21822500
C            1.68622400   -1.95119700   -1.18852800
C           -2.53037000    2.94590400   -0.75523500
C           -2.01391400   -2.92671500    2.29761400
Cl          -4.81148400    4.43993800   -0.63076100
F           -1.43734700    0.20547200   -2.76572400
F            2.20538600   -3.61598400    0.38176800
C            2.56424000   -2.90530200   -0.69216400
C           -4.60999000   -3.33885600    0.42762700
H           -4.59451700   -3.53127800    1.50331000
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C           -1.08836600    -3.97566100     2.24763400
H           -0.48517500    -4.13187900     1.34820600
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C           -3.79584400     3.19830200    -1.27610100
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H           -2.78014000    -1.83629700    -2.03789700
C            2.13504200    -1.25530400    -2.30257200
C           -4.63210900    -2.90260600    -2.33063900
H           -4.63495400    -2.73501100    -3.40989800
C           -2.60142600    -3.56236200     4.55278100
H           -3.19322900    -3.39788000     5.45666500
C            3.81712100    -3.16974900    -1.23703200
C           -0.93248100    -4.81755000     3.34442400
H           -0.21510300    -5.64059400     3.29555000
C           -2.76943600    -2.72137700     3.45629600
H           -3.49175300    -1.90282300     3.51268300
Cl           3.85549700    -0.60790100    -4.31832500
Cl          -3.97178100     0.45727200    -4.19280500
F            5.38145200    -2.67520500    -2.90448800
F           -5.42138100     2.62749000    -2.85825800
C            4.20627100    -2.44800600    -2.36119200
C            3.36766800    -1.48374300    -2.91121800
C           -3.42477800     1.40695700    -2.85715100
C           -1.68685600    -4.61084700     4.49685800
H           -1.56149000    -5.27158000     5.35831400
C           -5.64244800    -3.84922500    -0.35190800
H           -6.43918600    -4.43088200     0.11824000
C           -4.23173600     2.41575600    -2.34057600
C           -5.65482000    -3.62926100    -1.72774800
H           -6.46568000    -4.03683700    -2.33662200
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Model 3a T$_1$.

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Au          -0.52190100    -1.90567900    -0.28901300
Au           0.52877900     1.88073600    -0.29220300
Cu          -0.03417400     0.00400700     1.47165800
P           -2.57583400    -1.72864800     0.82782400
N           -1.79907600     0.66613800     1.77673000
C           -4.04611400    -2.30840100    -0.09256600
N            1.73736500    -0.67563000     1.83648100
C           -1.79007600    -3.92023000     2.36785800
H           -1.29579800    -4.25978900     1.45249600
C           -1.73120900    -4.69941200     3.51883600
H           -1.19568700    -5.65191900     3.50069100
C            2.85817000    -0.02813700     1.41437200
C           -2.90590200    -0.00409800     1.31964200
C           -2.48636100    -2.70527400     2.38289800
C           -5.03437600    -3.08429000     0.51909700
H           -4.94090600    -3.37599400     1.56801000
C           -6.25853700    -3.13254000    -1.56022300
H           -7.12717600    -3.45947300    -2.13718100
C           -3.03859800    -3.05406200     4.70662900
H           -3.52650700    -2.71357400     5.62330300
C           -3.10988800    -2.27254300     3.55640800
H           -3.65160700    -1.32300900     3.57468400
C           -4.15244300     0.60044900     1.25677100
H           -5.00080400     0.02904100     0.87352000
C           -1.96025100     1.94994000     2.19789200
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C           1.85946000    -1.93670000     2.30900400
H           0.93588300    -2.42604100     2.62768100
C          -3.17426400     2.59285600     2.17139200
H          -3.23749200     3.62340500     2.52489500
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H          -5.27441800     2.41648100     1.61675200
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H          -6.91363600    -4.10057500     0.25543800
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H          -5.35733600    -2.08475600    -3.22207000
C           3.07139600    -2.59165400     2.37011800
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H           5.19116700    -2.44407700     1.92384000
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H          -3.37751300    -1.36302800    -1.92787600
P           2.57234900     1.69134000     0.83554500
F           1.44924600    -4.28836800     0.10351800
C           4.08131900     2.17195700    -0.07999500
C           1.25404300    -2.36027700    -1.21606500
C          -1.24614700     2.39097700    -1.18418500
C           1.94719500    -3.51074400    -0.86057300
C           2.50301300     2.71166700     2.36174900
Cl          3.96861200    -5.34048800    -0.94402600
F           1.25817900    -0.45727300    -2.58292400
F          -1.23283100     4.39205300     0.03656400
C          -1.83836000     3.60431600    -0.85458100
C           5.09370300     2.92928300     0.51534600
H           4.99798400     3.26907000     1.54950600
C           1.79502800     3.91936400     2.32017200
H           1.28103600     4.22707400     1.40439000
C           1.84168400    -1.59299100    -2.21345900
C           3.14638200    -3.90622700    -1.44325300
Cl         -3.73178500     5.56498200    -0.92737000
F          -1.46210900     0.42028600    -2.43580800
C           4.19580500     1.76169400    -1.41272100
H           3.39400100     1.19120000    -1.88993500
C          -1.94234400     1.61460200    -2.10131300
C           5.33463300     2.09098900    -2.13893800
H           5.42328200     1.76625600    -3.17817100
C           3.08830300     3.13830300     4.66500100
H           3.59327800     2.83073100     5.58402600
C          -3.03902400     4.05342200    -1.39162600
C           1.74536900     4.73225800     3.44813900
H           1.19742500     5.67692900     3.40916500
C           3.14953500     2.32245200     3.53881000
H           3.70147100     1.37983700     3.58247700
Cl         -3.94424900     1.02713700    -3.86084700
Cl          3.69547800    -0.96491600    -4.11396200
F          -4.81668200     3.63261500    -2.85138600
F           4.80688400    -3.44932100    -3.02557500
C          -3.68117000     3.23976700    -2.32133300
C          -3.13870200     2.01258900    -2.69173000
C           3.02986000    -1.93968300    -2.85136000
C           2.38939100     4.34178600     4.61980500
H           2.34570100     4.98038200     5.50556100
C           6.22598900     3.26007200    -0.22292700
H           7.01756500     3.85477500     0.23944100
C           3.67707600    -3.10511200    -2.45112200
C           6.34793900     2.83965600    -1.54488100
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H                    7.23787600      3.10531800     -2.12080700
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Model **4a S$_0$**

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Au                  -2.10089300     -1.89780300      0.09424200
Cu                  -1.32272100      1.36037300      0.04692500
P                   -4.01305100     -0.60920000      0.36990800
P                    1.67702900      3.37390900     -0.12216100
Cl                   0.98318200     -5.49851200     -3.09467000
Cl                   2.44999400     -4.74236700      2.05888900
F                   -1.07400000     -3.53614300     -2.41331700
C                   -5.10097700      1.67942100     -2.89776500
F                    0.21484900     -2.85491400      2.03649300
F                    2.57517000     -5.85386300     -0.65179500
N                   -0.73962000      2.92551100     -1.32271100
C                   -0.27011100     -3.78809500     -1.38313100
C                   -4.15815800      0.36216400      1.92009000
C                    0.16894600      0.26850700      2.44555500
N                   -2.98096900      1.40851400     -1.11522200
C                   -1.70808700      3.09215500     -2.24592800
C                    1.41465300     -4.36708400      0.72775000
C                    0.37265200     -3.45456300      0.84772500
N                   -0.43783600      0.70030500      1.56697100
C                    0.90978100      3.90985200      1.46089900
C                    0.75740800     -4.70718000     -1.57830400
C                   -2.90638800      2.29758700     -2.12574000
C                   -0.26725200      4.65677900      1.53687300
C                    1.59736600     -4.98924300     -0.50433100
C                   -4.07813000      0.66899000     -0.97935500
C                   -5.17012600      0.78430500     -1.85347100
C                    4.08637700      4.26207000     -1.20292000
C                    2.95000200      4.64751100     -0.48482400
C                   -0.50137800     -3.13710000     -0.17873700
C                   -0.75781800      5.05494700      2.77851500
C                   -0.07293100      4.72007500      3.94236900
C                    0.35943300      3.66684800     -1.40671200
C                   -3.94814700      2.46558900     -3.06660500
C                   -4.75292400      1.62602200      1.96786700
C                    2.80662200      5.97286700     -0.06084800
C                    3.79177500      6.90568700     -0.36567900
C                   -1.59994500      4.00808600     -3.31730400
C                   -4.87413900      2.28956500      3.18555900
C                    4.91883900      6.52194700     -1.09004800
C                   -3.82027400      0.43260400      4.30950400
C                   -4.41179500      1.69277300      4.35535800
C                   -0.41665000      4.76178500     -3.39719300
C                    5.06606600      5.20258700     -1.50799300
C                    0.55986200      4.59744200     -2.44198200
C                   -3.68562700     -0.23082800      3.09473700
C                   -2.66727000      4.14105800     -4.25979600
C                    1.10621500      3.98136900      3.86793500
C                    1.59411300      3.56947500      2.63271800
C                    0.94792700     -0.26201700      3.53634400
Cl                   4.46948400     -3.56657700     -2.60525000
Cl                   5.65328900     -2.71838900      2.60498100
F                    3.01824500     -1.04446300     -2.30800100
F                    4.02743000     -0.32045600      2.20834500
F                    5.64831400     -4.11473100      0.02352800
C                   -5.58218200     -1.54421000      0.19517200
C                   -5.56404400     -2.69673800     -0.59814000
C                    4.12502000     -1.04758700      1.08514500
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C          4.33545300    -2.60031000    -1.18182900
C         -3.79949600     3.40209700    -4.13693600
C          4.86785100    -2.22101900     1.14998800
C         -7.92751100    -1.88843900     0.64118200
C         -7.91097700    -3.02875500    -0.15892600
C          4.96233000    -2.99539300    -0.00286300
C          3.61159500    -1.41059900    -1.17524400
C         -6.76641300    -1.14320900     0.82098800
C         -6.73101100    -3.43240500    -0.77799800
C          3.48506200    -0.59542000    -0.05856800
H          2.51733300     2.98413200     2.57512000
H          1.65348000     3.72613800     4.77915900
H         -0.45613100     5.04180300     4.91397500
H         -1.67932500     5.63995100     2.83319500
H         -0.81099400     4.93433700     0.63098200
H          1.93201400     6.27541300     0.52094600
H          3.68291300     7.93920500    -0.02757600
H          5.69390500     7.25695700    -1.32132000
H          5.95515600     4.89695400    -2.06470900
H          4.20990300     3.21936300    -1.51110700
H         -2.55234700     4.85404500    -5.07976700
H         -4.61605600     3.50743000    -4.85523500
H         -3.21213800    -1.21628800     3.05489000
H         -3.46079200    -0.03898500     5.22754100
H         -4.51597200     2.21264600     5.31104000
H         -5.34122600     3.27705300     3.22045100
H         -5.12671500     2.09971000     1.05619500
H         -6.78151700    -0.25890800     1.46311600
H         -8.85104800    -1.58004100     1.13741300
H         -8.82428300    -3.61414300    -0.29169500
H         -6.71278300    -4.33420300    -1.39465300
H         -4.63023200    -3.02542600    -1.06510300
H         -0.28295600     5.47735900    -4.21293100
H          1.48224300     5.17874900    -2.47827300
H         -6.05077700     0.15744200    -1.70406000
H         -5.93283300     1.78115600    -3.59995200
H          0.88515400     0.41841800     4.39615700
H          0.56921300    -1.25559900     3.80940000
H          1.99596000    -0.35548500     3.21472700
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Model 4a T$_1$

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Au         2.61466100     1.01536200     0.08470100
Au        -2.24487900    -1.76049800     0.02074200
Cu        -1.67404900     0.86026900    -0.15969200
P         -4.41981000    -0.91175200     0.16603800
P          1.40642500     3.01134100     0.17794600
Cl         2.20821800    -3.33342300    -3.22153300
Cl         2.38465600    -4.35169100     2.08817700
F         -0.36736600    -2.11501600    -2.52904000
C         -5.32544600     1.54448100    -3.02879500
F         -0.20946200    -2.98986800     2.06382200
F          3.30592800    -4.33528200    -0.69625100
N         -1.00653700     2.50723200    -1.16937900
C          0.24518400    -2.63103900    -1.46903900
C         -4.84304900    -0.08568400     1.74755500
C          0.07861600     0.12664700     2.26112600
N         -3.25715200     1.07982600    -1.18722000
C         -1.93806200     2.78800200    -2.15213400
C          1.56387300    -3.69637500     0.72020000
C          0.32631600    -3.07790100     0.83909100
N         -0.52048800     0.48895400     1.34807100
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C         0.57502500    3.43752900    1.76586600
C         1.48329400   -3.23674100   -1.66250600
C        -3.12646100    2.04849300   -2.15205300
C        -0.70445000    3.99020000    1.83744700
C         2.13254900   -3.76661900   -0.54980800
C        -4.42497400    0.37276700   -1.12832300
C        -5.45939000    0.58425100   -2.01272100
C         3.77357000    4.16725900   -0.75430300
C         2.58127600    4.40807300   -0.06388300
C        -0.37396800   -2.53808700   -0.22892600
C        -1.24844500    4.32391900    3.07676800
C        -0.51592400    4.12071300    4.24192600
C         0.10956400    3.26665100   -1.13706200
C        -4.14540000    2.29054500   -3.10791000
C        -5.57581800    1.10356100    1.77699400
C         2.31151100    5.68611100    0.43698900
C         3.22698700    6.71367200    0.23940700
C        -1.73306700    3.78441800   -3.14854600
C        -5.90129700    1.68322300    3.00018200
C         4.41066500    6.47321900   -0.45550500
C        -4.77397500   -0.10919000    4.16027600
C        -5.50456400    1.07674100    4.18913300
C        -0.54765400    4.50376500   -3.10921300
C         4.68300500    5.20212700   -0.95229400
C         0.36568400    4.24948700   -2.08904200
C        -4.43603700   -0.68904400    2.94213700
C        -2.75251500    4.00156300   -4.12842800
C         0.76782000    3.58187500    4.17115900
C         1.31129600    3.23500900    2.93849400
C         0.84446100   -0.33614500    3.38699500
Cl        6.15477600   -2.37727800   -2.82281800
Cl        5.96976900   -2.92405200    2.55225600
F         4.08224500   -0.36988300   -2.32406400
F         3.89857000   -0.86877000    2.32979800
F         6.85340900   -3.45925800   -0.19053100
C        -5.76767300   -2.08351500   -0.22520000
C        -5.52777700   -3.06462700   -1.19379200
C         4.40174400   -1.20085700    1.13103100
C         5.47989900   -1.92681000   -1.30067200
C        -3.90988900    3.29110500   -4.10573600
C         5.39247700   -2.17695300    1.10677900
C        -8.00955300   -2.91596700    0.06947300
C        -7.77402700   -3.88723800   -0.89950100
C         5.92340500   -2.53385500   -0.12928400
C         4.48936800   -0.95368700   -1.20029000
C        -7.00849900   -2.01148700    0.41213000
C        -6.53441900   -3.96158300   -1.53110600
C         3.91786200   -0.55739500    0.00289600
H         2.32180900    2.81699400    2.88355600
H         1.35458500    3.43851800    5.08249800
H        -0.94173600    4.39298900    5.21092800
H        -2.25080200    4.75657600    3.12750100
H        -1.28372400    4.16699900    0.92840700
H         1.38908200    5.87986600    0.98997700
H         3.01660000    7.70988900    0.63636300
H         5.12984800    7.28270400   -0.60374300
H         5.61434200    5.00779800   -1.48954500
H         3.99542600    3.16418600   -1.13107000
H        -2.57899700    4.76098000   -4.89471700
H        -4.68715200    3.47054100   -4.85255100
H        -3.85735500   -1.61757000    2.91980900
H        -4.46501300   -0.58711200    5.09325900
H        -5.76814800    1.53120500    5.14751000
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H          -6.47538800    2.61293100    3.02309700
H          -5.89197900    1.57845000    0.84403100
H          -7.19378700   -1.25648100    1.18000900
H          -8.98032200   -2.86210000    0.56818100
H          -8.56180700   -4.59804000   -1.16102500
H          -6.34632500   -4.72849600   -2.28620000
H          -4.55208500   -3.12848100   -1.68501100
H          -0.34236200    5.27245700   -3.85815700
H           1.28663900    4.82728100   -2.02545700
H          -6.36701100   -0.01622900   -1.92626100
H          -6.12766100    1.70756400   -3.75099300
H           0.80088500    0.41215400    4.18928600
H           0.43465100   -1.29595100    3.73015500
H           1.88767200   -0.48305200    3.06627800
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