Electronic Supporting Information

Structures and Luminescent Properties of Diethyldithiocarbamate-Bridged Polynuclear Gold(I) Cluster Complexes with Diphosphine/Triphosphine

Jia Li,[b] Xiao-Feng Zhu,[a] Li-Yi Zhang[b] and Zhong-Ning Chen[a,b*]

[a] *College of Chemistry, Fuzhou University, Fuzhou, Fujian 350002, China*

E-mail: czn@fjirsm.ac.cn

[b] *State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian, 350002, China*

Table S1. Crystallographic Data of **3**·CH_2Cl_2, **4**·$2CH_2Cl_2$, **5**·$2CH_2Cl_2$·H_2O and **6**.

	3 CH_2Cl_2	**4** $2CH_2Cl_2$	**5** $2CH_2Cl_2$ H_2O	**6**
empirical formula	$C_{50}H_{58}Au_4Cl_2F_6N_3O_3P_2S_6Sb$	$C_{55}H_{68}Au_{4.5}Cl_2F_9N_4P_2S_8Sb_{1.50}$	$C_{54}H_{60}Au_4Cl_2F_6N_3OP_2S_6Sb$	$C_{83}H_{96}Au_6F_{18}N_3P_6S_6Sb_3$
formula weight	2049.81	2414.43	2115.87	3402.86
crystal system	monoclinic	Triclinic	orthorhombic	monoclinic
space group	$P2_1/n$	$P\bar{1}$	$Pbcn$	$P2/c$
a, Å	18.670(4)	13.747(6)	15.586(4)	16.476(6)
b, Å	16.820(3)	14.952(6)	27.054(6)	19.474(8)
c, Å	22.720(5)	19.077(9)	33.449(8)	18.238(7)
α, °	90	93.190(5)	90	90
β, °	110.933(3)	107.365(6)	90	95.004(4)
γ, °	90	97.674(5)	90	90
V, $Å^3$	6664(2)	3690(3)	14104(6)	5830(4)
Z	4	2	8	2
$\rho_{calcd,}$ g/cm^{-3}	2.043	2.173	1.993	1.939
μ, mm^{-1}	9.542	9.855	9.021	8.457
radiation (λ /Å)	0.71073	0.71073	0.71073	0.71073
temp, (K)	293(2)	293(2)	293(2)	293(2)
R1(Fo)[a]	0.0624	0.0549	0.0509	0.0782
wR2(Fo^2)[b]	0.1842	0.1839	0.1522	0.2076
GOF	1.028	0.947	1.094	0.983

[a] $R1 = \Sigma|F_o - F_c|/\Sigma F_o$ [b] $wR2 = \Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)]^{1/2}$

Table S2. Selected Bonding Distances (Å) and Angles (°) of **3** CH_2Cl_2, **4** $2CH_2Cl_2$, **5** $2CH_2Cl_2$ H_2O and **6**.

3 $3H_2O$		**4** $2CH_2Cl_2$		**5** $2CH_2Cl_2$ H_2O		**6**	
Au1-P1	2.267(3)	Au1-P1	2.278(4)	Au1-P1	2.284(3)	Au1-P1	2.282(4)
Au1-S1	2.311(3)	Au1-S1	2.338(4)	Au1-S1	2.327(4)	Au1-S1	2.345(4)
Au1-Au2	2.9725(8)	Au1-Au2	3.1078(14)	Au1-Au2	3.0514(10)	Au1-Au2	2.9244(12)
Au2-S2	2.288(3)	Au2-S2	2.281(5)	Au2-S2	2.295(4)	Au1-Au1#2	3.1901(16)
Au2-S3	2.273(4)	Au2-S3	2.302(5)	Au2-S3	2.290(4)	Au2-P2	2.271(4)
Au2-Au3	2.9376(7)	Au2-Au3	2.9762(16)	Au2-Au3	2.9288(9)	Au2-S2	2.348(4)
Au3-S4	2.265(4)	Au3-S4	2.291(5)	Au3-S4	2.291(4)	Au2-Au3	3.1952(13)
Au3-S5	2.291(4)	Au3-S5	2.287(5)	Au3-S5	2.285(4)	Au3-P3	2.288(5)
Au3-Au4	2.9684(8)	Au3-Au4	2.9834(16)	Au3-Au4	2.9927(9)	Au3-S3	2.344(5)
Au4-P2	2.270(3)	Au4-P2	2.280(4)	Au4-P2	2.278(3)	Au3-Au3#1	2.9987(14)
Au4-S6	2.315(3)	Au4-S6	2.342(5)	Au4-S6	2.310(4)		
		Au5-S7	2.330(4)				
		Au5-S8	2.355(4)				
P1-Au1-S1	172.72(11)	P1-Au1-S1	172.76(15)			P1-Au1-S1	175.79(16)
P1-Au1-Au2	102.13(7)	P1-Au1-Au2	105.37(10)	P1-Au1-S1	166.47(12)	P1-Au1-Au2	97.67(10)
S1-Au1-Au2	82.95(7)	S1-Au1-Au2	81.81(11)	P1-Au1-Au2	112.74(8)	S1-Au1-Au2	81.95(11)
S2-Au2-S3	169.22(13)	S2-Au2-S3	166.87(17)	S1-Au1-Au2	80.64(10)	P1-Au1-Au1#2	108.15(10)
S2-Au2-Au3	97.01(7)	S2-Au2-Au3	94.51(12)	S2-Au2-S3	168.85(15)	S1-Au1-Au1#2	73.31(10)
S3-Au2-Au3	91.31(9)	S3-Au2-Au3	89.16(11)	S2-Au2-Au3	94.75(10)	Au2-Au1-Au1#	150.68(2)
S2-Au2-Au1	83.46(7)	S2-Au2-Au1	75.28(12)	S3-Au2-Au3	90.50(10)	P2-Au2-S2	177.81(14)
S3-Au2-Au1	92.53(9)	S3-Au2-Au1	113.27(12)	S2-Au2-Au1	79.71(11)	P2-Au2-Au1	96.02(10) .
Au1-Au2-Au3	151.25(2)	Au1-Au2-Au3	121.96(3)	S3-Au2-Au1	107.29(11)	S2-Au2-Au1	85.39(11)
S4-Au3-S5	172.63(10)	S4-Au3-S5	176.78(16)	Au1-Au2-Au3	112.78(3)	P2-Au2-Au3	103.05(10)
S5-Au3-Au2	95.01(9)	S5-Au3-Au2	96.22(12)	S4-Au3-S5	176.81(16)	S2-Au2-Au3	74.86(10)
S4-Au3-Au2	91.21(10)	S4-Au3-Au2	86.77(11)	S5-Au3-Au2	93.78(10)	P3-Au3-S3	172.34(16)
S5-Au3-Au2	95.01(9)	S5-Au3-Au2	96.22(12)	S4-Au3-Au2	85.65(10))	P3-Au3-Au3#1	101.82(11)
S4-Au3-Au4	94.41(10)	S4-Au3-Au4	94.41(11)	S5-Au3-Au4	81.82(11)	S3-Au3-Au3#1	79.19(12)
Au2-Au3-Au4	136.05(2)	Au2-Au3-Au4	163.23(3)	S4-Au3-Au4	98.12(9)	P3-Au3-Au2	110.21(10)
P2-Au4-S6	172.63(10)	P2-Au4-S6	171.52(14)	Au2-Au3-Au4	167.82(3)	S3-Au3-Au2	75.62(10)
P2-Au4-Au3	102.52(7)	P2-Au4-Au3	100.51(10)	P2-Au4-S6	169.86(13)	Au3#1-Au3-Au	116.66(4)
S6-Au4-Au3	84.78(7)	S6-Au4-Au3	86.55(11)	P2-Au4-Au3	102.27(8)	Au1-Au2-Au3	142.12(3)
P1-Au1-S1	172.72(11)	S7-Au5-S8	75.15(15)	S6-Au4-Au3	87.67(10)		

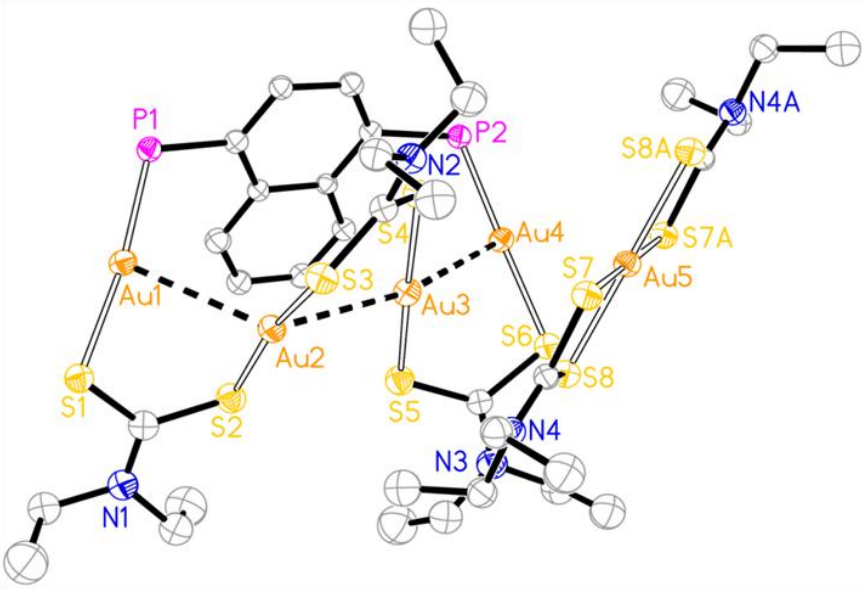

Fig. S1. ORTEP drawings of cationic complex **4** with atom-labeling scheme showing 30% thermal ellipsoids. Phenyl rings on the phosphorus atoms and all hydrogen atoms are omitted for clarity.

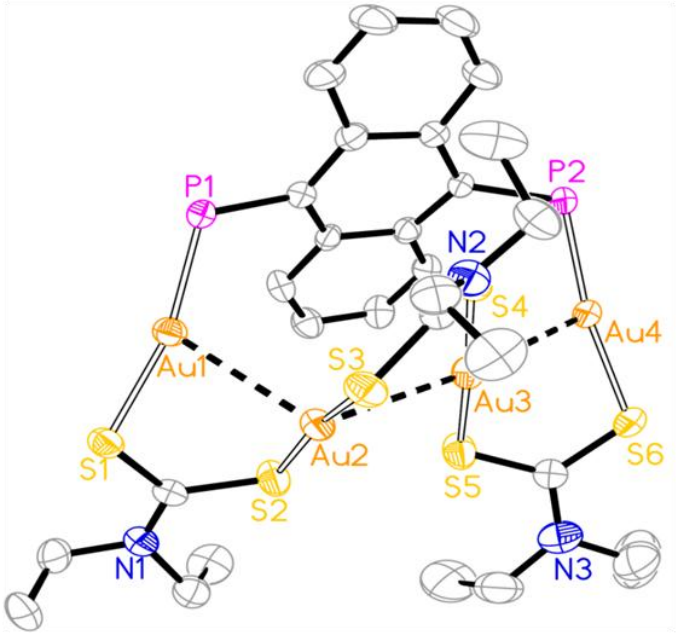

Fig. S2. ORTEP drawings of cationic complex **5** with atom-labeling scheme showing 30% thermal ellipsoids. Phenyl rings on the phosphorus atoms and all hydrogen atoms are omitted for clarity.

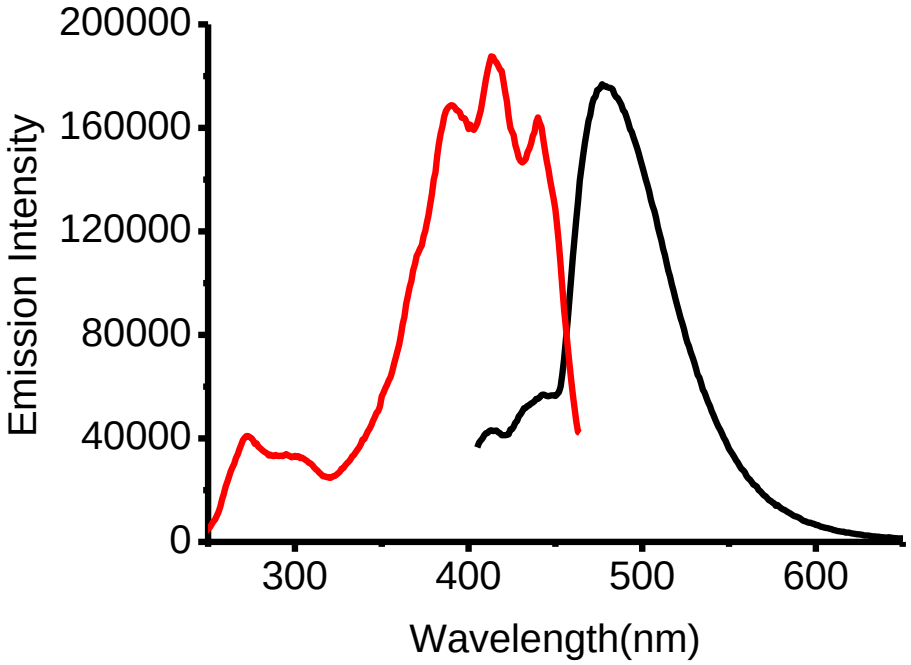

Fig. S3. Excitation and emission spectra of complex **5** in CH_2Cl_2 solution at 298 K.

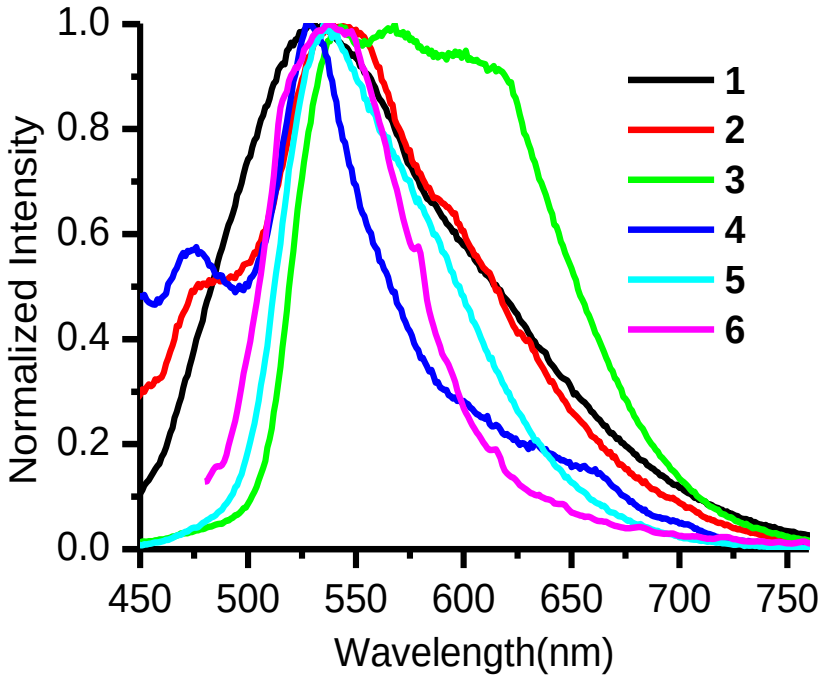

Fig. S4. Solid-state emission spectra of complexes **1–6** at 298 K.

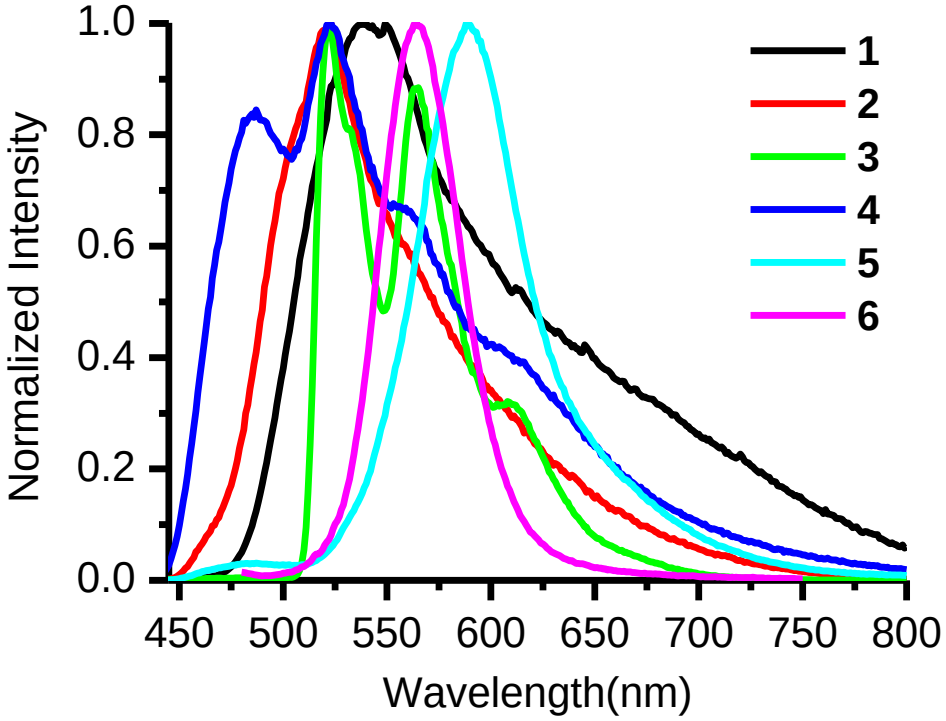

Fig. S5. Solid-state emission spectra of complexes **1**–**6** at 77 K.