Electronic supplementary information

Aurophilic interactions of dimeric bisphosphine gold(I) complexes pre-organized by the structure of the 1,5-diaza-3,7-diphosphacyclooctanes

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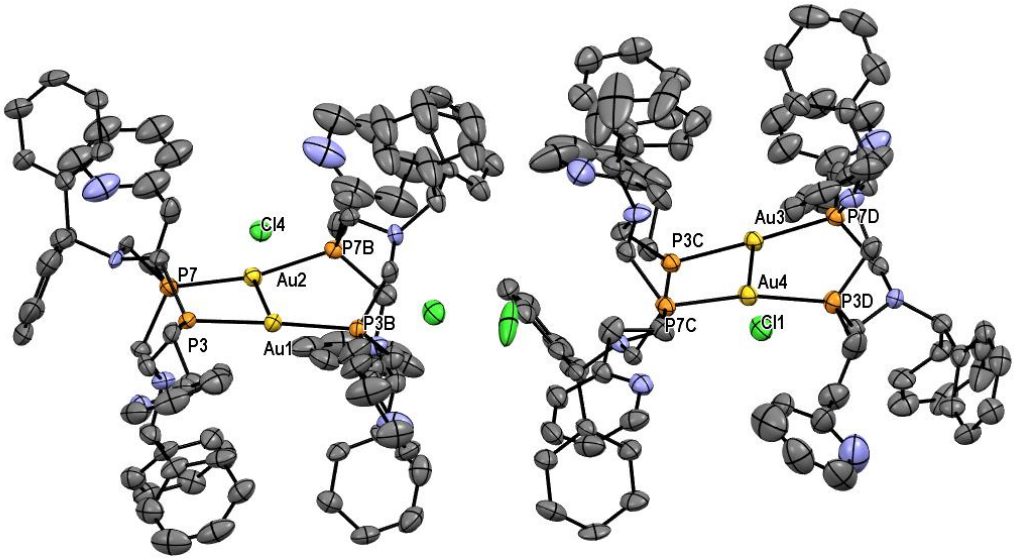


Figure S1. Unit cell of crystal of complex **2**

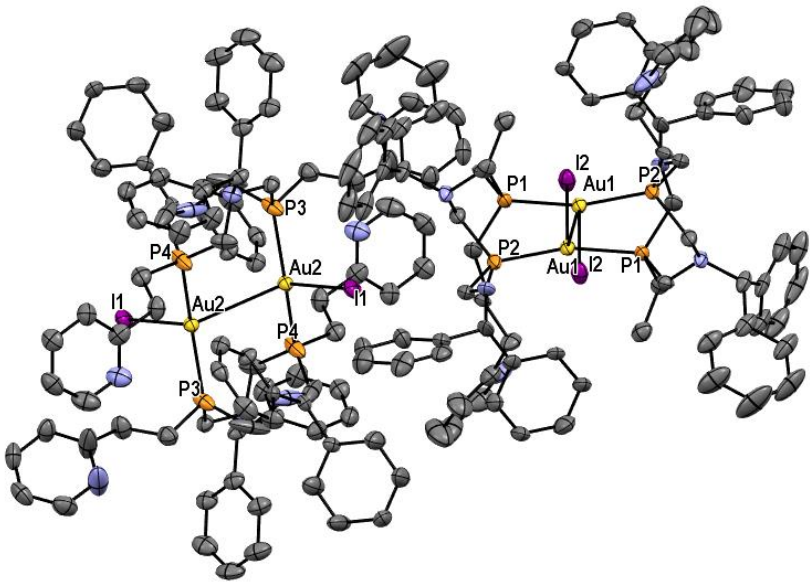


Figure S2. Unit cell of crystal of complex **3**

Table S1. Selected structural parameters of complexes **2** and **3**

	Molecule A					**Molecule B**			
Complex 2	**Bonds lengths and distances**								
	Atom1	Atom2	Distance (Å)			Atom1	Atom2	Distance (Å)	
	Au1	Au2	2.9977(6)			Au3	Au4	2.9870(6)	
	Au1	P3	2.316(3)			Au3	P3C	2.311(3)	
	Au1	P3B	2.298(3)			Au4	P7C	2.304(3)	
	Au2	P7	2.315(3)			Au4	P3D	2.317(3)	
	Au2	P7B	2.315(3)			Au3	P7D	2.308(3)	
	Au1	Cl4	3.036			Au3	Cl1	3.046	
	Angles								
	P3	Au1	P3B	169.4(1)		P3C	Au3	P7D	169.2(1)
	P7	Au2	P7B	165.3(1)		P7C	Au4	P3D	164.6(1)
	Molecule A					**Molecule B**			
Complex 3	**Bonds lengths and distances**								
	Atom1	Atom2	Distance (Å)			Atom1	Atom2	Distance (Å)	
	Au1	Au1	3.1680(5)			Au2	Au2	3.195(2)	
	Au1	P1	2.297(1)			Au2	P3	2.395(4)	
	Au1	P2	2.300(1)			Au2	P4	2.255(4)	
	Au1	I2	3.168(1)			Au2	I1	3.002(4)	
	Angles								
	P2	Au1	P1	164.18(5)		P3	Au2	P4	157.0(1)
	P1	Au1	I2	94.65(4)		P4	Au2	I1	101.1(1)
	I2	Au1	P2	91.31(4)		P3	Au2	I1	96.6(1)
						P4	Au2	I1A	100.1(1)
						I1A	Au2	P3	96.3(1)

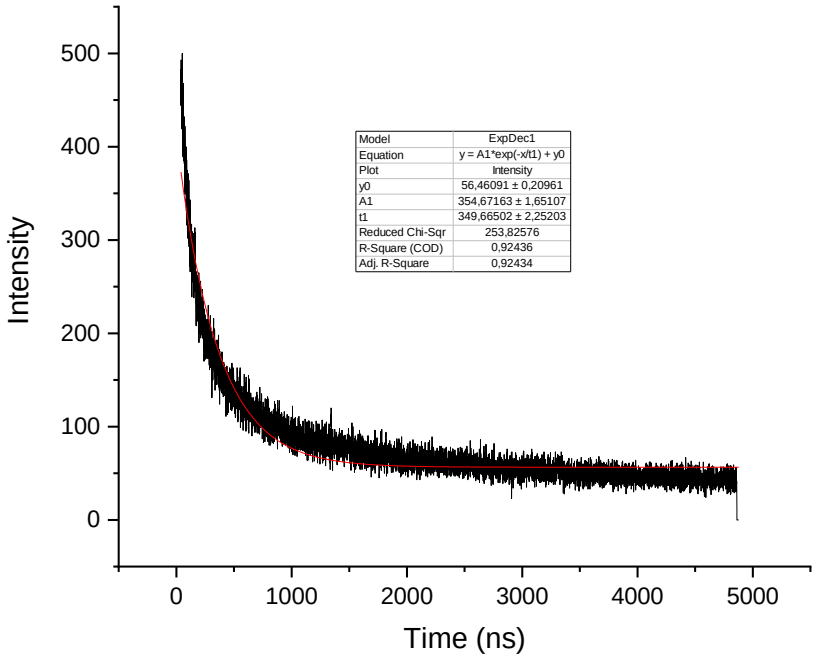


Figure S3. Luminescence decay curve of complex **2** measured for 505 nm emission band in solid state

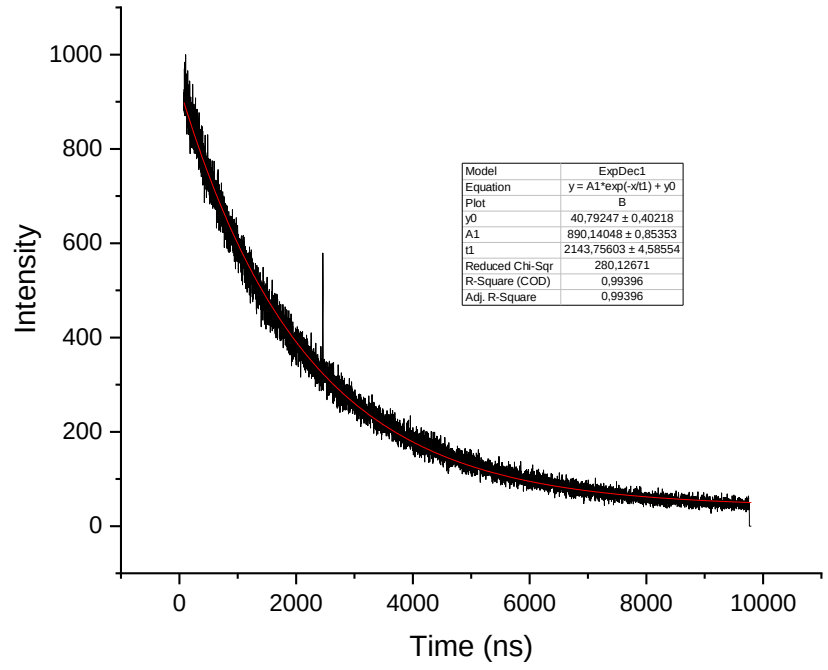
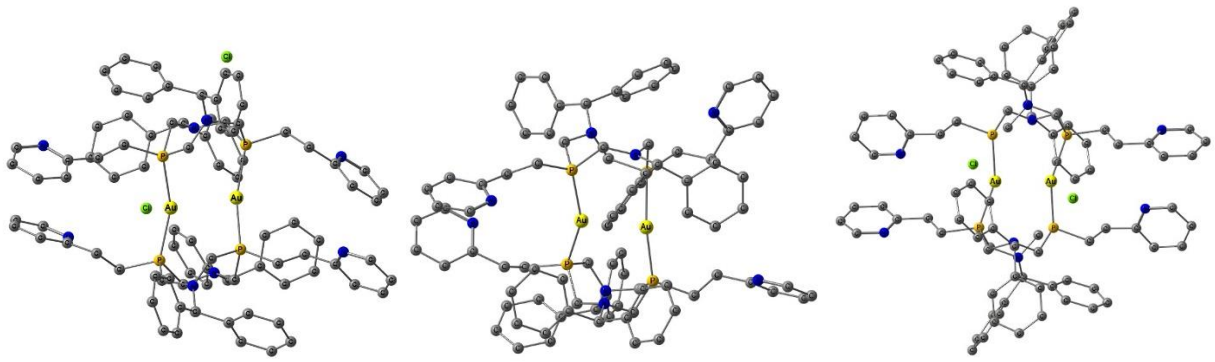
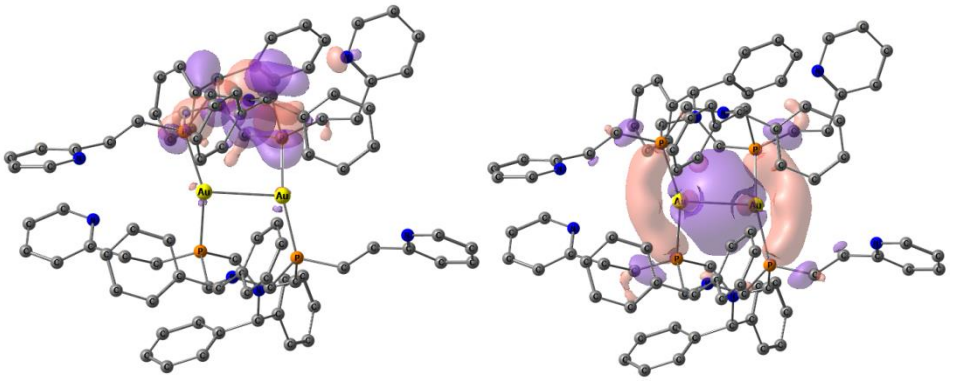


Figure S4. Luminescence decay curve of complex **3** measured for 530 nm emission band in solid state

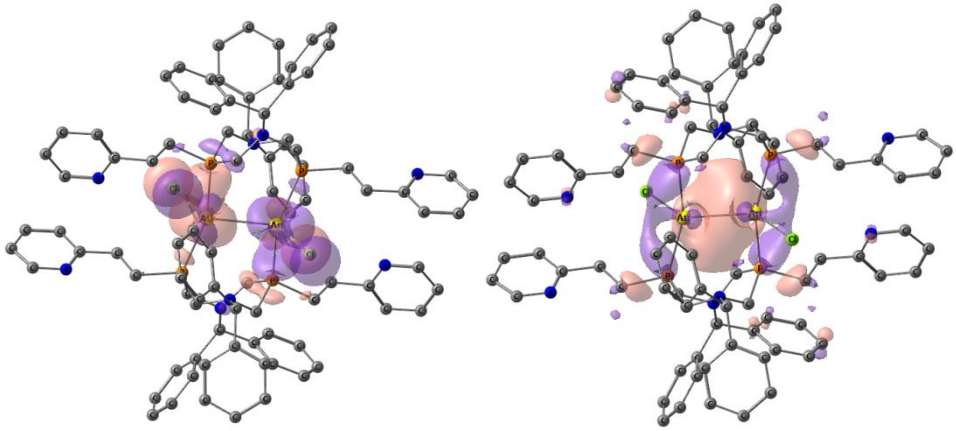


a **b** **c**

Figure S5. Optimized triplet structures of the singlet ground states (S_0) of considered models **2** (a), **2a** (b) and **2b** (c) of complex **2.**



HOMO (S_0@T_1 geometry of **2a**) LUMO (S_0@T_1 geometry of **2a**)



HOMO (S_0@T_1 geometry of **2b**) LUMO (S_0@T_1 geometry of **2b**)

Figure S6. Frontier orbitals of the singlet ground states (S_0) at the optimized T_1 (S_0@T_1, bottom) geometries of quantum-chemically considered models i and iii of complex **2.**

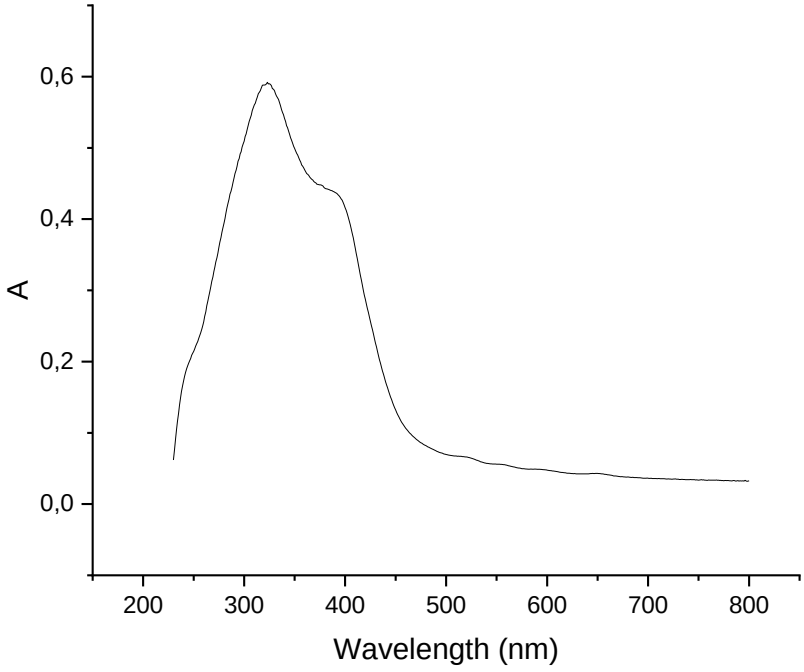


Figure S7. UV/Vis absorbance spectra of complex **2** measured in solid state

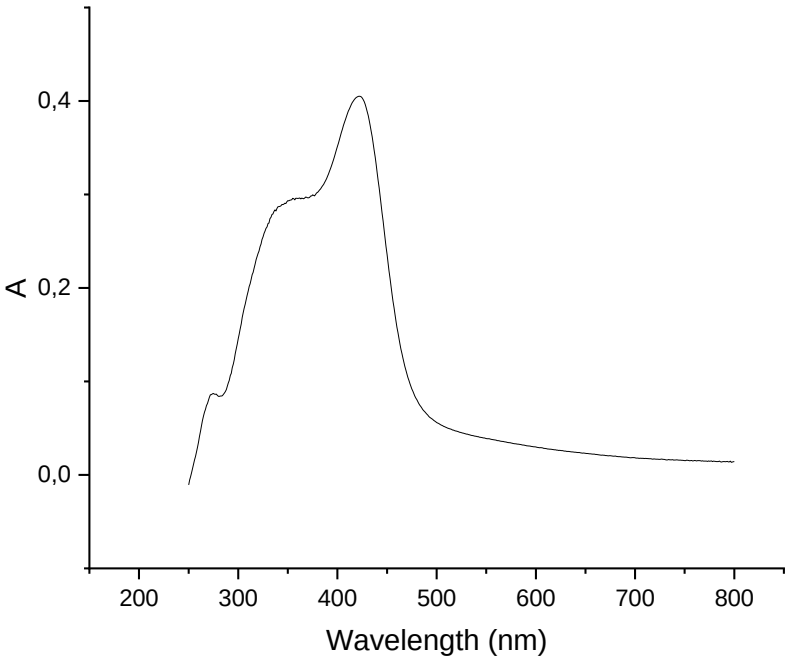


Figure S8. UV/Vis absorbance spectra of complex **3** measured in solid state