Photophysical and theoretical studies on luminescent tetranuclear coinage metals building blocks.

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SUPPORTING INFORMATION

Figure S1. View of the polymeric structure of complex **1** normal to the crystallographic *z* axis. Hydrogen atoms have been omitted for clarity.

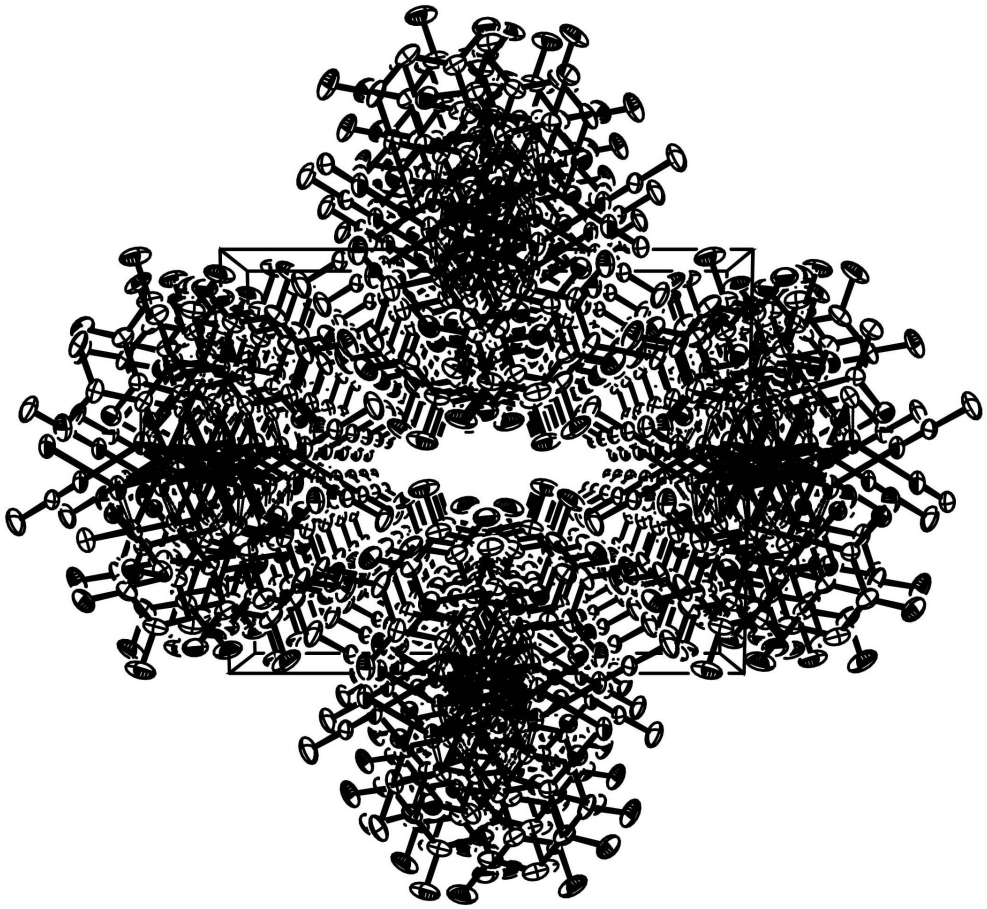


Figure S2. View of the polymeric structure of complex **2** normal to the crystallographic *z* axis. Hydrogen atoms have been omitted for clarity.

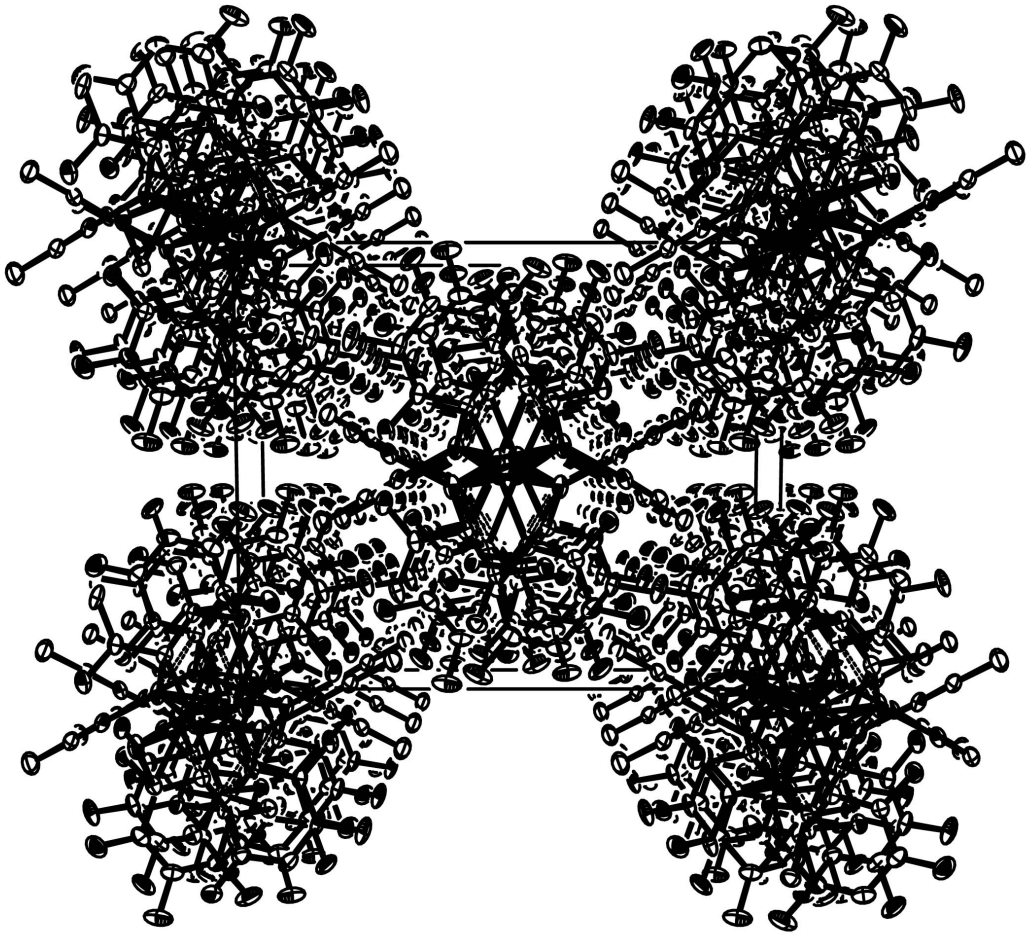
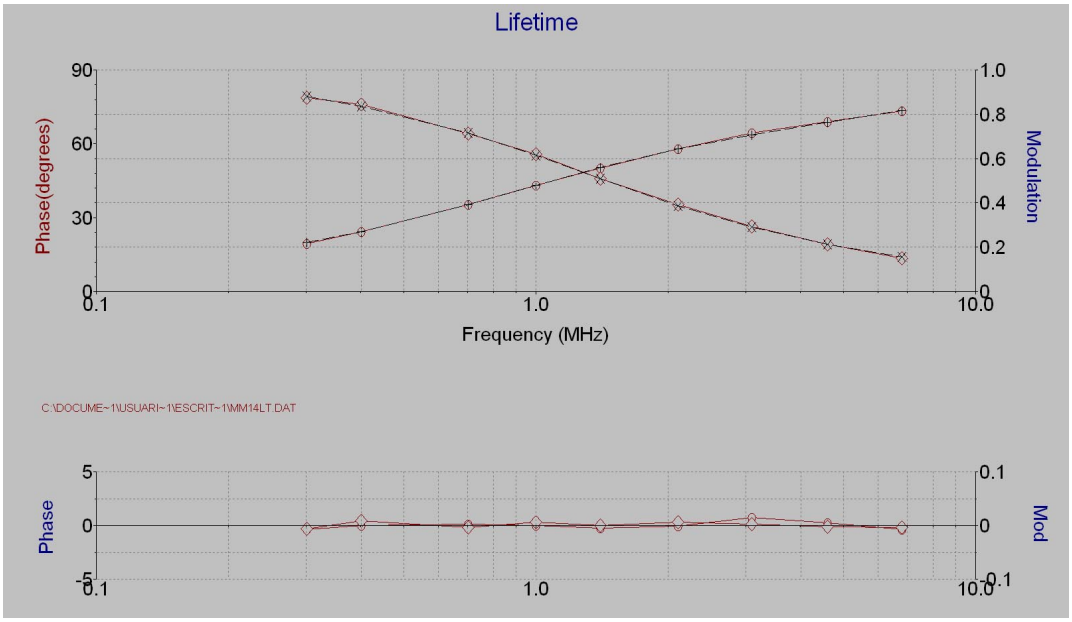
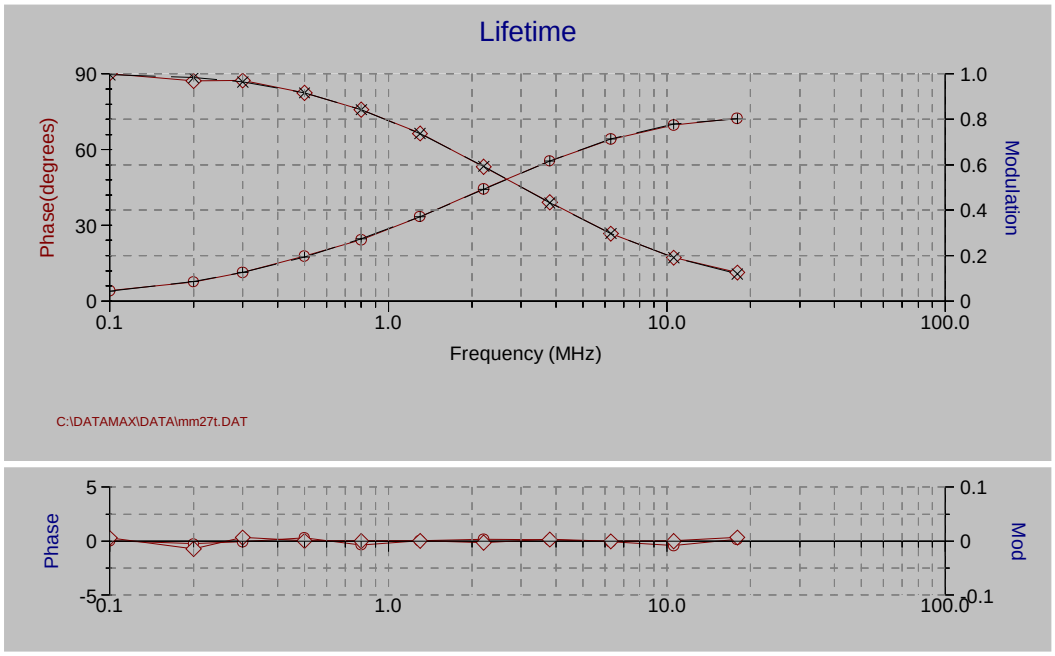


Figure S3. Phase and modulation data for complex $[Au_2Ag_2(C_6F_5)_4(N{\equiv}CCH_3)_2]_n$ (**1**) recorded at different frequencies in solid state at room temperature.



LIFETIME: τ_1 = 231 ns, τ_2 = 84 ns, (χ^2 = 1.5)

Figure S4. Phase and modulation data for complex $[Au_2Cu_2(C_6F_5)_4(N{\equiv}CCH_3)_2]_n$ (**2**) recorded at different frequencies in solid state at room temperature.



τ_1 = 592 ns, τ_2 = 163 ns (χ^2 = 1.3)

Figure S5. Experimental and excitation spectra of complex **2** in solid state at room temperature (black) and theoretical excitations (red) for model system $[Au_2Cu_2(C_6H_5)_4(N{\equiv}CCH_3)_2]_2$ **2a**.

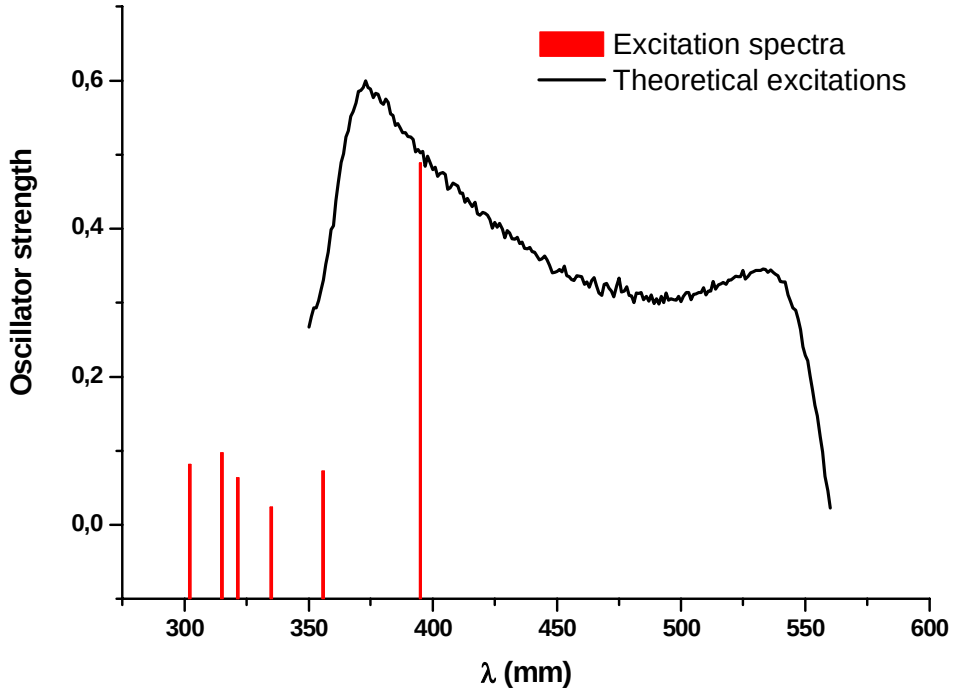


Table S1. Population analysis for the model system $[Au_2Ag_2(C_6H_5)_4(N{\equiv}CCH_3)_2]_2$ **1a**. Contribution from each part of the molecule to the occupied orbitals.

	Au	Ag	C_6H_5	CH_3CN
142b (HOMO)	51.8	13.0	34.9	0.3
140b (HOMO-4)	16.2	7.0	76.0	0.8
140a (HOMO-5)	5.0	3.2	91.8	-
139b (HOMO-7)	27.8	8.6	63.3	0.3
138b (HOMO-8)	3.4	3.0	93.6	-
137b (HOMO-10)	4.3	5.8	89.9	-
137a ((HOMO-11)	36.0	23.1	37.0	3.9
136b (HOMO-12)	53.7	36.9	6.0	3.4
135b (HOMO-14)	59.2	29.5	10.9	0.4
134b (HOMO-15)	71.1	17.5	11.3	0.1

Table S2. Population analysis for the model system $[Au_2Cu_2(C_6H_5)_4(N{\equiv}CCH_3)_2]_2$ **2a**. Contribution from each part of the molecule to the occupied orbitals.

	Au	Cu	C_6H_5	CH_3CN
152b (HOMO)	40.0	28.3	30.0	1.7
151b (HOMO-2)	7.0	35.9	55.4	1.7
150a (HOMO-4)	7.0	21.3	70.7	1.0
148b (HOMO-8)	7.3	24.3	67.7	0.7
147b (HOMO-10)	11.6	42.1	44.2	2.1
147a (HOMO-11)	10.8	26.9	61.9	0.4
146a ((HOMO-13)	9.0	51.5	38.3	1.2
144b (HOMO-16)	8.4	64.5	25.6	1.5
142b (HOMO-18)	34.1	49.9	15.4	0.9