"Host-guest" binding of luminescent dinuclear Au(I) complex based on cyclic diphosphine with organic substrates as a reason for luminescence tuneability

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Supporting Information

Content

Table S1 Crystallographic data for $(AuCl)_2L{\cdot}AN$ and $(AuCl)_2L{\cdot}DMSO$.

Compound	$(AuCl)_2L{\cdot}AN$	$(AuCl)_2L{\cdot}DMSO$
Formula	$C_{28}H_{30}Au_2Cl_2N_4P_2$, C_2H_3N	$C_{28}H_{30}Au_2Cl_2N_4P_2$, C_2H_6OS
Formula weight	990.39	1027.48
Crystal System	Monoclinic	
a (Å)	20.270(8)	8.9621(12)
b (Å)	18.845(11)	10.9006(15)
c (Å)	20.136(8)	17.225(2)
β (°)	119.588(6)	97.285(2)
V (Å^3)	6689(5)	1669.2(4)
Space group	C2/c	P2/c
Z (Z')	8 (1)	2 (1/2) Molecules on a special position on axe 2
D_{calc} (g/cm^3)	1.967	2.044
μ (mm^{-1})	9.046	9.128
Temperature (K)	296(2)	296(2)
Crystal size (mm^3)	0.10 × 0.10 × 0.20	0.2 × 0.1 × 0.12
Radiation, λ (Å)	Mo$K\alpha$, 0.71073	
Angle range θ (°)	1.6–23.5	1.9–26.0
Dataset	-23: 24 ; -22: 22 ; -24: 24	-11: 11 ; -13: 13 ; -21: 21
Total reflections	21538	12508
Unique reflections	6194	3289
R_{int}	0.088	0.048
Observed data [I > 2.0 σ(I)]	4025	2765
Refinement		
N_{ref}, N_{par}	6194, 373	3289, 197
R_1 ($\|F_o\| \geq 4\sigma_F$)	0.0519	0.0353
wR_2 ($\|F_o\| \geq 4\sigma_F$)	0.1634	0.0869
R_1 (all data)	0.1054	0.0461
wR_2 (all data)	0.2044	0.0920
S	1.044	1.063
ρ_{min}, ρ_{max}, e/Å^3	–2.557, 3.676	–1.097, 1.978

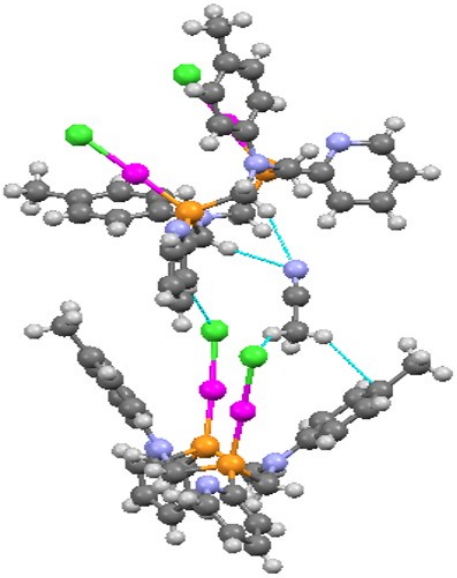

Fig. S1 X-ray structure of $(AuCl)_2L$ with AN, where short contacts are designated as blue lines.

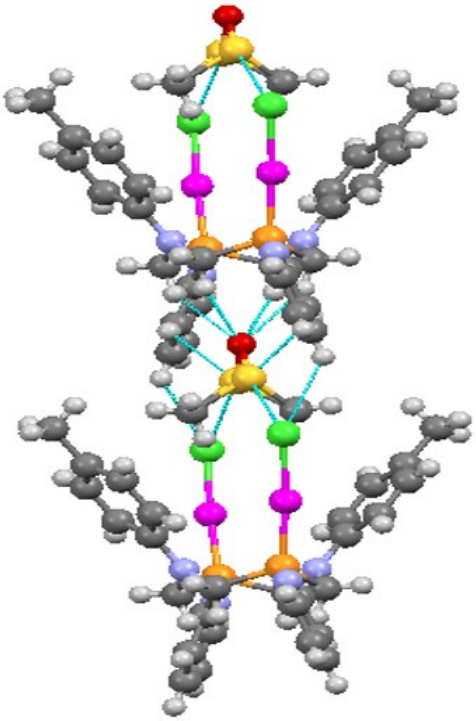

Fig. S2 X-ray structure of $(AuCl)_2L$ with DMSO, where short contacts are designated as blue lines.

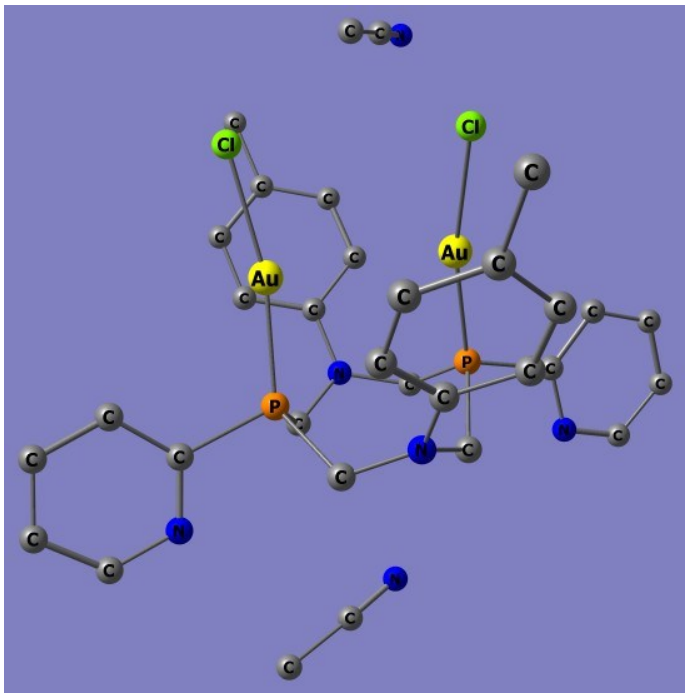

Fig. S3 The lowest energy PBE0/def-TZVP optimized structure of complex of $(AuCl)_2L$ with two acetonitrile molecules. Hydrogen atoms are omitted for clarity.

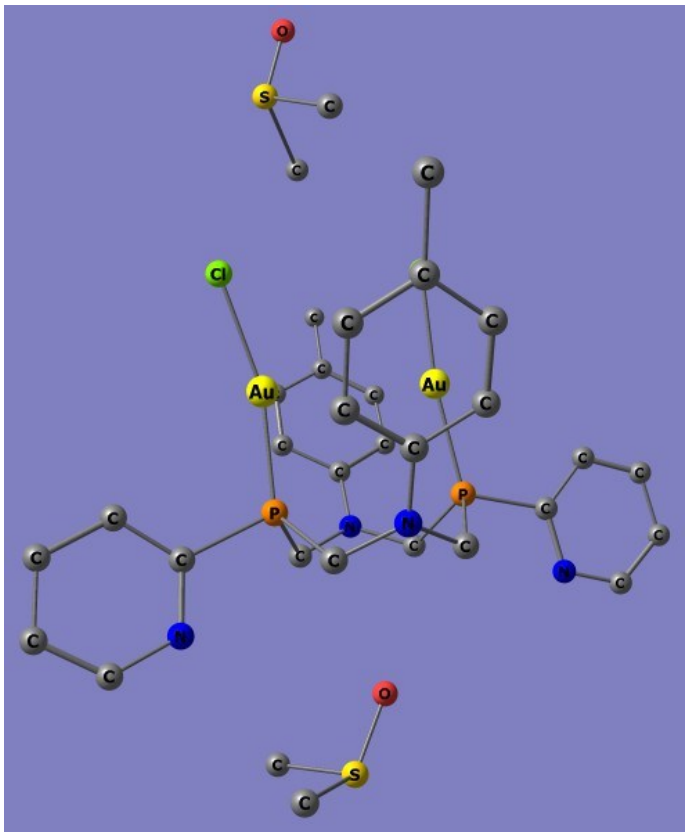

Fig. S4 The lowest energy PBE0/def-TZVP optimized structure of complex of $(AuCl)_2L$ with two DMSO molecules. Hydrogen atoms are omitted for clarity.

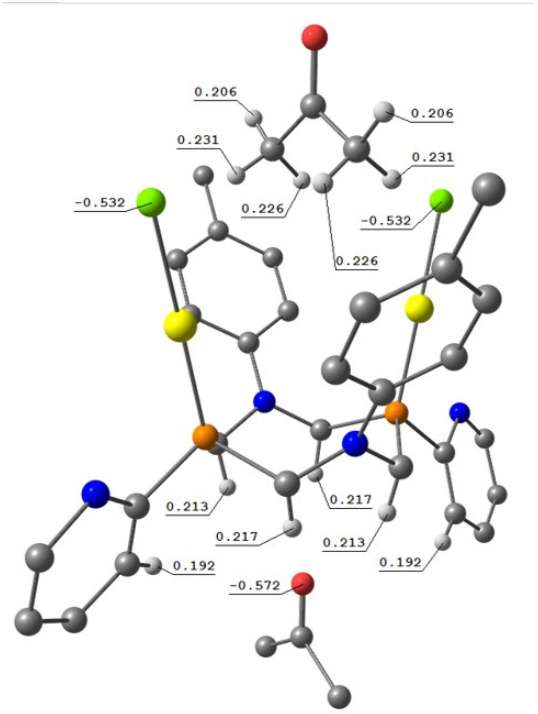

Fig. S5 The lowest energy PBE0/def-TZVP optimized structure of complex of $(AuCl)_2L$ with two acetone molecules. Hydrogen atoms that do not participate in the formation of the complex are omitted for clarity. Natural bond orbital charges on some atoms are shown.

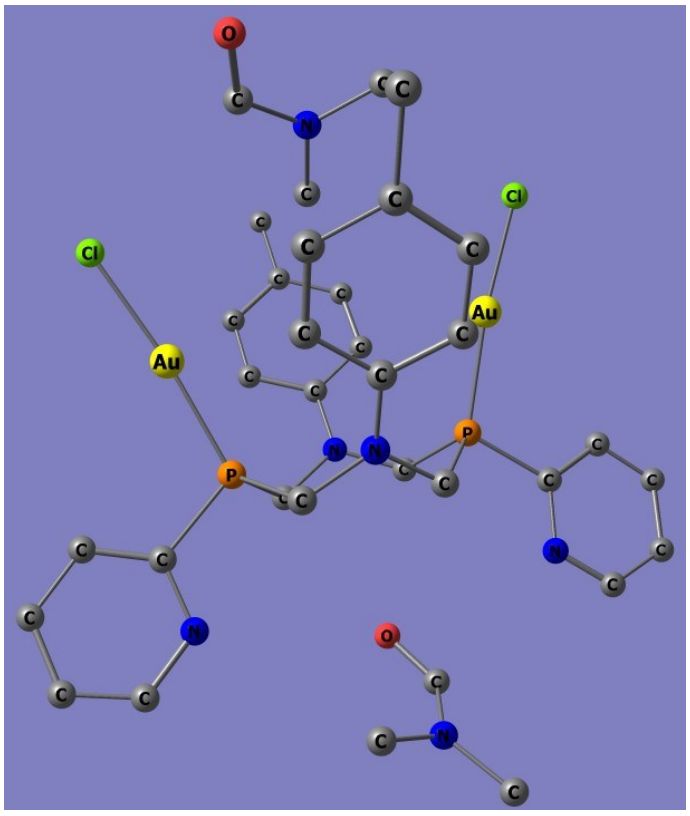

Fig. S6 The lowest energy PBE0/def-TZVP optimized structure of complex of $(AuCl)_2L$ with two DMF molecules. Hydrogen atoms are omitted for clarity.

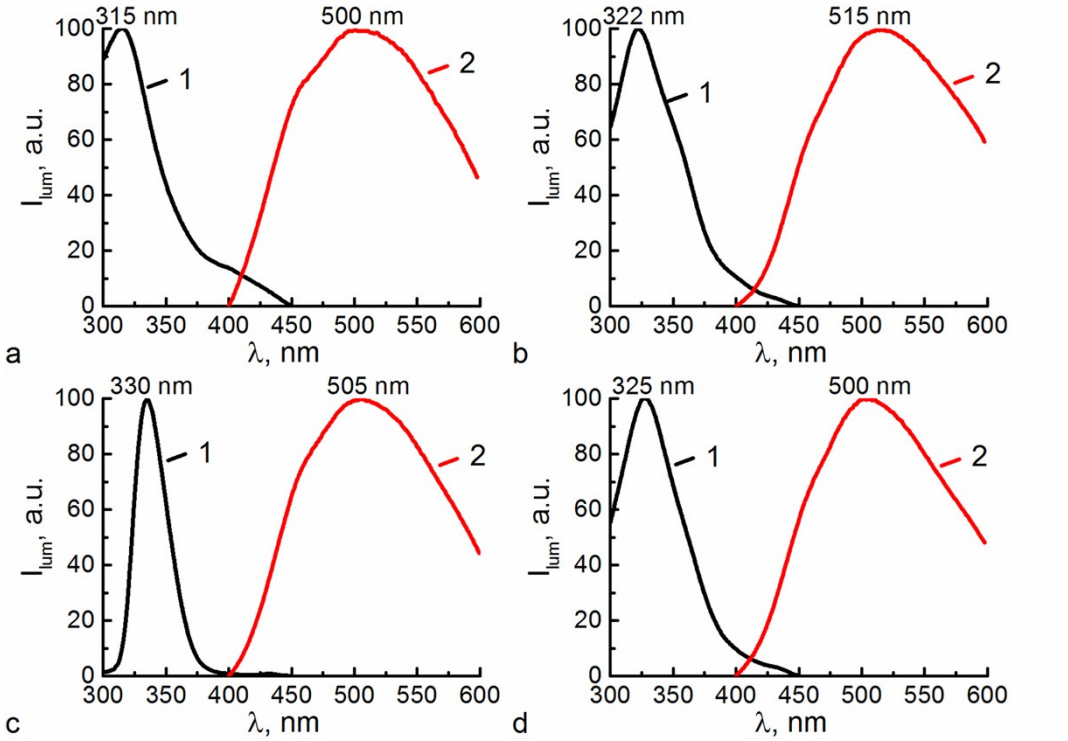

Fig. S7 Normalized excitation (1, λ_{em} = 500 nm) and emission (2, λ_{ex} = 340 nm) spectra of solutions of L in DCM (a), AN (b), acetone (c) and DMSO (d). C(L) = 0.2 mM

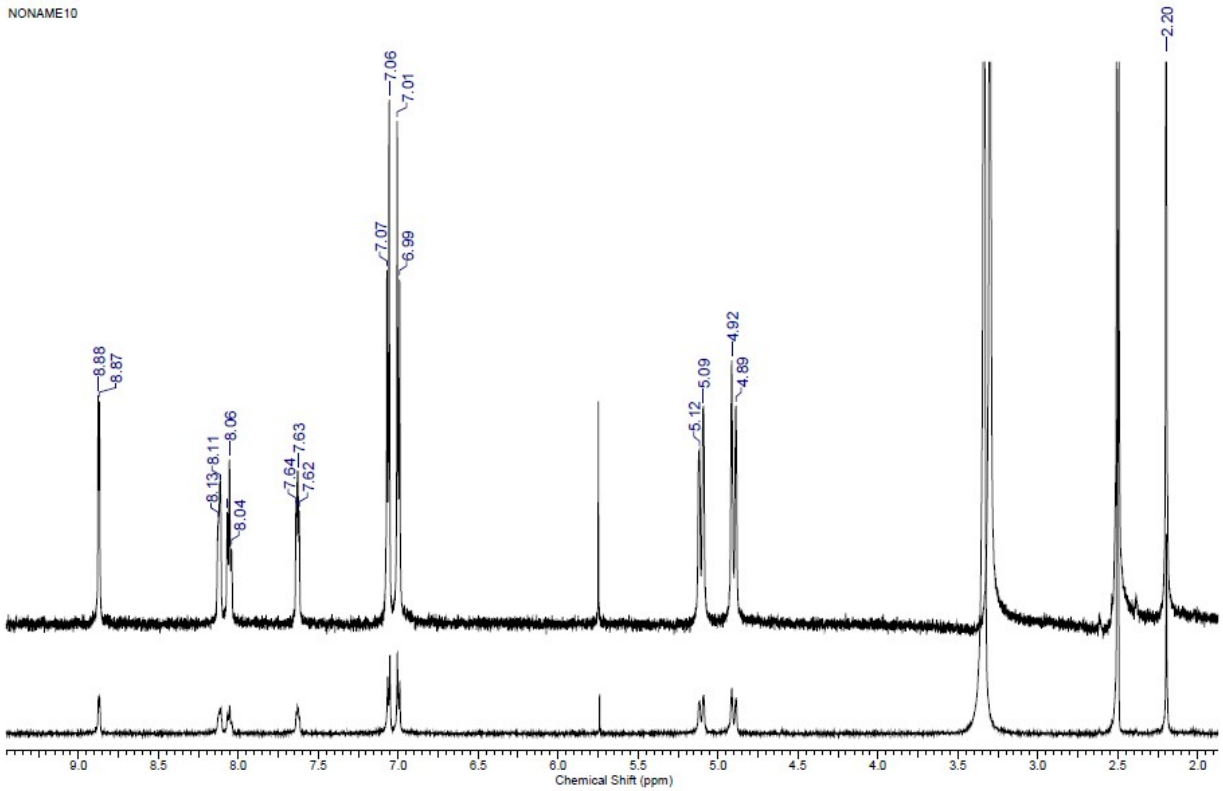

Fig. S8 ^{1}H NMR spectra (DMSO-d_6) of complex $(AuCl)_2L$ within one hour (top) and seven days after (bottom) the sample preparation.

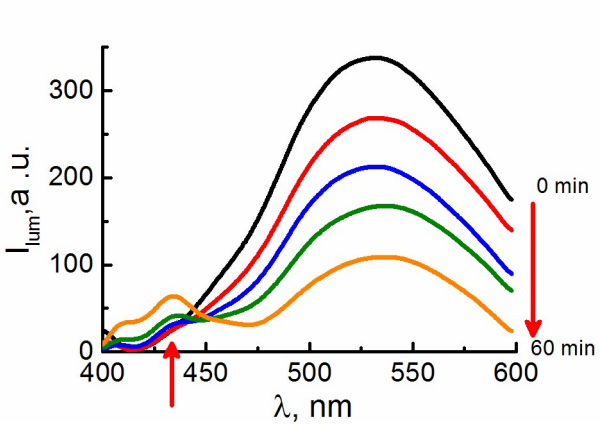

Fig. S9 Emission spectra of $(AuCl)_2L$ in DMSO at time storage of solution from 0 (black line) to 60 (orange line) minutes. C($(AuCl)_2L$) = 0.2 mM, λ_{ex} = 340 nm.

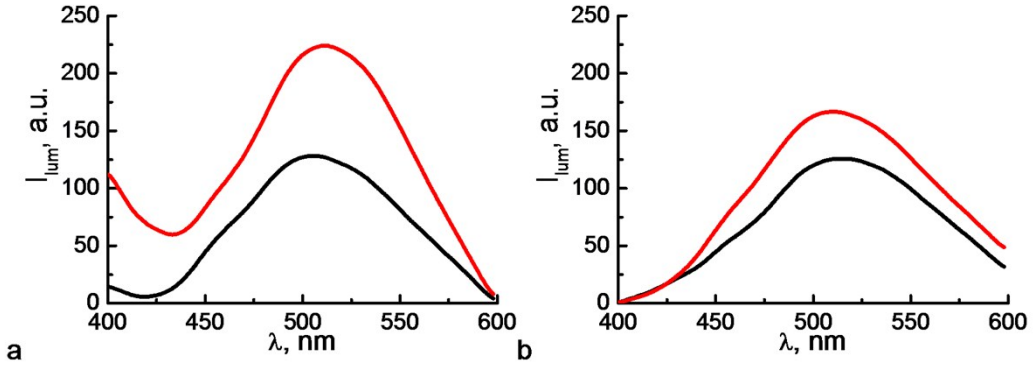

Fig. S10 Emission spectra of $(AuCl)_2L$ in acetone (a) and DMF (b) before (black line) and after (red line) deaeration of solutions by argon bubbling. C($(AuCl)_2L$) = 0.2 mM, λ_{ex} = 340 nm.

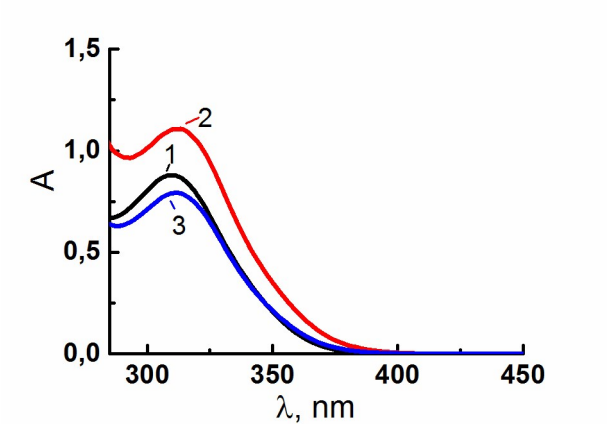

Fig. S11 Absorbance spectra of $(AuCl)_2L$ in AN (1), DMSO (2) and DMF (3). C($(AuCl)_2L$) = 0.05 mM.

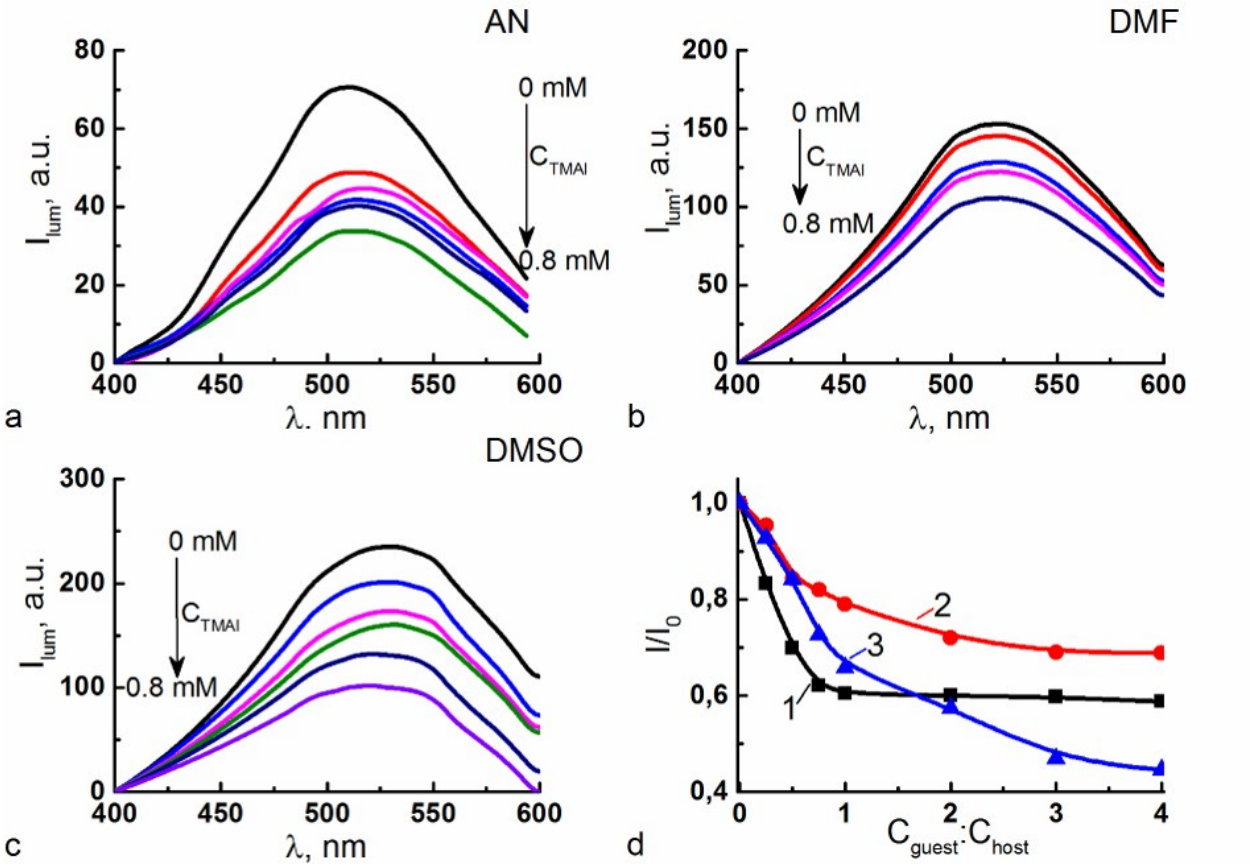

Fig. S12 (a-c) Emission spectra of $(AuCl)_2L$ (0.2 mM) at various concentrations (0–0.8 mM) of TMAI (guest) in AN (a), DMF (b) and DMSO (c). (d) I/I_0 of $(AuCl)_2L$ (host) versus guest:host concentration ratio in AN (1), DMF (2) and DMSO (3) solutions. λ_{ex} = 340 nm, λ_{em} = 500 nm.