Electronic supplementary material

1D and 2D silver-based coordination polymers with thiomorpholine-4-carbonitrile and aromatic polyoxoacids as co-ligands: structure, photocatalysis, photoluminescence and TD-DFT study

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Table S1. Crystallographic data and refinement parameters for SQUEEZED **3** with general formula $\{[Ag_2(H_2BTEC)(L)_2]\}_\infty$

Crystal data	
Chemical formula	$C_{30}H_{30}Ag_3N_6O_{12}S_3$
FW	1086.39
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	9.8212 (10)
b (Å)	26.3006 (4)
c (Å)	16.2293 (3)
α (°)	90
β (°)	93.666 (10)
γ (°)	90
V (Å^3)	4183.51 (11)
Z	4
D_x (mg m^{-3})	1.725
μ (mm^{-1})	13.09
Crystal size (mm)	0.37 × 0.16 × 0.07
Data collection	
Absorption correction	Analytical
T_{min}, T_{max}	0.094, 0.482
Reflections collected	16229
Independent reflections	7963
Observed reflections [$I > 2\sigma(I)$]	6801
R_{int}	0.026
Range of *h*, *k*, *l*	*h*=−12→11 *k*=−32→20 *l*=−19→19
θ values (°)	θ_{max} = 71.7, θ_{min} = 3.2
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$	0.0326, 0.0786
R[*all data*], *wR*2	0.0393, 0.0823
Goodness-of-fit (*S*)	1.037
No. of reflections	7963
No. of parameters	499
No. of restraints	118
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.76, –0.72
CCDC no.	1987948

Table S2. Pairwise interaction energies in the crystal structure of **1** based on B3LYP/ DGDZVP energy model.

N	Symmetry code	*R* (Å)	Interaction energies, kJ/mol				
			E_ele	E_pol	E_dis	E_rep	E_tot
2	x, y, z	13.16	11.1	–4.5	–12.1	7.2	2.3
2	x, y, z	13.89	6.5	–2.2	–11.3	10.1	1.7
1	x, y, z	18.61	13	–0.8	–1	0.3	12.4
2	x, y, z	4.43	–31.7	–16.3	–165.5	143.6	–101

Table S3. Pairwise interaction energies in the crystal structure of **2** based on B3LYP/ DGDZVP energy model.

N	Symmetry code	*R* (Å)	Interaction energies, kJ/mol				
			E_ele	E_pol	E_dis	E_rep	E_tot
1	–	7.12	–146.9	–41.1	–103.4	126.5	–197.7
1	–	14.04	4.8	–1.2	–8.6	0.8	–2.7
1	–	6.72	–93.7	–37.1	–158.5	160.7	–165.3
1	–	11.76	–1.6	–0.4	–0.9	0	–2.8
1	–	4.85	–28.5	–7.3	–77	71.8	–58.2
1	–	9.24	–9.2	–4.4	–20.7	18.5	–19.6
1	–	16.3	0.5	–0.7	–1.3	0	–1.2
1	–	5.02	–163.9	–36.4	–46.1	186.2	–125.4
1	–	7.74	–148.4	–37.4	–38.1	175.6	–109.3

Table S4. Pairwise interaction energies in the crystal structure of **3** based on B3LYP/ DGDZVP energy model.

N	Symmetry code	*R* (Å)	Interaction energies, kJ/mol				
			E_ele	E_pol	E_dis	E_rep	E_tot
1	x, y, z	16.6	0.2	–3.7	–11	17.3	–1.4
1	x, y, z	7.78	-145.1	–66.2	–185.9	110.3	–286.9

Table S5. Pairwise interaction energies in the crystal structure of **4** based on B3LYP/ DGDZVP energy model.

N	Symmetry code	*R* (Å)	Interaction energies, kJ/mol				
			E_ele	E_pol	E_dis	E_rep	E_tot
1	x, y, z	12.81	–20.9	–7.2	–20.6	8.6	–40.1
1	–	6.13	–200.5	–89.4	–311.2	288.6	–370.9
1	–	11.2	–11.2	–9.1	–83	56.7	–55.9

Powder X-ray diffraction analysis

All samples correspond to the single-phase X-ray powder patterns (Figure S1) in accordance with the structural model obtained by the single-crystal X-ray diffraction. It should be noted that the best overlap of peaks in the powder pattern for **3** was obtained using SQUEEZED cif single crystal data. According to the results of powder X-ray structural analysis, as well as thermogravimetric analysis, **3** readily loses solvent water molecules without change of the structure. For **1**, **2** and **4**, given the absence of any secondary phases, it can be concluded that all of the samples are stable in air under conditions of manual pulverization required to create powder samples from single crystals.

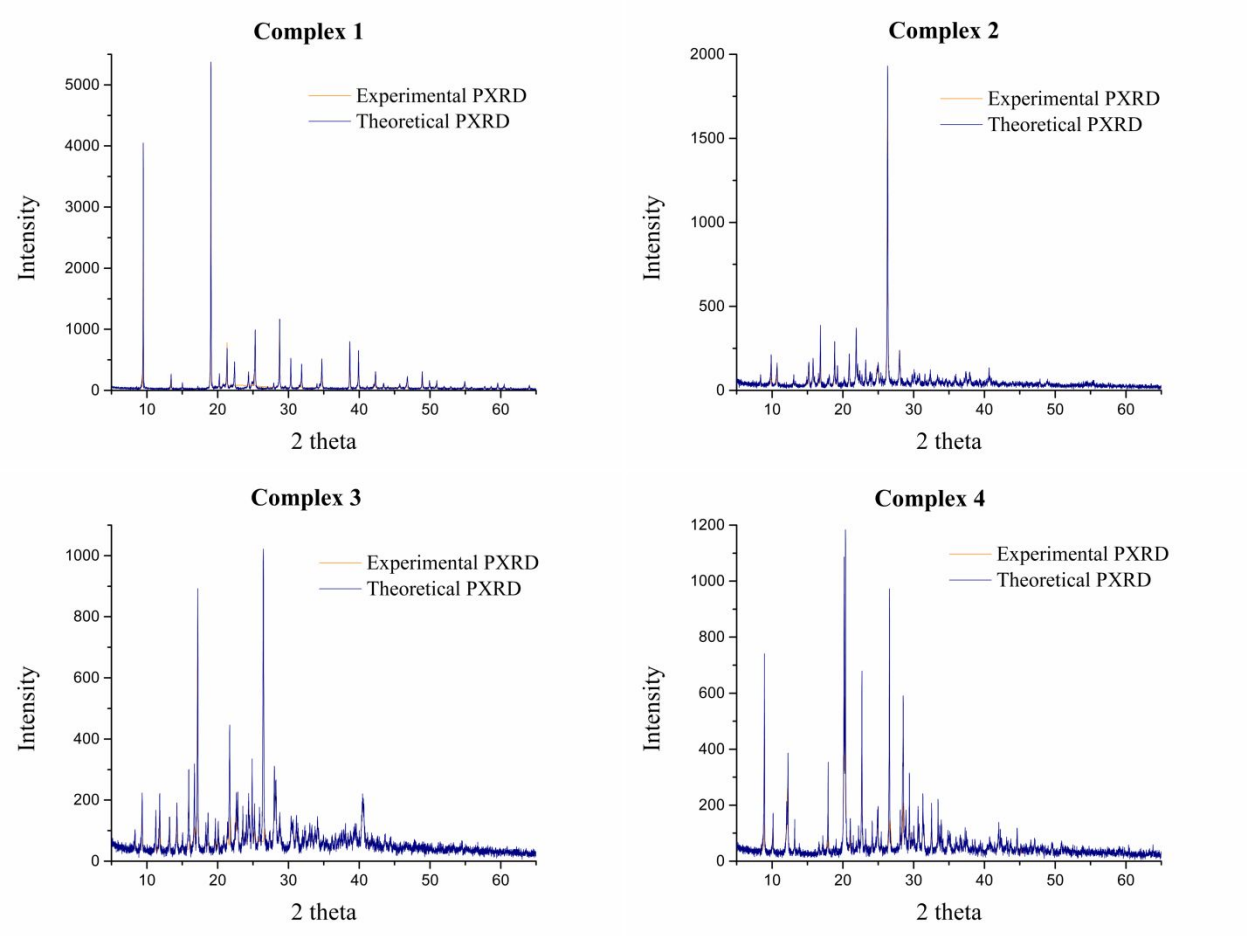

Figure S1. Overlapped experimental and theoretically obtained powder X-ray diffractograms.

Photocatalytic properties

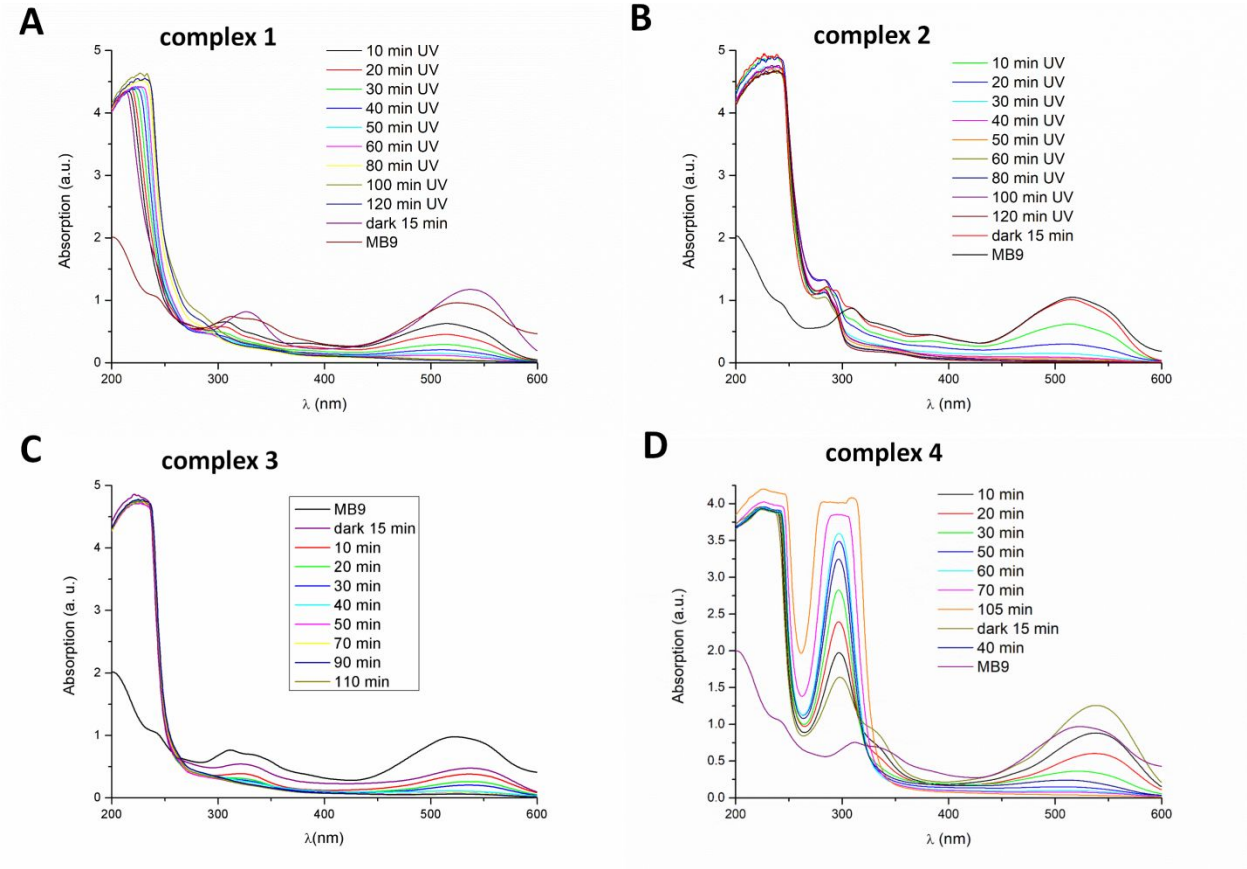

Figure S2. Photocatalytic degradation of MB9 dye using the complexes **1** (A), **2** (B), **3** (C) and **4** (D) monitored by UV-Vis spectroscopy.

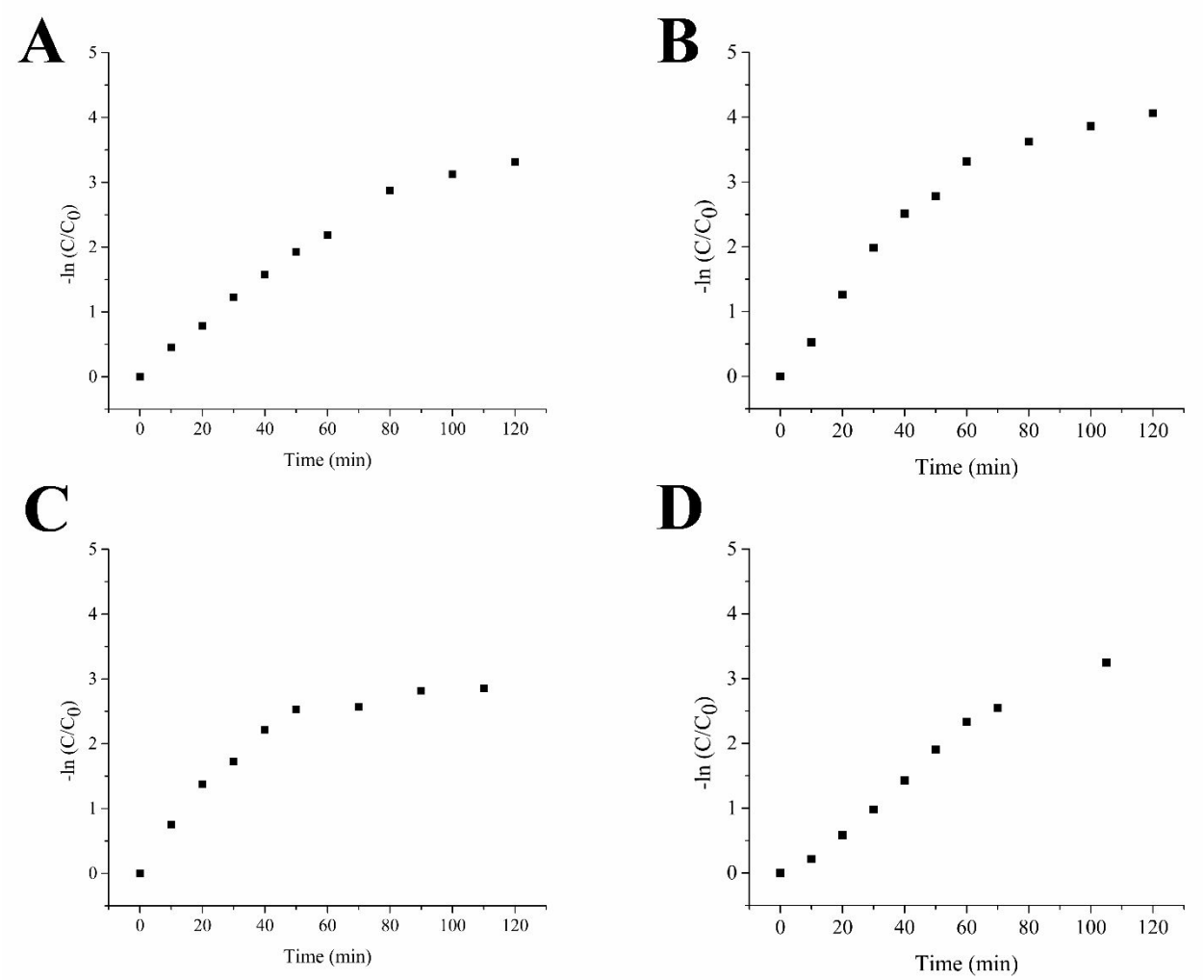

Figure S3. Dependence of –ln(C/C_0) on time for the photocatalytic degradation reaction of MB9 dye for the complexes **1** (A), **2** (B), **3** (C) and **4** (D).