

Supplementary Materials

Photocatalytic Degradation of Ciprofloxacin with Supramolecular Materials Consisting of Nitrogenous Organic Cations and Metal Salts

Chenfei Ren, Jian Li, Xingxing Zhang and Yunyin Niu *

Green catalysis center, and College of Chemistry, Zhengzhou University, Zhengzhou 450001, China

* Correspondence: niuyy@zzu.edu.cn

Table S1. Crystal data and structural refinement details of complexes 1–5.

Compounds	1	2	3	4	5
Empirical formula	C ₃₆ H ₄₀ Cu ₄ I ₈ N ₈	C ₃₆ H ₄₀ Ag ₄ I ₈ N ₈	C ₁₈ H ₂₀ Br ₄ N ₄ Zn	C ₃₆ H ₄₀ Ag ₄ I ₈ N ₈	C ₁₈ H ₂₀ Br ₃ CdClN ₄
Formula weight	1854.12	2031.44	677.39	1327.13	679.96
Temperature/K	300.00	300.00	291.00	292.00	300.00
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic	Triclinic
Space group	P2 ₁ /c	P2 ₁ /c	P2 ₁ /c	P-1	P-1
a/Å	17.852 (2)	18.2328 (19)	12.204	11.0705 (12)	9.9570 (4)
b/Å	19.295 (3)	19.478 (2)	11.732	11.9517 (13)	10.4582 (5)
c/Å	14.226 (2)	14.3224 (15)	16.659	17.722 (2)	11.6116 (5)
α/°	90	90	90	77.569 (4)	91.005 (2)
β/°	92.849 (5)	94.530 (4)	105.94	80.559 (4)	106.308 (2)
γ/°	90	90	90	67.721 (4)	104.270 (2)
Volume/Å ³	4894.1 (12)	5070.6 (9)	2293.4	2110.1 (4)	1119.78 (9)
Z	4	4	4	2	2
ρ _{calc} /cm ³	2.516	2.661	1.962	2.089	2.017
μ/mm ^{−1}	6.796	6.427	8.050	4.171	6.458
F(000)	3408.0	3696.0	1304.0	1248.0	652.0
Crystal size/mm ³	0.24 × 0.22 × 0.21	0.23 × 0.22 × 0.12	0.31 × 0.24 × 0.23	0.27 × 0.23 × 0.22	0.25 × 0.23 × 0.21
Reflections collected	142824	134714	104098	44704	18296
Independent reflections/R _{int} /R _{sigma}	11168 [R _{int} = 0.0617, R _{sigma} = 0.0260]	11660 [R _{int} = 0.1476, R _{sigma} = 0.0668]	5255 [R _{int} = 0.1046, R _{sigma} = 0.0356]	7438 [R _{int} = 0.0410, R _{sigma} = 0.0265]	3925 [R _{int} = 0.0545, R _{sigma} = 0.0402]
Data/restraints/parameters	11168/0/506	11660/0/507	5255/0/244	7438/36/472	3925/0/244
Goodness-of-fit on F ²	1.125	1.006	1.058	1.061	1.075
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0511, wR ₂ = 0.1314	R ₁ = 0.0388, wR ₂ = 0.0681	R ₁ = 0.0455, wR ₂ = 0.0720	R ₁ = 0.0367, wR ₂ = 0.1065	R ₁ = 0.0525, wR ₂ = 0.1592
Final R indexes [all data]	R ₁ = 0.0626, wR ₂ = 0.1359	R ₁ = 0.0895, wR ₂ = 0.0786	R ₁ = 0.0875, wR ₂ = 0.0845	R ₁ = 0.0433, wR ₂ = 0.1099	R ₁ = 0.0639, wR ₂ = 0.1674
Largest diff. peak/hole / e Å ^{−3}	1.75/−1.16	0.93/−1.06	0.94/−0.66	1.55/−1.66	1.07/−2.15

Table S2. The main bond length and bond angle of compounds 1–5.

Compound 1					
I2-Cu2-Cu1	110.46 (6)	I2-Cu2-Cu3	59.23 (5)	I2-Cu2-Cu4	58.91 (5)
I3-Cu2-Cu1	56.01 (5)	I3-Cu2-Cu3	58.33 (5)	I4-Cu2-I2	108.96 (6)
I4-Cu2-I3	104.39 (6)	I4-Cu2-I6	109.86 (6)	I4-Cu2-Cu1	140.29 (7)
I4-Cu2-Cu3	143.33 (7)	I4-Cu2-Cu4	148.46 (8)	I6-Cu2-I3	108.88 (6)
I6-Cu2-Cu1	57.77 (5)	I6-Cu2-Cu3	106.51 (6)	I6-Cu2-Cu4	59.13 (5)
Cu3-Cu2-Cu1	60.58 (6)	Cu4-Cu2-I3	107.15 (6)	Cu4-Cu2-Cu1	62.68 (5)
Cu4-Cu2-Cu3	59.62 (5)	I1-Cu3-I2	104.16 (6)	I1-Cu3-I3	106.75 (6)
I1-Cu3-I8	112.12 (6)	I1-Cu3-Cu1	147.37 (8)	I1-Cu3-Cu2	140.87 (7)
I1-Cu3-Cu4	143.98 (7)	I2-Cu3-I3	111.61 (6)	I2-Cu3-Cu1	108.12 (6)
I2-Cu3-Cu2	56.90 (5)	I2-Cu3-Cu4	58.17 (5)	I3-Cu3-Cu1	56.54 (4)
I3-Cu3-Cu2	60.64 (5)	I3-Cu3-Cu4	109.01 (6)	I8-Cu3-I2	113.01 (6)
I8-Cu3-I3	108.97 (6)	I8-Cu3-Cu1	58.63 (4)	I8-Cu3-Cu2	106.96 (6)
I8-Cu3-Cu4	59.33 (5)	Cu2-Cu3-Cu1	60.11 (5)	Cu4-Cu3-Cu1	62.50 (5)
Cu4-Cu3-Cu2	59.60 (5)	I2-Cu4-I6	110.97 (5)	I2-Cu4-I8	113.00 (6)
I2-Cu4-Cu1	106.91 (5)	I2-Cu4-Cu2	57.64 (4)	I2-Cu4-Cu3	59.26 (5)
I6-Cu4-I8	107.66 (6)	I6-Cu4-Cu1	56.49 (4)	I6-Cu4-Cu2	58.39 (5)
I6-Cu4-Cu3	106.86 (6)	I7-Cu4-I2	110.53 (6)	I7-Cu4-I6	107.74 (6)
I7-Cu4-I8	106.70 (5)	I7-Cu4-Cu1	142.56 (7)	I7-Cu4-Cu2	146.13 (7)
I7-Cu4-Cu3	145.17 (7)	I8-Cu4-Cu1	57.39 (4)	I8-Cu4-Cu2	107.03 (6)
I8-Cu4-Cu3	58.23 (5)	Cu2-Cu4-Cu1	59.61 (5)	Cu2-Cu4-Cu3	60.78 (6)
Cu3-Cu4-Cu1	59.91 (5)				
Compound 2					
I1-Ag1	2.7851 (8)	I2-Ag1	2.8605 (8)	I2-Ag2	2.9475 (8)
I2-Ag3	2.8952 (8)	I3-Ag2	2.7456 (7)	I4-Ag1	3.0278 (8)
I4-Ag2	2.9617 (8)	I4-Ag4	2.8817 (7)	I5-Ag2	2.8887 (7)
I5-Ag3	2.9580 (8)	I5-Ag4	2.9709 (8)	I6-Ag3	2.7597 (7)
I7-Ag4	2.7660 (8)	I8-Ag1	2.9169 (8)	I8-Ag3	2.9290 (8)
I8-Ag4	2.9107 (8)	Ag1-Ag2	3.1826 (9)	Ag1-Ag3	3.0621 (9)
Ag1-Ag4	3.1622 (9)	Ag2-Ag3	3.0862 (8)	Ag2-Ag4	3.1432 (9)
Ag3-Ag4	3.2632 (8)	Ag1-I2-Ag2	66.44 (2)	Ag1-I2-Ag3	64.28 (2)
Ag3-I2-Ag2	63.763 (18)	Ag2-I4-Ag1	64.185 (18)	Ag4-I4-Ag1	64.645 (19)
Ag4-I4-Ag2	65.07 (2)	Ag2-I5-Ag3	63.707 (18)	Ag2-I5-Ag4	64.86 (2)
Ag3-I5-Ag4	66.787 (19)	Ag1-I8-Ag3	63.17 (2)	Ag4-I8-Ag1	65.72 (2)
Ag4-I8-Ag3	67.944 (18)	I1-Ag1-I2	110.26 (2)	I1-Ag1-I4	105.51 (2)
I1-Ag1-I8	110.67 (2)	I1-Ag1-Ag2	144.49 (3)	I1-Ag1-Ag3	148.04 (3)
I1-Ag1-Ag4	140.18 (3)	I2-Ag1-I4	108.66 (2)	I2-Ag1-I8	113.06 (2)
I2-Ag1-Ag2	58.092 (18)	I2-Ag1-Ag3	58.410 (19)	I2-Ag1-Ag4	109.14 (2)
I4-Ag1-Ag2	56.899 (19)	I4-Ag1-Ag3	106.45 (2)	I4-Ag1-Ag4	55.440 (18)
I8-Ag1-I4	108.36 (2)	I8-Ag1-Ag2	104.45 (2)	I8-Ag1-Ag3	58.606 (19)
I8-Ag1-Ag4	57.044 (18)	Ag3-Ag1-Ag2	59.198 (19)	Ag3-Ag1-Ag4	63.21 (2)
Ag4-Ag1-Ag2	59.39 (2)	I2-Ag2-I4	108.13 (2)	I2-Ag2-Ag1	55.471 (19)
I2-Ag2-Ag3	57.294 (19)	I2-Ag2-Ag4	107.41 (2)	I3-Ag2-I2	102.17 (2)
I3-Ag2-I4	108.06 (2)	I3-Ag2-I5	115.15 (2)	I3-Ag2-Ag1	138.67 (3)
I3-Ag2-Ag3	143.19 (3)	I3-Ag2-Ag4	149.66 (3)	I4-Ag2-Ag1	58.916 (19)
I4-Ag2-Ag3	107.51 (2)	I4-Ag2-Ag4	56.239 (18)	I5-Ag2-I2	112.48 (2)
I5-Ag2-I4	110.36 (2)	I5-Ag2-Ag1	105.92 (2)	I5-Ag2-Ag3	59.240 (18)
I5-Ag2-Ag4	58.833 (17)	Ag3-Ag2-Ag1	58.45 (2)	Ag3-Ag2-Ag4	63.172 (18)
Ag4-Ag2-Ag1	59.980 (19)	I2-Ag3-I5	111.98 (2)	I2-Ag3-I8	111.69 (2)
I2-Ag3-Ag1	57.310 (18)	I2-Ag3-Ag2	58.943 (18)	I2-Ag3-Ag4	105.60 (2)

I5-Ag3-Ag1	107.31 (2)	I5-Ag3-Ag2	57.053 (18)	I5-Ag3-Ag4	56.795 (17)
I6-Ag3-I2	112.18 (2)	I6-Ag3-I5	106.36 (2)	I6-Ag3-I8	108.21 (2)
I6-Ag3-Ag1	146.11 (3)	I6-Ag3-Ag2	144.59 (3)	I6-Ag3-Ag4	142.21 (3)
I8-Ag3-I5	106.07 (2)	I8-Ag3-Ag1	58.220 (18)	I8-Ag3-Ag2	106.61 (2)
I8-Ag3-Ag4	55.761 (18)	Ag1-Ag3-Ag2	62.35 (2)	Ag1-Ag3-Ag4	59.889 (19)
Ag2-Ag3-Ag4	59.266 (19)	I4-Ag4-I5	110.30 (2)	I4-Ag4-I8	112.66 (2)
I4-Ag4-Ag1	59.914 (19)	I4-Ag4-Ag2	58.696 (17)	I4-Ag4-Ag3	104.92 (2)
I5-Ag4-Ag1	104.46 (2)	I5-Ag4-Ag2	56.305 (18)	I5-Ag4-Ag3	56.419 (18)
I7-Ag4-I4	114.27 (2)	I7-Ag4-I5	106.26 (2)	I7-Ag4-I8	106.63 (2)
I7-Ag4-Ag1	148.47 (3)	I7-Ag4-Ag2	146.77 (3)	I7-Ag4-Ag3	140.80 (2)
I8-Ag4-I5	106.21 (2)	I8-Ag4-Ag1	57.233 (19)	I8-Ag4-Ag2	105.60 (2)
I8-Ag4-Ag3	56.295 (18)	Ag1-Ag4-Ag3	56.896 (19)	Ag2-Ag4-Ag1	60.63 (2)
Ag2-Ag4-Ag3	57.561 (18)				
Compound 3					
Zn-Br1	2.3980 (8)	Br1-Zn-Br2	113.27 (3)	Br4-Zn-Br1	108.75 (3)
Zn-Br2	2.4085 (8)	Br3-Zn-Br1	108.27 (3)	Br4-Zn-Br2	105.96 (3)
Zn-Br3	2.3881 (9)	Br3-Zn-Br2	107.34 (3)		
Zn-Br4	2.3927 (8)	Br3-Zn-Br4	113.34 (3)		
Compound 4					
I4-Ag1	2.8756 (7)	I3-Ag1	2.8889 (12)	I1-Ag1	2.8567 (7)
I2-Ag1	2.8271 (7)	Ag1-I3A	3.16 (5)	I4-Ag1-I3	126.86 (5)
I4-Ag1-I3A	132.1 (4)	I1-Ag1-I4	109.49 (2)	I1-Ag1-I3	102.32 (3)
I1-Ag1-I3A	102.8 (3)	I2-Ag1-I4	103.21 (2)	I2-Ag1-I3	96.96 (6)
I2-Ag1-I1	118.75 (2)	I2-Ag1-I3A	90.6 (5)		
Compound 5					
Cd1-Cl1	2.4742 (18)	Cd1-Br2	2.5971 (10)	Cd1-Br3	2.5297 (10)
Cd1-Br4	2.5531 (12)	Cl1-Cd1-Br2	105.35 (6)	Cl1-Cd1-Br3	113.42 (5)
Cl1-Cd1-Br4	105.21 (6)	Br3-Cd1-Br2	112.06 (4)	Br3-Cd1-Br4	116.33 (4)
Br4-Cd1-Br2	103.39 (4)				