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Electronic Supplementary Information for

Structural Diversity and Photoluminescent Properties of Cadmium Thiophenedicarboxylate Coordination Polymers

Li-Ping Xue,[†] Xin-Hong Chang,[†] Shi-Hui Li, [†] Lu-Fang Ma,*[,†] and Li-Ya Wang*[,†,‡]

[†]*College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, P. R. China.*

[‡]*College of Chemistry and Pharmaceutical Engineering, Nanyang Normal University, Nanyang 473061, P. R. China*

Table S1 Crystal data and structure refinements for **1a–3b**

Compound	**1a**	**1b**	**2a**	**2b**	**3a**	**3b**
Formula	$C_{26}H_{28}CdN_8O_{12}S_2$	$C_{26}H_{22}CdN_8O_8S_2$	$C_{16}H_{16}CdN_4O_4S$	$C_{16}H_{18}CdN_4O_5S$	$C_{17}H_{13}CdN_5O_5S$	$C_{17}H_{13}CdN_5O_5S$
M_r	821.08	751.04	472.79	490.80	511.78	510.78
T (K)	293(2)	293(2)	293(2)	293(2)	293(2)	293(2)
Crystal system	triclinic	monoclinic	monoclinic	monoclinic	Tetragonal	Tetragonal
Space group	*P*−1	*C*2/*c*	*C*2/*c*	*C*2/*c*	*I*−42*d*	*I*−42*d*
a (Å)	8.768(2)	21.534(6)	15.539(3)	16.714(6)	9.4730(11)	9.4643(12)
b (Å)	8.851(2)	8.764(3)	8.9486(15)	16.289(6)	9.4730(11)	9.4643(12)
c (Å)	12.344(3)	16.832(5)	13.056(2)	13.976(5)	42.894(10)	42.890(11)
α (°)	76.950(2)	90.00	90.00	90.00	90	90
β (°)	77.453(2)	106.950(4)	103.428(2)	95.587(3)	90	90
γ (°)	63.795(2)	90.00	90.00	90.00	90	90
V (Å^3)	829.7(3)	3038.6(15)	1765.9(5)	3787(2)	3849.2(11)	3841.8(12)
Z	1	4	4	8	8	8
ρ(g cm^{-3})	1.643	1.642	1.778	1.722	1.766	1.766
μ (mm^{-1})	0.857	0.918	1.385	1.299	1.284	1.286
F(000)	416	1512	944	1968	2032	2024
GOF (F^2)	1.034	1.031	1.033	1.037	1.253	1.107
R_1[a] [$I>2\sigma(I)$]	0.0285	0.0447	0.0196	0.0516	0.0330	0.0367
wR_2[b] [$I>2\sigma(I)$]	0.0716	0.1288	0.0492	0.1329	0.0890	0.0962

[a] $R_1 = \sum\left||F_o|-|F_c|\right| / \sum|F_o|$. [b] $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]\}^{1/2}$

Tables S2 Selected Bond Distances (Å) and Angles (deg) for Complexes **1a−3b**

Compound **1a**[a]

Cd(1)−O(1)	2.3584(19)	Cd(1)−N(1)	2.328(2)	Cd(1)−N(4)#2	2.325(2)
N(4)#2−Cd(1)−N(4)#3)	180.0	N(4)#2−Cd(1)−N(1)	91.83(7)	N(4)#3−Cd(1)−N(1)	88.17(7)
N(1)−Cd(1)−N(1)#4	180.00(11)	N(4)#2−Cd(1)−O(1)	90.61(7)	N(4)#3−Cd(1)−O(1)	89.39(7)
N(1)−Cd(1)−O(1)	91.61(7)	N(1)#4−Cd(1)−O(1)	88.39(7)	O(1)−Cd(1)−O(1) #4	180.0

[a]Symmetry codes: #1 x+1, y−1, z #2 x-1, y+1, z #3 -x+1, -y+1, -z+1 #4 −x, −y+2, −z+1

Compound **1b**[b]

Cd(1)−O(1)	2.354(3)	Cd(1)−N(1)	2.338(4)	Cd(1)−N(4)#1	2.289(4)
N(4)#1−Cd(1)−N(4)#2	180.000(1)	N(4)#1−Cd(1)−N(1)	87.21(15)	N(4)#2−Cd(1)−N(1)	92.79(15)
N(1)−Cd(1)−N(1)#3	180.0	N(1)−Cd(1)−O(1)#3	95.43(15)	N(4)#1−Cd(1)−O(1)	88.66(16)
N(4)#2−Cd(1)−O(1)	91.34(16)	N(1)−Cd(1)−O(1)	84.57(15)	N(1)#3−Cd(1)−O(1)	84.57(15)
O(1)#3−Cd(1)−O(1)	180.00(9)				

[b]Symmetry codes: #1 −x+1/2, −y+1/2, −z+1 #2 x, y−1, z #3 −x+1/2, −y−1/2, −z+1

Compound **2a**[c]

Cd(1)−N(2)	2.2547(16)	Cd(1)−O(2)	2.3914(14)	Cd(1)−O(1)	2.3986(13)
N(2)#1−Cd(1)−N(2)	180.00(13)	N(2)−Cd(1)−O(2)#1	89.62(6)	N(2)−Cd(1)−O(2)	90.38(6)
O(2)#1−Cd(1)−O(2)	180.00(7)	N(2)−Cd(1)−O(1)	88.98(5)	O(2)−Cd(1)−O(1)	55.08(4)
N(2)−Cd(1)−O(1)#1	91.02(5)	O(2)−Cd(1)−O(1)#1	124.92(4)	O(1)−Cd(1)−O(1)#1	180.00(8)

[c]Symmetry codes: #1 −x+1, −y, −z

Compound **2b**[d]

Cd(1)−O(1)	2.215(5)	Cd(1)−N(1)	2.251(5)	Cd(1)−O(2)	2.642(5)

Cd(1)−O(3)#2	2.462(6)	Cd(1)−O(4)#2	2.401(5)	Cd(1)−N(4)#1	2.233(6)
O(1)−Cd(1)−N(4)#1	123.1(2)	O(1)−Cd(1)−N(1)	119.7(2)	N(4)#1−Cd(1)−N(1)	100.8(2)
O(1)−Cd(1)−O(4)#2	95.80(19)	N(4)#1−Cd(1)−O(4)#2	124.7(2)	N(1)−Cd(1)−O(4)#2	89.29(19)
O(1)−Cd(1)−O(3)#2	91.74(19)	N(4)#1−Cd(1)−O(3)#2	84.70(19)	N(1)−Cd(1)−O(3)#2	135.0(2)
O(4)#2−Cd(1)−O(3)#2	53.72(19)	O(1)−Cd(1)−O(2)	53.23(16)	N(4)#1−Cd(1)−O(2)	92.95(19)
N(1)−Cd(1)−O(2)	89.03(17)	O(4)#2−Cd(1)−O(2)	141.92(18)	O(3)#2−Cd(1)−O(2)	135.68(18)

[d]Symmetry codes: #1 −x+3/2, −y+1/2, −z+1 #2 −x+1/2, −y+1/2, −z+1

Compound **3a**[e]

Cd(1)−O(1)#1	2.342(4)	Cd(1)−O(1)	2.342(4)	Cd(1)−N(3)#2	2.345(4)
Cd(1)−N(3)#3	2.345(4)	Cd(1)−N(1)	2.439(5)	Cd(1)−O(2)	2.517(4)
Cd(1)−O(2)#1	2.517(4)				
O(1)#1−Cd(1)−O(1)	83.76(19)	O(1)#−Cd(1)−N(3)#2	89.88(15)	O(1)−Cd(1)−N(3)#2	99.91(14)
O(1)#1−Cd(1)−N(3)#3	99.91(14)	O(1)−Cd(1)−N(3)#3	89.88(15)	N(3)#2−Cd(1)−N(3)#3	166.9(2)
O(1)#1−Cd(1)−N(1)	138.12(10)	O(1)−Cd(1)−N(1)	138.12(10)	N(3)#2−Cd(1)−N(1)	83.45(10)
N(3)#3−Cd(1)−N(1)	83.45(10)	O(1)#1−Cd(1)−O(2)	136.88(13)	O(1)−Cd(1)−O(2)	53.66(13)
N(3)#2−Cd(1)−O(2)	91.11(15)	N(3)#3−Cd(1)−O(2)	87.69(15)	N(1)−Cd(1)−O(2)	84.71(9)
O(1)#1−Cd(1)−O(2)#1	53.66(13)	O(1)−Cd(1)−O(2)#1	136.88(13)	N(3)#2−Cd(1)−O(2)#1	87.69(15)
N(3)#3−Cd(1)−O(2)#1	91.11(15)	N(1)−Cd(1)−O(2)#1	84.71(9)	O(2)−Cd(1)−O(2)#1	169.42(17)

[e]Symmetry codes: #1 -x, -y+2, z #2 -x+1/2, y-1/2, -z+3/2 #3 -y+1/2,x+3/2,-z+3/2

Compound **3b**[f]

Cd1−O1#1	2.329(4)	Cd1−O1	2.329(4)	Cd1−N3#2	2.338(5)
Cd1−N3#3	2.338(5)	Cd1−N1	2.426(5)	Cd1−O2	2.562(6)
Cd1−O2#1	2.562(6)				
O1#1−Cd1−O1	83.8(2)	O1#1−Cd1−N3#2	88.68(17)	O1−Cd1−N3#2	100.31(17)
O1#1−Cd1−N3#3	100.31(17)	O1−Cd1−N3#3	88.68(17)	N3#2−Cd1−N3#3	168.0(2)
O1#1−Cd1−N1	138.09(11)	O1−Cd1−N1	138.09(11)	N3#2−Cd1−N1	83.99(12)
N3#3−Cd1−N1	83.99(12)	O1#1−Cd1−O2	135.68(15)	O1−Cd1−O2	52.81(15)
N3#2−Cd1−O2	90.5(2)	N3#3−Cd1−O2	88.6(2)	N1−Cd1−O2	85.72(11)
O1#1−Cd1−O2#1	52.81(15)	O1−Cd1−O2#1	135.68(15)	N3#2−Cd1−O2#1	88.6(2)
N3#3−Cd1−O2#1	90.5(2)	N1−Cd1−O2#1	85.72(11)	O2−Cd1−O2#1	171.4(2)

[f]Symmetry codes: #1 -x,-y+2,z #2 y-1/2,-x+1/2,-z+3/2 #3 -y+1/2,x+3/2,-z+3/2

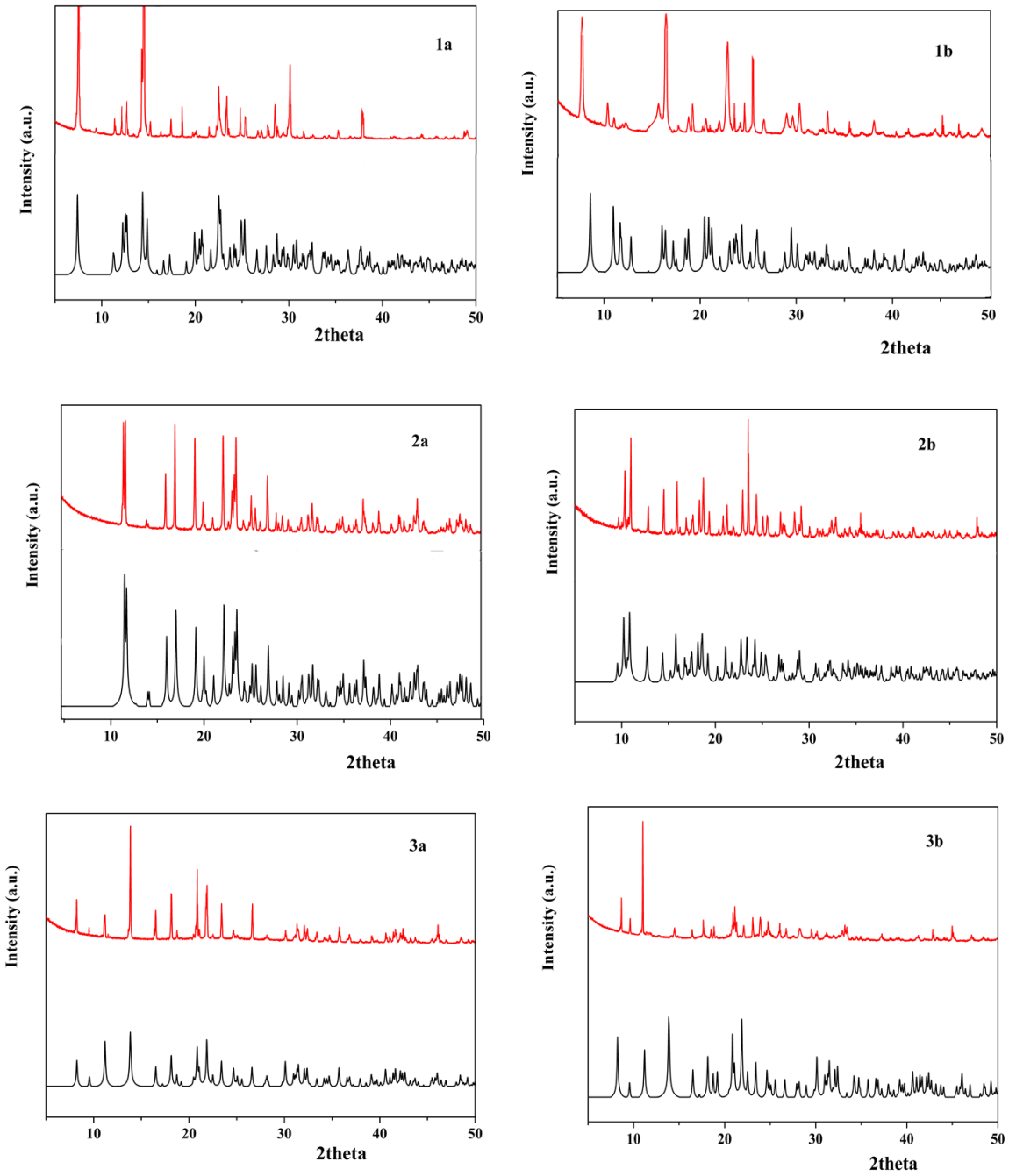

Fig. S1 PXRD patterns of **1a**–**3b** simulated from X−ray single−crystal diffraction data (bottom) and experimental data (upper).

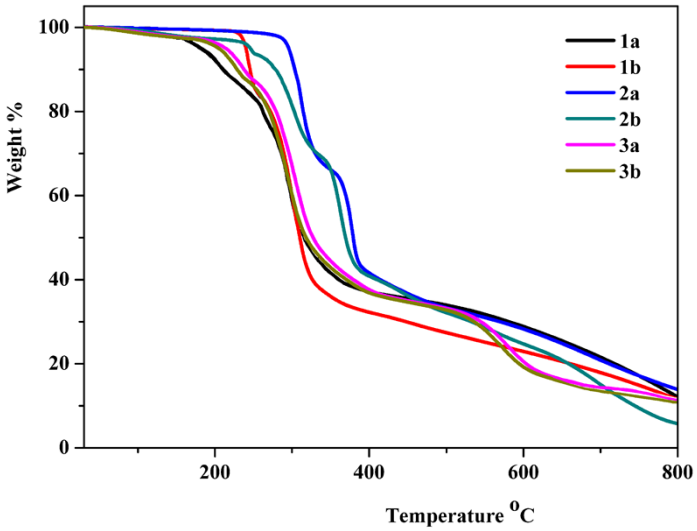

Fig. S2 TGA curves for complexes **1a**−**3b**.