

## Fluorescent Cadmium Complexes Based on N-Succinopyridine Ligand: Synthesis, Structures, and Tunable Photoluminescence by Variation of Excitation Light

Li-Zhen Cai,<sup>a,b</sup> Ming-Sheng Wang,<sup>a</sup> Ming-Jian Zhang,<sup>a</sup> Guan-E Wang,<sup>a</sup> Guo-Cong Guo,\*<sup>a</sup> and Jin-Shun Huang<sup>a</sup>

*a State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China*

*b Key Laboratory of Coal to Ethylene Glycol and Its Related Technology, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China*

**Table S1.** Selected bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ ) for **1** and **2**.

### **1**

Cd(1)-O(2W)	2.258(4)
Cd(1)-O(1W)	2.426(4)
Cd(1)-Cl(2)	2.561(2)
Cd(1)-Cl(1)	2.596(1)
Cd(1)-Cl(2)#1	2.613(1)
Cd(1)-Cl(1)#2	2.715(2)
O(2W)-Cd(1)-O(1W)	86.90(17)
O(2W)-Cd(1)-Cl(2)	172.60(13)
O(1W)-Cd(1)-Cl(2)	88.32(12)
O(2W)-Cd(1)-Cl(1)	90.78(11)
O(1W)-Cd(1)-Cl(1)	88.36(11)
Cl(2)-Cd(1)-Cl(1)	94.75(5)
O(2W)-Cd(1)-Cl(2)#1	85.71(12)
O(1W)-Cd(1)-Cl(2)#1	83.78(11)

---

\* Author to whom correspondence should be addressed. E-mail: gcguo@fjirsm.ac.cn (G.-C.Guo).

Cl(2)-Cd(1)-Cl(2)#1	88.15(4)
Cl(1)-Cd(1)-Cl(2)#1	171.55(4)
O(2W)-Cd(1)-Cl(1)#2	92.47(13)
O(1W)-Cd(1)-Cl(1)#2	172.71(10)
Cl(2)-Cd(1)-Cl(1)#2	91.55(5)
Cl(1)-Cd(1)-Cl(1)#2	98.91(3)
Cl(2)#1-Cd(1)-Cl(1)#2	88.93(5)

---

**2**

Cd(1)-O(1W)	2.297(5)
Cd(1)-O(2W)	2.318(5)
Cd(1)-Br(2)	2.757(1)
Cd(1)-Br(2)#1	2.780(1)
Cd(1)-Br(1)	2.781(1)
Cd(1)-Br(1)#2	2.781(1)
O(1W)-Cd(1)-O(2W)	176.29(19)
O(1W)-Cd(1)-Br(2)	89.96(13)
O(2W)-Cd(1)-Br(2)	89.20(14)
O(1W)-Cd(1)-Br(2)#1	88.97(14)
O(2W)-Cd(1)-Br(2)#1	92.10(14)
Br(2)-Cd(1)-Br(2)#1	176.30(4)
O(1W)-Cd(1)-Br(1)	86.75(13)
O(2W)-Cd(1)-Br(1)	89.75(13)
Br(2)-Cd(1)-Br(1)	96.54(4)
Br(2)#1-Cd(1)-Br(1)	86.93(4)
O(1W)-Cd(1)-Br(1)#2	91.64(13)
O(2W)-Cd(1)-Br(1)#2	91.93(14)
Br(2)-Cd(1)-Br(1)#2	87.37(4)
Br(2)#1-Cd(1)-Br(1)#2	89.13(4)
Br(1)-Cd(1)-Br(1)#2	175.77(4)

---

Symmetry codes for **1**: #1  $x -x+2, -y+2, -z$ ; #2  $x, -y+3/2, z-1/2$ ; #3  $x, -y+3/2, z+1/2$ ; for **2**: #1  $x+1/2, -y+3/2, -z+1$ ; #2  $x-1/2, -y+3/2, -z+1$ .

**Table S2.** Specified hydrogen bonds for **1** (with esds except fixed and riding H).

<b>1</b>				
D-H	H...A	D...A	$\angle$ (DHA)	D-H...A
0.847(10)	1.894(13)	2.736(5)	172(5)	O2W-H2WA...O4_\$3
0.842(10)	1.963(17)	2.793(5)	168(6)	O2W-H2WB...O4_\$2
0.82	1.62	2.425(5)	168.1	O3-H3B...O1_\$1
0.844(10)	2.53(3)	3.293(4)	150(5)	O1W-HIW...C11_\$4

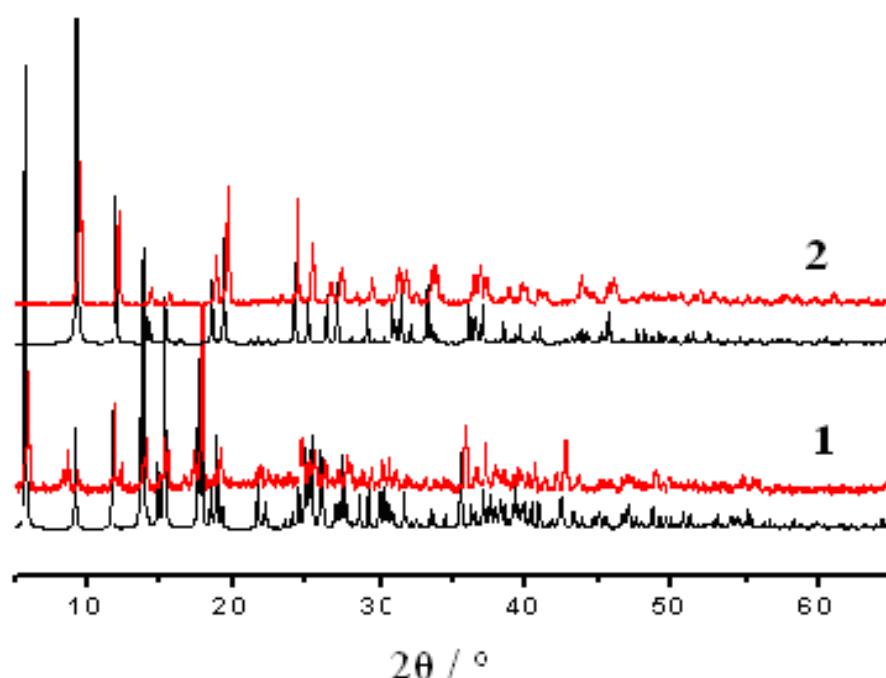
<b>2</b>				
D-H	H...A	D...A	$\angle$ (DHA)	D-H...A
0.82	1.65	2.465(8)	177.6	O3-H3B...O2_\$1
0.850(10)	2.39(3)	2.814(8)	111(8)	O1W-H1WA...O3_\$2
0.850(9)	2.48(4)	2.927(8)	114	O2W-H2WA...O4_\$3
0.850(9)	2.51(3)	3.232(8)	143	O2W-H2WA...O2
0.93	2.84	3.658(10)	147.0	C1-H1A...Br1_\$6

Symmetry codes for **1**: \$1  $x, y, z+1$ ; \$2  $x, y, z-1$ ; \$3  $x, -y+3/2, z-1/2$ ; \$4  $x, -y+3/2, z+1/2$ ; for **2**: \$1  $x+1, y, z$ ; \$2  $-x+3/2, -y+2, z-1/2$ ; \$3  $x-1, y, z$ ; \$4  $-x+1, y-1/2, -z+3/2$ ; \$5  $x-1/2, -y+3/2, -z+1$ ; \$6  $-x+3/2, -y+2, z+1/2$ .

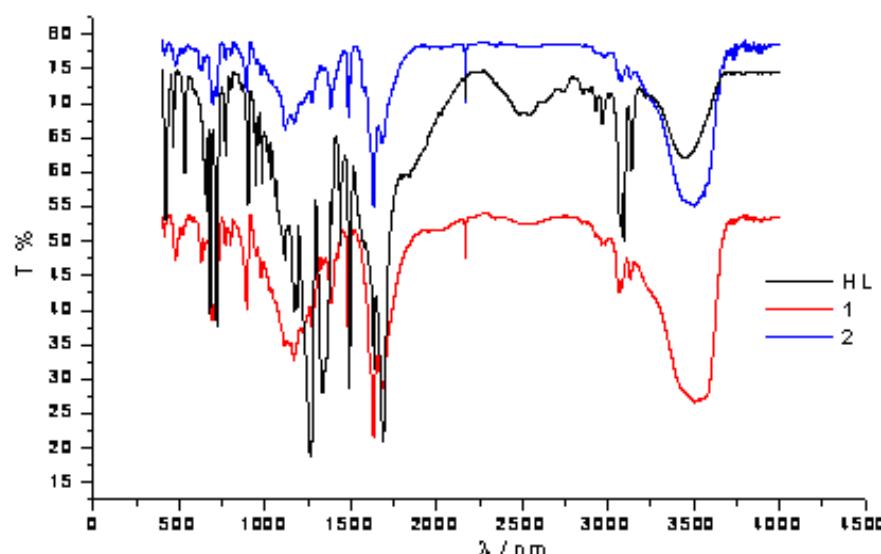
**Table S3.** emission peaks and its origin.

complex	$\lambda_{\text{em}}$ (nm)	VBs (HOMO)	CBs (LOMO)	origin
HL	375	p- $\pi$ of py <sup>+</sup>	p- $\pi^*$ of py <sup>+</sup>	intragroup $\pi$ - $\pi^*$
	485	p- $\pi$ of COO <sup>-</sup>	p- $\pi^*$ of py <sup>+</sup>	intergroup $\pi$ - $\pi^*$
<b>1</b>	391	p- $\pi$ of py <sup>+</sup>	p- $\pi^*$ of py <sup>+</sup>	intragroup $\pi$ - $\pi^*$
	425	orbital of inorganic layer	p- $\pi^*$ of py <sup>+</sup>	MLCT
<b>2</b>	425	orbital of inorganic chain	p- $\pi^*$ of py <sup>+</sup>	MLCT
	463	orbital of inorganic chain	p- $\pi^*$ of py <sup>+</sup>	MLCT and

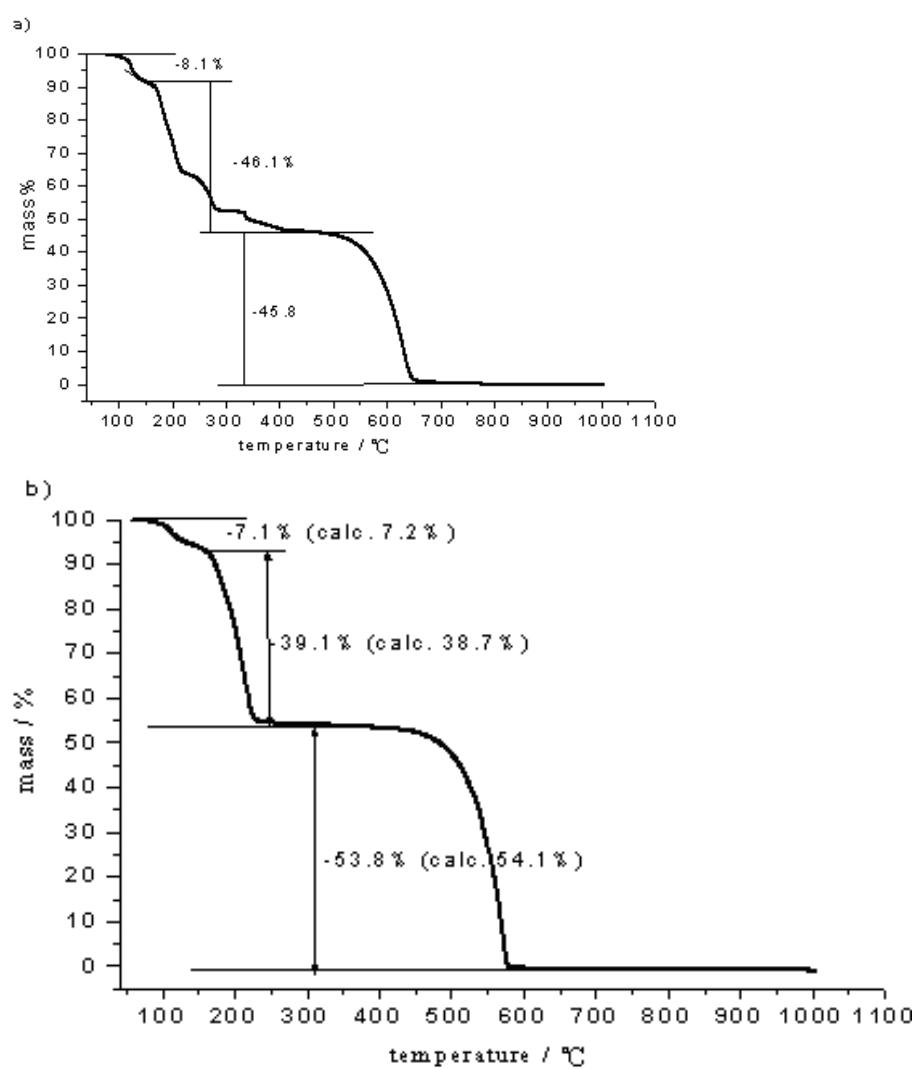
		and p- $\pi$ of COO <sup>-</sup>		intergroup $\pi$ - $\pi^*$
	500	p- $\pi$ of COO <sup>-</sup>	p- $\pi^*$ of py <sup>+</sup>	intergroup $\pi$ - $\pi^*$



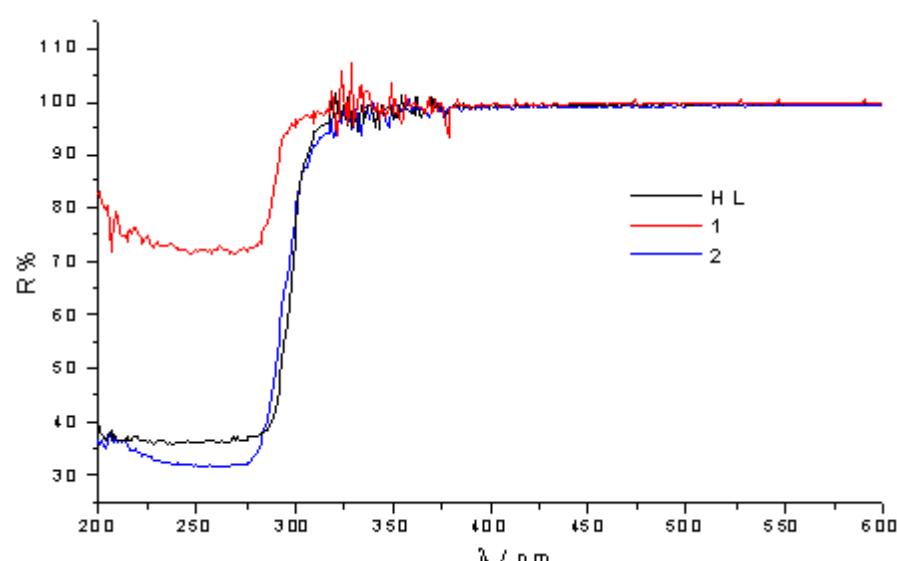
**Fig. S1.** PXRD patterns of **1** and **2**.



**Fig. S2.** IR spectra of HL, **1** and **2**.



**Fig. S3.** TGA spectra of **1** (a), **2** (b).



**Fig. S4.** Optical diffuse reflectance spectra for HL, **1** and **2**.