Electronic Supplementary Material (ESI) for Dalton Transactions.

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The effect of conjugation degree of aromatic carboxylic acids on electronic and photo-responsive behaviors of naphthalenediimide-based coordination polymers

Ming Kang, Bohong Gao, Shimin Zhang, Pengfei Hao,* Gaopeng Li, Junju Shen and Yunlong Fu*

Key Laboratory of Magnetic Molecules and Magnetic Information Materials of Ministry of Education & School of Chemistry and Materials Science of Shanxi Normal University, Taiyuan 030031, China

Supplementary Information Contents

1. Figures

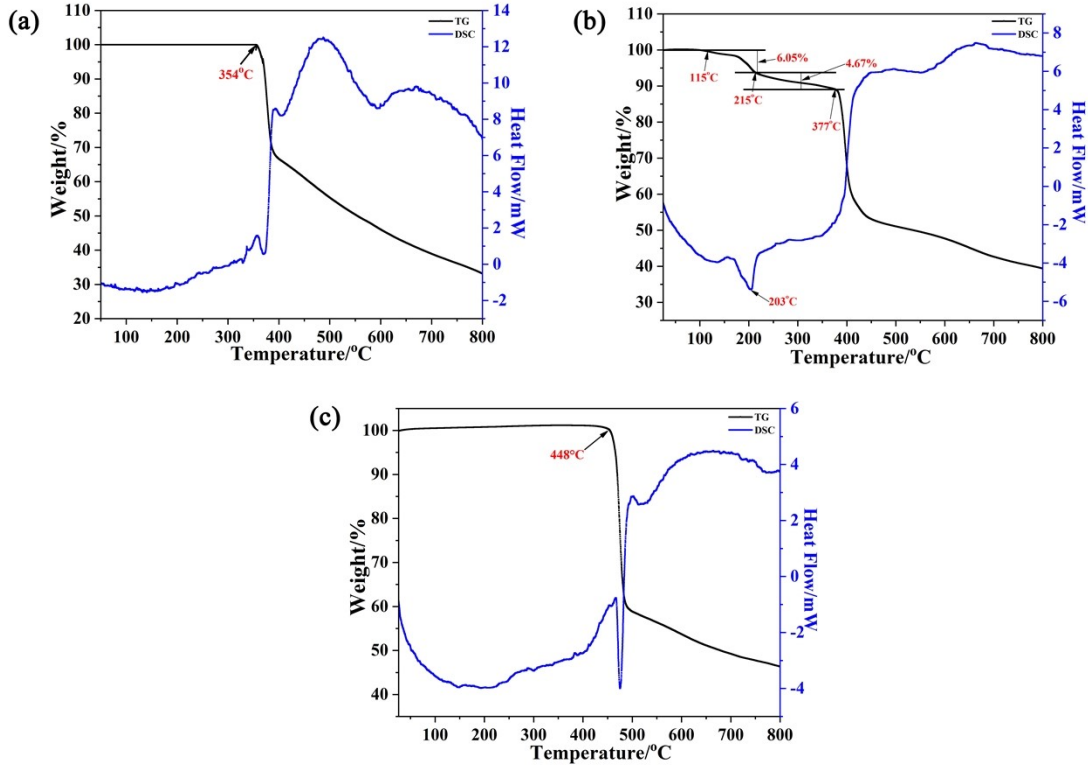

Fig. S1 Thermo-gravimetric (TG) and Differential scanning calorimetry (DSC) curves of **1**-**3**.

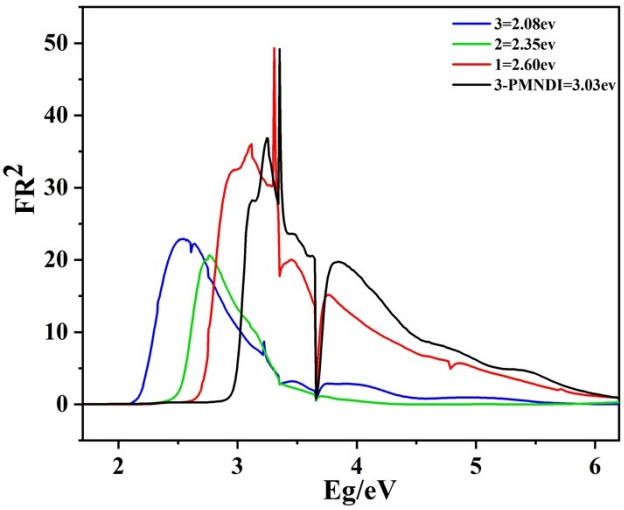

Fig. S2 Kubelka-Munk transformed reflectivity *vs* energy of complexes **1**-**3**.

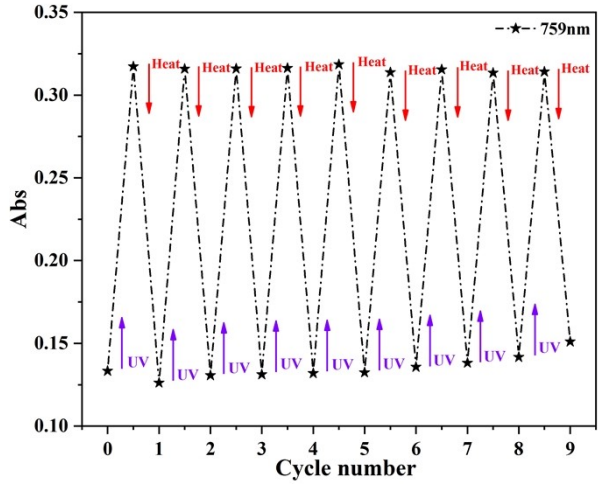

Fig. S3 The switching cycles of coloration-decoloration processes of **2** (759 nm) upon alternating Xe light illumination and thermal treatment.

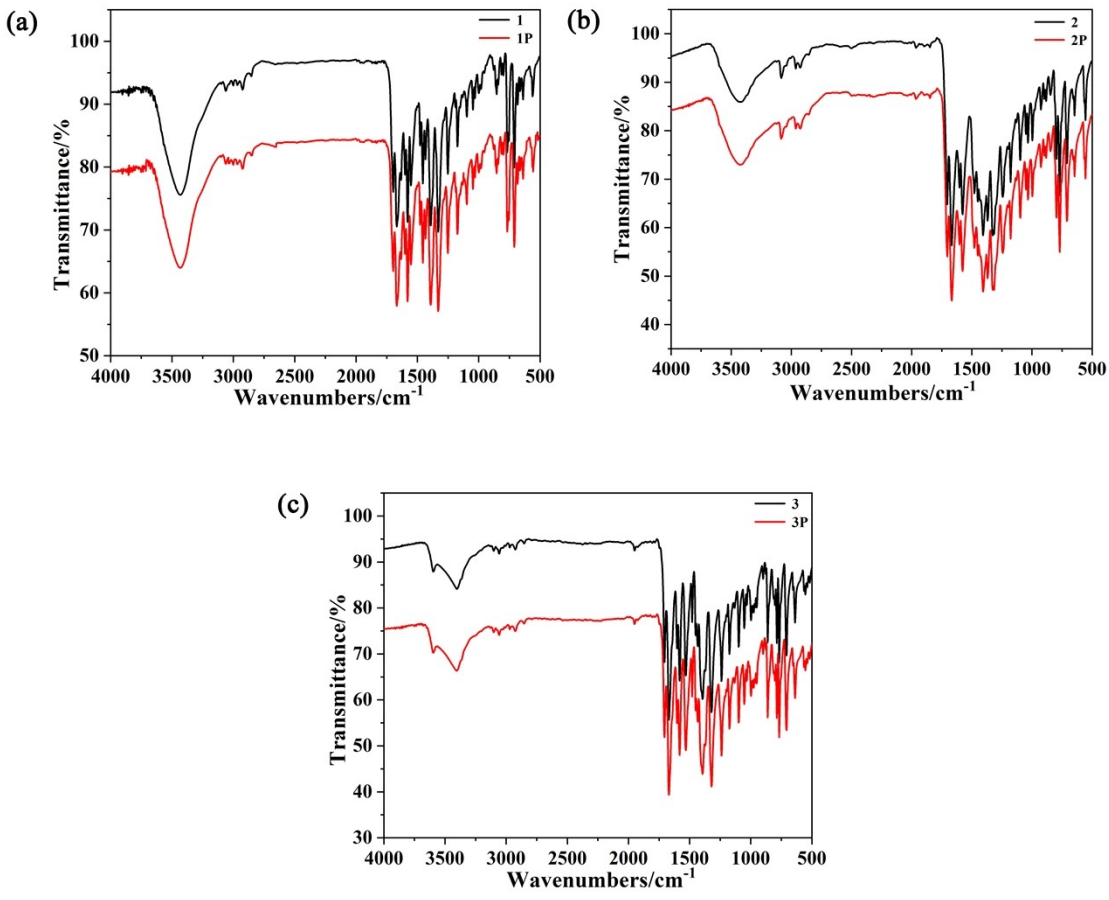

Fig. S4 FT-IR spectra of **1**-**3** as-synthesized samples and after irradiation samples.

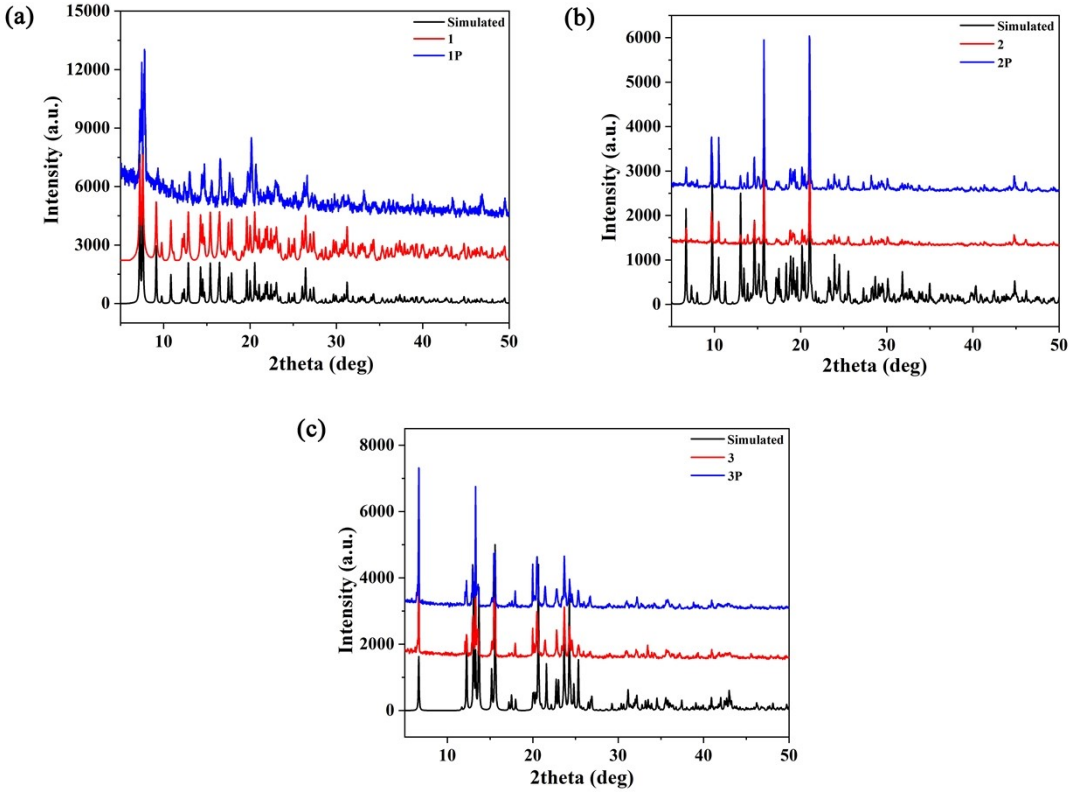

Fig. S5 PXRD patterns of **1**-**3** simulated from the X-ray single-crystal structures, as-synthesized samples and after irradiation samples.

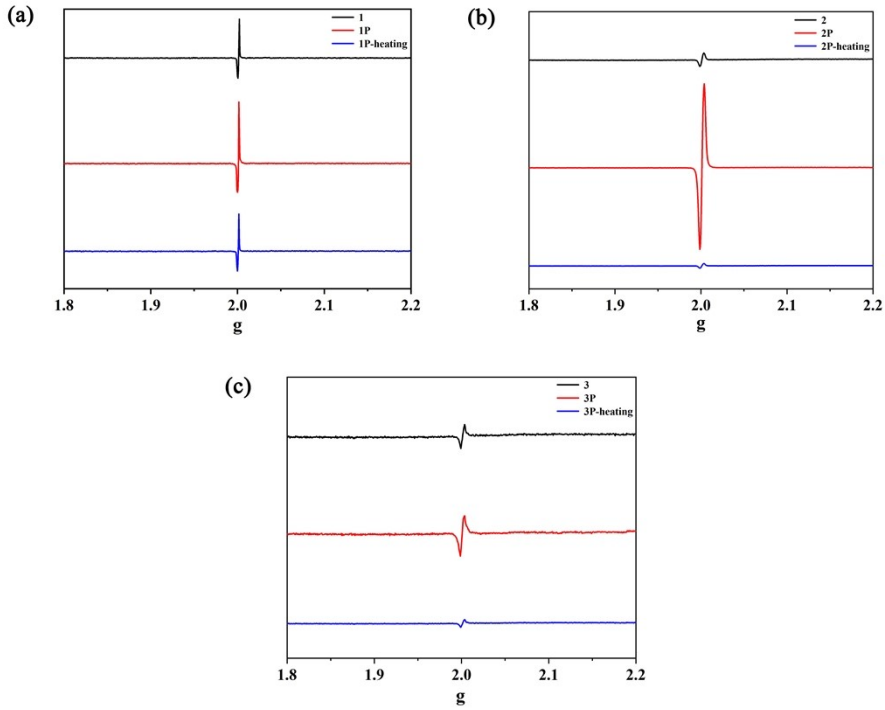

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Fig. S6 The EPR spectra of **1**, **1P**-UV and **1P**-UV-heating (a), **2**, **2P**-UV and **2P**-UV-heating (b) and **3**, **3P**-UV and **3P**-UV-heating (c).

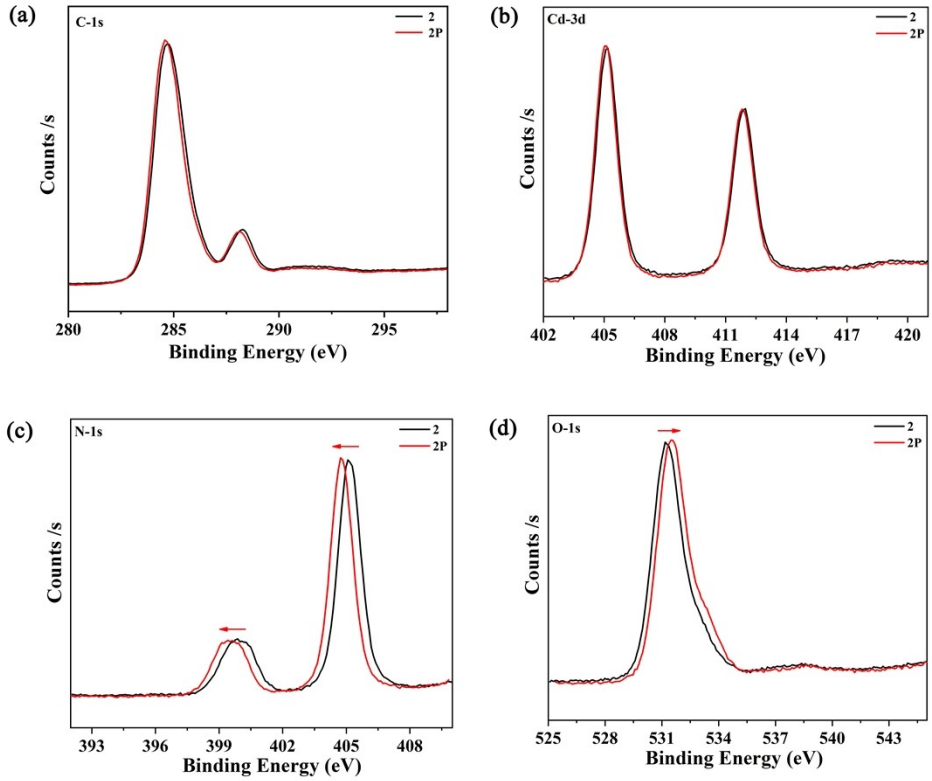

Fig. S7 Cd 3d (a), C 1s (b), N 1s (c) and O 1s (d) XPS core-level spectra of **2** and **2P**.

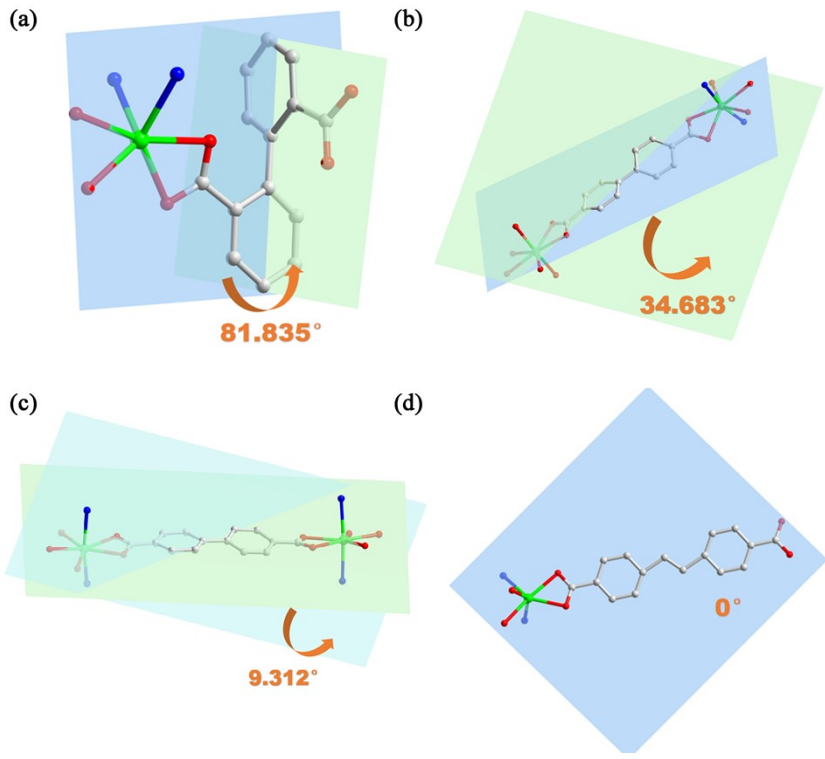

Fig. S8 The dihedral angle between the two benzene rings of the 2,2′-$BPDC^{2-}$ (a)， (b)，4,4′-$BPDC^{2-}$ (c) and 4,4′-SDC^{2-} (d).

2. Tables

Table S1. Crystallographic data and refinement of **1**-**3**.

Compound	**1**	**2**	**3**
CCDC code	2263419	2263420	2263421
Temperature (K)	293(2)	293(2)	293(2)
Empirical formula	$C_{40}H_{24}CdN_4O_8$	$C_{68}H_{53}Cd_2N_9O_{18}$	$C_{42}H_{26}CdN_4O_8$
Formula weight	801.03	1508.99	827.07
Crystal size (mm)	0.25 × 0.08 × 0.06	0.341 ×0.259 × 0.058	0.24 × 0.16 × 0.06
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$C2/c$	$C2/c$
a (Å)	9.8114(4)	37.305(2)	15.2689(9)
b (Å)	14.3212(7)	12.4534(8)	8.7100(5)
c (Å)	23.6696(11)	27.1003(17)	26.6400(15)
α (°)	90	90	90
β (°)	99.800(4)	103.182(2)	93.109(2)
γ (°)	90	90	90
V (Å^3)	3277.3(3)	12258.4(13)	3537.7(4)
Z	4	8	4
D_c (g cm^{-3})	1.623	1.635	1.553
μ (mm^{-1})	0.731	0.779	0.680
F (000)	1616.0	6112.0	1672.0
Reflections collected	18496	111451	21567
Independent reflections	8981	15319	4384
R_{int}	0.0418	0.0390	0.0261
Goodness-of-fit on F^2	1.010	1.022	1.107
R_1/wR_2, [$I \geq 2\sigma(I)$][a,b]	0.0553/0.0837	0.0358/0.0819	0.0308/0.0787
R_1/wR_2, (all data)	0.1121/0.1016	0.0588/0.0918	0.0380/0.0816

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

Table S2. Selected bond lengths (Å) and angles (°) for **1**-**3**.

Compound **1**			
Cd1-N1	2.395(3)	Cd1-O2	2.302(2)
Cd1-N4#2	2.373(3)	Cd1-O3#1	2.328(2)
Cd1-O1	2.411(3)	Cd1-O4#1	2.401(3)
N1-Cd1-O1	83.55(10)	N42-Cd1-N1	81.01(10)
N1-Cd1-O4#1	81.26(10)	N42-Cd1-O1	85.53(11)
#1 -x,+y,-1/2-z; #2 -1+x,1+y,+z			

Compound **2**			
Cd1-O1	2.3467(17)	Cd2-O5	2.340(3)
Cd1-O2	2.507(2)	Cd2-O5#3	2.340(3)
Cd1-O7	2.3306(17)	Cd2-O6	2.285(3)
Cd1-O8	2.4117(16)	Cd3-O10#1	2.3417(16)
Cd1-O9	2.4152(17)	Cd3-O10	2.3416(16)
Cd1-N1	2.358(2)	Cd3-O11	2.4304(18)
Cd1-N4#2	2.327(2)	Cd3-O11#1	2.4304(18)
Cd2-O3	2.384(2)	Cd3-O12	2.271(3)
Cd2-O3#3	2.384(2)	Cd3-N7#1	2.393(2)
Cd2-O4#3	2.388(2)	Cd3-N7	2.393(2)
Cd2-O4	2.388(2)		
O8-Cd1-O9	54.16(6)	O6-Cd2-O5	93.12(8)
O8-Cd1-O2	136.26(6)	O5#3-Cd2-O3	90.77(9)
O9-Cd1-O2	82.12(6)	O5#3-Cd2-O3#3	90.17(9)
O1-Cd1-O8	163.80(7)	O5-Cd2-O3#3	90.78(9)
O1-Cd1-O9	133.29(6)	O5-Cd2-O3	90.17(9)
O1-Cd1-O2	53.54(6)	O5-Cd2-O4#3	85.15(10)
O1-Cd1-N1	82.87(7)	O5-Cd2-O4	90.41(10)
O7-Cd1-O8	87.50(6)	O5#3-Cd2-O4	85.15(10)
O7-Cd1-O9	141.66(6)	O5#3-Cd2-O4#3	90.41(10)
O7-Cd1-O1	83.78(7)	O5-Cd2-O5#3	173.77(15)
O7-Cd1-O2	136.22(6)	O10-Cd3-O10#1	167.72(9)

O7-Cd1-N1	87.69(7)	O10-Cd3-O11	54.69(6)
N1-Cd1-O8	83.15(7)	O10#1-Cd3-O11	137.55(6)
N1-Cd1-O9	88.01(7)	O10#1-Cd3-O11#1	54.69(6)
N1-Cd1-O2	95.26(7)	O10-Cd3-O11#1	137.55(6)
N4#2-Cd1-O8	84.92(7)	O10-Cd3-N7	93.18(7)
N4#2-Cd1-O9	86.49(7)	O10#1-Cd3-N7	87.69(7)
N4#2-Cd1-O1	108.65(7)	O10#1-Cd3-N7#1	93.18(7)
N4#2-Cd1-O7	89.98(7)	O10-Cd3-N7#1	87.69(7)
N4#2-Cd1-O2	94.62(7)	O11#1-Cd3-O11	83.32(8)
N4#2-Cd1-N1	167.93(7)	N7#1-Cd3-O11	88.73(7)
O3-Cd2-O3#3	162.53(11)	N7#1-Cd3-O11#1	85.16(7)
O3#3-Cd2-O4	143.16(7)	N7-Cd3-O11	85.16(7)
O3#3-Cd2-O4#3	54.27(7)	N7-Cd3-O11#1	88.73(7)
O3-Cd2-O4	54.27(7)	N7#1-Cd3-N7	171.82(11)
O3-Cd2-O4#3	143.16(7)	O12-Cd3-O10	83.86(4)
O4#3-Cd2-O4	89.17(10)	O12-Cd3-O10#1	83.86(4)
O6-Cd2-O3#3	81.26(5)	O12-Cd3-O11#1	138.34(4)
O6-Cd2-O3	81.26(5)	O12-Cd3-O11	138.34(4)
O6-Cd2-O4	135.41(5)	O12-Cd3-O7	94.09(6)
O6-Cd2-O4#3	135.41(5)	O12-Cd3-O7#1	94.09(6)
O6-Cd2-O5#3	93.12(8)		
#1 -x,+y,-1/2-z; #2 +x,-y,1/2+z; #3 1-x,+y,3/2-z			

Compound **3**

Cd1 N1#1	2.3209(18)	Cd1-O1#1	2.2795(17)
Cd1-N1	2.3210(18)	Cd1-O2#1	2.3665(18)
Cd1-O1	2.2796(17)	Cd1-O2	2.3666(18)
N11-Cd1-N1	81.44(10)	N1-Cd1-O2#1	102.90(7)
N11-Cd1-O2#1	89.27(7)	N1-Cd1-O2	89.27(7)
#1 1-x,+y,1/2-z			

Table S3. Hydrogen bonds of for **1**-**3** (Å and °)

Compound **1**				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C15-H15···O4#1	0.93	2.36	3.026(5)	128.8
C19-H19···O1	0.93	2.47	3.098(4)	124.7
C20-H20A···O3	0.97	2.32	3.259(5)	162.2
C35-H35A···O2#2	0.97	2.60	3.479(4)	151.4
C35-H35B···O5#3	0.97	2.65	3.383(5)	133.0
C39-H39···O1#4	0.93	2.54	3.187(5)	127.2
#1 1-x,1/2+y,3/2-z; #2 2-x,-1/2+y,3/2-z; #3 2-x,-y,1-z; #4 1+x,-1+y,+z				

Compound **2**				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O7-H7A···O9#1	0.85	2.01	144.6	2.750(2)
O7-H7B···O2#1	0.85	2.09	143.1	2.818(3)
O6-H6B···O11#2	0.86	1.95	157.9	2.765(3)
O6-H6A···O11#3	0.86	1.95	158.6	2.765(3)
O5-H5A···O19#4	0.81	1.88	175.5	2.691(5)
O12-H12B···O4#5	0.85	1.93	154.0	2.716(3)
O12-H12A···O4#2	0.84	1.96	148.2	2.716(3)
#1 1/2-x,1/2+y,1/2-z; #2 1/2-x,1/2+y,1/2-z; #3 1/2+x,-1/2+y,1+z; #4 1/2-x,1/2-y,1-z; #5 1/2+x,-1/2+y，-1+z				

Compound **3**				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C1-H1···O3#1	0.93	2.51	3.176(3)	128.3
#1 1/2-x,1/2+y,1/2-z				