Electronic Supplementary Information for

Construction of Cd(II) Coordination Polymers Based on R-isophthalate (R = -CH_3 or –OCH_3) and Flexible N-donor Co-ligands: Syntheses, Structures, and Photoluminescence

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Table S1. Selected Bond Lengths (Å) and Angles (º) for **1–6**[a].

1			
Cd(1)-O(1)	2.2298(14)	Cd(1)-N(1)	2.3400(18)
Cd(1)-N(12)#1	2.2964(18)	Cd(1)-O(6)	2.3574(16)
Cd(1)-O(11)	2.3299(16)	Cd(1)-O(7)	2.4706(14)
Cd(2)-O(12)	2.3032(15)	Cd(2)-O(4)#3	2.3562(15)
Cd(2)-O(9)	2.3137(14)	Cd(2)-O(3)#3	2.4664(14)
Cd(2)-N(7)	2.3213(17)	Cd(2)-N(6)#2	2.3268(17)
O(9)-Cd(2)-O(3)#3	140.62(5)	N(12)#1-Cd(1)-N(1)	95.66(6)
O(1)-Cd(1)-N(12)#1	137.99(6)	O(11)-Cd(1)-N(1)	169.06(5)
O(1)-Cd(1)-O(11)	81.30(6)	O(1)-Cd(1)-O(6)	86.00(5)
N(12)#1-Cd(1)-O(11)	91.98(6)	N(12)#1-Cd(1)-O(6)	135.45(6)
O(1)-Cd(1)-N(1)	87.79(6)	O(11)-Cd(1)-O(7)	89.23(5)
O(11)-Cd(1)-O(6)	87.97(6)	N(1)-Cd(1)-O(7)	99.61(6)
N(1)-Cd(1)-O(6)	92.04(6)	O(6)-Cd(1)-O(7)	53.85(5)
O(1)-Cd(1)-O(7)	139.14(6)	N(12)#1-Cd(1)-O(7)	81.60(6)
O(12)-Cd(2)-O(9)	81.10(5)	O(4)#3-Cd(2)-O(3)#3	54.06(5)
O(12)-Cd(2)-N(7)	170.91(6)	N(7)-Cd(2)-O(3)#3	91.34(5)
O(9)-Cd(2)-N(7)	90.95(6)	N(6)#2-Cd(2)-O(3)#3	82.79(5)

O(12)-Cd(2)-N(6)#2	92.53(6)	O(9)-Cd(2)-O(4)#3	86.82(5)
O(9)-Cd(2)-N(6)#2	135.91(6)	N(7)-Cd(2)-O(4)#3	87.14(6)
N(7)-Cd(2)-N(6)#2	96.26(6)	N(6)#2-Cd(2)-O(4)#3	136.82(5)
O(12)-Cd(2)-O(4)#3	88.02(6)	O(12)-Cd(2)-O(3)#3	92.04(5)
2			
Cd(1)-N(1)	2.248(2)	Cd(1)-O(4)#1	2.249(2)
Cd(1)-O(1)#2	2.2958(19)	Cd(1)-N(4)#3	2.355(2)
Cd(1)-O(2)	2.449(2)		
N(4)#3-Cd(1)-O(2)	171.64(8)	N(1)-Cd(1)-O(1)#2	129.77(8)
N(1)-Cd(1)-O(3)#1	85.37(7)	O(1)#2-Cd(1)-O(3)#1	144.42(7)
N(4)#3-Cd(1)-O(3)#1	94.97(8)	N(1)-Cd(1)-N(4)#3	91.00(9)
O(3)#1-Cd(1)-O(2)	93.37(6)	O(1)#2-Cd(1)-N(4)#3	80.96(8)
N(1)-Cd(1)-O(2)	89.55(8)	O(1)#2-Cd(1)-O(2)	92.29(7)
3			
Cd(1)-O(4)#1	2.240(3)	Cd(1)-N(1)	2.271(3)
Cd(1)-O(1)	2.289(3)	Cd(1)-O(6)	2.336(3)
Cd(1)-O(3)#2	2.402(3)	Cd(1)-O(2)	2.573(3)
O(4)#1-Cd(1)-N(1)	128.81(12)	O(4)#1-Cd(1)-O(1)	93.79(10)
N(1)-Cd(1)-O(1)	137.07(11)	O(4)#1-Cd(1)-O(6)	82.72(12)
N(1)-Cd(1)-O(6)	88.49(13)	O(1)-Cd(1)-O(6)	92.60(13)
O(4)#1-Cd(1)-O(3)#2	97.06(11)	N(1)-Cd(1)-O(3)#2	89.47(11)
O(1)-Cd(1)-O(3)#2	90.23(11)	O(6)-Cd(1)-O(3)#2	177.17(11)
O(4)#1-Cd(1)-O(2)	141.95(10)	N(1)-Cd(1)-O(2)	84.60(11)
O(1)-Cd(1)-O(2)	53.48(9)	O(6)-Cd(1)-O(2)	80.40(11)
O(3)#2-Cd(1)-O(2)	101.36(10)		
4			
Cd(1)-O(1)	2.233(2)	Cd(1)-N(6)#1	2.304(3)
Cd(1)-O(5)	2.326(2)	Cd(1)-N(1)	2.335(3)
Cd(1)-O(4)#2	2.370(2)	Cd(1)-O(3)#2	2.471(2)
O(1)-Cd(1)-N(6)#1	135.27(10)	O(1)-Cd(1)-O(5)	81.08(9)
N(6)#1-Cd(1)-O(5)	93.46(9)	O(1)-Cd(1)-N(1)	88.03(9)
N(6)#1-Cd(1)-N(1)	97.75(9)	O(5)-Cd(1)-N(1)	168.05(8)
O(1)-Cd(1)-O(4)#2	89.87(9)	N(6)#1-Cd(1)-O(4)#2	134.39(8)
O(5)-Cd(1)-O(4)#2	86.76(9)	N(1)-Cd(1)-O(4)#2	88.32(9)
O(1)-Cd(1)-O(3)#2	143.47(9)	N(6)#1-Cd(1)-O(3)#2	80.75(9)
O(5)-Cd(1)-O(3)#2	92.62(8)	N(1)-Cd(1)-O(3)#2	93.24(8)
O(4)#2-Cd(1)-O(3)#2	53.72(7)		
5			
Cd(1)-O(4)#1	2.2859(18)	Cd(1)-N(1)	2.297(2)
Cd(1)-N(4)	2.310(2)	Cd(1)-O(5)	2.324(2)
Cd(1)-O(1)	2.3468(17)	Cd(1)-O(2)	2.5062(17)
O(1)-Cd(1)-O(2)	53.61(6)	O(4)#1-Cd(1)-N(1)	92.95(8)
O(4)#1-Cd(1)-N(4)	97.49(8)	N(1)-Cd(1)-N(4)	169.49(8)
O(4)#1-Cd(1)-O(5)	128.41(7)	N(1)-Cd(1)-O(5)	85.76(9)

N(4)-Cd(1)-O(5)	86.82(9)	O(4)#1-Cd(1)-O(1)	83.67(6)
N(1)-Cd(1)-O(1)	92.77(8)	N(4)-Cd(1)-O(1)	89.57(8)
O(5)-Cd(1)-O(1)	147.92(7)	O(4)#1-Cd(1)-O(2)	137.14(6)
N(1)-Cd(1)-O(2)	86.58(8)	N(4)-Cd(1)-O(2)	86.57(8)
O(5)-Cd(1)-O(2)	94.33(7)		
6			
Cd(1)-O(2)#1	2.2315(15)	Cd(1)-N(1)	2.2835(8)
Cd(1)-O(5)	2.3006(8)	Cd(1)-O(3)#2	2.3637(16)
Cd(1)-O(4)#2	2.4321(16)	Cd(1)-O(1)	2.4363(17)
O(2)#1-Cd(1)-N(1)	127.66(4)	O(2)#1-Cd(1)-O(5)	83.80(5)
N(1)-Cd(1)-O(5)	87.17(3)	O(2)#1-Cd(1)-O(3)#2	91.31(6)
N(1)-Cd(1)-O(3)#2	141.00(4)	O(5)-Cd(1)-O(3)#2	96.85(5)
O(2)#1-Cd(1)-O(4)#2	143.47(6)	N(1)-Cd(1)-O(4)#2	87.10(4)
O(5)-Cd(1)-O(4)#2	87.65(5)	O(3)#2-Cd(1)-O(4)#2	54.53(5)
O(2)#1-Cd(1)-O(1)	93.10(6)	N(1)-Cd(1)-O(1)	89.06(4)
O(5)-Cd(1)-O(1)	172.16(4)	O(3)#2-Cd(1)-O(1)	90.40(6)
O(4)#2-Cd(1)-O(1)	99.02(6)		

[a] Symmetry codes: **1**: #1 *x*, *y* - 1, *z*; #2 *x*, *y*, *z* + 1; #3: *x*, *y* + 1, *z* + 1; **2**: #1: – *x* + 2, - *y* + 2, - z + 2; #2: – *x* + 2,- *y* + 1,- *z* + 2; #3: *x*, *y*, *z* + 1; **3**: #1: *x* - 1, *y* + 1, *z*; #2: - *x* + 1, - *y*, - *z*; **4**: #1: *x*, *y*, *z* + 1; #2: *x* + 1, *y*, *z*; **5**: #1: *x* + 1, *y*, *z*; **6**: #1: - *x* + 1, - *y*, - *z*; #2: - *x*, - *y* + 1, - *z*.

Table S2. Distance (Å) and angles (°) of hydrogen bonding for **1–6**[a].

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
1				
O(19)-H(18W)···O(10)#7	0.84	2.09	2.918(3)	169.7
O(19)-H(17W)···O(8)	0.83	2.03	2.794(3)	151.7
O(14)-H(8W)···O(8)#8	0.83	2.09	2.875(3)	158.4
O(18)-H(16W)···O(15)	0.86	1.99	2.758(4)	148.4
O(18)-H(15W)···O(19)#8	0.83	1.92	2.742(4)	171.1
O(15)-H(9W)···O(17)#8	0.83	1.91	2.734(3)	177.0
O(15)-H(10W)···O(13)#9	0.83	2.15	2.801(3)	134.8
O(17)-H(14W)···O(5)#8	0.84	2.57	3.309(3)	148.4
O(17)-H(13W)···N(5)#2	0.83	2.23	3.025(3)	159.4
O(16)-H(11W)···O(18)#10	0.85	1.91	2.758(4)	179.4
O(13)-H(5W)···O(16)	0.83	2.10	2.885(3)	157.0
O(13)-H(6W)···O(2)#6	0.83	1.91	2.722(3)	166.1
O(12)-H(4W)···O(3)#8	0.83	1.86	2.685(2)	172.9
O(12)-H(3W)···O(13)#7	0.83	2.00	2.809(2)	162.6
O(11)-H(2W)···O(14)	0.83	1.92	2.749(2)	173.8
O(11)-H(1W)···O(7)#8	0.84	1.90	2.722(2)	168.3
2				

O(6)-H(1W)···O(4)#5	0.83	2.21	2.972(7)	153.0
O(6)-H(2W)···O(1)	0.84	2.42	2.902(5)	117.5
3				
O(7)-H(4W)···O(8)#5	0.85	1.90	2.747(13)	173.5
O(7)-H(3W)···O(1)#6	0.85	1.95	2.803(7)	176.5
O(6)-H(2W)···O(7)#7	0.84	1.85	2.684(7)	176.1
O(6)-H(1W)···O(2)#8	0.83	1.97	2.749(4)	157.0
O(8)-H(5W)···N(3)	0.81	2.22	2.867(12)	137.9
O(8)-H(6W)···N(3)#9	0.84	2.26	3.027(12)	150.9
4				
O(6)-H(4W)···O(2)#5	0.84	1.88	2.716(5)	175.7
O(5)-H(2W)···O(6)#6	0.84	2.12	2.853(4)	146.0
O(5)-H(1W)···O(3)#7	0.83	1.89	2.694(3)	162.6
5				
O(6)-H(4W)···O(3)#5	0.85	2.36	2.910(3)	123.4
O(6)-H(3W)···O(3)#6	0.84	1.97	2.804(3)	173.6
O(5)-H(2W)···O(2)#7	0.83	1.87	2.682(3)	163.8
O(5)-H(1W)···O(6)#8	0.82	2.06	2.881(4)	178.7
6				
O(6)-H(4W)···O(1)#4	0.82	1.97	2.7557(17)	159.7
O(6)-H(3W)···O(3)#5	0.83	2.16	2.871(2)	143.7
O(5)-H(2W)···O(4)#6	0.83	1.93	2.7411(18)	165.9
O(5)-H(1W)···O(6)#7	0.83	1.93	2.748	166.9

[a] Symmetry codes: **1**: #2: *x*, *y*, *z* + 1; #6: *x*, *y* + 1, *z*; #7: – *x* + 1, - *y* + 1, - *z* + 1; #8: – *x* + 1, - *y*, - *z* + 1; #9: *x* - 1, *y* - 1, *z*; #10: *x* + 1, *y* + 1, *z*; **2**: #5: *x*, *y* - 1, *z*; **3**: #5: *x* + 1, *y*, *z*; #6: *x*, *y*, *z* + 1; #7: *x* - 1, *y*, *z* – 1; #8: - *x*, - *y*, - *z*; #9: – *x* - 1, - *y* + 1, -*z* + 1; **4**: #5: - *x* + 1,- *y* + 1, - *z* + 2; #6: *x* - 1, *y*, *z* + 1; #7: - *x*, - *y* + 1, - *z* + 3; **5**: #5: - *x* + 1, - *y* + 1, - *z*; #6: *x* + 1, *y* + 1, *z*; #7: - *x* + 1, - *y*, - *z*; #8: - *x* + 2, - *y* + 1, - *z*; **6**: #4: *x*, *y*, *z* + 1; #5: - *x*, - *y* + 1, - *z* + 1; #6: *x* + 1, *y*, *z*; #7: *x* + 1, *y*, *z* - 1.

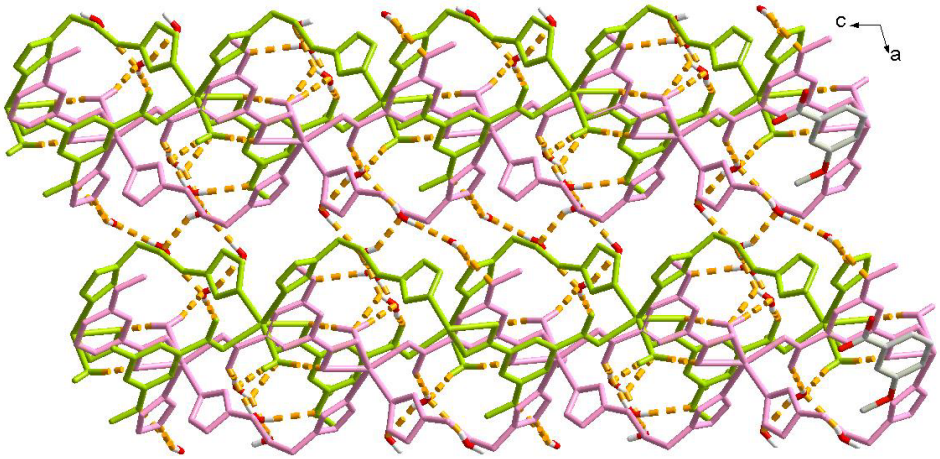

Fig. S1 View of the 3-D supramolecular architecture of **1**. Hydrogen bonds are represented as light orange dash line.

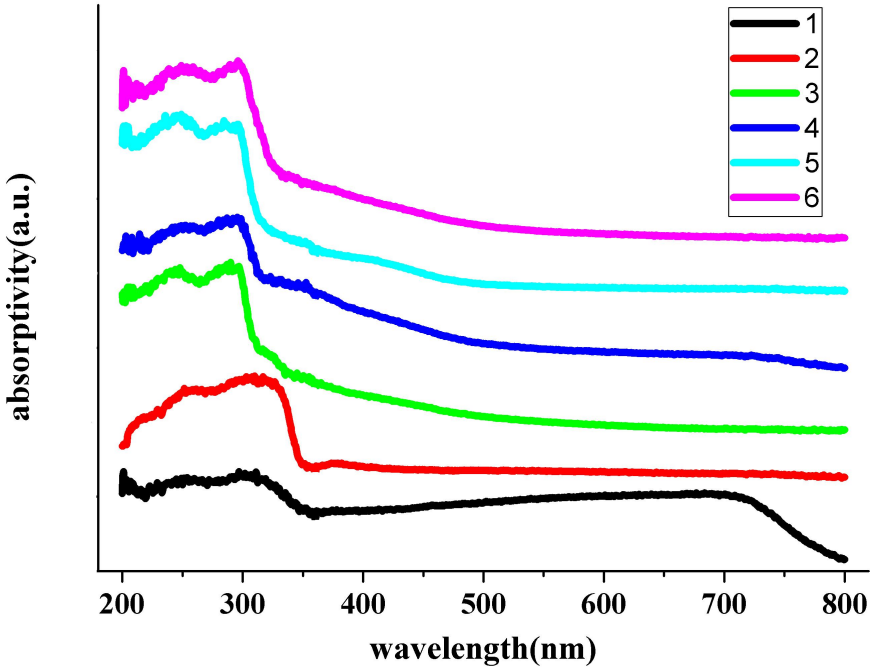

Fig. S2 The UV-vis absorption spectra for **1**–**6** in the solid state at room temperature.