Solvothermal Synthesis, Structure, and Fluorescence Property of Three d^{10} Polymers Assembled From Semi-rigid V-shaped Aza -Bridged Multicarboxylate

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Table SI **Crystal data and structure refinement for 1-3**

Complex	1	2	3
Empirical formula	$C_{43}H_{34}Cd_2N_5O_{10}$	$C_{24}H_{19}CdN_3O_4$	$C_{28}H_{18}Zn_2N_2O_8$
Formula weight	1005.55	525.82	641.18
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	*P-1*	*P21/C*	*P21/C*
a (Å)	9.2272(3)	11.667(4)	11.5015(7)
b (Å)	10.9734(4)	9.677(3)	12.6151(6)
c (Å)	20.8598(6)	19.320(6)	19.6648(13)
α (deg)	78.118(3)	90	90
β (deg)	84.743(3)	96.150(4)	117.658(4)
γ (deg)	72.358(4)	90	90
V (Å^3)	1968.70(11)	2168.7(11)	2527.2(3)
Dcalca / Mgm-3	1.696	1.610	1.685
Z	2	4	4
μ (mm-1)	1.148	1.043	1.955
F(000)	1006	1056	1296
Data / restraints / parameters	6902 / 6 / 547	3711 / 1 / 289	5757 / 22 / 361
GOF	1.072	1.071	1.101
R_1[I > 2σ(I)]	R_1 = 0.0435, wR_2 = 0.0998	R_1 = 0.0319, wR_2 = 0.0643	R_1 = 0.0634, wR_2 = 0.1356
wR_2 (all data)	R_1 = 0.0621, wR_2 = 0.1122	R_1 = 0.0385, wR_2 = 0.0674	R_1 = 0.0697, wR_2 = 0.1392
$\triangle\rho max$ / $\triangle\rho min$ (eÅ^{-3})	1.610 /-1.032	0.446 /-0.359	2.452 / -1.936

Table SII Bond lengths [Å] and angles [°] for **1-3**

Complex 1			
Bond lengths			
Cd(1)-N(1)	2.278(5)	Cd(1)-O(4)	2.315(4)
Cd(1)-O(3)	2.323(4)	Cd(1)-O(1)	2.347(4)
Cd(1)-N(2)	2.355(4)	Cd(1)-O(2)	2.389(4)
Cd(2)-O(6)	2.222(4)	Cd(2)-O(7)	2.2661(18)
Cd(2)-O(5)	2.3411(18)	Cd(2)-N(2)	2.267(4)
Cd(2)-N(3)	2.290(4)	Cd(2)-O(8)	2.313(4)
Cd(2)-O(5)	2.339(4)	Cd(2)-O(3)	2.350(4)
Bond angles			
N(1)-Cd(1)-O(4)	81.34(17)	N(1)-Cd(1)-O(3)	85.36(15)
O(4)-Cd(1)-O(3)	112.37(15)	N(1)-Cd(1)-O(1)	107.63(17)
O(4)-Cd(1)-O(1)	155.35(15)	O(3)-Cd(1)-O(1)	91.52(13)
N(1)-Cd(1)-N(2)	170.11(17)	O(4)-Cd(1)-N(2)	91.52(15)
O(3)-Cd(1)-N(2)	91.10(14)	O(1)-Cd(1)-N(2)	81.66(14)
N(1)-Cd(1)-O(2)	94.35(16)	O(4)-Cd(1)-O(2)	102.27(14)
O(3)-Cd(1)-O(2)	144.85(12)	O(1)-Cd(1)-O(2)	55.02(12)
N(2)-Cd(1)-O(2)	93.84(14)	O(6)-Cd(2)-O(7)	100.62(18)
O(6)-Cd(2)-N(3)	89.27(16)	O(7)-Cd(2)-N(3)	139.77(17)
O(6)-Cd(2)-O(8)	131.50(18)	O(7)-Cd(2)-O(8)	56.03(15)
N(3)-Cd(2)-O(8)	88.34(14)	O(6)-Cd(2)-O(5)	133.55(16)

O(7)-Cd(2)-O(5)	109.03(19)	N(3)-Cd(2)-O(5)	90.32(15)
O(8)-Cd(2)-O(5)	94.90(15)	O(6)-Cd(2)-O(3)	83.48(17)
O(7)-Cd(2)-O(3)	105.04(16)	N(3)-Cd(2)-O(3)	114.84(14)
O(8)-Cd(2)-O(3)	139.81(15)	O(5)-Cd(2)-O(3)	55.07(12)
Complex 2			
Bond lengths			
Cd(1)-N(2)	2.294(3)	Cd(1)-O(4)	2.325(2)
Cd(1)-N(1)	2.326(3)	Cd(1)-O(2)	2.328(2)
Cd(1)-O(1)	2.351(2)	Cd(1)-O(3)	2.375(2)
Bond angles			
N(2)-Cd(1)-O(4)	141.90(9)	N(2)-Cd(1)-N(1)	107.65(10)
O(4)-Cd(1)-N(1)	88.77(9)	N(2)-Cd(1)-O(2)	97.44(10)
O(4)-Cd(1)-O(2)	118.11(9)	N(1)-Cd(1)-O(2)	86.64(9)
N(2)-Cd(1)-O(1)	92.57(10)	O(4)-Cd(1)-O(1)	96.69(9)
N(1)-Cd(1)-O(1)	139.22(9)	O(2)-Cd(1)-O(1)	55.21(8)
N(2)-Cd(1)-O(3)	86.81(9)	O(4)-Cd(1)-O(3)	55.42(8)
N(1)-Cd(1)-O(3)	104.83(9)	O(2)-Cd(1)-O(3)	166.02(8)
O(1)-Cd(1)-O(3)	111.47(8)		
Complex 3			
Bond lengths			
Zn(1)-O(1)	1.900(4)	Zn(1)-O(5)	1.927(4)
Zn(1)-O(7)#1	1.930(3)	Zn(1)-O(3)	2.004(4)
Zn(2)-O(8)#1	1.937(4)	Zn(2)-O(6)#2	1.963(4)
Zn(2)-O(2)	2.002(4)	Zn(2)-O(4)#2	2.090(4)
Zn(2)-O(3)#2	2.245(6)	O(7)-Zn(1)#2	1.930(3)
O(3)-Zn(2)#1	2.245(6)	O(4)-Zn(2)#1	2.090(4)
O(6)-Zn(2)#1	1.963(4)	O(8)-Zn(2)#2	1.937(4)
Bond angles			
O(1)-Zn(1)-O(5)	113.99(18)	O(1)-Zn(1)-O(7)#1	116.47(18)
O(5)-Zn(1)-O(7)#1	110.58(16)	O(1)-Zn(1)-O(3)	103.4(2)
O(5)-Zn(1)-O(3)	102.61(18)	O(7)#1-Zn(1)-O(3)	108.42(16)
O(8)#1-Zn(2)-O(6)#2	93.64(16)	O(8)#1-Zn(2)-O(2)	135.8(2)
O(6)#2-Zn(2)-O(2)	100.27(17)	O(8)#1-Zn(2)-O(4)#2	93.99(17)
O(6)#2-Zn(2)-O(4)#2	150.60(19)	O(2)-Zn(2)-O(4)#2	93.84(17)
O(8)#1-Zn(2)-O(3)#2	122.32(18)	O(6)#2-Zn(2)-O(3)#2	93.52(16)
O(2)-Zn(2)-O(3)#2	98.61(18)	O(4)#2-Zn(2)-O(3)#2	58.69(16)

Symmetry transformations: #1 -x,y+1/2,-z+3/2 ; #2 -x,y-1/2,-z+3/2

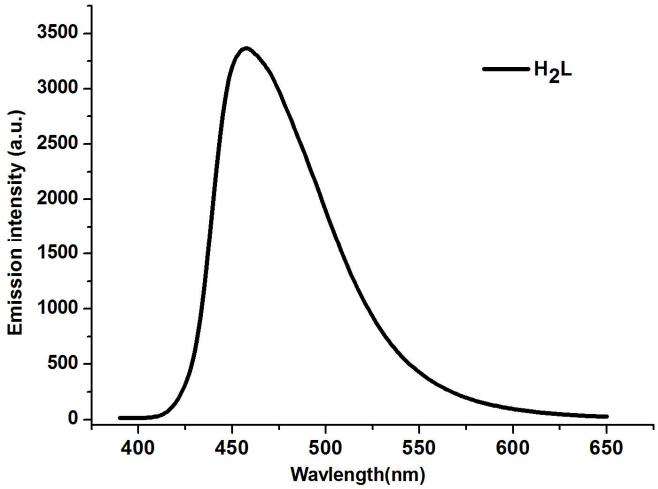

Figure S1 Fluorescent emission spectra of H_2L ligand in solid state at room temperature.

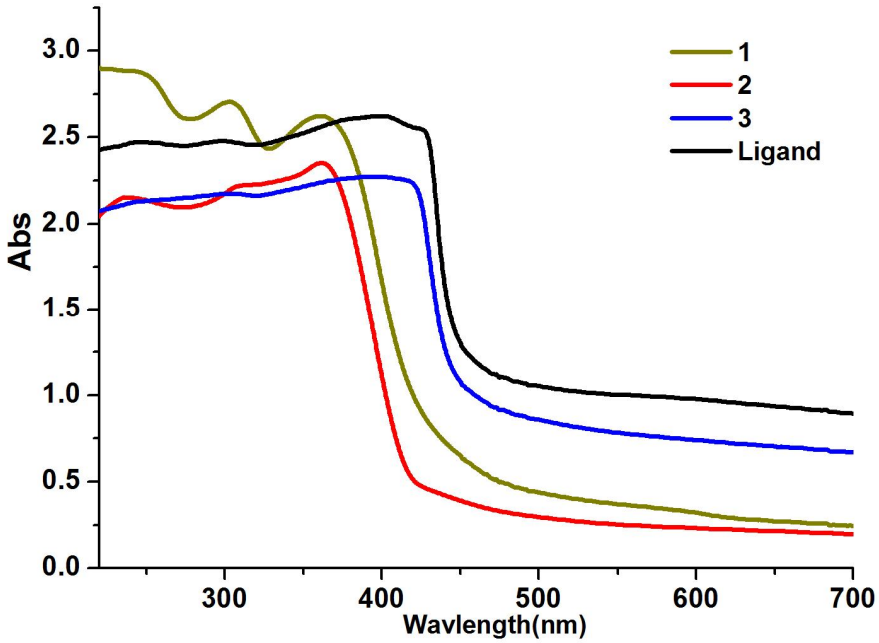

Figure S2 Absorption spectra of free ligand and their respective complexes 1−3 i at ambient temperature.