Supporting Information

Novel (3,6)-connected network and (4,6)-connected framework in two Copper(II) and Cadmium(II) complexes of flexible (2*S*,3*S*,4*R*,5*R*)-tetrahydrofurantetracarboxylic acid: synthesis, structure, thermostability, and luminescence studies

Lei Zhang, Zhao-Ji Li, Qi-Pu Lin, Jian Zhang, Pei-Xiu Yin, Ye-Yan Qin, Jian-Kai Cheng and Yuan-Gen Yao*

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, The Chinese Academy of Sciences, Fuzhou, Fujian 350002, China. E-mail: yyg@fjirsm.ac.cn

Graduate School of The Chinese Academy of Sciences, Beijing, China.

Table S1. Selected Band Lengths (Å) and Band Angles (°) for Complexes **1** and **2**

Complex **1**			
Cu(1)-O(3)#1	1.931(3)	Cu(2)-O(5)#2	1.954(3)
Cu(1)-O(6)#2	1.944(3)	Cu(2)-O(2)#3	1.979(3)
Cu(1)-O(1)	1.971(3)	Cu(2)-N(1)	2.005(4)
Cu(1)-O(8)	1.996(3)	Cu(2)-N(2)	2.019(4)
Cu(1)-O(9)	2.264(3)	Cu(2)-O(8)	2.268(3)
O(3)#1-Cu(1)-O(6)#2	91.01(14)	O(5)#2-Cu(2)-O(2)#3	92.86(13)
O(3)#1-Cu(1)-O(1)	87.94(14)	O(5)#2-Cu(2)-N(1)	165.04(15)
O(6)#2-Cu(1)-O(1)	171.10(13)	O(2)#3-Cu(2)-N(1)	94.40(16)
O(3)#1-Cu(1)-O(8)	149.27(14)	O(5)#2-Cu(2)-N(2)	88.80(15)
O(6)#2-Cu(1)-O(8)	98.56(13)	O(2)#3-Cu(2)-N(2)	172.44(15)
O(1)-Cu(1)-O(8)	86.74(13)	N(1)-Cu(2)-N(2)	82.37(17)
O(3)#1-Cu(1)-O(9)	129.11(13)	O(5)#2-Cu(2)-O(8)	97.89(12)
O(6)#2-Cu(1)-O(9)	96.01(12)	O(2)#3-Cu(2)-O(8)	84.96(12)
O(1)-Cu(1)-O(9)	77.90(11)	N(1)-Cu(2)-O(8)	95.77(14)
O(8)-Cu(1)-O(9)	79.06(11)	N(2)-Cu(2)-O(8)	102.12(13)

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

Complex **2**			
O(1W)-Cd(1)	2.255(4)	O(3W)-Cd(2)	2.320(3)
O(1)-Cd(1)	2.439(2)	O(8)-Cd(2)	2.224(3)
O(2W)-Cd(1)	2.313(3)	Cd(2)-O(6)#6	2.304(3)
O(2)-Cd(1)	2.334(3)	Cd(2)-O(5)#7	2.345(3)
O(2)-Cd(1)#1	2.460(3)	Cd(2)-O(7)#4	2.359(3)

O(3)-Cd(1)#1	2.407(3)	Cd(2)-O(4)#7	2.520(3)
O(9)-Cd(1)	2.295(3)	Cd(2)-O(6)#4	2.580(3)
O(1W)-Cd(1)-O(9)	164.87(13)	O(8)-Cd(2)-O(6)#6	91.51(10)
O(1W)-Cd(1)-O(2W)	89.98(14)	O(8)-Cd(2)-O(3W)	170.42(10)
O(9)-Cd(1)-O(2W)	85.46(12)	O(6)#6-Cd(2)-O(3W)	86.71(10)
O(1W)-Cd(1)-O(2)	83.84(12)	O(8)-Cd(2)-O(5)#7	93.37(10)
O(9)-Cd(1)-O(2)	92.89(10)	O(6)#6-Cd(2)-O(5)#7	104.19(9)
O(2W)-Cd(1)-O(2)	149.92(10)	O(3W)-Cd(2)-O(5)#7	77.97(10)
O(1W)-Cd(1)-O(3)#5	96.85(15)	O(8)-Cd(2)-O(7)#4	99.78(9)
O(9)-Cd(1)-O(3)#5	96.94(11)	O(6)#6-Cd(2)-O(7)#4	124.09(9)
O(2W)-Cd(1)-O(3)#5	131.77(10)	O(3W)-Cd(2)-O(7)#4	88.98(10)
O(2)-Cd(1)-O(3)#5	78.27(9)	O(5)#7-Cd(2)-O(7)#4	129.16(9)
O(1W)-Cd(1)-O(1)	96.14(12)	O(8)-Cd(2)-O(4)#7	87.39(10)
O(9)-Cd(1)-O(1)	68.98(8)	O(6)#6-Cd(2)-O(4)#7	157.42(9)
O(2W)-Cd(1)-O(1)	82.66(10)	O(3W)-Cd(2)-O(4)#7	90.64(10)
O(2)-Cd(1)-O(1)	68.86(8)	O(5)#7-Cd(2)-O(4)#7	53.43(9)
O(3)#5-Cd(1)-O(1)	142.96(8)	O(7)#4-Cd(2)-O(4)#7	78.22(9)
O(1W)-Cd(1)-O(2)#5	100.89(13)	O(8)-Cd(2)-O(6)#4	106.77(10)
O(9)-Cd(1)-O(2)#5	92.35(10)	O(6)#6-Cd(2)-O(6)#4	72.14(10)
O(2W)-Cd(1)-O(2)#5	78.59(10)	O(3W)-Cd(2)-O(6)#4	81.65(10)
O(2)-Cd(1)-O(2)#5	131.49(5)	O(5)#7-Cd(2)-O(6)#4	159.49(10)
O(3)#5-Cd(1)-O(2)#5	53.22(8)	O(7)#4-Cd(2)-O(6)#4	52.11(8)
O(1)-Cd(1)-O(2)#5	154.54(8)	O(4)#7-Cd(2)-O(6)#4	129.63(9)

Symmetry codes: #1 = x,-y-1/2,z-1/2; #4 = -x,-y,-z+2; #5 = x,-y-1/2,z+1/2;

#6 = x-1,y,z; #7 = x,y,z+1.

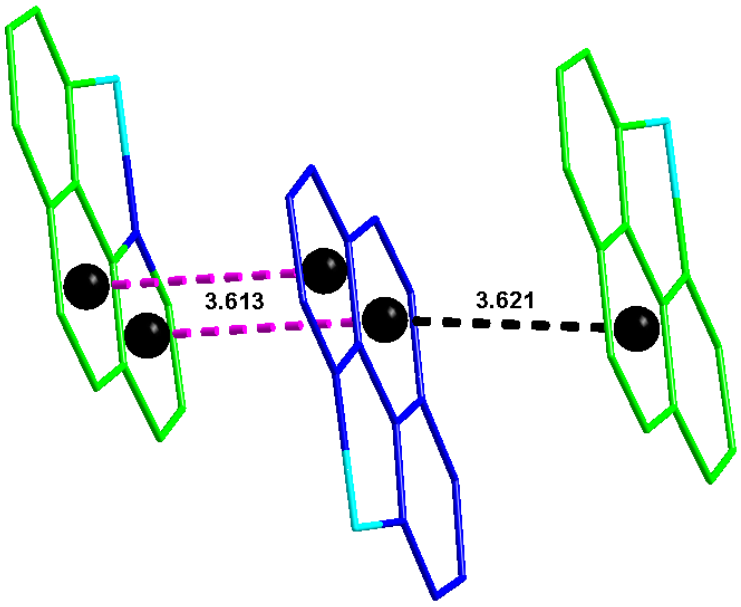

Fig. S1 π-π interactions of phen in complexes **1.**

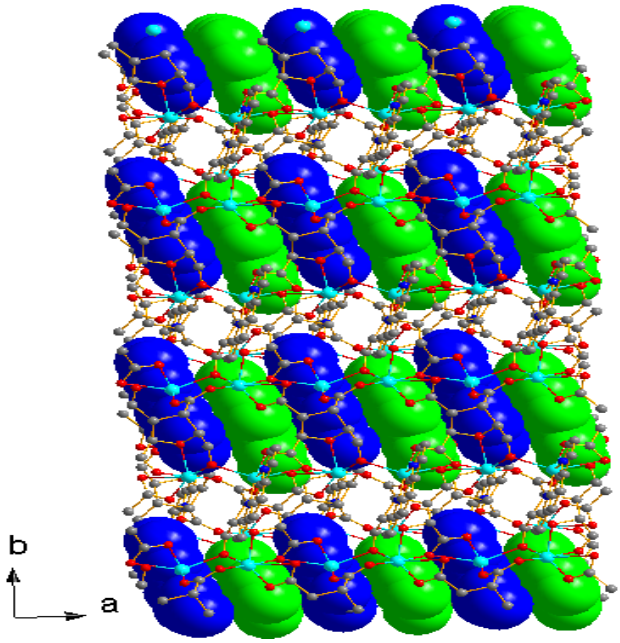

Fig. S2 View of the π-π stacking of phen in complexes **1** (green and blue are phen ligands in different layers).

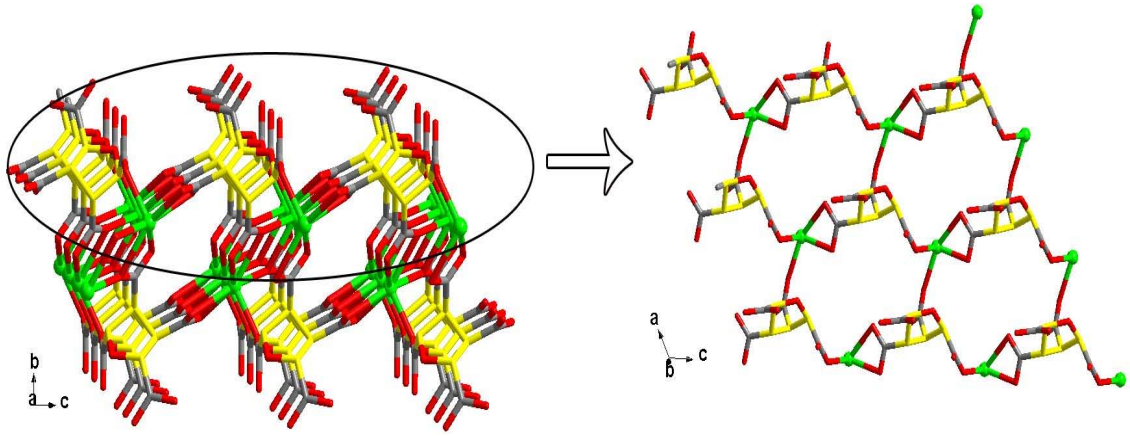

Fig. S3 View of the (6,3)-(THFTCA-Cd2)-sheet (right) and the 2D THFTCA-Cd2-THFTCA double-layer (left) in complexes **2**.