Supporting Information for

Structural and luminescent modulation in 8-hydroxyquinolinate-based coordination polymers by varying dicarboxylic acids

Guozan Yuan*, Guoli Hu, Weilong Shan, Suo Jin, Qingyun Gu and Jing Chen

School of Chemistry and Chemical Engineering, Anhui University of Technology, Maanshan,

243002, P. R. China

E-mail: yuanguozan@163.com

Table of Content

- 1. Table S1-6 Selected Bond lengths [Å] and angles [°] for 1-6.
- 2. Fig. S1-16. Views of the crystal structures of coordination polymers 1-6.
- 3. Fig. S17 and S18. NMR spectra of HL.
- 4. Fig. S19-24. IR spectra of complexes 1-6.
- 5. Fig. S25. Emission spectra of HL ligand in the solid state.
- 6. Fig. S26-31. Fluorescence decay and fit curves of complexes 1-6.

1.1. Table S1 Selected Bond lengths [Å] and angles [°] for 1.

1.993(2)	
1.993(2)	
2.260(2)	
2.260(2)	
2.279(3)	
2.279(3)	
2.279(3)	
180.0	
79.98(9)	
100.02(9)	
100.02(9)	
79.98(9)	
180.0	
88.75(11)	
91.25(11)	
89.34(10)	
90.66(10)	
91.25(11)	
88.75(11)	
90.66(10)	
89.34(10)	
180.00(11)	
	1.993(2) 1.993(2) 2.260(2) 2.260(2) 2.279(3) 2.279(3) 2.279(3) 180.0 79.98(9) 100.02(9) 100.02(9) 100.02(9) 79.98(9) 180.0 88.75(11) 91.25(11) 89.34(10) 90.66(10) 91.25(11) 88.75(11) 90.66(10) 91.25(11) 88.75(11) 90.66(10) 89.34(10) 180.00(11)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z #2 x,-y+3/2,z-1/2 #3 -x+1,y-1/2,-z+1/2 #4 -x+1,y+1/2,-z+1/2

1.2. Table S2 Selected Bond lengths [Å] and angles [°] for $\mathbf{2}$.

Cd(1)-O(1)	2.2403(18)
Cd(1)-O(1)#1	2.2871(18)
Cd(1)-N(2)#2	2.341(2)
Cd(1)-O(2)	2.347(2)
Cd(1)-O(3)	2.375(2)
Cd(1)-N(1)	2.385(2)
Cd(1)-C(17)	2.697(3)

O(1)-Cd(1)-O(1)#1	72.60(8)
O(1)-Cd(1)-N(2)#2	107.33(9)
O(1)#1-Cd(1)-N(2)#2	92.25(8)
O(1)-Cd(1)-O(2)	110.19(8)
O(1)#1-Cd(1)-O(2)	98.38(8)
N(2)#2-Cd(1)-O(2)	142.47(9)
O(1)-Cd(1)-O(3)	164.51(8)
O(1)#1-Cd(1)-O(3)	104.00(7)
N(2)#2-Cd(1)-O(3)	87.74(8)
O(2)-Cd(1)-O(3)	54.79(8)
O(1)-Cd(1)-N(1)	72.47(7)
O(1)#1-Cd(1)-N(1)	144.90(7)
N(2)#2-Cd(1)-N(1)	94.84(7)
O(2)-Cd(1)-N(1)	96.65(8)
O(3)-Cd(1)-N(1)	110.58(8)
O(1)-Cd(1)-C(17)	137.18(10)
O(1)#1-Cd(1)-C(17)	99.95(8)
N(2)#2-Cd(1)-C(17)	115.16(10)
O(2)-Cd(1)-C(17)	27.56(9)
O(3)-Cd(1)-C(17)	27.47(9)
N(1)-Cd(1)-C(17)	107.84(8)
C(1)-O(1)-Cd(1)	117.74(16)
C(1)-O(1)-Cd(1)#1	134.37(16)
Cd(1)-O(1)-Cd(1)#1	107.40(8)
C(9)-N(1)-Cd(1)	128.89(17)

Symmetry transformations used to generate equivalent atoms: #1 -x, -y+1, -z #2 -x+1/2, y-1/2, -z+1/2 #3 -x+1/2, y+1/2, -z+1/2

1.3. Table S3 Selected Bond lengths [Å] and angles [°] for ${\bf 3}.$

Zn(1)-O(1)	2.0208(15)
Zn(1)-O(2)	2.039(2)
Zn(1)-N(2)#1	2.1191(19)
Zn(1)-O(1)#2	2.1321(16)
Zn(1)-N(1)	2.1888(19)
Zn(1)-C(20)	2.546(3)
O(1)-Zn(1)-O(2)	149.55(10)
O(1)-Zn(1)-N(2)#1	103.49(7)
O(2)-Zn(1)-N(2)#1	106.03(11)
O(1)-Zn(1)-O(1)#2	76.56(7)
O(2)-Zn(1)-O(1)#2	94.12(7)

N(2)#1-Zn(1)-O(1)#2	93.77(7)
O(1)-Zn(1)-N(1)	78.41(7)
O(2)-Zn(1)-N(1)	106.71(8)
N(2)#1-Zn(1)-N(1)	93.74(7)
O(1)#2-Zn(1)-N(1)	154.90(7)
O(1)-Zn(1)-C(20)	121.67(11)
O(2)-Zn(1)-C(20)	27.97(12)
N(2)#1-Zn(1)-C(20)	133.61(12)
O(1)#2-Zn(1)-C(20)	87.33(8)
N(1)-Zn(1)-C(20)	104.45(9)
C(1)-O(1)-Zn(1)	116.61(14)
C(1)-O(1)-Zn(1)#2	139.65(14)
Zn(1)-O(1)-Zn(1)#2	103.45(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2, y+1/2, -z+1/2	#2 -x, -y+2, -z
#3 -x+1/2, y-1/2, -z+1/2	#4 -x, -y+1, -z

1.4. Table S4 Selected Bond lengths [Å] and angles [°] for 4.

I(1)-Zn(2)	2.5391(6)
Zn(1)-O(2)	1.991(2)
Zn(1)-O(1)	1.999(3)
Zn(1)-O(4)	2.069(4)
Zn(1)-O(1)#1	2.071(3)
Zn(1)-N(1)	2.181(3)
O(1)-Zn(1)#1	2.071(3)
Zn(2)-N(2)	2.068(3)
Zn(2)-N(2)#2	2.068(3)
Zn(2)-I(1)#2	2.5391(6)
O(2)-Zn(1)-O(1)	149.03(15)
O(2)-Zn(1)-O(4)	99.17(16)
O(1)-Zn(1)-O(4)	111.42(15)
O(2)-Zn(1)-O(1)#1	97.34(10)
O(1)-Zn(1)-O(1)#1	75.61(11)
O(4)-Zn(1)-O(1)#1	95.48(15)
O(2)-Zn(1)-N(1)	104.81(10)
O(1)-Zn(1)-N(1)	78.86(10)
O(4)-Zn(1)-N(1)	93.38(14)
O(1)#1-Zn(1)-N(1)	154.47(11)
N(2)-Zn(2)-N(2)#2	95.90(18)
N(2)-Zn(2)-I(1)#2	107.69(9)
N(2)#2-Zn(2)-I(1)#2	108.35(8)

N(2)- $Zn(2)$ - $I(1)$	108.35(8)
N(2)#2-Zn(2)-I(1)	107.69(9)
I(1)#2-Zn(2)-I(1)	124.99(4)

Symmetry transformations used to generate equivalent atoms: #1 -x+3/2,-y+3/2,-z #2 -x+2,y,-z+1/2 #3 -x+3/2,-y+5/2,-z

1.5. Table S5 Selected Bond lengths [Å] and angles [°] for 5.

Cd(1)-O(1)#1	2.247(2)	
Cd(1)-O(1)	2.281(2)	
Cd(1)-O(3)	2.329(3)	
Cd(1)-N(2)#2	2.332(3)	
Cd(1)-N(1)#1	2.340(3)	
Cd(1)-O(2)	2.389(3)	
Cd(1)-C(20)	2.705(3)	
O(1)#1-Cd(1)-O(1)	76.37(10)	
O(1)#1-Cd(1)-O(3)	155.90(11)	
O(1)-Cd(1)-O(3)	97.74(9)	
O(1)#1-Cd(1)-N(2)#2	98.65(11)	
O(1)-Cd(1)-N(2)#2	90.02(10)	
O(3)-Cd(1)-N(2)#2	104.76(12)	
O(1)#1-Cd(1)-N(1)#1	72.32(10)	
O(1)-Cd(1)-N(1)#1	148.25(10)	
O(3)-Cd(1)-N(1)#1	113.02(10)	
N(2)#2-Cd(1)-N(1)#1	89.56(10)	
O(1)#1-Cd(1)-O(2)	101.80(12)	
O(1)-Cd(1)-O(2)	91.46(10)	
O(3)-Cd(1)-O(2)	54.55(12)	
N(2)#2-Cd(1)-O(2)	159.26(13)	
N(1)#1-Cd(1)-O(2)	99.84(11)	
O(1)#1-Cd(1)-C(20)	129.10(11)	
O(1)-Cd(1)-C(20)	92.66(10)	
O(3)-Cd(1)-C(20)	26.89(11)	
N(2)#2-Cd(1)-C(20)	131.37(12)	
N(1)#1-Cd(1)-C(20)	111.06(10)	
O(2)-Cd(1)-C(20)	27.89(11)	
C(1)-O(1)-Cd(1)#1	117.0(2)	
C(1)-O(1)-Cd(1)	137.5(2)	
Cd(1)#1-O(1)-Cd(1)	103.63(10)	

Symmetry transformations used to generate equivalent atoms: #1 -x, -y, -z #2 x+1/2, -y-1/2, z+1/2 #3 x-1/2, -y-1/2, z-1/2 #4 -x, -y+1, -z

Cd(1)-O(1)	2.259(4)	
Cd(1)-O(1)#1	2.260(4)	
Cd(1)-O(3)	2.325(5)	
Cd(1)-N(2)#2	2.332(5)	
Cd(1)-N(1)	2.353(4)	
Cd(1)-O(2)	2.414(4)	
O(1)-Cd(1)#1	2.260(4)	
N(2)-Cd(1)#4	2.332(5)	
O(1)-Cd(1)-O(1)#1	76.52(17)	
O(1)-Cd(1)-O(3)	97.27(17)	
O(1)#1-Cd(1)-O(3)	105.24(18)	
O(1)-Cd(1)-N(2)#2	103.73(17)	
O(1)#1-Cd(1)-N(2)#2	89.80(17)	
O(3)-Cd(1)-N(2)#2	156.59(19)	
O(1)-Cd(1)-N(1)	71.78(15)	
O(1)#1-Cd(1)-N(1)	147.19(15)	
O(3)-Cd(1)-N(1)	87.19(17)	
N(2)#2-Cd(1)-N(1)	89.61(17)	
O(1)-Cd(1)-O(2)	150.96(16)	
O(1)#1-Cd(1)-O(2)	99.84(16)	
O(3)-Cd(1)-O(2)	55.34(17)	
N(2)#2-Cd(1)-O(2)	105.07(17)	
N(1)-Cd(1)-O(2)	111.96(16)	

1.6. Table S6 Selected Bond lengths [Å] and angles [°] for **6**.

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,-z+9/4 #2 y-1,-x+1,-z+2 #3 -x+1,-y+2,z #4 -y+1,x+1,-z+2 2.1 Fig. S1. View of the asymmetric unit in 1.



2.2 Fig. S2. Perspective view of C–H $^{...}$ O intermolecular interactions in 1.



2.3 Fig. S3. View of 3D supramolecular structure in 1.



2.4 Fig. S4. View of the asymmetric unit in **2**.



2.5 Fig. S5. View of the asymmetric unit in **3**.



2.6 Fig. S6. The π ... π stacking between quinoline and pyridine rings of adjacent 2D layer networks in **3**.



2.7 Fig. S7.View of the 3D structure in **3**.



2.8 Fig. S8. View of the asymmetric unit in 4.



2.9 Fig. S9. Perspective view of $\pi \cdots \pi$ stacking and C-H $\cdots \pi$ intermolecular interactions in 4.



2.10 Fig. S10. View of the asymmetric unit in 5.



2.11 Fig. S11. View of the coordination geometries of Cd(II) atoms in 5.



2.12 Fig. S12. The 2D network structure of 5.



2.13 Fig. S13. View of the asymmetric unit in 6.



2.14 Fig. S14. (a) View of a cyclic tetramer Zn_6L_4 in 6; (b) Two types of $\pi \cdots \pi$ interactions Between the adjacent cyclic tetramers are observed in 6



2.15 Fig. S15. View of 3D supramolecular structure in 6.







3.1 Fig. S17. ¹H NMR spectrum of HL (d₆-DMSO).



3.2 Fig. S18. 13 C NMR spectrum of HL (d₆-DMSO).



4.2 Fig. S20. IR spectrum of complex 2.



4.3 Fig. S21. IR spectrum of complex 3.



4.4 Fig. S22. IR spectrum of complex 4.



4.5 Fig. S23. IR spectrum of complex 5.



4.6 Fig. S24. IR spectrum of complex 6.



5 Fig. S25. Emission spectra of HL ligand in the solid state.



6.1 Fig. S26. Fluorescence decay and fit curves of complex 1.



6.2 Fig. S27. Fluorescence decay and fit curves of compound 2.



6.3 Fig. S28. Fluorescence decay and fit curves of compound **3**.



6.4 Fig. S29. Fluorescence decay and fit curves of compound 4.



6.5 Fig. S30. Fluorescence decay and fit curves of compound 5.



6.6 Fig. S31. Fluorescence decay and fit curves of compound 6.

