Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information for

Assembly of four 8-quinolinate-based multinuclear complexes: the effect of substituents on core structures and photoluminescent properties

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

I(1)-Cd(1)	2.6965(6)
Cd(1)-O(1)	2.232(3)
Cd(1)-O(1)#1	2.260(3)
Cd(1)-O(2)	2.266(4)
Cd(1)-N(1)	2.351(4)
O(1)-Cd(1)-O(1)#1	72.08(14)
O(1)-Cd(1)-O(2)	128.45(15)
O(1)#1-Cd(1)-O(2)	87.49(14)
O(1)-Cd(1)-N(1)	72.71(13)
O(1)#1-Cd(1)-N(1)	139.05(13)
O(2)-Cd(1)-N(1)	98.47(15)
O(1)-Cd(1)-I(1)	121.40(10)
O(1)#1-Cd(1)-I(1)	108.94(10)
O(2)-Cd(1)-I(1)	109.87(11)
N(1)-Cd(1)-I(1)	106.90(9)
C(1)-O(1)-Cd(1)	117.3(3)
C(1)-O(1)-Cd(1)#1	133.1(3)
Cd(1)-O(1)-Cd(1)#1	107.91(14)
C(9)-N(1)-Cd(1)	126.0(3)
C(6)-N(1)-Cd(1)	112.6(3)

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

1.2 Table S2 Selected Bond lengths [Å] and angles [º] for **2**.

Cd(1)-O(1)	2.199(3)
Cd(1)-O(2)	2.235(2)
Cd(1)-N(1)	2.326(3)
Cd(1)-O(3)#1	2.332(2)
Cd(1)-N(2)	2.384(3)
Cd(2)-O(3)#1	2.257(2)
Cd(2)-N(3)	2.329(3)
Cd(2)-N(3)#1	2.329(3)
Cd(2)-O(2)#1	2.332(2)
Cd(2)-O(2)	2.332(2)
O(3)-Cd(1)#1	2.332(2)
O(1)-Cd(1)-O(2)	173.02(11)
O(1)-Cd(1)-N(1)	75.76(13)
O(2)-Cd(1)-N(1)	110.82(11)
O(1)-Cd(1)-O(3)#1	103.26(11)

O(2)-Cd(1)-O(3)#1	73.72(9)
N(1)-Cd(1)-O(3)#1	100.01(10)
O(1)-Cd(1)-N(2)	107.75(12)
O(2)-Cd(1)-N(2)	72.91(10)
N(1)-Cd(1)-N(2)	108.27(11)
O(3)#1-Cd(1)-N(2)	142.08(9)
C(1)-O(1)-Cd(1)	114.5(3)
C(9)-N(1)-C(6)	120.6(4)
C(9)-N(1)-Cd(1)	129.3(3)
C(6)-N(1)-Cd(1)	110.0(3)
O(3)-Cd(2)-O(3)#1	172.45(13)
O(3)-Cd(2)-N(3)	73.86(9)
O(3)#1-Cd(2)-N(3)	111.05(9)
O(3)-Cd(2)-N(3)#1	111.05(9)
O(3)#1-Cd(2)-N(3)#1	73.86(9)
N(3)-Cd(2)-N(3)#1	103.79(14)
O(3)-Cd(2)-O(2)#1	73.33(9)
O(3)#1-Cd(2)-O(2)#1	100.85(9)
N(3)-Cd(2)-O(2)#1	146.18(9)
N(3)#1-Cd(2)-O(2)#1	95.42(9)
O(3)-Cd(2)-O(2)	100.85(9)
O(3)#1-Cd(2)-O(2)	73.33(9)
N(3)-Cd(2)-O(2)	95.42(9)
N(3)#1-Cd(2)-O(2)	146.18(9)
O(2)#1-Cd(2)-O(2)	82.87(13)
C(18)-O(2)-Cd(1)	116.4(2)
C(18)-O(2)-Cd(2)	122.2(2)
Cd(1)-O(2)-Cd(2)	104.03(10)
C(26)-N(2)-C(23)	119.7(3)
C(26)-N(2)-Cd(1)	129.2(3)
C(23)-N(2)-Cd(1)	110.9(2)
C(35)-O(3)-Cd(2)	115.2(2)
C(35)-O(3)-Cd(1)#1	131.9(2)
Cd(2)-O(3)-Cd(1)#1	103.33(9)
C(43)-N(3)-Cd(2)	127.8(2)
C(40)-N(3)-Cd(2)	112.3(2)

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

1.3 Table S3 Selected Bond lengths [Å] and angles [º] for **3**.

Cd(1)-O(3)	2.239(4)
Cd(1)-O(1)	2.253(4)
Cd(1)-N(1)	2.318(5)

Cd(1)-O(5)#1	2.356(5)
Cd(1)-N(2)	2.364(6)
Cd(1)-O(5)	2.516(4)
Br(1)-Cd(2)	2.5499(10)
O(1)-Cd(2)	2.195(4)
Cd(2)-O(3)#1	2.243(5)
Cd(2)-N(3)	2.333(6)
Cd(2)-O(5)	2.342(4)

O(3)-Cd(1)-O(1)	167.94(15)
O(3)-Cd(1)-N(1)	117.61(17)
O(1)-Cd(1)-N(1)	72.55(17)
O(3)-Cd(1)-O(5)#1	73.92(15)
O(1)-Cd(1)-O(5)#1	97.85(15)
N(1)-Cd(1)-O(5)#1	104.26(16)
O(3)-Cd(1)-N(2)	72.53(18)
O(1)-Cd(1)-N(2)	113.62(18)
N(1)-Cd(1)-N(2)	99.31(18)
O(5)#1-Cd(1)-N(2)	145.17(17)
O(3)-Cd(1)-O(5)	91.59(14)
O(1)-Cd(1)-O(5)	78.12(14)
N(1)-Cd(1)-O(5)	150.66(16)
O(5)#1-Cd(1)-O(5)	80.03(17)
N(2)-Cd(1)-O(5)	91.77(17)
C(1)-O(1)-Cd(2)	137.3(4)
C(1)-O(1)-Cd(1)	117.4(4)
Cd(2)-O(1)-Cd(1)	105.29(17)
C(9)-N(1)-Cd(1)	126.4(4)
C(6)-N(1)-Cd(1)	112.9(4)
O(1)-Cd(2)-O(3)#1	94.74(17)
O(1)-Cd(2)-N(3)	93.65(18)
O(3)#1-Cd(2)-N(3)	142.47(19)
O(1)-Cd(2)-O(5)	83.12(15)
O(3)#1-Cd(2)-O(5)	74.11(15)
N(3)-Cd(2)-O(5)	70.71(19)
O(1)-Cd(2)-Br(1)	123.64(11)
O(3)#1-Cd(2)-Br(1)	101.94(11)
N(3)-Cd(2)-Br(1)	103.51(15)
O(5)-Cd(2)-Br(1)	153.22(11)
C(19)-O(3)-Cd(1)	114.9(4)
C(19)-O(3)-Cd(2)#1	129.4(4)
Cd(1)-O(3)-Cd(2)#1	109.55(19)
C(45)-N(3)-C(42)	120.0(7)
C(45)-N(3)-Cd(2)	126.0(5)

C(42)-N(3)-Cd(2)	112.8(5)
C(37)-O(5)-Cd(2)	113.2(4)
C(37)-O(5)-Cd(1)#1	128.9(4)
Cd(2)-O(5)-Cd(1)#1	102.40(17)
C(37)-O(5)-Cd(1)	112.7(4)
Cd(2)-O(5)-Cd(1)	93.31(14)
Cd(1)#1-O(5)-Cd(1)	99.97(17)

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

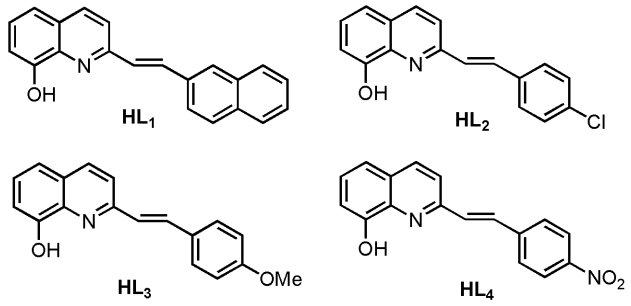
1.4 Table S4 Selected Bond lengths [Å] and angles [º] for **4**.

Cd(1)-O(4)#1	2.280(3)
Cd(1)-O(7)	2.285(3)
Cd(1)-O(1)	2.370(3)
Cd(1)-O(10)	2.383(3)
Cd(1)-N(1)	2.401(3)
Cd(1)-Br(1)	2.6147(6)
O(1)-Cd(2)	2.356(3)
O(1)-Cd(2)#1	2.385(3)
Cd(2)-O(7)	2.239(3)
Cd(2)-O(4)	2.252(3)
Cd(2)-N(3)	2.336(4)
Cd(2)-O(1)#1	2.385(3)
Cd(2)-N(5)	2.403(4)
O(4)-Cd(1)#1	2.280(3)
O(4)#1-Cd(1)-O(7)	93.26(12)
O(4)#1-Cd(1)-O(1)	79.03(10)
O(7)-Cd(1)-O(1)	75.06(10)
O(4)#1-Cd(1)-O(10)	156.81(12)
O(7)-Cd(1)-O(10)	88.51(12)
O(1)-Cd(1)-O(10)	79.11(11)
O(4)#1-Cd(1)-N(1)	88.73(12)
O(7)-Cd(1)-N(1)	143.60(11)
O(1)-Cd(1)-N(1)	69.67(11)
O(10)-Cd(1)-N(1)	76.48(12)
O(4)#1-Cd(1)-Br(1)	108.98(8)
O(7)-Cd(1)-Br(1)	107.26(8)
O(1)-Cd(1)-Br(1)	171.27(7)
O(10)-Cd(1)-Br(1)	92.46(9)
N(1)-Cd(1)-Br(1)	106.35(8)
C(1)-O(1)-Cd(2)	127.1(2)
C(1)-O(1)-Cd(1)	111.6(2)

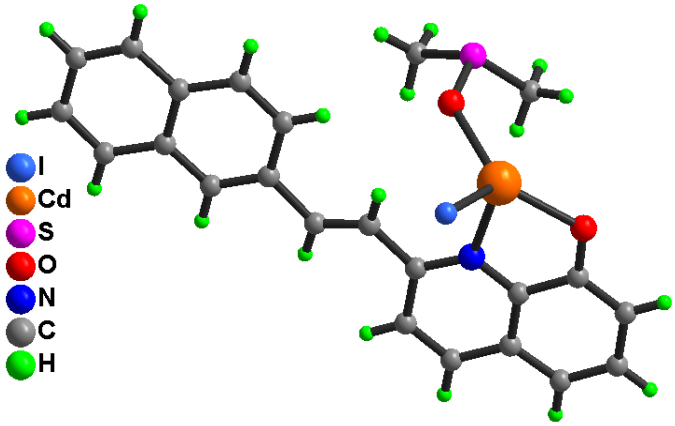
Cd(2)-O(1)-Cd(1)	100.89(10)
C(1)-O(1)-Cd(2)#1	113.9(2)
Cd(2)-O(1)-Cd(2)#1	101.20(10)
Cd(1)-O(1)-Cd(2)#1	97.52(10)
C(9)-N(1)-Cd(1)	125.3(3)
C(6)-N(1)-Cd(1)	110.1(3)
O(7)-Cd(2)-O(4)	170.43(12)
O(7)-Cd(2)-N(3)	116.07(13)
O(4)-Cd(2)-N(3)	72.92(13)
O(7)-Cd(2)-O(1)	76.19(10)
O(4)-Cd(2)-O(1)	99.04(11)
N(3)-Cd(2)-O(1)	103.36(12)
O(7)-Cd(2)-O(1)#1	91.62(11)
O(4)-Cd(2)-O(1)#1	79.25(10)
N(3)-Cd(2)-O(1)#1	152.09(12)
O(1)-Cd(2)-O(1)#1	78.80(10)
O(7)-Cd(2)-N(5)	72.53(12)
O(4)-Cd(2)-N(5)	110.76(12)
N(3)-Cd(2)-N(5)	96.85(13)
O(1)-Cd(2)-N(5)	147.86(12)
O(1)#1-Cd(2)-N(5)	94.77(11)
C(18)-O(4)-Cd(2)	117.5(3)
C(18)-O(4)-Cd(1)#1	138.3(3)
Cd(2)-O(4)-Cd(1)#1	104.18(12)

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

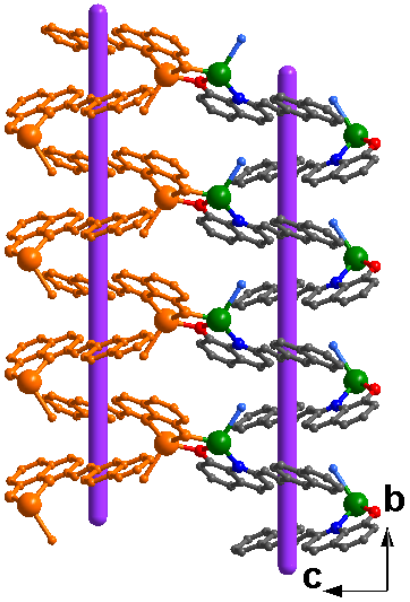
2.1 Fig. S1. The structures of four ligands HL_1-HL_4



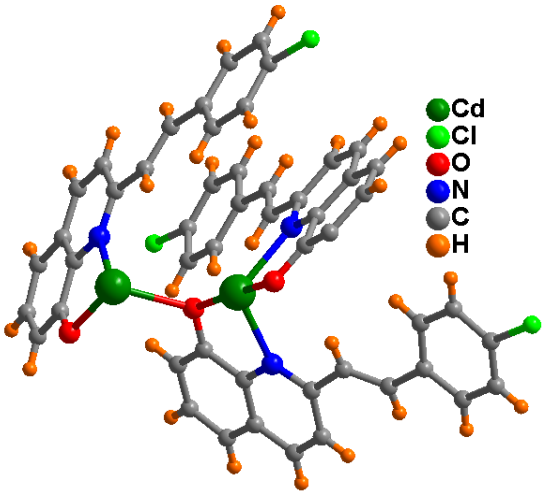
2.2 Fig. S2. View of the asymmetric unit in **1**.



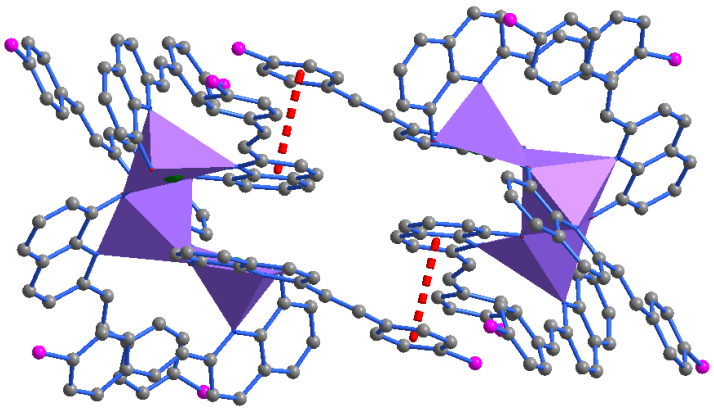
2.3 Fig. S3. The *meso*-helical chains (*P* + *M*) along the *b* axis in **1**.



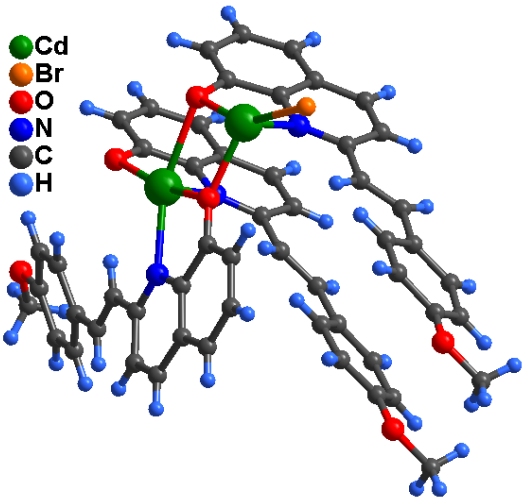
2.4 Fig. S4. View of the asymmetric unit in **2**.



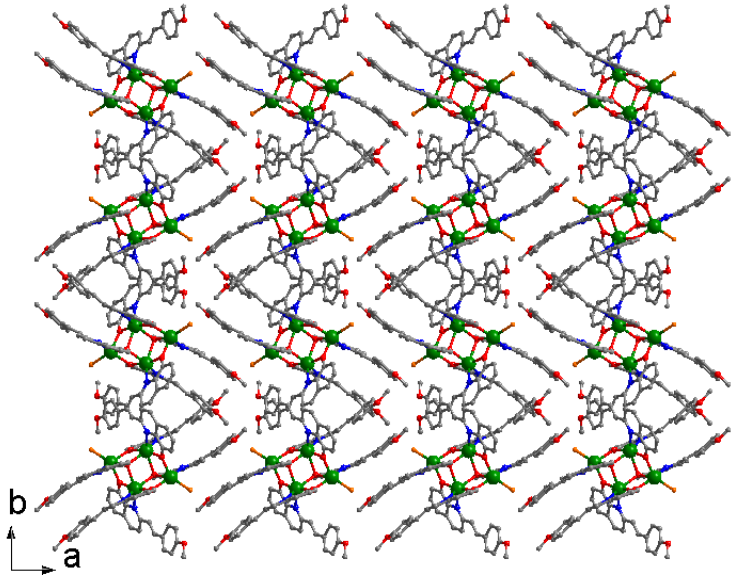
2.5 Fig. S5. The π···π stacking interactions (red dashed lines) between chlorophenyl and pyridyl rings of adjacent units in **2.**



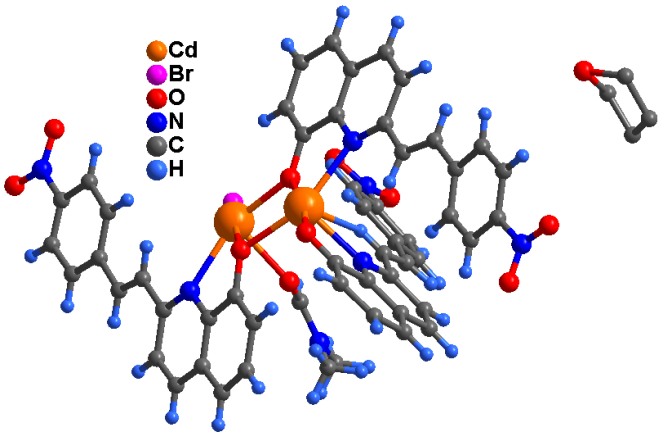
2.6 Fig. S6. View of the asymmetric unit in **3**.



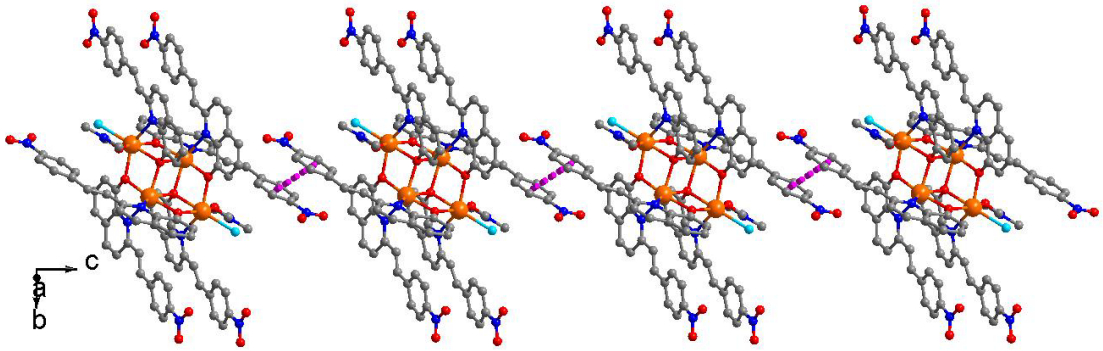
2.7 Fig. S7. View of 3D supramolecular structure in **3**.



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

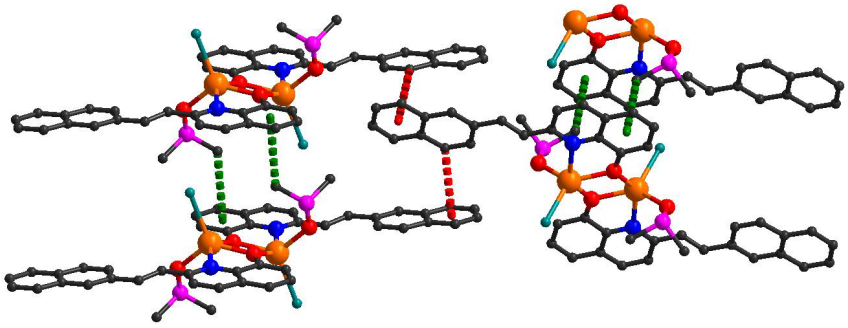


2.9 Fig. S9. Adjacent tetranuclear units in **4** are linked into 1D infinite chain by π···π interactions (pink dashed lines)

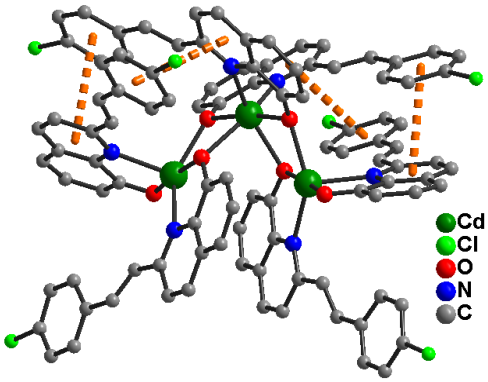


3 In order to investigate the effect of substituents on the structures of M(II)-quinolinate complexes, the noncovalent interactions fabricated by the substituents of different ligands in **1**-**4** were explored.

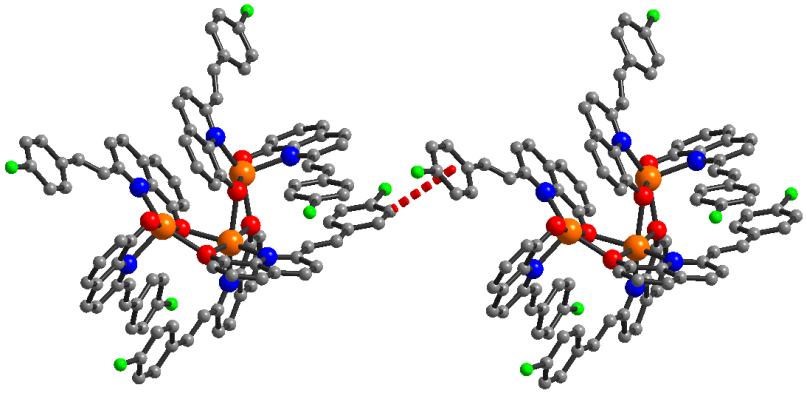
3.1 Fig. S10. Two kinds of C–H···π intermolecular interactions in **1**: C(14)–H(14A)···π interactions between adjacent naphthyl groups (red dashed lines) and C(22)–H(22C)···π interactions between $–CH_3$ group of DMSO molecule and phenolate ring (green dashed lines).



3.2 Fig. S11. In the trinuclear building unit of **2**, there are two kinds of face-to-face π···π stacking interactions (yellow dashed lines) between adjacent chlorophenyl and pyridyl rings (face-to-face distance of ca. 3.70 and 3.83 Å).

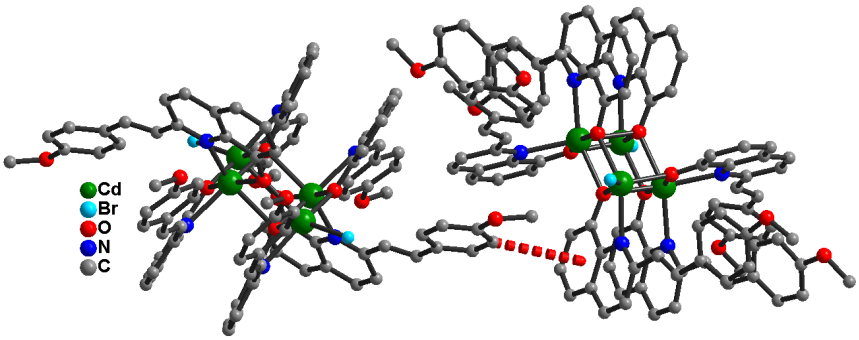


3.3 Fig. S12. In the adjacent building units of **2**, there one kind of C–H···π interaction between adjacent chlorophenyl groups (red dashed lines).



3.4 Fig. S13. In the adjacent building units of **3**, there one kind of C–H···π interaction between C-H

group of methoxyphenyl and quinoline ring (red dashed lines).



3.5 Fig. S14. In complex **4**, the intermolecular C–H···O hydrogen-bonding (green dashed lines) between the vinylene C–H groups and nitryl oxygen atoms (C···O, 3.540(7) Å) was observed.