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Hydrothermal syntheses，structures and luminescent properties of d^{10} metal-organic frameworks based on rigid 3, 3', 5, 5' - azobenzenetetracarboxylic acid

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Electronic Supporting Information

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Table S1 Selected bond lengths (Å) and angles (°) for complexes **1**[a], **2**[b], **3**[c] and **4**[d]

1			
Cd-O1	2.317(3)	Cd2-O1	2.371(3)
Cd1-O7	2.296(3)	Cd2-O2	2.465(3)
Cd1-O5#1	2.508(3)	Cd2-O8	2.660(1)
Cd1-O6#1	2.378(3)	Cd2-O3#2	2.788(1)
Cd1-O8	2.627(3)	Cd2-O4#2	2.181(3)
Cd1-N3	2.289(3)	Cd2-N7	2.314(3)
Cd1-N4	2.372(3)	Cd2-N8	2.292(3)
N3-Cd1-O7	146.53(11)	O7-Cd1-O8	51.74(9)
N3-Cd1-O1	79.63(10)	O1-Cd1-O8	74.77(9)
O7-Cd1-O1	94.42(10)	N4-Cd1-O8	91.92(10)
N3-Cd1-N4	73.30(11)	O6#1-Cd1-O8	177.48(8)
O7-Cd1-N4	99.35(11)	O5#1-Cd1-O8	124.14(9)
O1-Cd1-N4	148.58(11)	O4#2-Cd2-N8	133.94(11)
N3-Cd1-O6#1	86.89(10)	O4#2-Cd2-N7	118.00(11)
O7-Cd1-O6#1	126.24(10)	N8-Cd2-N7	73.88(11)
O1-Cd1-O6#1	104.41(9)	O4#2-Cd2-O1	123.75(10)
N4-Cd1-O6#1	89.94(10)	N8-Cd2-O1	94.82(10)
N3-Cd1-O5#1	137.27(10)	N7-Cd2-O1	98.62(11)
O7-Cd1-O5#1	75.66(10)	O4#2-Cd2-O2	82.33(10)
O1-Cd1-O5#1	94.29(9)	N8-Cd2-O2	143.70(10)
N4-Cd1-O5#1	116.40(11)	N7-Cd2-O2	91.37(11)
O6#1-Cd1-O5#1	53.41(8)	O1-Cd2-O2	54.00(9)
N3-Cd1-O8	95.27(10)		
2			
Cd1-O1	2.268(3)	Cd1-O4#2	2.293(3)
Cd1-O2	2.510(3)	Cd1-N2	2.296(3)
Cd1-O3#1	2.230(3)	Cd1-N3	2.360(3)
O3#1-Cd1-O1	91.73(11)	O4#2-Cd1-N3	89.92(10)
O3#1-Cd1-O4#2	83.66(11)	N2-Cd1-N3	72.26(12)
O1-Cd1-O4#2	100.58(10)	O3#1-Cd1-O2	99.10(12)
O3#1-Cd1-N2	105.57(12)	O1-Cd1-O2	54.34(10)
O1-Cd1-N2	138.57(10)	O4#2-Cd1-O2	154.68(10)
O4#2-Cd1-N2	118.26(10)	N2-Cd1-O2	85.46(10)
O3#1-Cd1-N3	171.23(10)	N3-Cd1-O2	89.26(12)
O1-Cd1-N3	95.33(12)		
3			
Zn1-N2	2.177(4)	Zn1-O3#1	2.015(2)
Zn1-N3	2.089(4)	Zn1-O4#2	2.066(3)
Zn1-O1	1.980(3)	O1-Zn1-O3#1	105.46(11)
O1-Zn1-O4#2	92.95(11)	O1-Zn1-N2	96.34(12)
O3#1-Zn1-O4#2	88.79(12)	O3#1-Zn1-N2	87.69(12)
O1-Zn1-N3	124.73(12)	O4#2-Zn1-N2	170.65(13)
O3#1-Zn1-N3	128.87(13)	N3-Zn1-N2	78.51(13)
O4#2-Zn1-N3	97.06(13)		
4			
Zn1-O1	1.950(3)	Zn2-O5#2	1.936(3)
Zn1-N2	2.035(3)	Zn2-O3	1.953(2)
Zn2-O5	1.917(3)	Zn2-N3	2.058(3)
O1-Zn1-O1#1	107.04(17)	O5-Zn2-O3	116.37(12)
O1-Zn1-N2#1	100.29(12)	O5#2-Zn2-O3	107.93(11)
O1-Zn1-N2	121.64(12)	O5-Zn2-N3	111.32(12)
O1#1-Zn1-N2	100.28(12)	O5#2-Zn2-N3	105.34(12)
N2#1-Zn1-N2	107.50(18)	O3-Zn2-N3	106.34(12)
O5-Zn2-O5#2	108.93(6)		

[a]Symmetry codes: #1 x, 1+y, z; #2 x, -1+y, z. [b] Symmetry codes: #1 -0.5+x, -0.5-y, -0.5+z; #2 0.5-x, -0.5-y, 1-z.

[c] Symmetry codes: #1 -x, 1-y, 1-z; #2 x, 1-y,-0.5+z. [d] Symmetry codes: #1 -x, *y*, 0.5-*z*; #2 0.5-*x*, 0.5+*y*, 1.5-z.

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Table S2 Hydrogen bond distances [Å] and angles [°] in complexes **1**[a], **2**[b], **3**[c] and **4**[d]. (D, donor atom; A, acceptor atom).

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
1					
N5-H5	0.860	1.885	156.37	2.695	O6#1
N6-H6A	0.860	2.127	128.31	2.744	O3#2
N9-H9	0.860	2.150	151.26	2.933	O5#3
N10-H10A	0.860	2.031	152.10	2.820	O7#4
2					
O1W-H1B	0.837	2.20	146	2.930	O4#1
O2W-H2A	0.844(10)	2.05	165	2.878	O1W#1
3					
O1W-H1A	0.850	2.544	136.34	3.213	O1 #1
O1W-H1A	0.850	2.629	143.61	3.351	O4
O1W-H1B	0.850	2.521	117.04	3.004	O1#2
4					
O5-H5	0.831	1.964	174.58	2.792	O4#1

[a]Symmetry codes: #1 -*x*, -*y*, -*z* ; #2 -*x*, -*y*+1, -*z*; #3 *x*-1, *y*+1, *z*; #4 *x*-1, *y*, *z*.
[b]Symmetry codes: #1 -*x*+1/2, *y*+1/2,-*z*+3/2. [c]Symmetry codes: #1 *x*, -*y*+1, *z*+1/2; #2 -*x*, *y*, -*z*+3/2.
[d]Symmetry codes: #1 -*x*+1/2, *y*+1/2, -*z*+3/2.

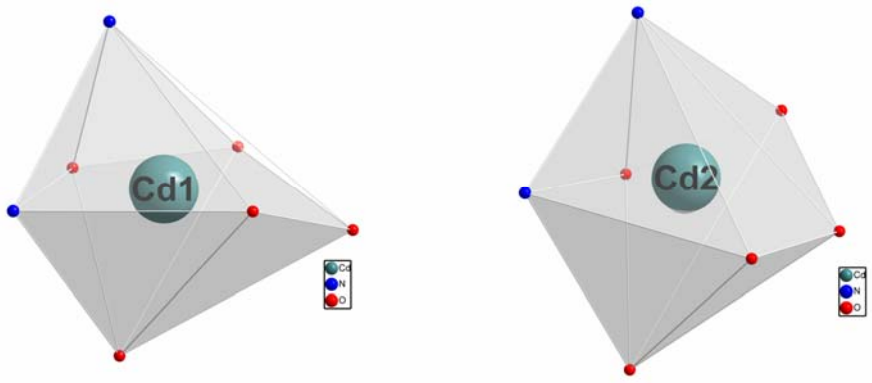

Fig.S1 The coordination geometries of Cd1 and Cd2 in **1**.

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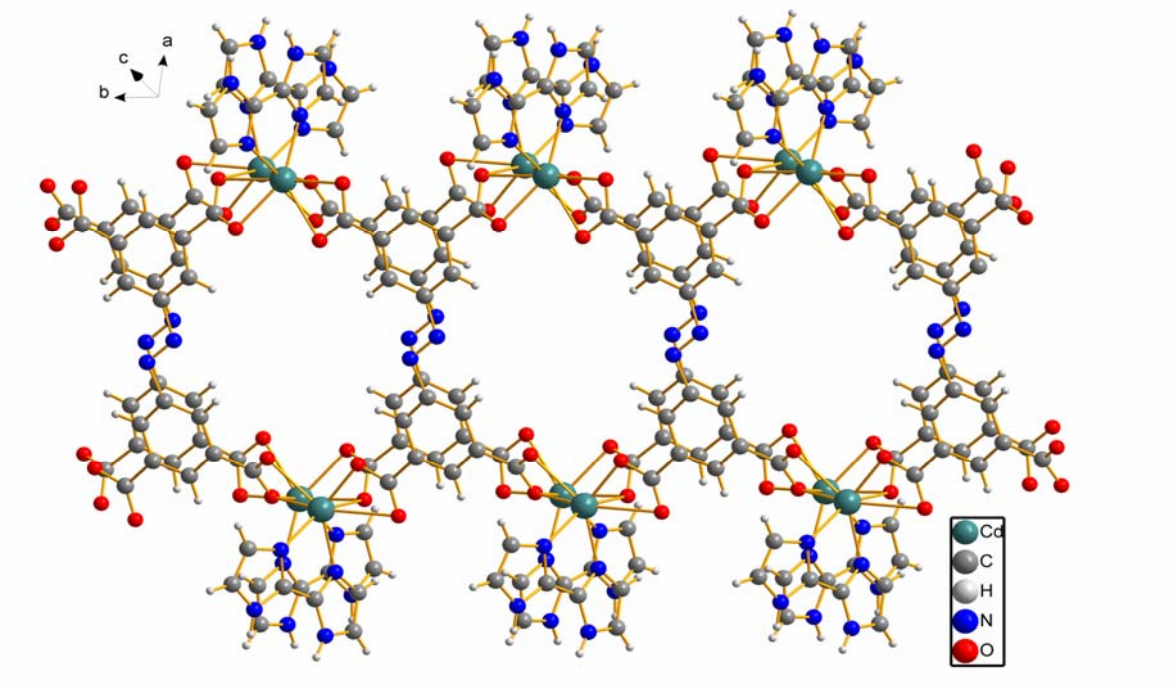

Fig. S2 A representation of the 1D tubular structure from the side view in **1**.

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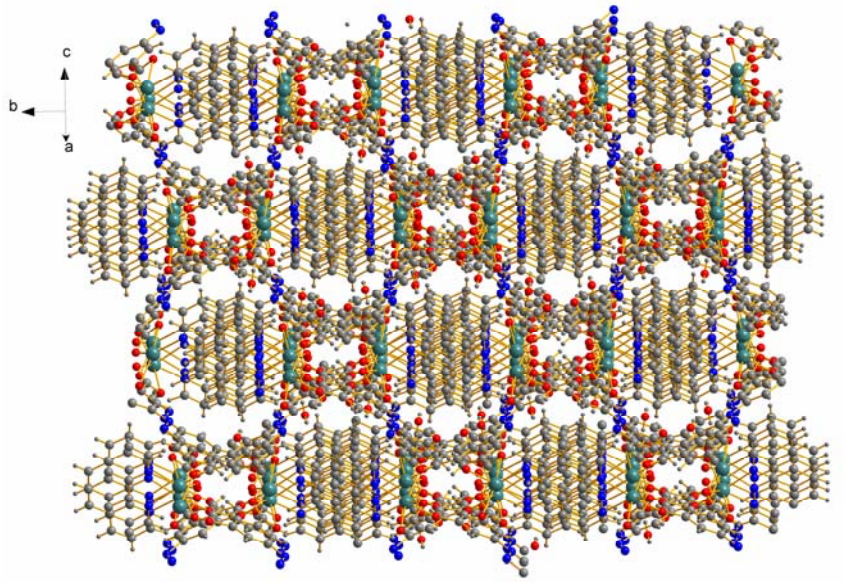

Fig.S3 An illustration of the 3D stacking of **2**.

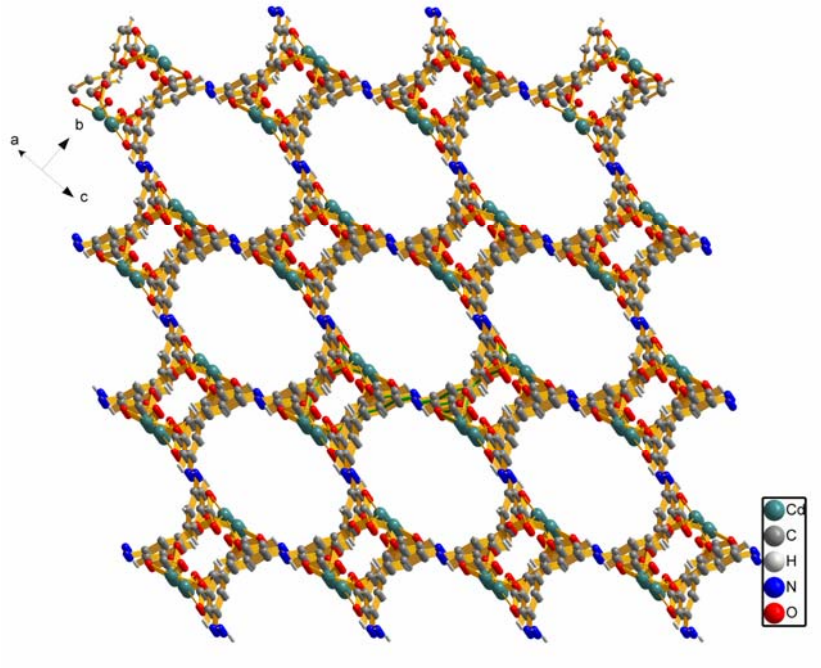

Fig. S4 Parking diagram of the 3D network with elliptical channels of **2**. (Hydrogen atoms, coordinated phen and free water molecules are omitted for clarity).

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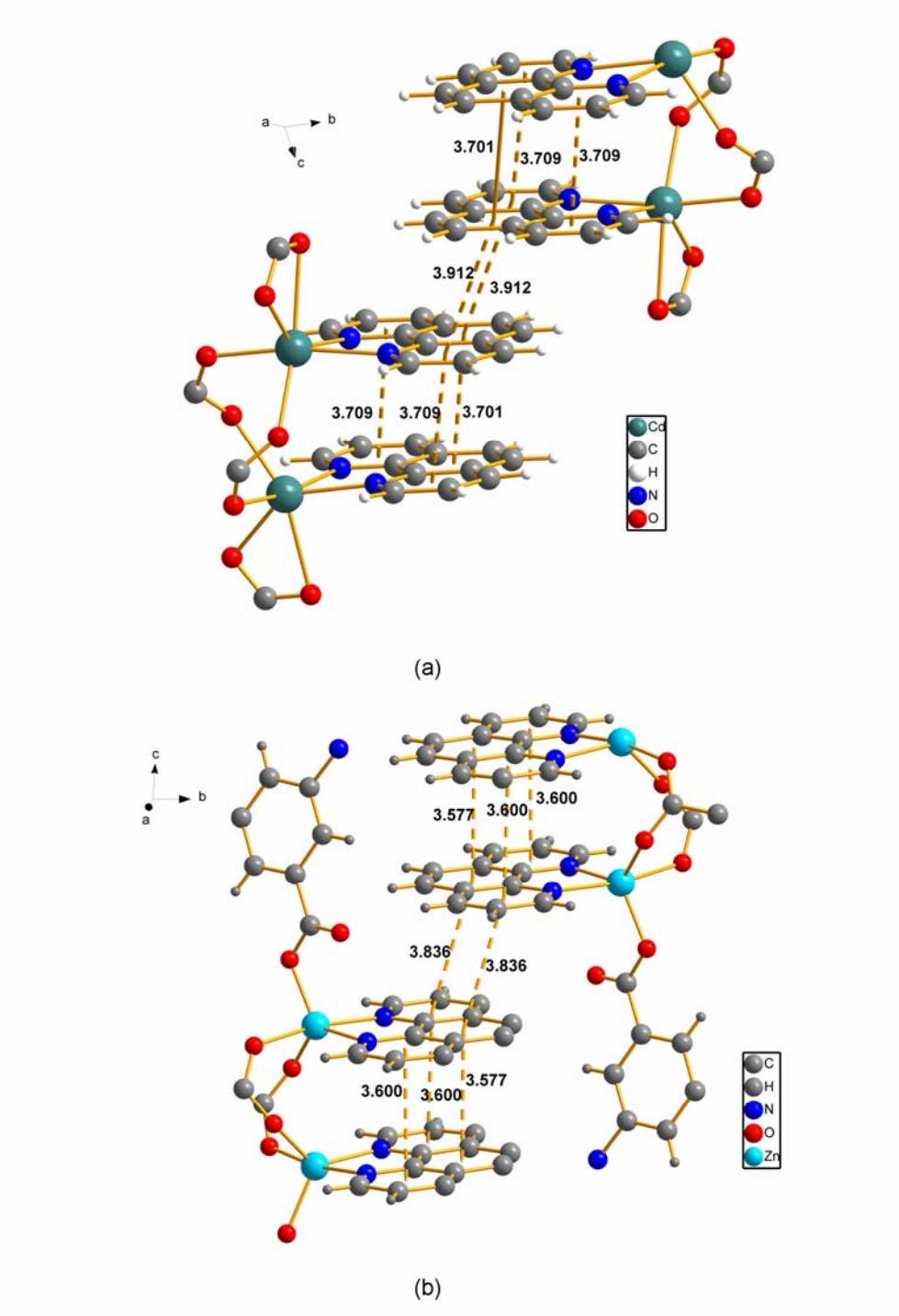

Fig.S5 The offset face-to-face π-π interreactions of the auxiliary phen ligands in **2**(a) and **3**(b).

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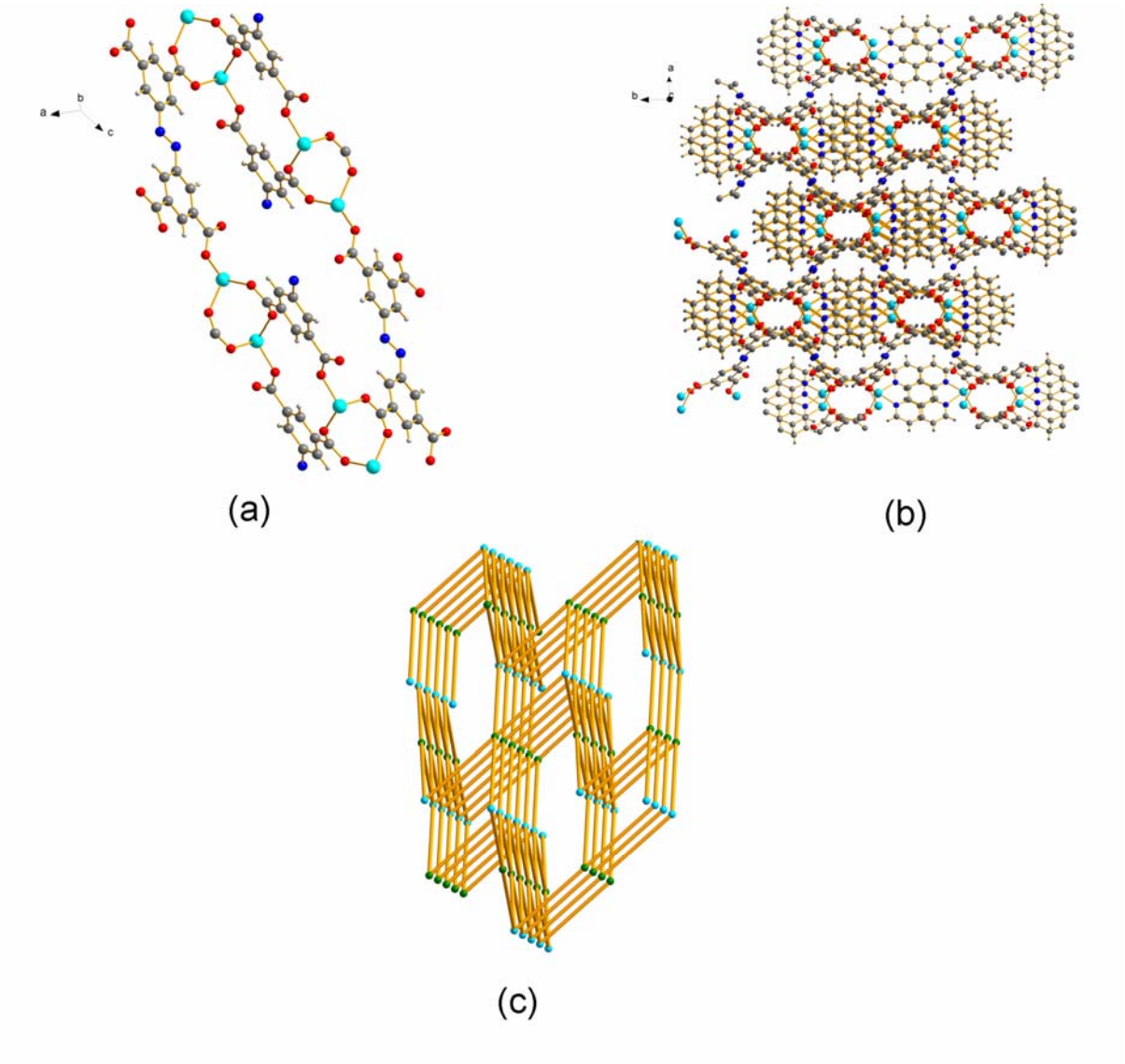

Fig.S6 (a) An illustration of the unit with three kinds of rings in **3**. (Hydrogen atoms, coordinated phen and free water molecules are omitted for clarity). (b) Packing diagram of the 3D network of **3** viewed down the crystallographic *c*-axis. (c) Topology representation of **3**. Green spheres represent the $(abtc)^{4-}$ ligands and blue spheres represent the Zn bimetallic units

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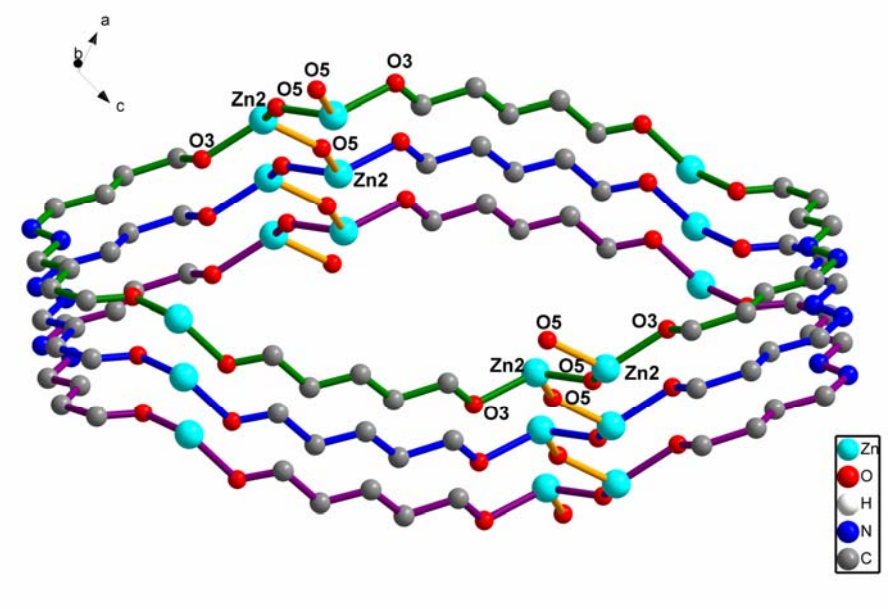

Fig S7. The connecting mode of the 46-member macrocycles and 1D zigzag zinc chains in **4**.

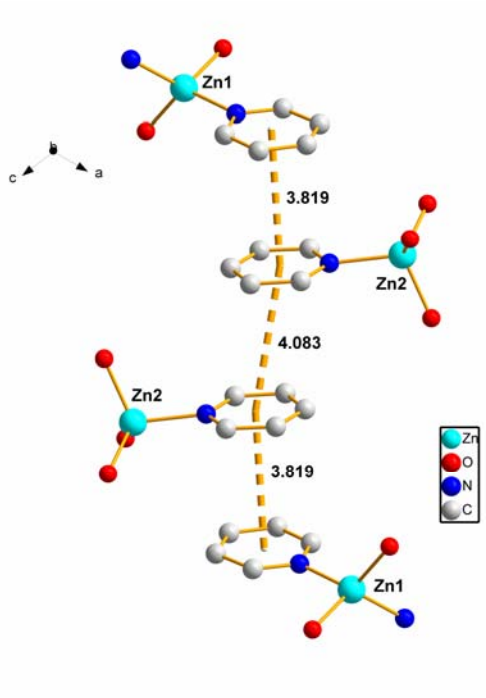

Fig.S8 The offset face-to-face π-π interreactions of the auxiliary py ligands in **4**

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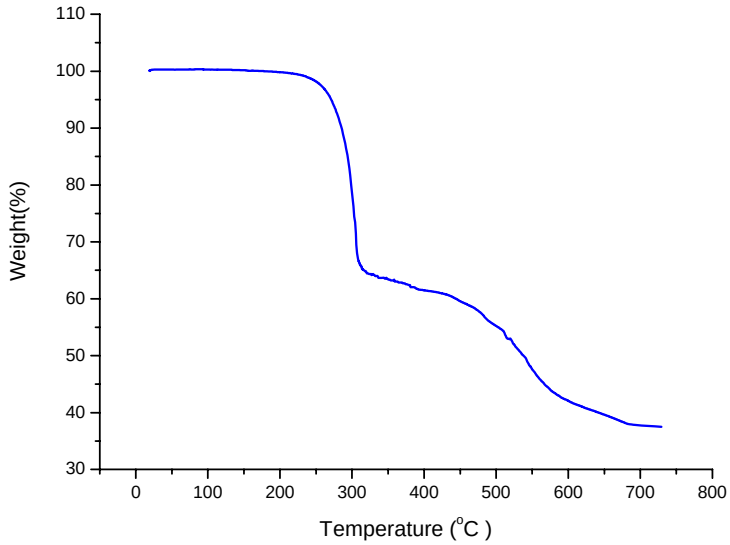
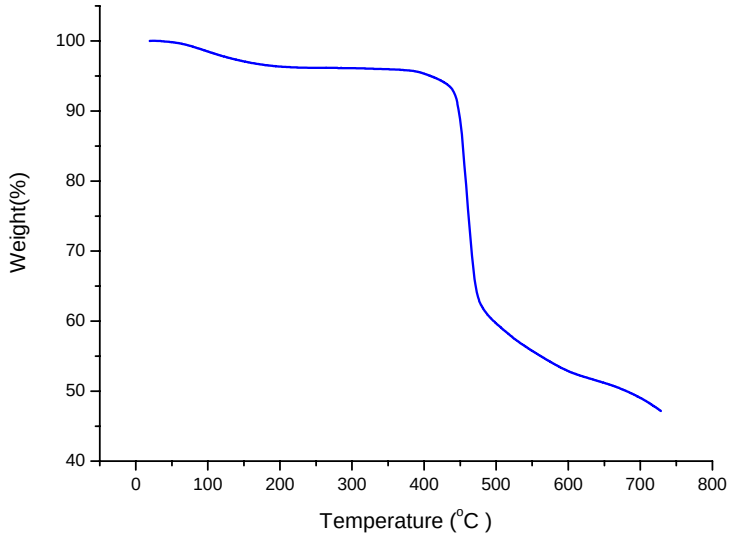


(a) TG curve of **1.**



(b) TG curve of **2.**

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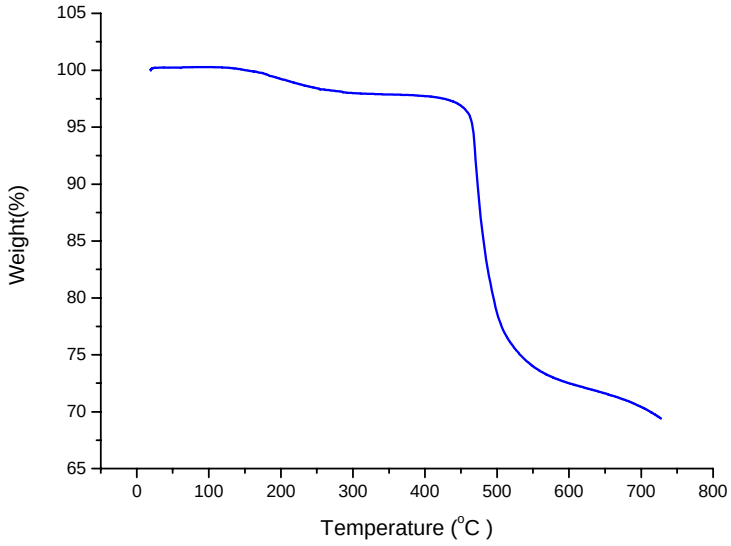
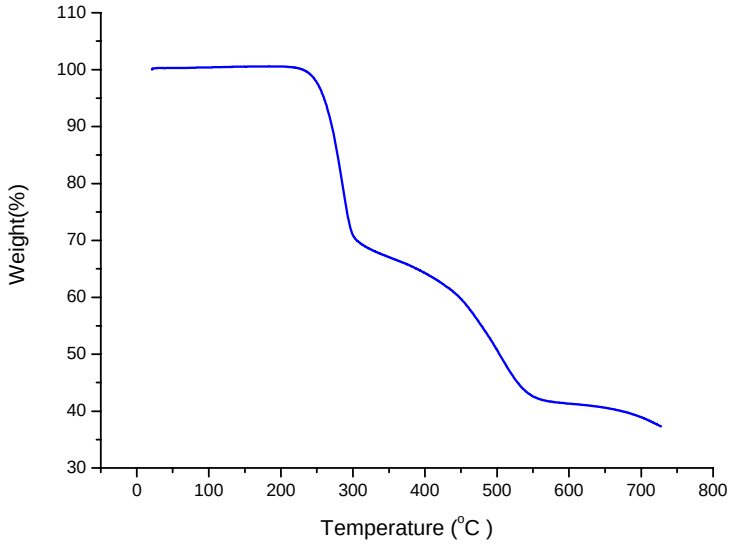


(c) TG curve of **3.**



(d) TG curve of **4.**

Fig S9 The TG figures of complexes **1-4**.