

***Supporting Information for***

**Isomeric phenylenediacetates as modular tecton for a series of Zn<sup>II</sup>/Cd<sup>II</sup>  
coordination polymers incorporating flexible bis (imidazole) co-ligands**

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**Table S1. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for complex 1.**

Complex 1			
Zn1-O2	1.932(4)	Zn1-N1	1.998(4)
Zn1-O3#1	1.943(3)	Zn1-N4#2	1.994(4)
O2-Zn1-N1	119.64(17)	O3#1-Zn1-N1	106.10(16)
O2-Zn1-N4#2	106.32(16)	O3#1-Zn1-N4#2	117.69(16)
O2-Zn1-O3#1	100.05(15)	N4#2-Zn1-N1	107.59(18)

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

**Table S2. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for complex 2.**

Complex 2			
Cd1-O1	2.442(7)	Cd1-O4#2	2.269(6)
Cd1-O2	2.365(6)	Cd1-N1	2.239(7)
Cd1-O3#2	2.592(6)	Cd1-N4#1	2.225(6)
N4#1-Cd1-N1	115.4(2)	N4#1-Cd1-O4#2	109.0(2)
N1-Cd1-O4#2	114.2(2)	N4#1-Cd1-O2	134.0(2)
N1-Cd1-O2	93.3(2)	O4#2-Cd1-O2	88.4(2)
N4#1-Cd1-O1	86.2(2)	N1-Cd1-O1	98.8(3)
O4#2-Cd1-O1	130.9(3)	O2-Cd1-O1	52.9(2)
N4#1-Cd1-O3#2	83.2(2)	N1-Cd1-O3#2	87.1(2)
O4#2-Cd1-O3#2	52.5(2)	O2-Cd1-O3#2	136.1(2)
O1-Cd1-O3#2	169.3(2)		

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

**Table S3. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for complex 3.**

Complex 3			
Zn1-O1	1.962(2)	Zn1-N1	1.996(3)
Zn1-O3#1	1.986(2)	Zn1-N3	2.025(3)
O1-Zn1-N3	107.35(12)	N3-Zn1-N1	110.49(11)
O1-Zn1-N1	118.59(11)	O3#1-Zn1-N3	98.27(11)
O1-Zn1-O3#1	113.26(11)	O3#1-Zn1-N1	98.27(11)

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

**Table S4. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for complex 4.**

Complex 4			
Cd1-O1	2.2617(16)	Cd1-O4#2	2.3147(18)
Cd1-O2	2.2884(17)	Cd1-O5#2	2.3531(18)
Cd1-O3#1	2.3961(17)	Cd1-N1	2.261(2)
O2-Cd1-O1	93.48(6)	N1-Cd1-O3#1	92.52(7)
O2-Cd1-N1	86.45(7)	O2-Cd1-O3#1	111.56(6)
N1-Cd1-O1	100.18(7)	O2-Cd1-O4#2	166.92(7)
N1-Cd1-O4#2	94.17(8)	O5-Cd1-O3	86.88(6)
O3#1-Cd1-O1	152.62(6)	O4#2-Cd1-O1	99.26(6)
O2-Cd1-O5#2	85.37(6)	N1-Cd1-O5#2	170.94(7)
O4-Cd1-O3	55.36(6)	O4#2-Cd1-O5#2	92.93(7)
O1-Cd1-O5#2	84.21(6)	O1-Cd1-O5	84.21(6)

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

**Table S5. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for complex 5.**

Complex 5			
Cd1-O1	2.357(3)	Cd1-O4#2	2.396(2)
Cd1-O2	2.465(3)	Cd1-N1	2.270(2)
Cd1-O3#2	2.331(2)	Cd1-N4#1	2.242(2)
O1-Cd1-O2	52.89(8)	N1-Cd1-O1	94.17(10)
O1-Cd1-O4#2	125.38(9)	N1-Cd1-O2	92.03(10)
O3#2-Cd1-O1	90.10(9)	N1-Cd1-O3#2	134.97(9)
O3#2-Cd1-O2	124.73(9)	N1-Cd1-O4#2	87.30(9)
O4#2-Cd1-O2	178.11(8)	N4#1-Cd1-O1	135.10(9)
O3#2-Cd1-O4#2	55.06(8)	N4#1-Cd1-O2	85.66(9)
N4#1-Cd1-N1	104.92(9)	N4#1-Cd1-O3#2	103.10(9)
N4#1-Cd1-O4#2	96.22(10)		

Symmetry transformations used to generate equivalent atoms: #1  $x+1, y, z+1$ ; #2  $x+1, y, z$ .

**Table S6. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for complex 6.**

Complex 6			
Zn1-O1	1.941(5)	Zn1-N1	2.019(5)
Zn1-O4	1.943(5)	Zn1-N4	2.012(5)
O1-Zn1-N1	119.1(2)	O1-Zn1-O4#1	96.9(3)
O1-Zn1-N4	112.3(3)	O4#1-Zn1-N4	116.9(2)
N1-Zn1-N4	98.0(2)	O4#1-Zn1-N1	114.8(2)

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

**Table S7. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for complex 7.**

Complex 7			
Cd1-O1	2.343(3)	Cd1-O3#2	2.375(3)
Cd1-O2	2.624(4)	Cd1-N1	2.258(5)
Cd1-O3#1	2.400(3)	Cd1-N4#3	2.285(4)
Cd1-O4#1	2.518(5)		
O1-Cd1-O2	51.99(13)	N1-Cd1-O1	89.95(17)
O1-Cd1-O3#1	159.84(12)	N1-Cd1-O2	87.57(15)
O1-Cd1-O4#1	148.36(13)	N1-Cd1-N4#3	171.91(18)
O1-Cd1-O3#2	90.17(12)	N1-Cd1-O3#2	87.99(15)
O3#2-Cd1-O2	147.80(12)	N1-Cd1-O3#1	88.99(18)
O3#2-Cd1-O3#1	69.75(13)	N1-Cd1-O4#3	88.5(2)
O3#2-Cd1-O4#1	121.38(12)	N4#3-Cd1-O3#2	99.10(13)
O3#1-Cd1-O4#1	51.64(12)	N4#3-Cd1-O3#1	94.80(13)
N4#3-Cd1-O1	90.01(13)	N4#3-Cd1-O4#1	87.34(16)
N4#3-Cd1-O2	86.03(12)	O4-Cd1-O2	96.36(13)
O3-Cd1-O2	141.98(12)		

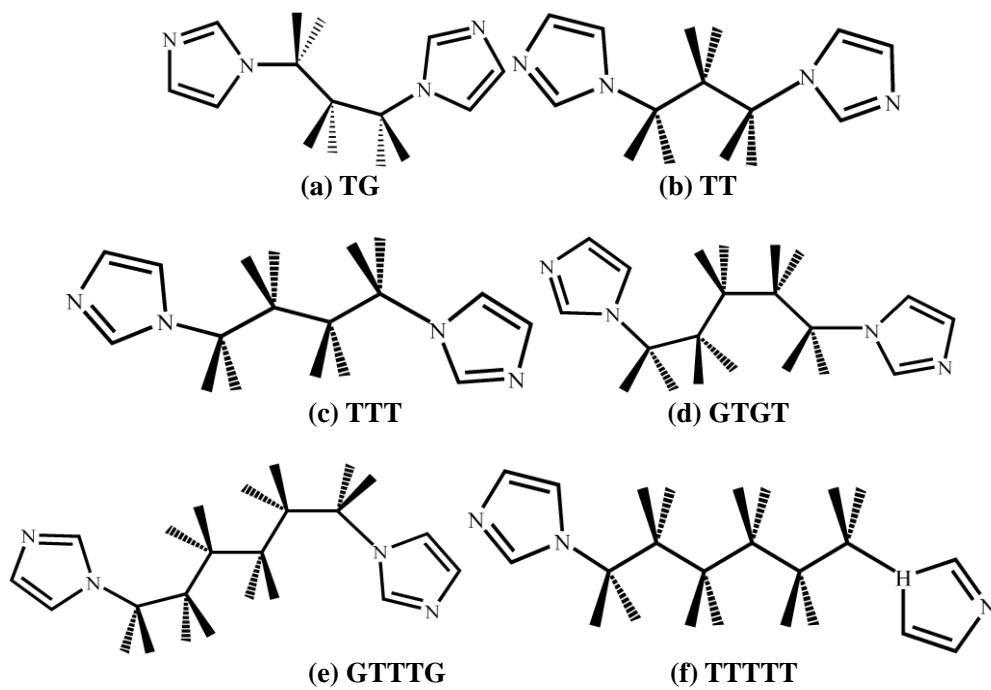
Symmetry transformations used to generate equivalent atoms: #1  $x+1/2, y-1/2, z$ ; #2  $-x, -y+2, -z+1$ ; #3  $x-1/2, -y+3/2, z+1/2$ .

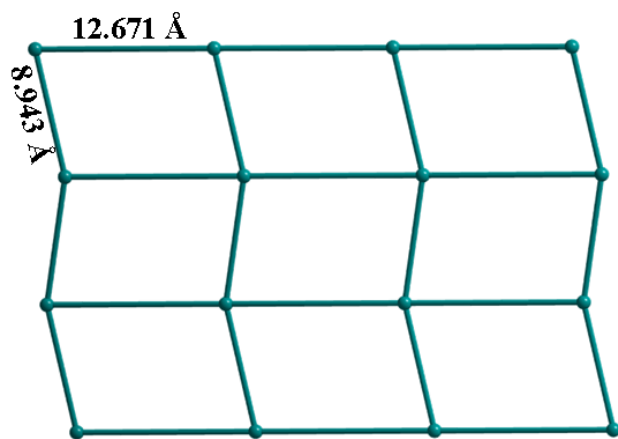
**Table S8. Geometrical Parameters ( $\text{\AA}, ^\circ$ ) of Hydrogen Bonds for the  $(\text{H}_2\text{O})_6$  cluster <sup>a</sup>**

D-H...A	d(D-H)	d(H...A)	d(D-A)	<(DHA)
O2W-H2WB...O1W	0.70	2.31	2.835(2)	136.5
O3W#2-H3WB...O2W	0.89	2.01	2.826(2)	151.7
O1W#3-H1WA...O3W#2	0.90	1.97	2.830(2)	159.1
O2W#3-H2WB...O1W#3	0.70	2.31	2.835(2)	136.5
O3W#1-H3WB...O2W#3	0.89	2.01	2.826(2)	151.7
O1W-H1WA...O3W#1	0.90	1.97	2.830(2)	159.1

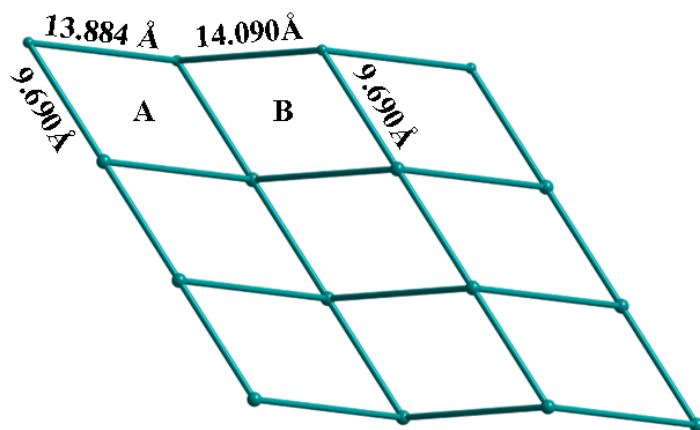
<sup>a</sup> Symmetry transformations used to generate equivalent atoms: #1:  $1-x, 1-y, 2-z$ ; #2:  $1+x, y, z$ ; #3:  $2-x, 1-y, 2-z$ .

**Scheme S1. Conformations of biim-n (n=3, 4, 5, 6) in coordination complexes (T = trans and G =gauche)**

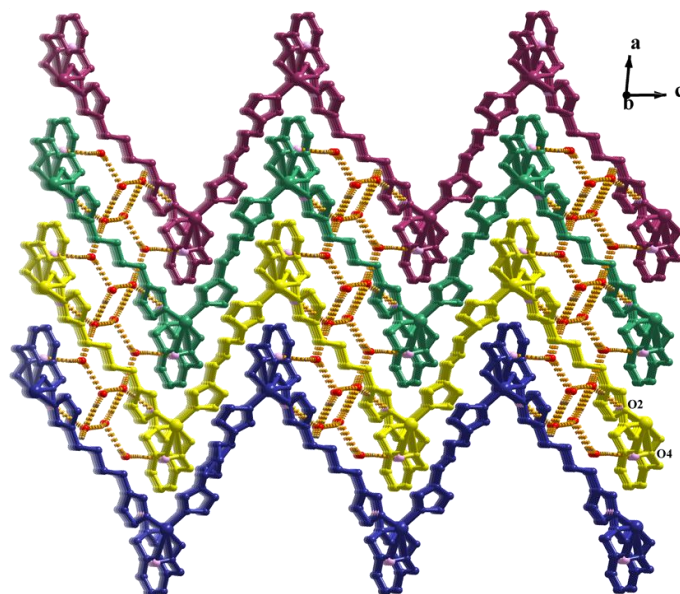




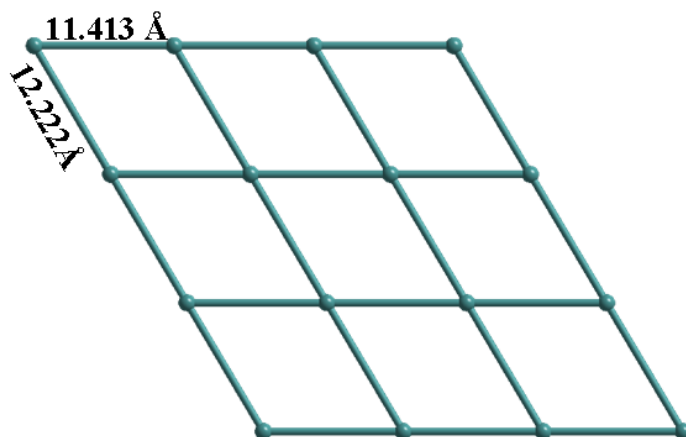
**Fig. S1** Schematic representation of undulated 4-sql net in **2**.



**Fig. S2** Schematic representation of undulated 4-sql net in **3**.

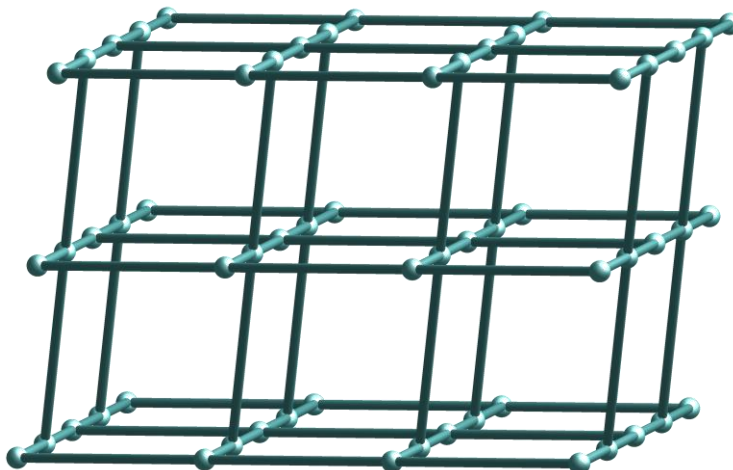


**Fig. S3** Packing diagram of the 3D supramolecular network in **3** viewed along the crystallographic *b* axis, all the hydrogen atoms were omitted for clarity.

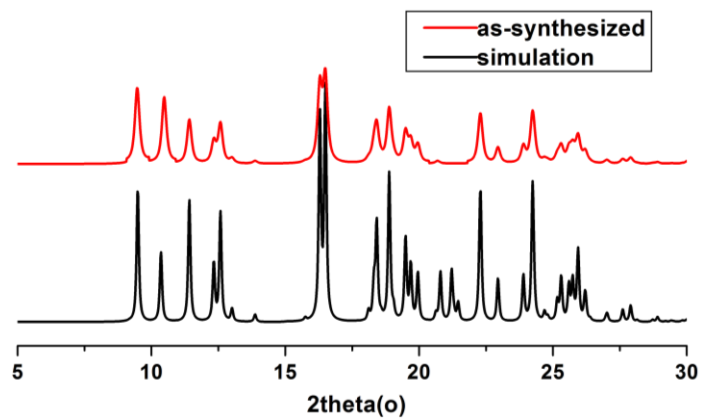


**Fig. S4** Schematic representation of planar 4-sqI net in **5**.

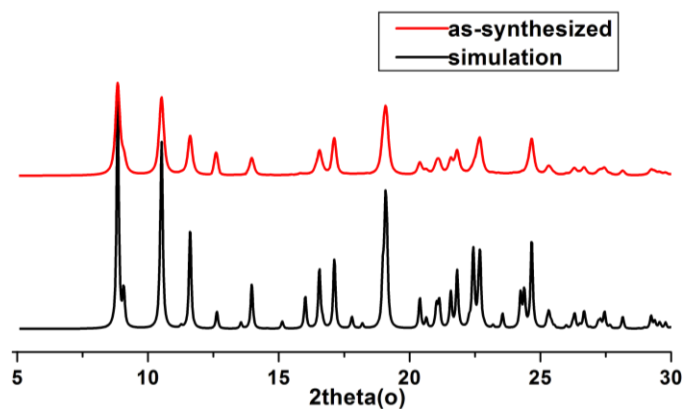




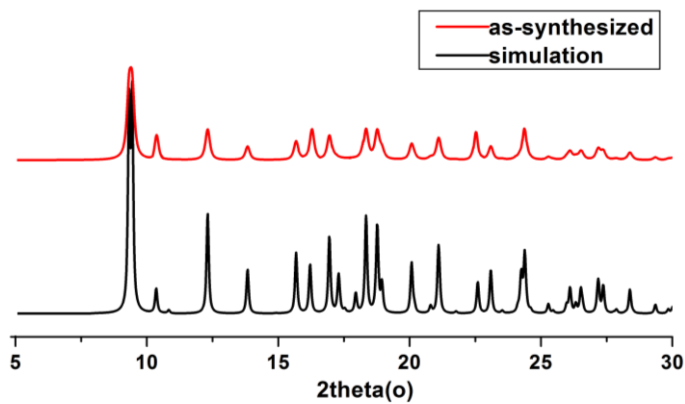
**Fig. S5** Schematic representation of 3D 4-connected CdS topology with point symbol of  $(4^2 \cdot 6)(4^2 \cdot 6^3 \cdot 8^3)$ .



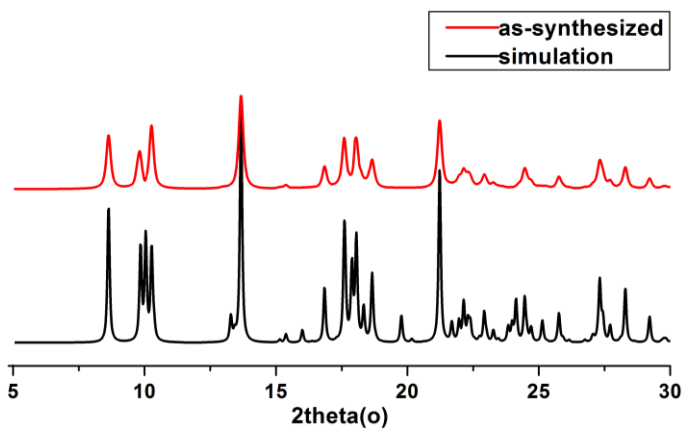
**Fig. S6** X-Ray power diffraction profiles of complex 1.



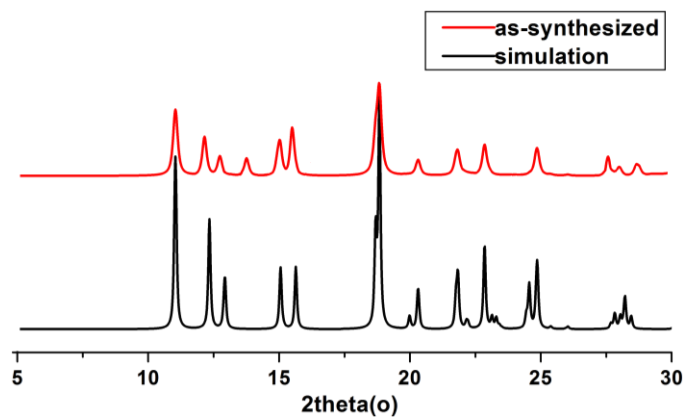
**Fig. S7** X-Ray power diffraction profiles of complex 2.



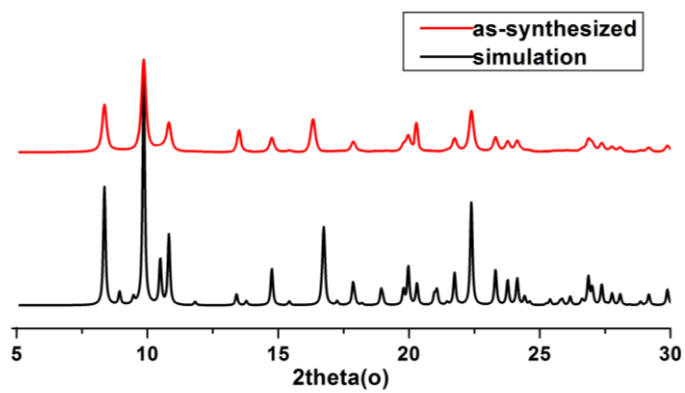
**Fig. S8** X-Ray power diffraction profiles of complex 4.



**Fig. S9** X-Ray power diffraction profiles of complex 5.



**Fig. S10** X-Ray power diffraction profiles of complex **6**.



**Fig.S11** X-Ray power diffraction profiles of complex **7**.

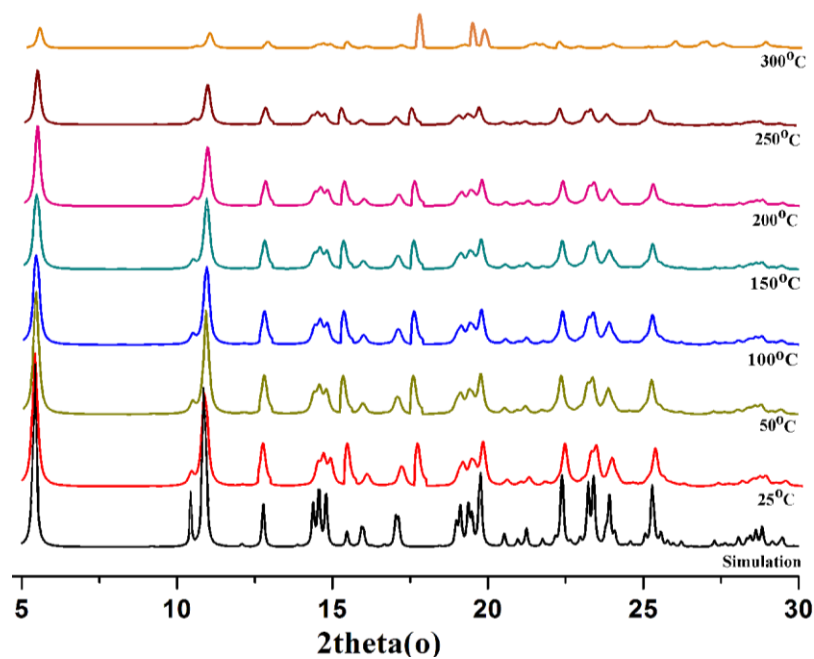


Fig. S12 Variable-temperature XRD patterns of complex 3.

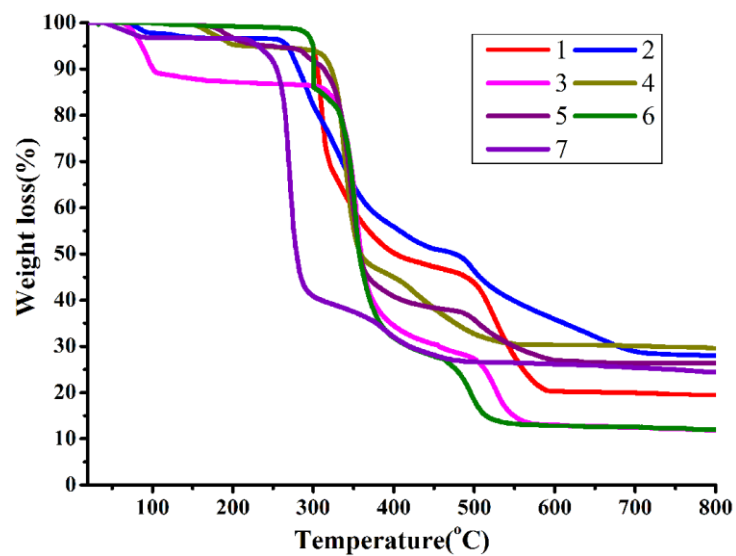


Fig. S13 The TGA of complexes 1-7.