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A series of metal-organic frameworks based on flexible (3,5-dicarboxyl-phenyl)-(4-(2′-carboxyl-phenyl)-benzyl) ether and various N-donor ligands: syntheses, topological structures, photoluminescence, and surface photovoltage properties

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Table S1. Hydrogen bonds for **H_3L** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(2)-H(2')···O(8)$^{\#1}$	0.82	1.76	2.575(3)	171.4
O(3)-H(3')···O(6)$^{\#2}$	0.82	1.84	2.652(3)	171.2
O(7)-H(7')···O(4)$^{\#3}$	0.82	1.88	2.697(3)	174.5
O(8)-H(8)···O(1)$^{\#4}$	0.82	1.92	2.699(5)	158.8
O(8)-H(8)···O(1')$^{\#4}$	0.82	2.00	2.820(5)	174.9

Symmetry codes for H_3L: $^{\#1}$ -x-7/4,y+1/4,z+1/4; $^{\#2}$ x-1/4,-y-3/4,z-1/4; $^{\#3}$ x+1/4,-y-3/4,z+1/4; $^{\#4}$ x+1/4,-y-1/4,z-1/4.

Table S1. Selected bond distances (Å) and angles (°) for **1**.

Zn(1)-O(8)	1.919(4)	Zn(1)-O(17)	1.926(4)
Zn(1)-O(11)$^{\#1}$	1.968(5)	Zn(1)-O(15)	2.012(5)
Zn(2)-O(17)	1.975(4)	Zn(2)-O(18)	2.071(4)
Zn(2)-O(7)$^{\#2}$	2.088(5)	Zn(2)-O(16)	2.098(5)
Zn(2)-O(13)$^{\#3}$	2.140(4)	Zn(2)-O(10)$^{\#1}$	2.367(5)
Zn(3)-O(19)	1.912(4)	Zn(3)-O(14)$^{\#3}$	1.942(5)
Zn(3)-O(18)	1.965(4)	Zn(3)-O(6)$^{\#2}$	1.987(5)
Zn(4)-O(16)	2.028(4)	Zn(4)-O(2)	2.047(4)
Zn(4)-O(18)$^{\#4}$	2.052(5)	Zn(4)-O(16)$^{\#4}$	2.140(4)
Zn(4)-O(15)	2.156(4)	Zn(4)-O(10)$^{\#1}$	2.237(5)
Zn(5)-O(1)$^{\#1}$	1.974(4)	Zn(5)-O(19)$^{\#5}$	1.972(5)
Zn(5)-O(4)	1.987(4)	Zn(5)-O(15)$^{\#1}$	2.020(4)
O(8)-Zn(1)-O(17)	115.4(2)	O(8)-Zn(1)-O(11)$^{\#1}$	112.2(2)
O(17)-Zn(1)-O(11)$^{\#1}$	108.9(2)	O(8)-Zn(1)-O(15)	106.87(19)
O(17)-Zn(1)-O(15)	109.2(2)	O(11)$^{\#1}$-Zn(1)-O(15)	103.4(2)
O(17)-Zn(2)-O(18)	169.89(18)	O(17)-Zn(2)-O(7)$^{\#2}$	92.78(19)
O(18)-Zn(2)-O(7)$^{\#2}$	90.22(17)	O(17)-Zn(2)-O(16)	94.73(19)
O(18)-Zn(2)-O(16)	80.78(17)	O(7)$^{\#2}$-Zn(2)-O(16)	167.75(18)
O(17)-Zn(2)-O(13)$^{\#3}$	88.88(19)	O(18)-Zn(2)-O(13)$^{\#3}$	100.44(17)
O(7)$^{\#2}$-Zn(2)-O(13)$^{\#3}$	95.71(19)	O(16)-Zn(2)-O(13)$^{\#3}$	94.09(18)

O(17)-Zn(2)-O(10)$^{\#1}$	85.55(17)	O(18)-Zn(2)-O(10)$^{\#1}$	84.74(15)
O(7)$^{\#2}$-Zn(2)-O(10)$^{\#1}$	91.11(18)	O(16)-Zn(2)-O(10)$^{\#1}$	79.87(17)
O(13)$^{\#3}$-Zn(2)-O(10)$^{\#1}$	171.40(17)	O(19)-Zn(3)-O(14)$^{\#3}$	112.2(2)
O(19)-Zn(3)-O(18)	106.73(19)	O(14)$^{\#3}$-Zn(3)-O(18)	117.71(19)
O(19)-Zn(3)-O(6)$^{\#2}$	114.7(2)	O(14)$^{\#3}$-Zn(3)-O(6)$^{\#2}$	109.9(2)
O(18)-Zn(3)-O(6)$^{\#2}$	94.69(19)	O(16)-Zn(4)-O(2)	170.9(2)
O(16)-Zn(4)-O(18)$^{\#4}$	96.60(18)	O(2)-Zn(4)-O(18)$^{\#4}$	90.50(19)
O(16)-Zn(4)-O(16)$^{\#4}$	82.44(18)	O(2)-Zn(4)-O(16)$^{\#4}$	93.18(16)
O(18)$^{\#4}$-Zn(4)-O(16)$^{\#4}$	80.21(16)	O(16)-Zn(4)-O(15)	94.53(16)
O(2)-Zn(4)-O(15)	90.50(16)	O(18)$^{\#4}$-Zn(4)-O(15)	95.23(17)
O(16)$^{\#4}$-Zn(4)-O(15)	174.15(17)	O(16)-Zn(4)-O(10)#1	84.54(18)
O(2)-Zn(4)-O(10)$^{\#1}$	87.69(19)	O(18)$^{\#4}$-Zn(4)-O(10)$^{\#1}$	172.52(15)
O(16)$^{\#4}$-Zn(4)-O(10)$^{\#1}$	92.65(16)	O(15)-Zn(4)-O(10)$^{\#1}$	92.04(16)
O(1)$^{\#1}$-Zn(5)-O(19)$^{\#5}$	104.5(2)	O(1)$^{\#1}$-Zn(5)-O(4)	107.92(19)
O(19)$^{\#5}$-Zn(5)-O(4)	106.68(19)	O(1)$^{\#1}$-Zn(5)-O(15)$^{\#1}$	103.71(18)
O(19)$^{\#5}$-Zn(5)-O(15)$^{\#1}$	111.42(19)	O(4)-Zn(5)-O(15)$^{\#1}$	121.3(2)

Symmetry codes for **1**: $^{\#1}$ x-1,y,z; $^{\#2}$ x,y,z-1; $^{\#3}$ –x+2,-y+1,-z+1; $^{\#4}$ -x+1,-y,-z+1; $^{\#5}$ -x,-y,-z+1.

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Zn(1)-O(14)$^{\#1}$	1.931(4)	Zn(1)-O(8)	1.958(3)
Zn(1)-O(1)	1.964(3)	Zn(1)-O(15)	1.998(3)
Zn(2)-O(13)$^{\#1}$	2.020(4)	Zn(2)-O(15)	2.030(3)
Zn(2)-O(10)$^{\#2}$	2.036(3)	Zn(2)-O(6)$^{\#3}$	2.040(4)
Zn(2)-O(2)	2.145(3)	Zn(2)-O(7)$^{\#3}$	2.328(4)
Zn(3)-O(4)$^{\#4}$	1.918(4)	Zn(3)-O(11)$^{\#2}$	1.923(3)
Zn(3)-O(15)	1.966(3)	Zn(3)-O(9)	2.007(3)
O(14)$^{\#1}$-Zn(1)-O(8)	111.35(15)	O(14)$^{\#1}$-Zn(1)-O(1)	113.07(15)
O(8)-Zn(1)-O(1)	114.83(14)	O(14)#1-Zn(1)-O(15)	111.75(13)
O(8)-Zn(1)-O(15)	103.55(13)	O(1)-Zn(1)-O(15)	101.43(14)

O(13)$^{\#1}$-Zn(2)-O(15)	110.83(14)	O(13)$^{\#1}$-Zn(2)-O(10)$^{\#2}$	87.09(16)
O(15)-Zn(2)-O(10)$^{\#2}$	93.35(15)	O(13)$^{\#1}$-Zn(2)-O(6)$^{\#3}$	99.62(15)
O(15)-Zn(2)-O(6)$^{\#3}$	148.59(15)	O(10)$^{\#2}$-Zn(2)-O(6)$^{\#3}$	95.73(15)
O(13)$^{\#1}$-Zn(2)-O(2)	88.34(16)	O(15)-Zn(2)-O(2)	85.48(13)
O(10)$^{\#2}$-Zn(2)-O(2)	174.54(17)	O(6)$^{\#3}$-Zn(2)-O(2)	87.97(14)
O(13)$^{\#1}$-Zn(2)-O(7)$^{\#3}$	157.32(15)	O(15)-Zn(2)-O(7)$^{\#3}$	91.42(14)
O(10)$^{\#2}$-Zn(2)-O(7)$^{\#3}$	87.27(16)	O(6)$^{\#3}$-Zn(2)-O(7)$^{\#3}$	59.17(14)
O(2)-Zn(2)-O(7)$^{\#3}$	98.08(15)	O(4)$^{\#4}$-Zn(3)-O(11)$^{\#2}$	115.72(14)
O(4)$^{\#4}$-Zn(3)-O(15)	114.66(15)	O(11)$^{\#2}$-Zn(3)-O(15)	115.00(14)
O(4)$^{\#4}$-Zn(3)-O(9)	105.82(16)	O(11)$^{\#2}$-Zn(3)-O(9)	108.98(15)
O(15)-Zn(3)-O(9)	93.67(13)		

Symmetry codes for **2**: $^{\#1}$ -x,-y,-z+1; $^{\#2}$ -x+0.5,-y+0.5,-z+0.5; $^{\#3}$ x+0.5,-y+0.5,z-0.5; $^{\#4}$ –x-0.5,y-0.5,-z+0.5.

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Zn(1)-O(1)	2.208(6)	Zn(1)-O(1)$^{\#1}$	2.208(6)
Zn(1)-O(7)$^{\#2}$	2.264(7)	Zn(1)-O(7)$^{\#3}$	2.264(7)
Zn(2)-O(6)$^{\#2}$	2.221(9)	Zn(2)-N(1)	2.249(9)
Zn(2)-O(3)$^{\#4}$	2.273(6)	Zn(2)-O(2)	2.285(7)
Zn(2)-O(1W)	2.344(7)	Zn(2)-O(4)$^{\#4}$	2.417(6)
O(1)-Zn(1)-O(1)$^{\#1}$	137.5(4)	O(1)-Zn(1)-O(7)$^{\#2}$	111.8(2)
O(1)$^{\#1}$-Zn(1)-O(7)$^{\#2}$	111.8(2)	O(1)-Zn(1)-O(7)$^{\#3}$	97.4(4)
O(1)$^{\#1}$-Zn(1)-O(7)$^{\#3}$	111.8(2)	O(7)$^{\#2}$-Zn(1)-O(7)$^{\#3}$	97.4(4)
O(6)$^{\#2}$-Zn(2)-N(1)	154.0(3)	O(6)$^{\#2}$-Zn(2)-O(3)$^{\#4}$	108.5(3)
N(1)-Zn(2)-O(3)$^{\#4}$	93.9(3)	O(6)$^{\#2}$-Zn(2)-O(2)	80.8(3)
N(1)-Zn(2)-O(2)	86.3(3)	O(3)#4-Zn(2)-O(2)	90.1(2)
O(6)$^{\#2}$-Zn(2)-O(1W)	78.1(3)	N(1)-Zn(2)-O(1W)	90.4(3)
O(3)$^{\#4}$-Zn(2)-O(1W)	146.9(2)	O(2)-Zn(2)-O(1W)	123.0(2)
O(6)$^{\#2}$-Zn(2)-O(4)$^{\#4}$	115.3(3)	N(1)-Zn(2)-O(4)$^{\#4}$	88.0(3)
O(3)$^{\#4}$-Zn(2)-O(4)$^{\#4}$	55.6(2)	O(2)-Zn(2)-O(4)$^{\#4}$	144.6(2)

O(1W)-Zn(2)-O(4)$^{\#4}$	91.9(2)		

Symmetry codes for **3**: $^{\#1}$ –x-0.5,y,-z-0.5; $^{\#2}$ –x-1,-y+2,-z; $^{\#3}$ x+0.5,-y+2,z-0.5; $^{\#4}$ –x,-y+1,-z.

Table S4. Selected bond distances (Å) and angles (°) for **4**.

Cd(1)-O(2)$^{\#1}$	2.188(2)	Cd(1)-O(2)	2.188(2)
Cd(1)-O(6)$^{\#2}$	2.264(3)	Cd(1)-O(6)$^{\#3}$	2.264(3)
Cd(2)-O(7)$^{\#3}$	2.207(3)	Cd(2)-N(1)	2.234(4)
Cd(2)-O(3)$^{\#4}$	2.281(3)	Cd(2)-O(1)	2.285(2)
Cd(2)-O(1W)	2.324(3)	Cd(2)-O(4)$^{\#4}$	2.417(3)
O(2)$^{\#1}$-Cd(1)-O(2)	137.20(16)	O(2)$^{\#1}$-Cd(1)-O(6)$^{\#2}$	112.09(11)
O(2)-Cd(1)-O(6)$^{\#2}$	96.06(10)	O(2)$^{\#1}$-Cd(1)-O(6)$^{\#3}$	96.06(10)
O(2)-Cd(1)-O(6)$^{\#3}$	112.09(11)	O(6)$^{\#2}$-Cd(1)-O(6)$^{\#3}$	97.42(16)
O(7)$^{\#3}$-Cd(2)-N(1)	154.29(15)	O(7)$^{\#3}$-Cd(2)-O(3)$^{\#4}$	107.87(13)
N(1)-Cd(2)-O(3)$^{\#4}$	94.03(13)	O(7)$^{\#3}$-Cd(2)-O(1)	80.44(11)
N(1)-Cd(2)-O(1)	86.30(11)	O(3)$^{\#4}$-Cd(2)-O(1)	90.26(10)
O(7)$^{\#3}$-Cd(2)-O(1W)	79.52(12)	N(1)-Cd(2)-O(1W)	89.74(13)
O(3)$^{\#4}$-Cd(2)-O(1W)	146.38(10)	O(1)-Cd(2)-O(1W)	123.33(10)
O(7)#3-Cd(2)-O(4)$^{\#4}$	115.37(12)	N(1)-Cd(2)-O(4)$^{\#4}$	87.95(11)
O(3)$^{\#4}$-Cd(2)-O(4)$^{\#4}$	55.43(9)	O(1)-Cd(2)-O(4)$^{\#4}$	144.69(10)
O(1W)-Cd(2)-O(4)$^{\#4}$	91.42(9)		

Symmetry codes for **4**: $^{\#1}$ –x+1.5,y,-z+1.5; $^{\#2}$ x-0.5,-y+1,z+0.5; $^{\#3}$ -x+2,-y+1,-z+1; $^{\#4}$ –x+1,-y,-z+1.

Table S5. Selected bond distances (Å) and angles (°) for **5**.

Pb(1)-O(2)	2.591(9)	Pb(1)-O(2)$^{\#1}$	2.591(9)
Pb(1)-O(15)	2.688(8)	Pb(1)-O(15)$^{\#1}$	2.688(8)
Pb(1)-O(11)$^{\#2}$	2.697(8)	Pb(1)-O(11)$^{\#3}$	2.697(8)
Pb(1)-O(10)$^{\#2}$	2.735(10)	Pb(1)-O(10)$^{\#3}$	2.735(10)
Pb(2)-O(15)	2.335(7)	Pb(2)-O(13)$^{\#4}$	2.387(7)
Pb(2)-O(11)$^{\#2}$	2.468(9)	Pb(2)-O(9)	2.554(9)

Pb(2)-O(1)	2.684(10)	Pb(3)-O(15)	2.287(7)
Pb(3)-O(1W)	2.466(10)	Pb(3)-O(8)	2.569(8)
Pb(3)-O(9)	2.667(9)	Pb(3)-O(10)$^{\#3}$	2.667(8)
Pb(4)-O(6)$^{\#5}$	2.388(9)	Pb(4)-O(3)	2.412(13)
Pb(4)-O(2W)$^{\#6}$	2.45(3)	Pb(4)-O(7)$^{\#5}$	2.515(10)
Pb(4)-O(4)	2.695(9)	Pb(4)-O(6)$^{\#7}$	2.729(10)
Pb(4)-O(2W')$^{\#6}$	2.75(2)	Pb(4)-C(22)$^{\#5}$	2.833(14)
O(2)-Pb(1)-O(15)	93.7(3)	O(2)$^{\#1}$-Pb(1)-O(15)	86.3(3)
O(2)-Pb(1)-O(15)$^{\#1}$	86.3(3)	O(2)$^{\#1}$-Pb(1)-O(15)$^{\#1}$	93.7(3)
O(2)-Pb(1)-O(11)$^{\#2}$	83.1(3)	O(2)$^{\#1}$-Pb(1)-O(11)$^{\#2}$	96.9(3)
O(15)-Pb(1)-O(11)$^{\#2}$	66.3(2)	O(15)$^{\#1}$-Pb(1)-O(11)$^{\#2}$	113.7(2)
O(2)-Pb(1)-O(11)$^{\#3}$	96.9(3)	O(2)$^{\#1}$-Pb(1)-O(11)$^{\#3}$	83.1(3)
O(15)-Pb(1)-O(11)$^{\#3}$	113.7(2)	O(15)$^{\#1}$-Pb(1)-O(11)$^{\#3}$	66.3(2)
O(2)-Pb(1)-O(10)$^{\#2}$	85.5(3)	O(2)$^{\#1}$-Pb(1)-O(10)$^{\#2}$	94.5(3)
O(15)-Pb(1)-O(10)$^{\#2}$	112.7(3)	O(15)$^{\#1}$-Pb(1)-O(10)$^{\#2}$	67.3(3)
O(11)$^{\#2}$-Pb(1)-O(10)$^{\#2}$	46.7(3)	O(11)$^{\#3}$-Pb(1)-O(10)$^{\#2}$	133.3(3)
O(2)-Pb(1)-O(10)$^{\#3}$	94.5(3)	O(2)$^{\#1}$-Pb(1)-O(10)$^{\#3}$	85.5(3)
O(15)-Pb(1)-O(10)$^{\#3}$	67.3(3)	O(15)$^{\#1}$-Pb(1)-O(10)$^{\#3}$	112.7(3)
O(11)$^{\#2}$-Pb(1)-O(10)$^{\#3}$	133.3(3)	O(11)$^{\#3}$-Pb(1)-O(10)$^{\#3}$	46.7(3)
O(15)-Pb(2)-O(13)$^{\#4}$	88.3(3)	O(15)-Pb(2)-O(11)$^{\#2}$	75.6(3)
O(13)$^{\#4}$-Pb(2)-O(11)$^{\#2}$	83.1(3)	O(15)-Pb(2)-O(9)	72.7(3)
O(13)$^{\#4}$-Pb(2)-O(9)	89.1(3)	O(11)$^{\#2}$-Pb(2)-O(9)	147.5(3)
O(15)-Pb(2)-O(1)	66.2(3)	O(13)#4-Pb(2)-O(1)	153.2(3)
O(11)$^{\#2}$-Pb(2)-O(1)	97.5(3)	O(9)-Pb(2)-O(1)	76.0(3)
O(15)-Pb(3)-O(1W)	86.0(3)	O(15)-Pb(3)-O(8)	94.8(3)
O(1W)-Pb(3)-O(8)	75.7(3)	O(15)-Pb(3)-O(9)	71.2(3)
O(1W)-Pb(3)-O(9)	116.8(3)	O(8)-Pb(3)-O(9)	50.0(2)
O(15)-Pb(3)-O(10)$^{\#3}$	74.1(3)	O(1W)-Pb(3)-O(10)$^{\#3}$	77.1(3)
O(8)-Pb(3)-O(10)$^{\#3}$	151.2(3)	O(9)-Pb(3)-O(10)$^{\#3}$	141.2(3)

O(6)$^{\#5}$-Pb(4)-O(3)	84.7(4)	O(6)$^{\#5}$-Pb(4)-O(2W)$^{\#6}$	120.2(7)
O(3)-Pb(4)-O(2W)$^{\#6}$	95.0(9)	O(6)$^{\#5}$-Pb(4)-O(7)$^{\#5}$	53.6(3)
O(3)-Pb(4)-O(7)$^{\#5}$	74.1(4)	O(2W)$^{\#6}$-Pb(4)-O(7)$^{\#5}$	68.9(7)
O(6)$^{\#5}$-Pb(4)-O(4)	77.6(3)	O(3)-Pb(4)-O(4)	49.8(3)
O(2W)$^{\#6}$-Pb(4)-O(4)	141.2(9)	O(7)$^{\#5}$-Pb(4)-O(4)	108.2(4)
O(6)$^{\#5}$-Pb(4)-O(6)$^{\#7}$	68.2(3)	O(3)-Pb(4)-O(6)$^{\#7}$	119.3(4)
O(2W)$^{\#6}$-Pb(4)-O(6)$^{\#7}$	145.9(8)	O(7)$^{\#5}$-Pb(4)-O(6)$^{\#7}$	119.3(4)
O(4)-Pb(4)-O(6)$^{\#7}$	70.9(3)	O(6)$^{\#5}$-Pb(4)-O(2W')$^{\#6}$	126.0(5)
O(3)-Pb(4)-O(2W')$^{\#6}$	64.8(6)	O(2W)$^{\#6}$-Pb(4)-O(2W')$^{\#6}$	33.2(8)
O(7)$^{\#5}$-Pb(4)-O(2W')$^{\#6}$	74.9(5)	O(4)-Pb(4)-O(2W')$^{\#6}$	108.0(6)
O(6)$^{\#7}$-Pb(4)-O(2W')$^{\#6}$	165.6(5)		

Symmetry codes for **5**: $^{\#1}$ –x,-y,-z+2; $^{\#2}$ -x-1,-y,-z+2; $^{\#3}$ x+1,y,z; $^{\#4}$ x,y-1,z; $^{\#5}$ -x,-y,-z+1; $^{\#6}$ -x,-y+2,-z+2.

Table S6. Selected bond distances (Å) and angles (°) for **6**.

Zn(1)-O(8)	1.940(4)	Zn(1)-N(1)	1.945(6)
Zn(1)-N(1)$^{\#1}$	1.945(6)	Zn(1)-O(1)$^{\#1}$	2.102(4)
Zn(1)-O(1)	2.102(4)	Zn(1)-O(7)$^{\#2}$	2.243(7)
Zn(1)-O(7)$^{\#3}$	2.243(7)	Zn(2)-O(2)	1.950(3)
Zn(2)-O(8)	1.9513(17)	Zn(2)-O(4)$^{\#4}$	1.966(3)
Zn(3)-N(4)$^{\#4}$	2.018(14)	Zn(3)-N(4)$^{\#5}$	2.018(14)
Zn(3)-O(3)$^{\#5}$	2.072(4)	Zn(3)-O(3)$^{\#4}$	2.072(4)
Zn(3)-O(7')$^{\#2}$	2.158(7)	Zn(3)-O8	1.961(4)
O(8)-Zn(1)-N(1)	153.3(2)	O(8)-Zn(1)-N(1)$^{\#1}$	153.3(2)
N(1)-Zn(1)-N(1)$^{\#1}$	26.2(4)	O(8)-Zn(1)-O(1)$^{\#1}$	99.67(13)
N(1)-Zn(1)-O(1)$^{\#1}$	88.2(2)	N(1)$^{\#1}$-Zn(1)-O(1)$^{\#1}$	106.3(2)
O(8)-Zn(1)-O(1)	99.67(13)	N(1)-Zn(1)-O(1)	106.3(2)
N(1)$^{\#1}$-Zn(1)-O(1)	88.2(2)	O(1)$^{\#1}$-Zn(1)-O(1)	86.7(2)
O(8)-Zn(1)-O(7')$^{\#2}$	89.3(2)	N(1)-Zn(1)-O(7')$^{\#2}$	65.5(2)
N(1)$^{\#1}$-Zn(1)-O(7')$^{\#2}$	85.9(3)	O(1)$^{\#1}$-Zn(1)-O(7')$^{\#2}$	169.8(2)

O(1)-Zn(1)-O(7')$^{\#2}$	87.0(2)	O(8)-Zn(1)-O(7')$^{\#3}$	89.3(2)
N(1)-Zn(1)-O(7')$^{\#3}$	65.5(2)	N(1)$^{\#1}$-Zn(1)-O(7')$^{\#3}$	65.5(2)
O(1)$^{\#1}$-Zn(1)-O(7')$^{\#3}$	169.8(2)	O(1)-Zn(1)-O(7')$^{\#3}$	87.0(2)
O(7)$^{\#2}$-Zn(1)-O(7')$^{\#3}$	98.1(4)	O(2)-Zn(2)-O(8)	112.36(16)
O(2)-Zn(2)-O(4)$^{\#4}$	110.28 (15)	O(8)-Zn(2)-O(4)$^{\#4}$	112.00(16)
O(2)-Zn(2)-O(6)$^{\#2}$	108.45(16)	O(8)-Zn(2)-O(6)$^{\#2}$	108.44(16)
O(4)$^{\#4}$-Zn(2)-O(6)$^{\#3}$	104.97(15)	O(8)-Zn(3)-N(4)$^{\#4}$	150.4(4)
O(8)-Zn(3)-N(4)$^{\#5}$	150.4(4)	N(4)$^{\#5}$-Zn(3)-N(4)$^{\#4}$	31.0(8)
O(8)-Zn(3)-O(3)$^{\#5}$	100.66(14)	N(4)$^{\#4}$-Zn(3)-O(3)$^{\#5}$	86.0(4)
N(4)$^{\#5}$-Zn(3)-O(3)$^{\#5}$	108.1(4)	O(8)-Zn(3)-O(3)$^{\#4}$	100.66(14)
N(4)$^{\#4}$-Zn(3)-O(3)$^{\#4}$	108.1(4)	N(6)$^{\#5}$-Zn(3)-O(3)$^{\#4}$	86.0(4)
O(3)$^{\#4}$-Zn(3)-O(3)$^{\#5}$	90.9(2)	O(8)-Zn(3)-O(7)$^{\#2}$	88.8(2)
N(4)$^{\#4}$-Zn(3)-O(7)$^{\#2}$	62.4(4)	N(4)$^{\#5}$-Zn(3)-O(7)$^{\#2}$	85.0(4)
O(3)$^{\#4}$-Zn(3)-O(7)$^{\#2}$	88.9(2)	O(3)$^{\#4}$-Zn(3)-O(7)$^{\#3}$	170.5(2)
O(8)-Zn(3)-O(7)$^{\#3}$	88.8(2)	N(4)$^{\#4}$-Zn(3)-O(7)$^{\#3}$	85.0(5)
N(4)$^{\#5}$-Zn(3)-O(7)$^{\#3}$	62.4(4)	O(3)$^{\#4}$-Zn(3)-O(7)$^{\#3}$	170.5(2)
O(3)$^{\#5}$-Zn(3)-O(7)$^{\#3}$	88.9(2)	O(7)$^{\#3}$-Zn(3)-O(7')$^{\#3}$	89.7(4)

Symmetry codes for **6**: $^{\#1}$ x,-y+0.5,z; $^{\#2}$ –x+1,-y,-z+1; $^{\#3}$ -x+1,y+0.5,-z+1; $^{\#4}$ x,y,z-1; $^{\#5}$ x,-y+0.5,z-1.

Table S7. Selected bond distances (Å) and angles (°) for **7**.

Zn(1)-N(1)	2.005(4)	Zn(1)-O(1)	2.012(3)
Zn(1)-O(2)$^{\#1}$	2.031(3)	Zn(1)-O(7)$^{\#2}$	2.063(3)
Zn(1)-O(6)$^{\#3}$	2.073(3)	N(1)-Zn(1)-O(1)	102.93(14)
N(1)-Zn(1)-O(2)$^{\#1}$	97.98(14)	O(1)-Zn(1)-O(2)$^{\#1}$	159.09(14)
N(1)-Zn(1)-O(7)$^{\#2}$	102.98(14)	O(1)-Zn(1)-O(7)$^{\#2}$	86.21(15)
O(2)$^{\#1}$-Zn(1)-O(7)$^{\#2}$	89.57(14)	N(1)-Zn(1)-O(6)$^{\#3}$	97.50(14)
O(1)-Zn(1)-O(6)$^{\#3}$	87.73(14)	O(2)$^{\#1}$-Zn(1)-O(6)$^{\#3}$	89.14(14)
O(7)$^{\#2}$-Zn(1)-O(6)$^{\#3}$	159.46(13)		

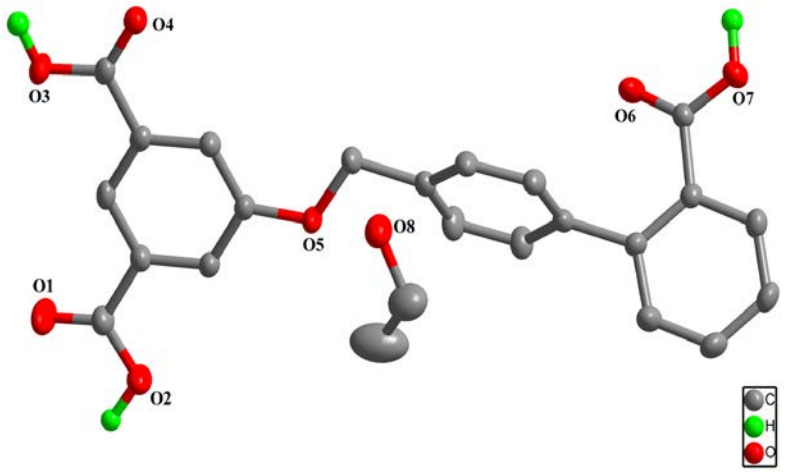
Symmetry codes for **7**: $^{\#1}$ –x+1,-y+1,-z+1; $^{\#2}$ –x,-y+1,-z; $^{\#3}$ x+1,y,z+1.

Table S8. Selected bond distances (Å) and angles (°) for **8**.

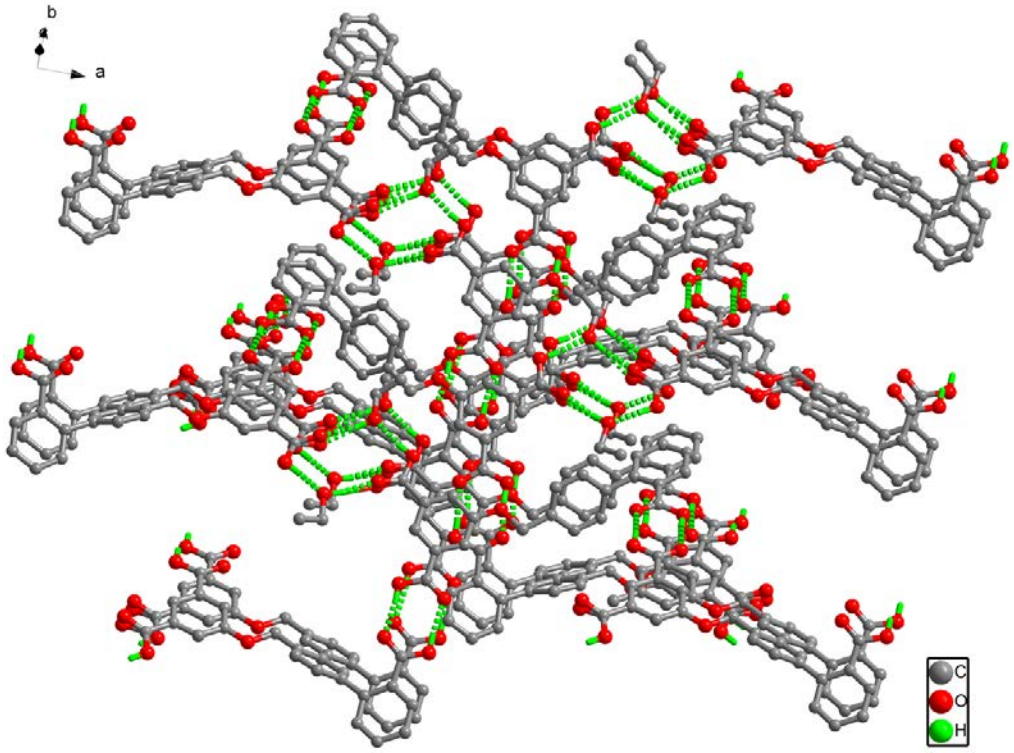
Zn(1)-O(1)	1.999(3)	Zn(1)-O(2)$^{\#1}$	2.003(3)
Zn(1)-N(1)	2.022(3)	Zn(1)-O(7)$^{\#2}$	2.070(3)
Zn(1)-O(6)$^{\#3}$	2.129(3)	Zn(1)-Zn(1)$^{\#1}$	2.9891(8)
Zn(2)-O(3)	1.953(2)	Zn(2)-O(3)$^{\#4}$	1.953(3)
Zn(2)-N(3)$^{\#4}$	2.036(4)	Zn(2)-N(3)	2.036(4)
O(1)-Zn(1)-O(2)$^{\#1}$	157.63(12)	O(1)-Zn(1)-N(1)	100.76(13)
O(2)$^{\#1}$-Zn(1)-N(1)	101.59(13)	O(1)-Zn(1)-O(7)$^{\#2}$	87.83(12)
O(2)$^{\#1}$-Zn(1)-O(7)$^{\#2}$	86.56(12)	N(1)-Zn(1)-O(7)$^{\#2}$	107.03(12)
O(1)-Zn(1)-O(6)$^{\#3}$	89.66(11)	O(2)$^{\#1}$-Zn(1)-O(6)$^{\#3}$	87.92(11)
N(1)-Zn(1)-O(6)$^{\#3}$	93.84(12)	O(7)$^{\#2}$-Zn(1)-O(6)$^{\#3}$	159.09(11)
O(3)$^{\#4}$-Zn(2)-O(3)	101.04(19)	O(3)-Zn(2)-N(3)$^{\#4}$	116.63(14)
O(3)$^{\#4}$-Zn(2)-N(3)$^{\#4}$	111.02(16)	O(3)-Zn(2)-N(3)	111.02(16)
O(3)$^{\#4}$-Zn(2)-N(3)	116.63(14)	N(3)$^{\#4}$-Zn(2)-N(3)	101.2(3)

Symmetry codes for **8**: $^{\#1}$ –x+0.5,-y+0.5,-z; $^{\#2}$ –x-0.5,y+0.5,z; $^{\#3}$ -x+1,-y,-z; $^{\#4}$ –x+1,y,-z-0.5.

Structure of $H_3L \cdot 0.5CH_3CH_2OH$. Single-crystal X-ray diffraction analysis reveals that **H_3L** crystallizes in the orthorhombic space group *Fdd2* and displays a discrete structure. As illustrated in Figure 1a, the discrete structure of **H_3L** consists of one L molecule, and a half ethanol molecule.

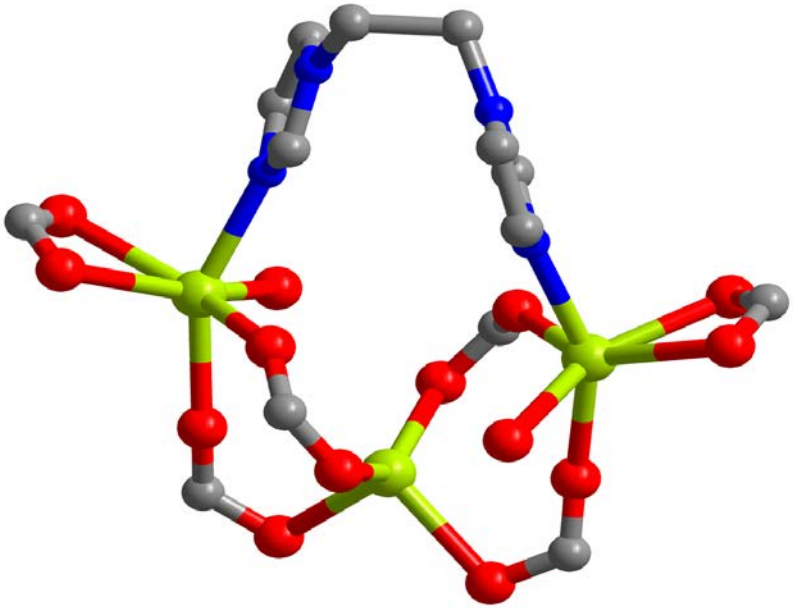


(a)

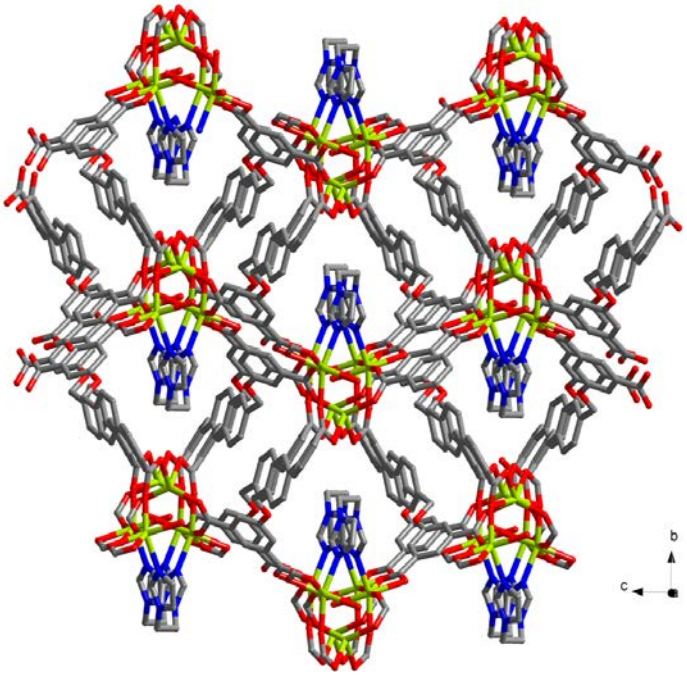


(b)

Fig. S1 (a) Crystal structure of H_3L with hydrogen atoms of the carbon atoms omitted for clarity molecules are omitted for clarity (30% probability displacement ellipsoids). (b) 3D supramolecular structure generated by O-H···O hydrogen-bonding interaction in H_3L, and H_3L interaction with alcohol molecules.

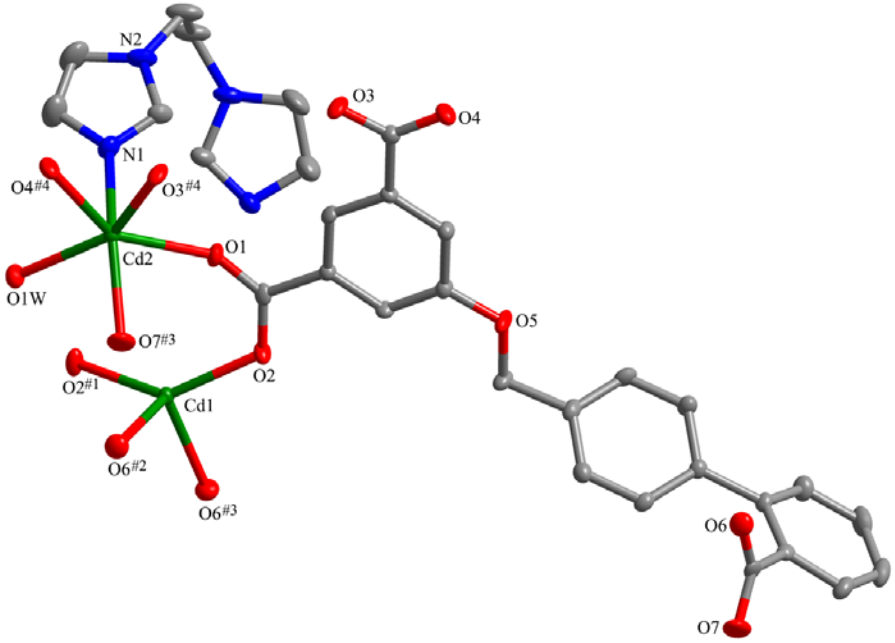


(a)

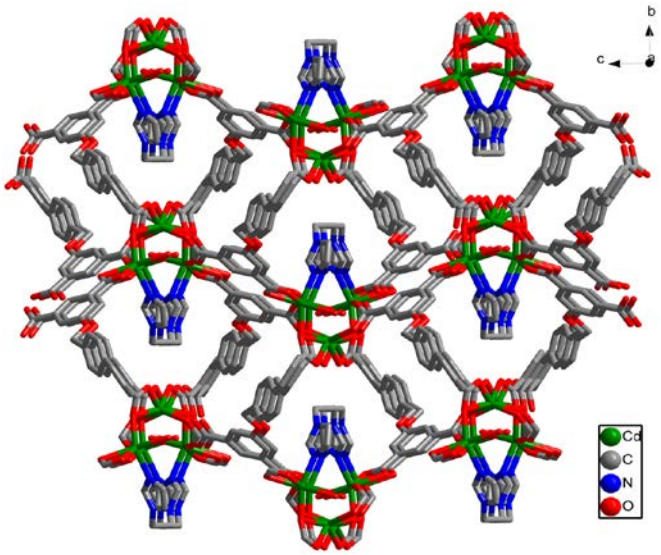


(b)

Fig. S2 (a) Ball-and-stick view of the trinuclear zinc cluster of **3**. (b) 3D framework formed by trinuclear zinc units, L anions, and BIME ligands.



(a)



(b)

Fig. S3 (a) Coordination environments of the Cd(II) ions in **4** with the free solvent water molecules are omitted for clarity (30% probability displacement ellipsoids). Symmetry codes: $^{\#1}$ = -x+1.5, y, -z+1.5; $^{\#2}$ = x-0.5, -y+1, z+0.5; $^{\#3}$ = -x+2, -y+1, -z+1; $^{\#4}$ = -x+1, -y, -z+1. (b) Schematic representation of the 3D heart-shaped framework formed by trinuclear cadmium clusters, L anions, and BIME ligands.

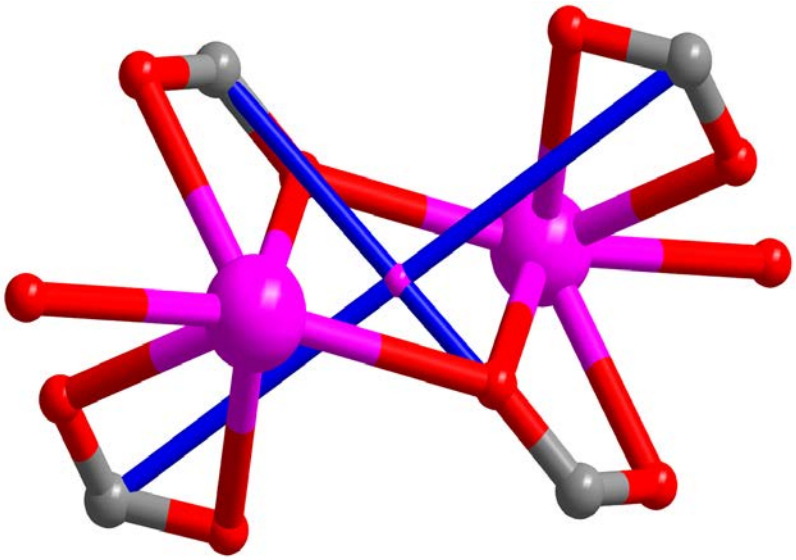


Fig. S4 The paddle-wheel-like dimer of **5**.

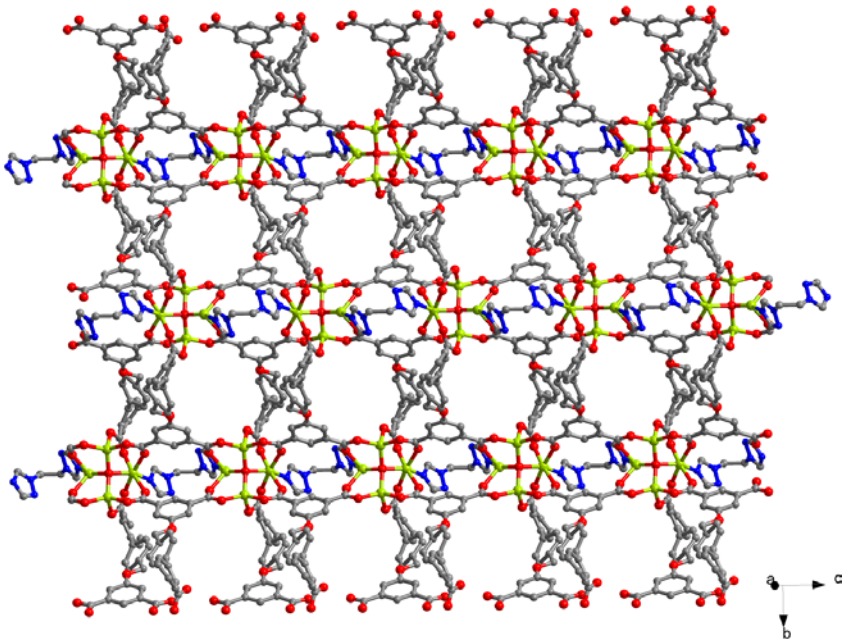


Fig. S5 Schematic representation of the 2D layer formed by tetranuclear zinc units, L anions and BIME ligands of **6**.

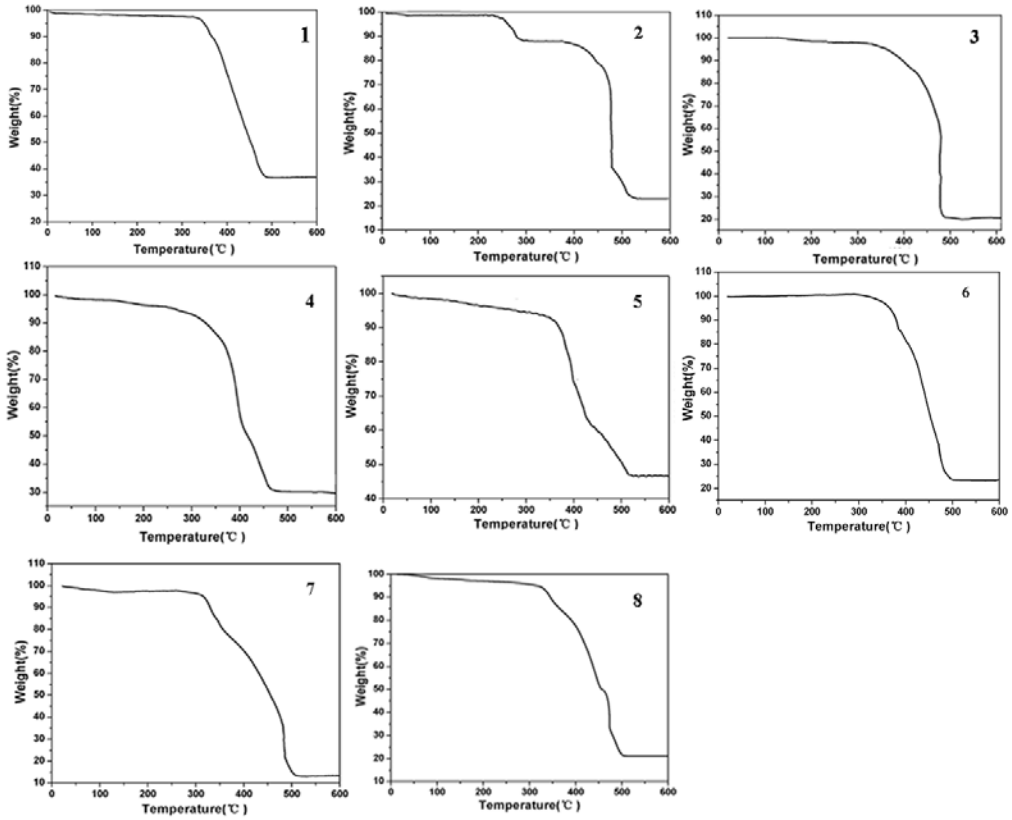


Fig. S6 The TGA curves of compounds **1-8**.

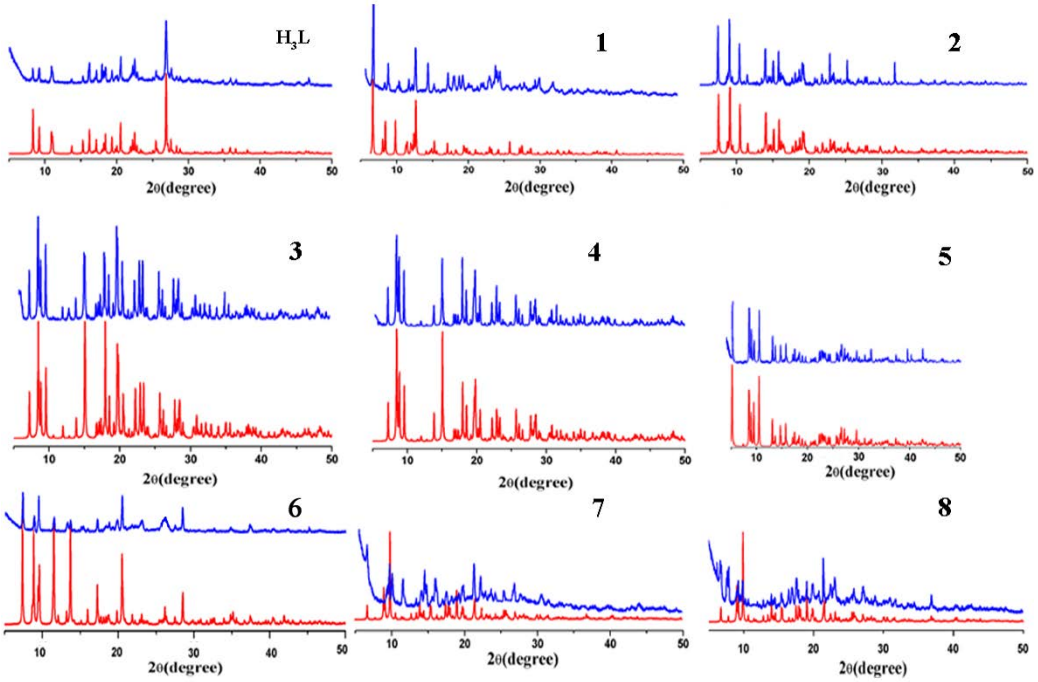


Fig. S7 Simulated (red) and experimental (blue) PXRD patterns of H_3L and compounds **1**–**8**.