Supplementary Material (ESI) for CrystEngComm

Supporting Information Available:

Molecular tectonics of metal-organic frameworks based on ligand-modulated polynuclear zinc SBUs and aromatic multicarboxylic acids

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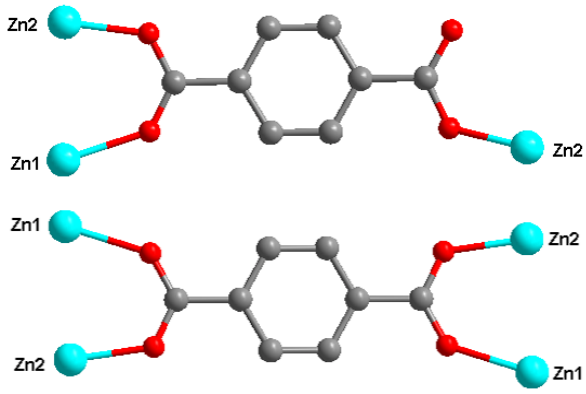


Fig. S1 Ball-stick representations of the different coordination modes of BDC ligands in **1**.

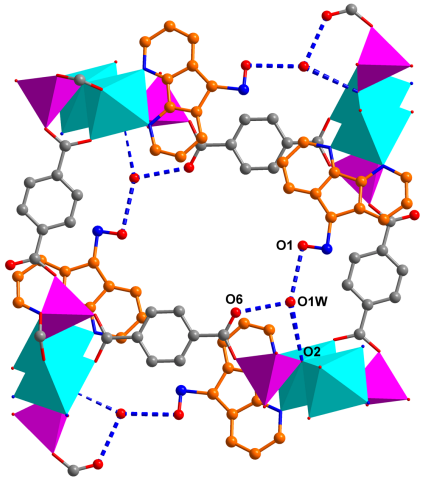


Fig. S2 Ball-stick and polyhedral representations of the hydrogen bond interactions about L ligands in compound **1**.

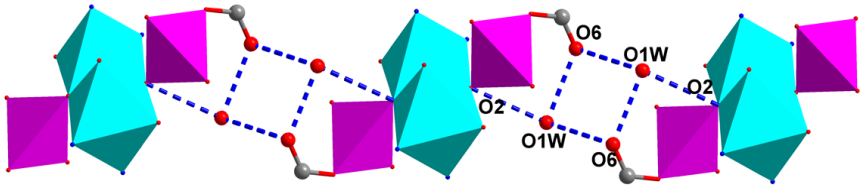
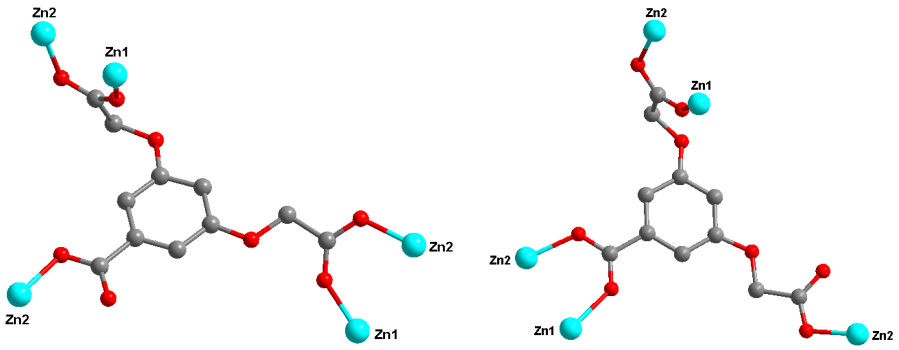


Fig. S3 View of the hydrogen bond interactions between the tetranuclear zinc clusters



(a) **(b)**

Fig. S4 Ball-stick representation of the different conformations of two kinds of BOABA ligands.

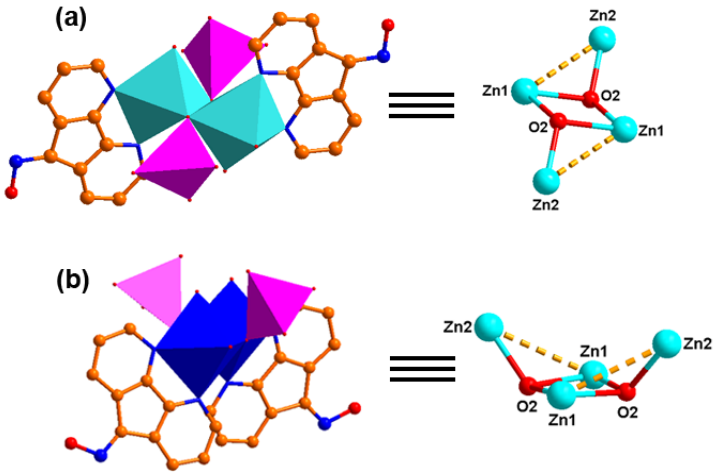


Fig. S5 Polyhedral and ball-and-stick representation of (a) chair conformation tetranuclear zinc cluster, (b) boat conformation tetranuclear zinc cluster.

Table S1 Selected Bond Lengths [Å] and Angles [°] for **1**~**5**

		1[a]	
Zn(1)-O(7)	2.065(3)	Zn(1)-O(3)	2.076(3)
Zn(1)-O(2)#3	2.090(2)	Zn(1)-O(2)	2.092(2)
Zn(1)-N(1)	2.312(3)	Zn(1)-N(2)	2.220(3)
Zn(2)-O(5)#4	1.905(3)	Zn(2)-O(4)	1.949(3)
Zn(2)-O(8)	1.950(3)	Zn(2)-O(2)	1.959(2)
O(7)-Zn(1)-O(3)	91.26(12)	O(7)-Zn(1)-O(2)#3	177.12(10)
O(3)-Zn(1)-O(2)#3	88.55(10)	O(7)-Zn(1)-O(2)	96.15(10)
O(3)-Zn(1)-O(2)	97.65(10)	O(2)#3-Zn(1)-O(2)	81.02(9)
O(7)-Zn(1)-N(2)	91.20(12)	O(3)-Zn(1)-N(2)	89.70(12)
O(2)#3-Zn(1)-N(2)	91.68(11)	O(2)-Zn(1)-N(2)	169.46(11)
O(7)-Zn(1)-N(1)	85.24(11)	O(3)-Zn(1)-N(1)	168.25(12)
O(2)#3-Zn(1)-N(1)	95.48(10)	O(2)-Zn(1)-N(1)	93.87(11)
N(2)-Zn(1)-N(1)	79.18(13)	O(5)#4-Zn(2)-O(4)	101.55(13)
O(5)#4-Zn(2)-O(8)	119.45(12)	O(4)-Zn(2)-O(8)	102.55(13)
O(5)#4-Zn(2)-O(2)	115.42(11)	O(4)-Zn(2)-O(2)	109.66(11)
O(8)-Zn(2)-O(2)	106.99(11)		
		2[b]	
Zn(1)-O(2)	2.079(2)	Zn(1)-O(10)#3	2.071(2)
Zn(1)-O(2)#1	2.074(2)	Zn(1)-O(6)	2.088(2)
Zn(1)-N(2)	2.171(3)	Zn(1)-N(1)	2.307(3)
Zn(2)-O(2)	1.956(2)	Zn(2)-O(3)#2	1.925(2)
Zn(2)-O(9)#3	1.981(2)	Zn(2)-O(7)	1.983(2)

O(10)#3-Zn(1)-O(2)#1	174.60(8)	O(2)#1-Zn(1)-N(2)	96.42(10)
O(10)#3-Zn(1)-O(2)	92.81(9)	O(2)-Zn(1)-N(2)	178.72(10)
O(2)#1-Zn(1)-O(2)	82.39(9)	O(6)-Zn(1)-N(2)	86.26(11)
O(10)#3-Zn(1)-O(6)	88.75(11)	O(10)#3-Zn(1)-N(1)	89.14(11)
O(2)#1-Zn(1)-O(6)	89.12(9)	O(2)#1-Zn(1)-N(1)	94.11(9)
O(2)-Zn(1)-O(6)	94.17(8)	O(2)-Zn(1)-N(1)	99.67(10)
O(10)#3-Zn(1)-N(2)	88.40(10)	O(6)-Zn(1)-N(1)	166.09(10)
N(2)-Zn(1)-N(1)	79.94(12)	O(3)#2-Zn(2)-O(7)	99.45(11)
O(3)#2-Zn(2)-O(2)	119.83(9)	O(2)-Zn(2)-O(7)	112.21(10)
O(3)#2-Zn(2)-O(9)#3	117.66(11)	O(9)#3-Zn(2)-O(7)	99.92(12)
O(2)-Zn(2)-O(9)#3	105.85(10)		
		3[c]	
Zn(1)-O(9)#2	2.067(2)	Zn(1)-O(2)	2.0962(19)
Zn(1)-O(3)	2.080(2)	Zn(1)-N(1)	2.202(2)
Zn(1)-O(2)#3	2.086(2)	Zn(1)-N(2)	2.322(3)
Zn(2)-O(6)#1	1.932(2)	Zn(2)-O(4)	1.982(2)
Zn(2)-O(2)	1.9493(19)	Zn(2)-O(10)#2	1.990(2)
O(9)#2-Zn(1)-O(3)	92.40(9)	O(3)-Zn(1)-N(1)	87.63(9)
O(9)#2-Zn(1)-O(2)#3	173.08(8)	O(2)#3-Zn(1)-N(1)	91.71(9)
O(3)-Zn(1)-O(2)#3	87.29(8)	O(2)-Zn(1)-N(1)	170.50(9)
O(9)#2-Zn(1)-O(2)	92.56(8)	O(9)#2-Zn(1)-N(2)	88.12(10)
O(3)-Zn(1)-O(2)	97.54(8)	O(3)-Zn(1)-N(2)	167.10(9)
O(2)#3-Zn(1)-O(2)	80.63(8)	O(2)#3-Zn(1)-N(2)	93.73(9)
O(9)#2-Zn(1)-N(1)	95.18(10)	O(2)-Zn(1)-N(2)	95.31(8)
N(1)-Zn(1)-N(2)	79.49(9)	O(6)#1-Zn(2)-O(10)#2	108.78(9)
O(6)#1-Zn(2)-O(2)	123.19(9)	O(2)-Zn(2)-O(10)#2	101.50(9)
O(6)#1-Zn(2)-O(4)	105.57(9)	O(4)-Zn(2)-O(10)#2	99.59(10)
O(2)-Zn(2)-O(4)	115.41(8)		
		4[d]	
Zn(1)-O(2)#2	1.885(2)	Zn(1)-O(13)	1.9626(17)
Zn(1)-O(5)#3	1.9508(19)	Zn(1)-O(3)	1.9643(18)
Zn(2)-O(7)#4	1.9214(18)	Zn(2)-O(13)	1.9908(17)
Zn(2)-O(6)#3	1.9276(19)	Zn(2)-O(12)	1.9429(19)
Zn(3)-O(11)	1.9780(19)	Zn(3)-O(4)	1.9517(19)
Zn(3)-O(9)#5	1.9319(19)	Zn(3)-O(13)	1.9772(17)
O(2)#2-Zn(1)-O(5)#3	115.02(9)	O(2)#2-Zn(1)-O(3)	101.74(9)
O(2)#2-Zn(1)-O(13)	121.53(8)	O(5)#3-Zn(1)-O(3)	105.68(9)
O(5)#3-Zn(1)-O(13)	107.50(8)	O(13)-Zn(1)-O(3)	103.32(8)
O(7)#4-Zn(2)-O(6)#3	114.69(9)	O(7)#4-Zn(2)-O(13)	103.76(8)
O(7)#4-Zn(2)-O(12)	112.80(8)	O(6)#3-Zn(2)-O(13)	109.48(8)
O(6)#3-Zn(2)-O(12)	106.60(9)	O(12)-Zn(2)-O(13)	109.45(7)

O(9)#5-Zn(3)-O(4)	111.58(9)	O(9)#5-Zn(3)-O(11)	103.10(8)
O(9)#5-Zn(3)-O(13)	116.48(8)	O(4)-Zn(3)-O(11)	107.86(8)
O(4)-Zn(3)-O(13)	112.86(8)	O(13)-Zn(3)-O(11)	103.79(8)
		5[e]	
Zn(1)-O(2)	2.0596(18)	Zn(1)-O(6)	1.914(2)
Zn(1)-O(7)	1.900(2)	Zn(1)-N(1)	2.066(2)
Zn(2)-O(7)#1	1.910(2)	Zn(2)-O(3)	2.0049(17)
Zn(2)-O(6)	1.926(2)	Zn(2)-O(5)	2.0250(18)
O(7)-Zn(1)-O(6)	128.19(10)	O(7)-Zn(1)-N(1)	113.24(9)
O(7)-Zn(1)-O(2)	101.33(10)	O(6)-Zn(1)-N(1)	112.09(10)
O(6)-Zn(1)-O(2)	97.90(9)	O(2)-Zn(1)-N(1)	95.62(9)
O(7)#1-Zn(2)-O(6)	113.73(11)	O(7)#1-Zn(2)-O(5)	119.84(9)
O(7)#1-Zn(2)-O(3)	104.59(9)	O(6)-Zn(2)-O(5)	113.66(10)
O(6)-Zn(2)-O(3)	102.32(9)	O(3)-Zn(2)-O(5)	99.26(8)

[a]Symmetry transformations used to generate equivalent atoms: #1 x-1/2,-y+1/2,z+1/2; #2 -x+2,-y+1,-z+1; #3 -x+1,-y+1,-z; #4 x+1/2,-y+1/2,z-1/2. [b]Symmetry transformations used to generate equivalent atoms:#1 -x,-y,-z+1; #2 x-1,y,z; #3 -x+1/2,y-1/2,-z+1/2; #4 x+1,y,z; #5 -x+1/2,y+1/2,-z+1/2. [c] Symmetry transformations used to generate equivalent atoms: #1 x,-y,z+1/2; #2 -x+3/2,y+1/2,z; #3 -x+1,y,-z+3/2; #4 -x+3/2,y-1/2,z; #5 x,-y,z-1/2. [d]Symmetry transformations used to generate equivalent atoms: #1 -x+1,y+1/2,-z+3/2; #2 -x+1,-y,-z+2; #3 x+1/2,-y+1/2,-z+2; #4 -x+1,y-1/2,-z+3/2; #5 -x+1/2,y-1/2,z. [e]Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z.

Table S2. Hydrogen bonds lengths [Å] and angles [˚] for **1**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...O(1W)	0.82	2.15	2.906(6)	152.6
O(2)-H(2O)...O(1W)	0.82	2.24	2.972(3)	147.6
O(1W)-H(1A)...O(6)	0.85	1.89	2.733(4)	171.0
O(1W)-H(1B)...O(6)	0.85	2.13	2.882(4)	148.7

Symmetry transformations used to generate equivalent atoms: #1 x-1/2,-y+1/2,z+1/2; #2 -x+2,-y+1,-z+1; #3 -x+1,-y+1,-z; #4 x+1/2,-y+1/2,z-1/2; #5 x-1/2,-y+3/2,z-1/2; #6 x,y,z-1; #7 x+1/2,-y+1/2,z+1/2; #8 -x+3/2,y+1/2,-z+3/2.