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Controlling Interpenetration in Metal-Organic Frameworks by Tuning the Conformations of Flexible Bis(triazole) Ligands

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Table S1. Selected bond distances (Å) and angles (º) for compounds **1**-**2**

Compound **1**					
N(1)-Zn(1)	2.057(4)	O(2)-Zn(1)-N(1)	114.57(13)	O(2)-Zn(1)-O(7)	84.00(14)
O(2)-Zn(1)	1.967(3)	O(2)-Zn(1)-O(3)#4	148.32(12)	N(1)-Zn(1)-O(7)	85.74(15)
O(3)-Zn(1)#1	2.106(3)	N(1)-Zn(1)-O(3)#4	96.40(13)	O(3)#4-Zn(1)-O(7)	92.25(13)
O(6)-Zn(1)	2.128(3)	O(2)-Zn(1)-O(6)	95.73(13)	O(6)-Zn(1)-O(7)	179.59(14)
O(7)-Zn(1)	2.230(3)	N(1)-Zn(1)-O(6)	94.66(14)	O(3)#4-Zn(1)-O(6)	87.82(13)
Compound **2**					
N(1)-Zn(1)#1	2.020(6)	Zn(1)-O(4)#3	1.990(4)	O(4)#3-Zn(1)-N(1)#1	104.8(2)
N(4)-Zn(1)	2.017(6)	Zn(1)-N(1)#1	2.020(6)	O(1)-Zn(1)-N(1)#1	105.1(2)
O(1)-Zn(1)	1.986(4)	O(4)#3-Zn(1)-O(1)	96.83(18)	N(4)-Zn(1)-N(1)#1	118.0(2)
O(4)-Zn(1)#2	1.990(4)	O(1)-Zn(1)-N(4)	114.1(2)	O(4)#3-Zn(1)-N(4)	115.4(2)

Symmetry transformations used to generate equivalent atoms: #1 x, y-1, z, #2 -x-1/2, -y+3/2, -z, #3 -x+1, -y+3, -z+1, #4 x, y+1, z for **1**; #1 -x+2, -y+2, -z, #2 x-1, y, z, #3 x+1, y, z, #4 -x, -y, -z for **2**;

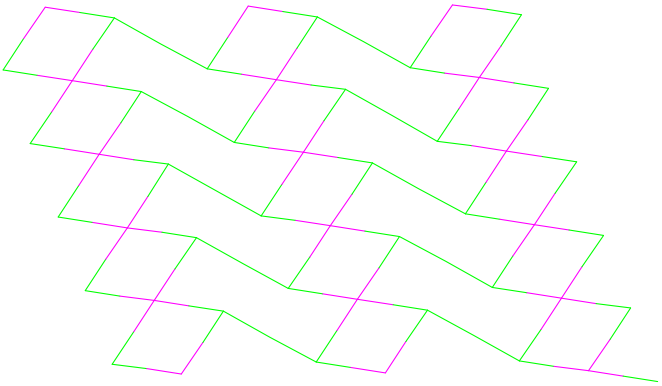

Fig. S1 New (3,4)-connected 2-nodal topologic structure of **1** with a $(4.6^2)_2(4^2.6^2.8^2)$ network in the Schlafli notation. (green for 3-connected node and purple for 4-connected node)

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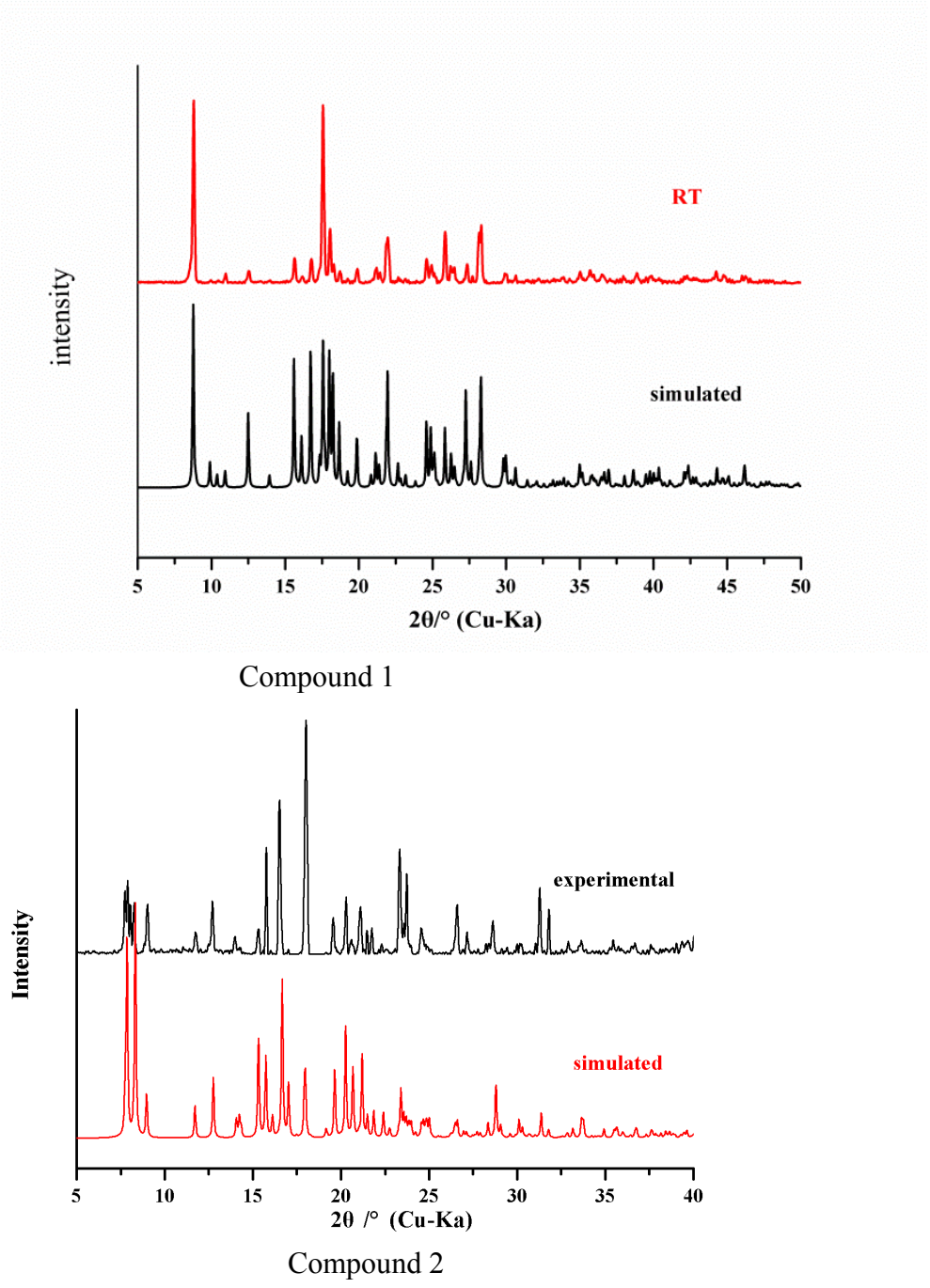

Fig S2 Powder X-ray diffractions (PXRD) for complexes **1-2.**

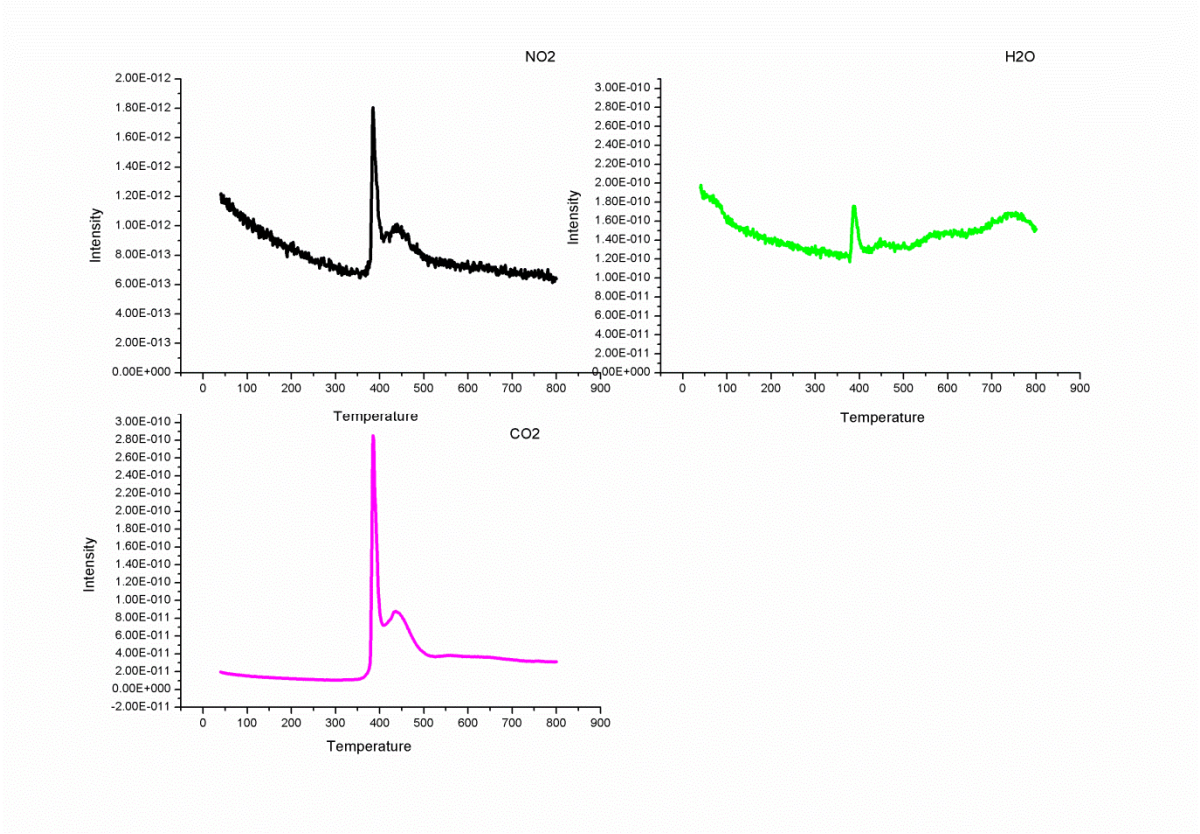

Fig S3 MS curves of the decomposed products for **2**.

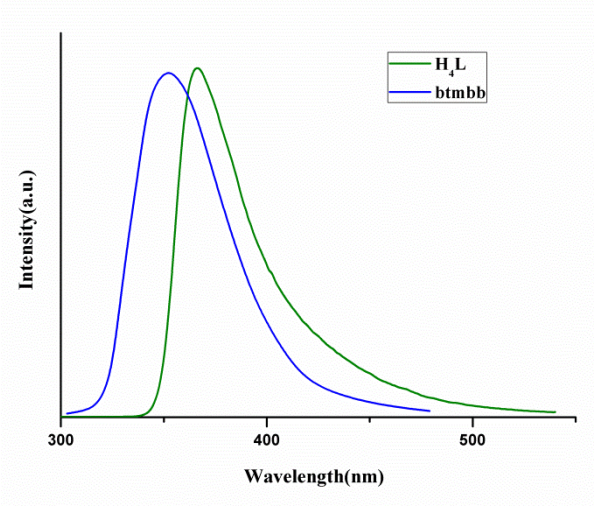

Fig. S4 Solid-state emission spectra of the free ligands btmbb and H_4L_1 at room temperature.