

Supporting information

A novel [4+3] topological net containing 7-fold interlocking *pseudo-helical* chains and exceptional catenane-like motifs

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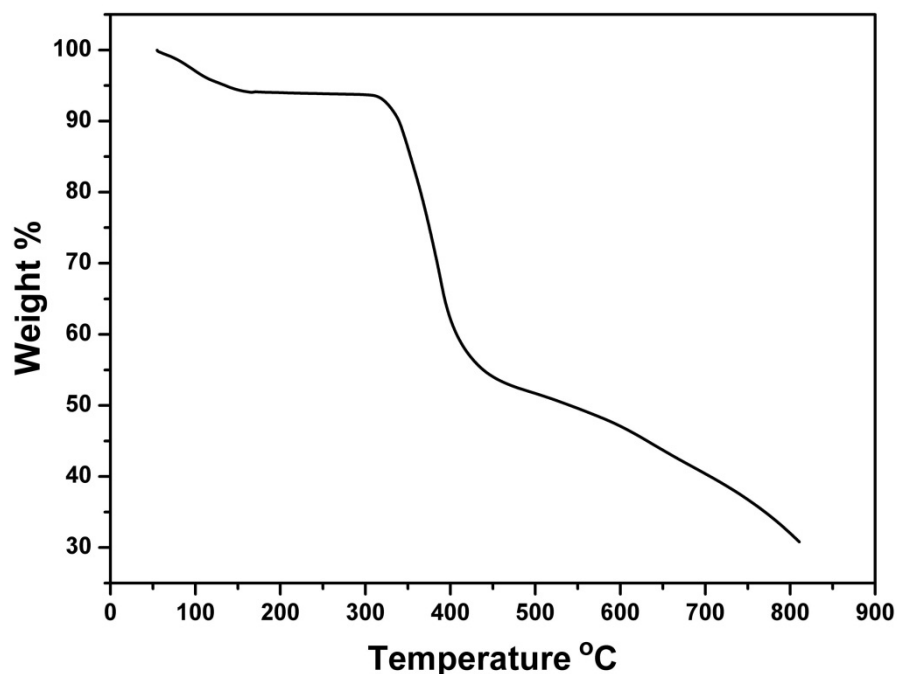
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Table S1. Selected bond lengths (Å) and bond angles (°)

Bond lengths (Å)			
Zn(1)-O(11)#1	1.956(3)	Zn(2)-O(2W)	1.959(4)
Zn(1)-O(4)	1.977(3)	Zn(2)-N(16)	2.036(4)
Zn(1)-N(1)	2.010(4)	Zn(3)-O(2)	1.946(4)
Zn(1)-N(8)#2	2.015(4)	Zn(3)-O(1W)	2.008(4)
Zn(2)-O(7)	1.921(4)	Zn(3)-O(14)	2.011(4)
Zn(2)-O(8)	1.934(4)	Zn(3)-N(9)	2.044(5)
Bond angles (°)			
O(11)#1-Zn(1)-O(4)	112.53(15)	O(2W)-Zn(2)-N(16)	111.4(2)
O(11)#1-Zn(1)-N(1)	101.51(15)	O(2)-Zn(3)-O(1W)	113.67(17)
O(4)-Zn(1)-N(1)	101.64(15)	O(2)-Zn(3)-O(14)	116.06(18)
O(11)#1-Zn(1)-N(8)#2	101.25(16)	O(1W)-Zn(3)-O(14)	123.95(19)
O(4)-Zn(1)-N(8)#2	129.71(15)	O(2)-Zn(3)-N(9)	104.89(18)
N(1)-Zn(1)-N(8)#2	106.96(16)	O(1W)-Zn(3)-N(9)	96.26(17)
O(7)-Zn(2)-O(8)	119.77(18)	O(14)-Zn(3)-N(9)	94.63(18)
O(7)-Zn(2)-O(2W)	109.6(2)	O(1W)-Zn(3)-O(15A)	93.0(7)
O(8)-Zn(2)-O(2W)	108.57(19)	O(14)-Zn(3)-O(15A)	57.9(6)
O(7)-Zn(2)-N(16)	111.50(18)	N(9)-Zn(3)-O(15A)	151.1(7)
O(8)-Zn(2)-N(16)	95.22(17)		

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

**Fig. S1** TGA curves of compound 1.

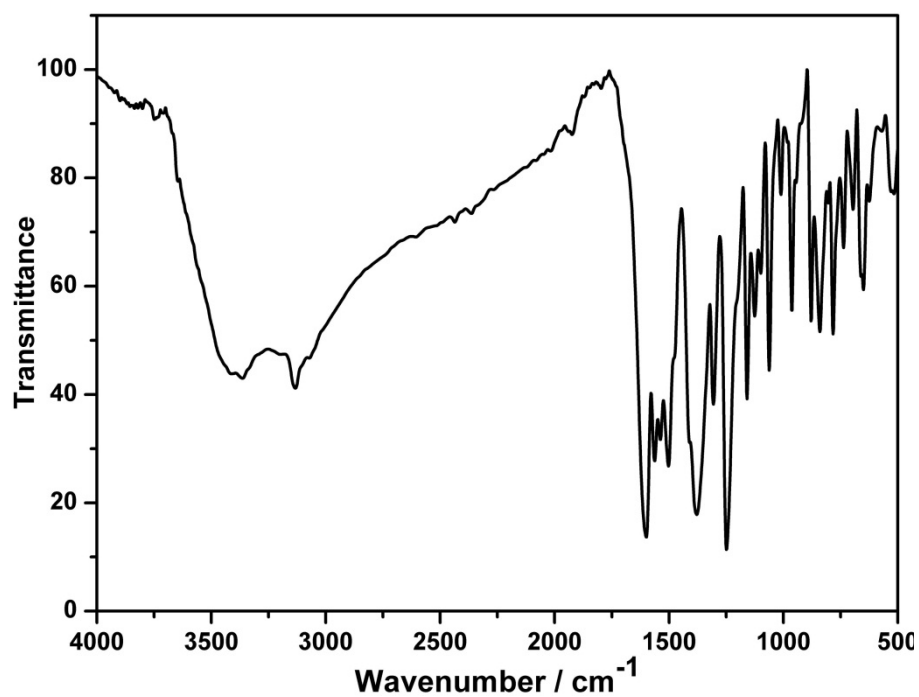


Fig. S2 Infrared spectrum of fresh **1**.

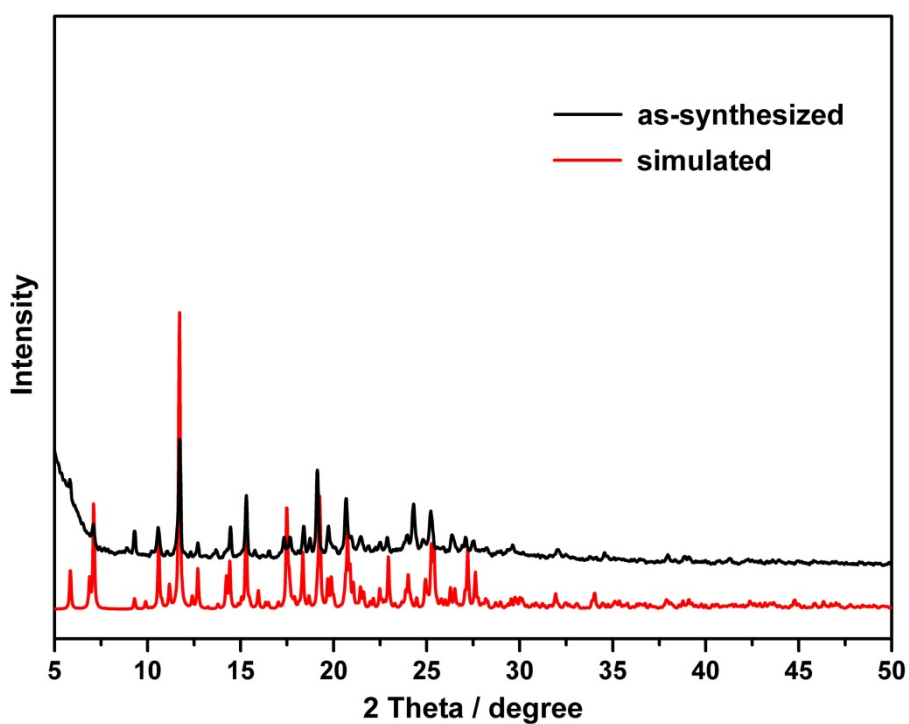


Fig. S3 PXRD profiles of as-synthesized (**1**) with the simulated one.

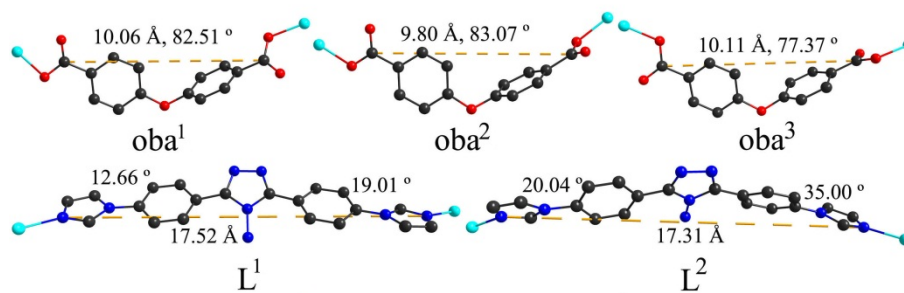


Fig. S4 Different conformers of ligand **L** and ligand **oba** in **1**.

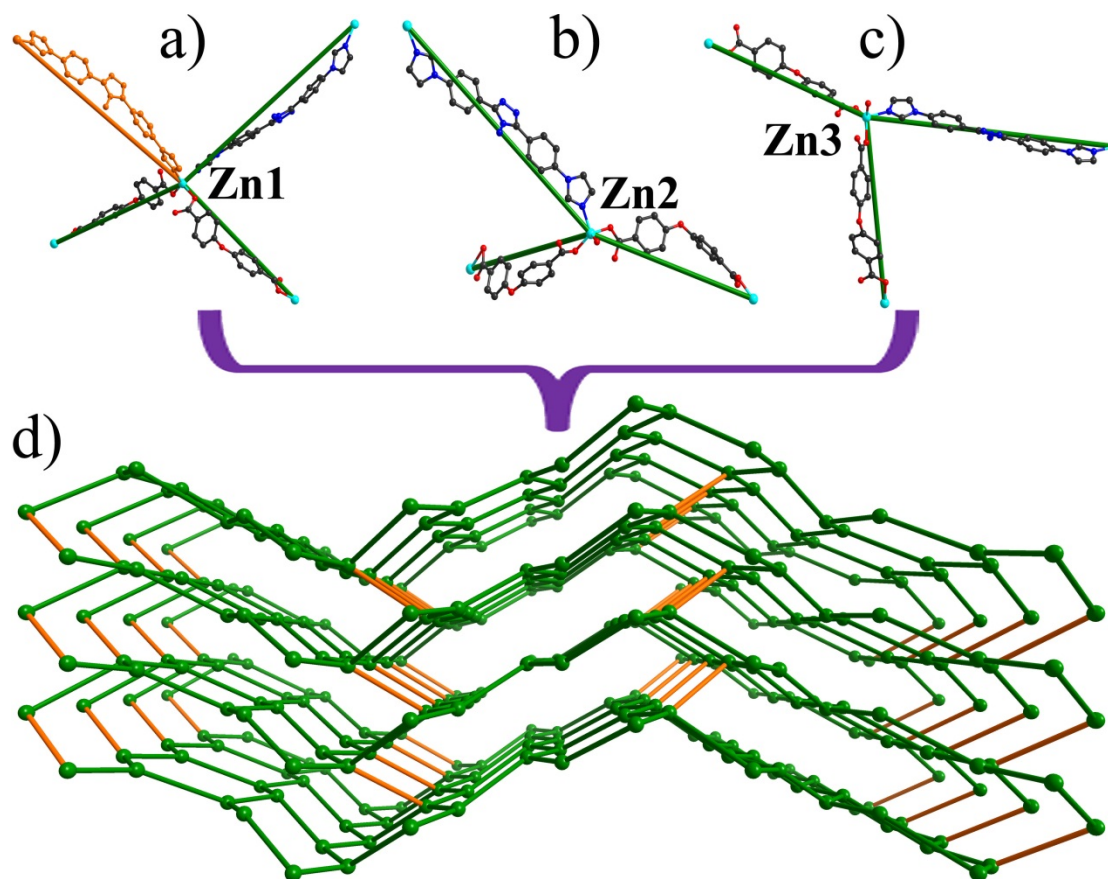


Fig. S5 a), b), c) Three kinds of nodes found in **1**, where the ligand **L** linking the adjacent layers is highlighted as orange; d) The entire 3D framework formed by the nodes and linkers.

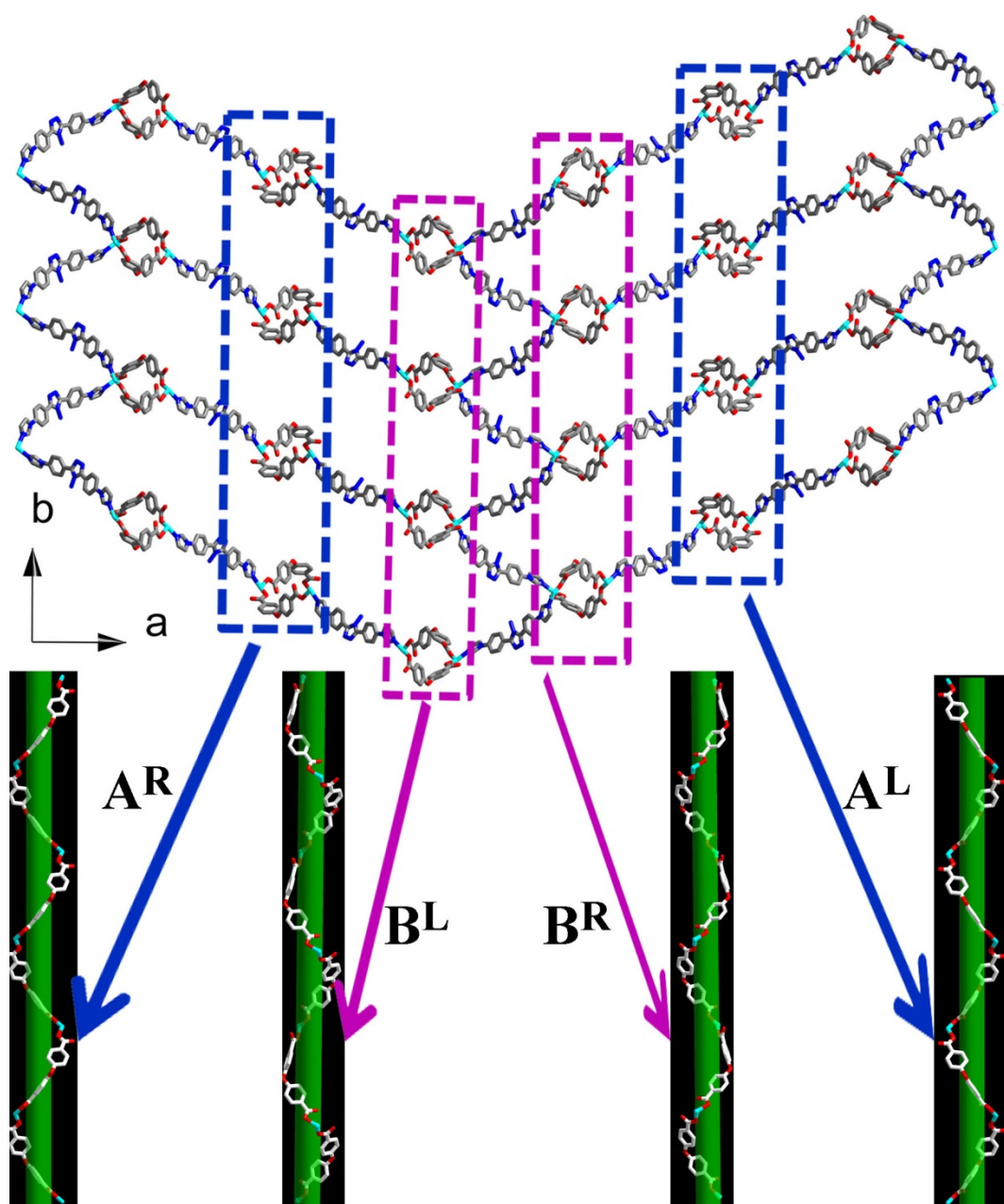


Fig. S6 The first type (code A^L) and the second type (code A^R) of helix and the first (code B^L) and the second (code B^R) type of *pseudo*-helical chains in **1**.

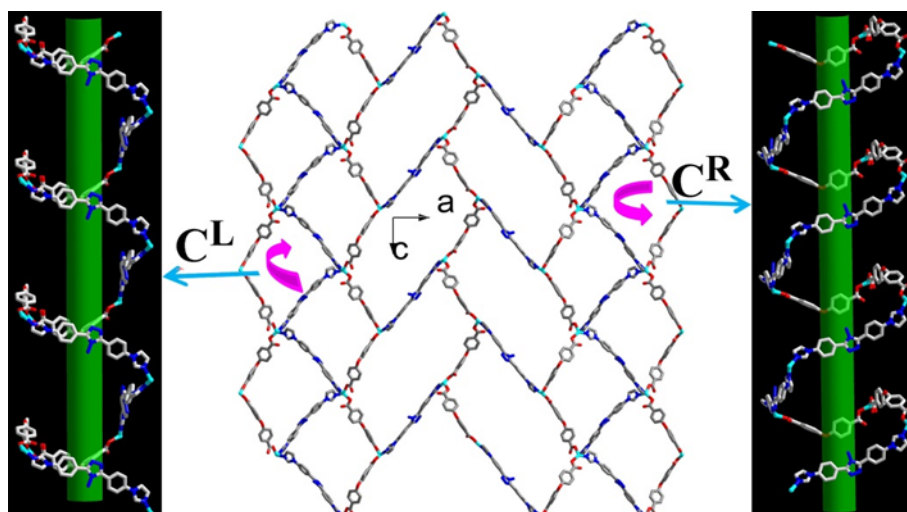


Fig. S7 The third type (code C^L) and the fourth type (code C^R) of *pseudo*-helical chains in **1**.

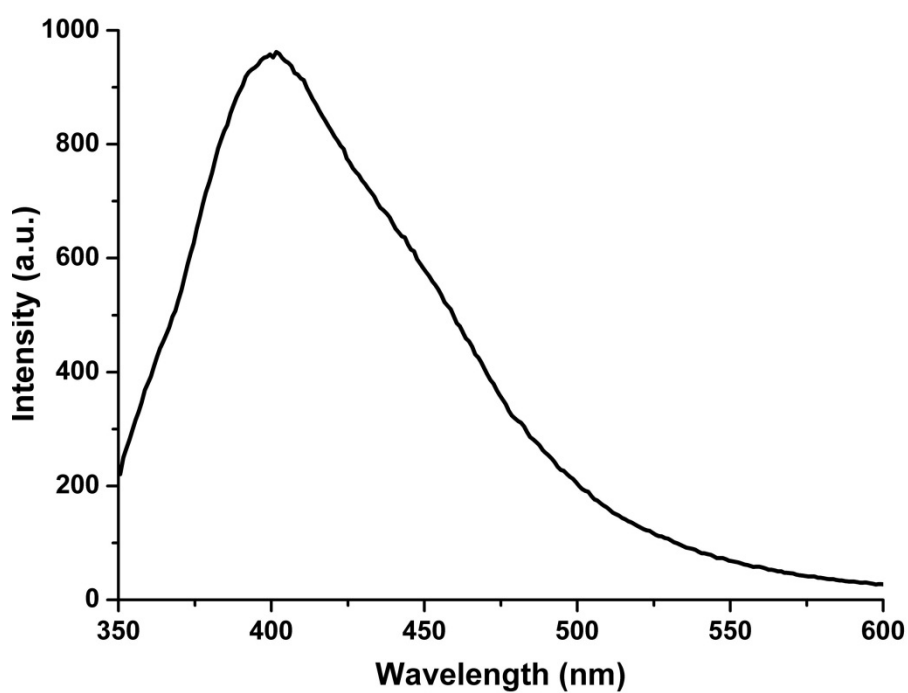


Fig. S8 Photoluminescent spectra of 4-amino-3,5-bis(4-imidazol-1-ylphenyl)-1,2,4-triazole (**L**) in solid state at room temperature ($\lambda_{\text{ex}} = 330$ nm).