

Electronic Supporting Information (ESI)

Two New Zinc(II) Coordination Complexes with Helix Characteristics Showing Both Interpenetration and Self-catenation Features: a Platform for Synthesis of Chiral and Catenated Structures Assembled by Length-Modulated Dicarboxylates

Yue Wang,^{a*} Yan Qi^a, Vladislav A. Blatov^{b,c}, Jimin, Zheng^d, Qun Li^a and Chao Zhang^a

^a College of Chemical Science and Engineering, Qingdao University, 308 Ningxia Road, Qingdao 266071, China.

^b Samara Center for Theoretical Materials Science (SCTMS), Samara State University, Ac. Pavlov St. 1, Samara 443011, Russia.

^c Chemistry Department, Faculty of Science, King Abdulaziz University P. O. Box 80203, Jeddah 21589, Saudi Arabia.

^d Chemistry Department, Nankai University, 300071, Tianjin, China.

Table S1 Selected bond distances (Å) and angles (°) for compounds 1-2^a

1					
N(1)-Zn(1)	1.959(4)	N(3)-Zn(1)	2.053(5)	O(8)-Zn(1)#2	1.964(4)
O(6)-Zn(1)	1.926(4)	N(7)-Zn(2)	2.051(4)	N(5)-Zn(2)	2.003(5)
O(2)-Zn(2)	1.995(4)	O(3)-Zn(2)#1	1.955(4)		
O(6)-Zn(1)-N(1)	111.38(17)	O(6)-Zn(1)-O(8)#3	104.66(17)	O(3)#4-Zn(2)-O(2)	96.98(16)
N(1)-Zn(1)-O(8)#3	124.95(18)	O(6)-Zn(1)-N(3)	113.99(19)	O(3)#4-Zn(2)-N(5)	104.49(17)
N(1)-Zn(1)-N(3)	109.02(16)	O(8)#3-Zn(1)-N(3)	91.63(15)	O(3)#4-Zn(2)-N(7)	119.21(18)
O(2)-Zn(2)-N(5)	128.60(16)	O(2)-Zn(2)-N(7)	109.48(16)	N(5)-Zn(2)-N(7)	99.71(17)
2					
Zn(1)-O(5)#5	1.931(5)	Zn(1)-N(1)	1.998(5)	Zn(1)-N(3)	2.007(5)
Zn(1)-O(1)	1.943(4)				
O(5)#5-Zn(1)-O(1)	111.2(2)	O(5)#5-Zn(1)-N(3)	116.6(2)	O(1)-Zn(1)-N(1)	107.54(19)
O(5)#5-Zn(1)-N(1)	96.8(2)	O(1)-Zn(1)-N(3)	111.1(2)	N(1)-Zn(1)-N(3)	112.7(2)

^a: Symmetry transformations used to generate equivalent atoms: #1 -x+y+1,-x+1,z+1; #2 -y,x-y,z+1; #3 -x+y,-x,z-

1; #4 -y+1,x-y,z-1 for 1; #5 x-2/3,x-y-1/3,z+1/6 for 2.

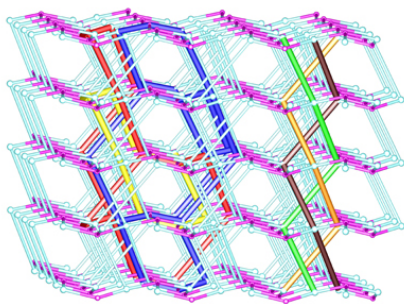
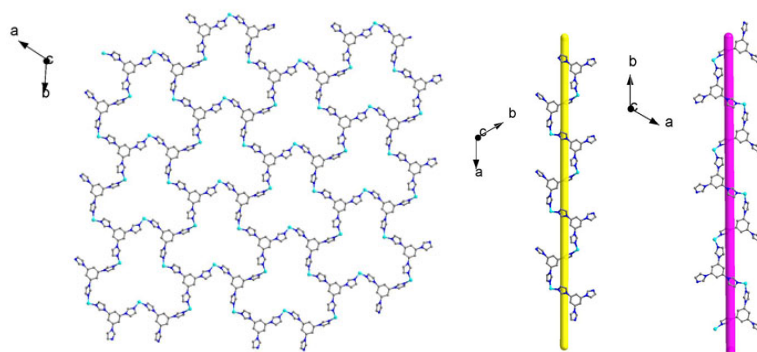
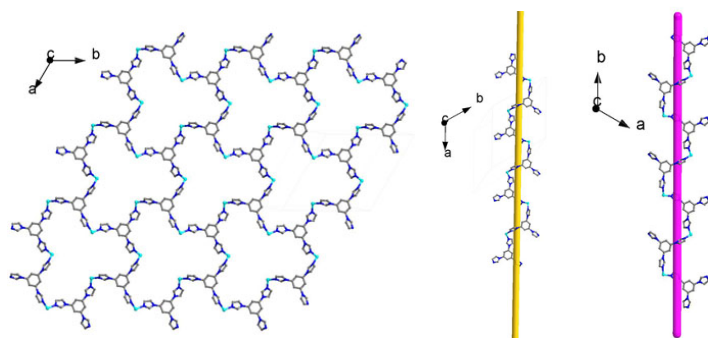


Fig. S1. Schematic description of the chiral (3,4)-coordinated self-catenated 3D motif β : light cyan spheres represent Zn₂ nodes, purple spheres represent tib ligands. One triple-stranded left-handed [Zn₂(L²)] helical chains are highlighted in green, orange and brown. One 10-ring in yellow is catenated by five other 10-rings, including three in blue and two in red.



(a)



(b)

Fig. S2. Stick and spheres view of (a) the 2D chiral [Zn(tib)_{2/3}]²⁺ layer (left) in **2** containing two types of left-handed helical chains viewing along the *a*-axis (middle) and *b*-axis (right), respectively; (b) the 2D chiral [Zn(tib)_{2/3}]²⁺ layer (left) in **2** containing two types of right-handed helical chains viewing along the *a*-axis (middle) and *b*-axis (right), respectively.

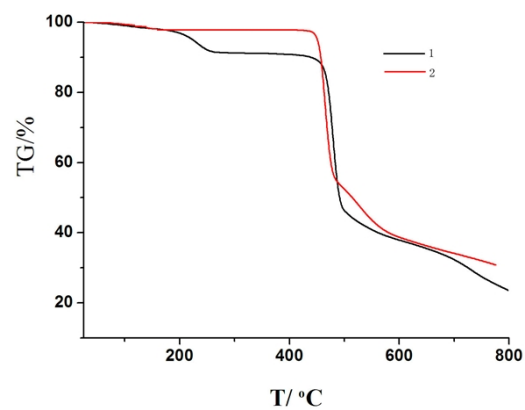


Fig. S3. TG plots of compounds 1-2.

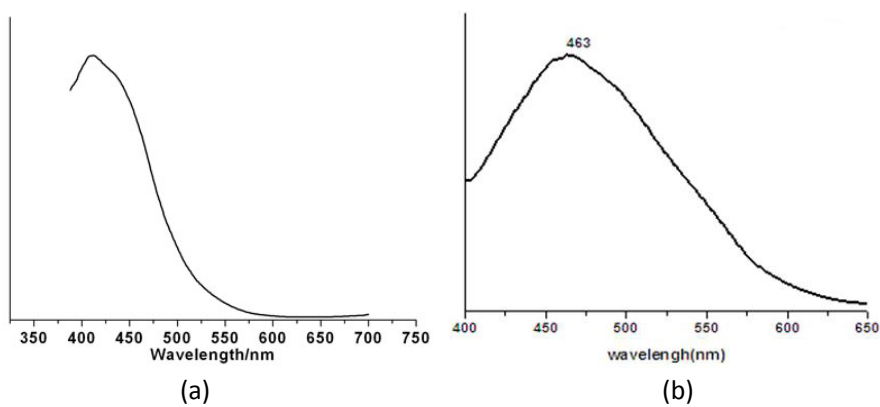


Fig. S4 Solid-state emission spectra of compounds 1-2 (a-b).