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Electronic Supplementary Information

Unusual 3D Zn^{II} Coordination Networks with Mixed Tetrahedral and Square-Planar Building Units: From 2-Fold Interpenetrating bbf Architecture to Self-Penetrating 8^6 Topological Framework

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Materials and General Methods

All the solvents and reagents for syntheses were commercially available and used as received. FT-IR spectra were recorded as KBr pellets on a Thermo Nicolet Nexus 670 FT-IR spectrometer. Elemental analyses were performed on a Perkin-Elmer 2400 Series II analyzer. Powder X-ray diffraction (PXRD) patterns were taken on a Rigaku D/max-2500 diffractometer (Cu Kα radiation, λ = 1.5406 Å), with a scan speed of 2 °/min and a step size of 0.02° in 2θ. The calculated PXRD patterns were simulated by using the single-crystal X-ray diffraction data. Thermogravimetric (TG) curves were recorded on a NETZSCH STA 449C microanalyzer in nitrogen atmosphere at a heating rate of 10 ºC·min^{-1}. Solid-state fluorescent spectra were measured on a Perkin-Elmer LS50B luminescence spectrophotometer.

Single Crystal X-ray Crystallography

Single-crystal X-ray diffraction data for complexes **1** and **2** were collected on a Bruker APEX II CCD diffractometer with graphite monochromated Mo Ka radiation (0.71073 Å) at 291(2) K. Empirical absorption corrections were applied using the SADABS program.[1] The structures were solved by direct methods and refined based on F^2 by the full matrix least-squares methods using SHELXTL.[2,3] All non-H atoms were refined anisotropically. The H atoms were located geometrically and refined as riding. Selected bond geometries for **1** and **2** are listed in Table S1.

References

1 Sheldrick, G M. SADABS, *Program for Empirical Absorption Correction of Area Detector Data*, University of Göttingen, Germany, 1997.

2 Sheldrick, G. M. SHELXS-97, *Program for the Solution of Crystal Structures*; University of Göttingen, Germany, 1997.

3 Sheldrick, G. M. SHELXL, *Program for the Refinement of Crystal Structures*, University of Göttingen, Germany, 1997.

Table S1 Selected Bond Distances (Å) and Angles (deg) for **1** and **2**

1[a]			
Zn1-O1	1.911(4)	Zn1-N2	2.009(4)
Zn1-O3#1	1.950(4)	Zn1-N5#2	2.014(4)
O1-Zn1-O3#1	122.44(2)	O1-Zn1-N5#2	117.40(2)
O1-Zn1-N2	100.79(2)	O3#1-Zn1-N5#2	99.84(2)
O3#1-Zn1-N2	106.73(2)	N2-Zn1-N5#2	109.01(2)
2[b]			
Zn1-O1	1.945(3)	Zn1-N2	2.007(4)
Zn1-O4#1	1.982(3)	Zn1-N4	2.017(4)
O1-Zn1-O4#1	112.09(2)	O1-Zn1-N4	96.14(2)
O1-Zn1-N2	118.78(2)	O4#1-Zn1-N4	112.46(2)
O4#1-Zn1-N2	99.19(2)	N2-Zn1-N4	118.94(2)

[a] Symmetry codes for **1**: #1 = -0.5 + x, 0.5 - y, -0.5 + z; #2 = -0.5 - x, -0.5 + y, 0.5 – z.

[b] Symmetry codes for **2**: #1 = 0.5 + x, 1.5 - y, 0.5 + z.

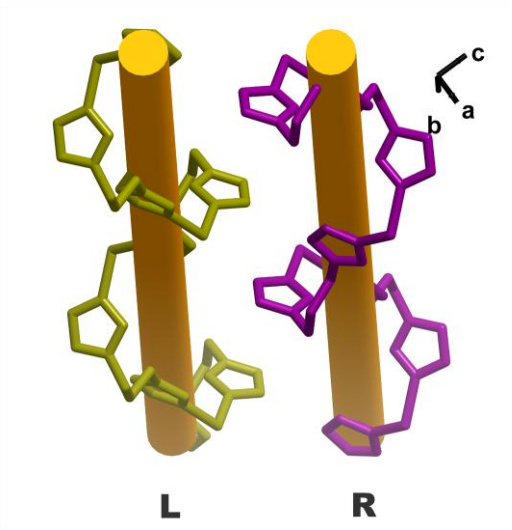


Figure S1. The left- and right-hand helical pillars constructed from Zn^{II} centers and bip ligands.

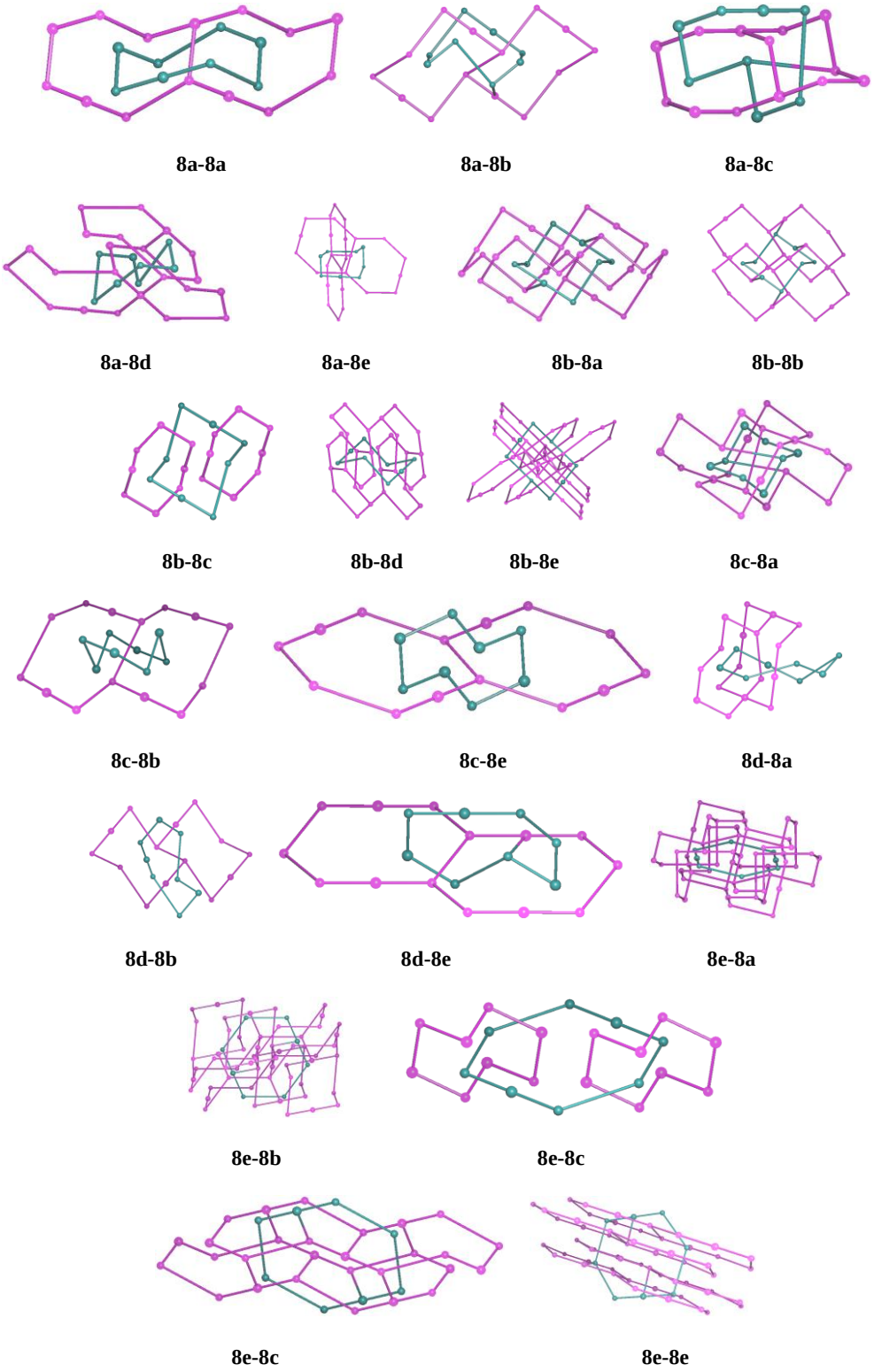
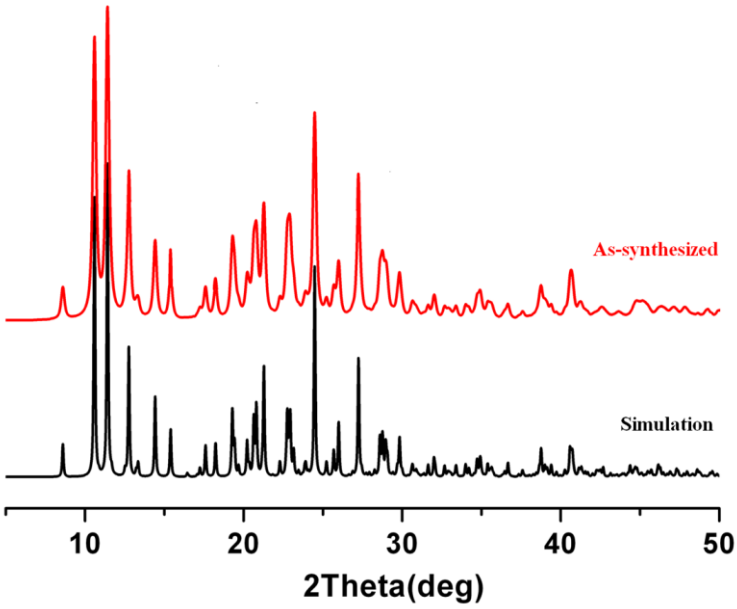
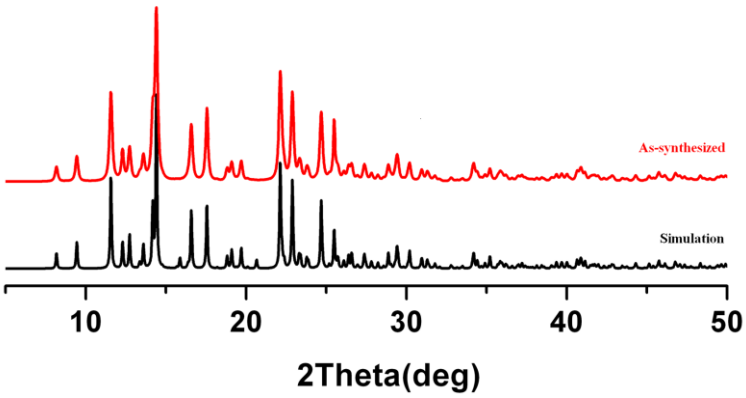


Figure S2. Different self-catenated patterns consisting of five types of 8-membered circuits analyzed by TOPOS progarm. Five types of 8-membered circuits are shown as following: Circuit no 1, type=8a, centroid: (0.500,0.500,0.500); Circuit no 2, type=8b, centroid: (0.091,0.293,0.915); Circuit no 3, type=8c, centroid: (0.596,0.769,0.398); Circuit no 4, type=8d, centroid: (0.500,0.500,0.000); Circuit no 5, type=8e, centroid: (0.500,0.500,0.500).



(a)



(b)

Figure S3. PXRD patterns for (a) **1** and (b) **2**.

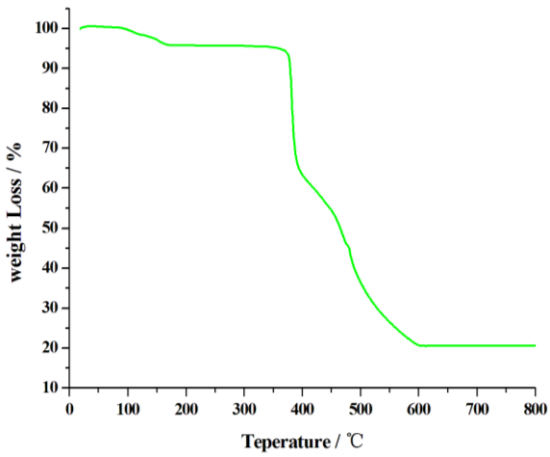


Figure S4. TG curve of **1**

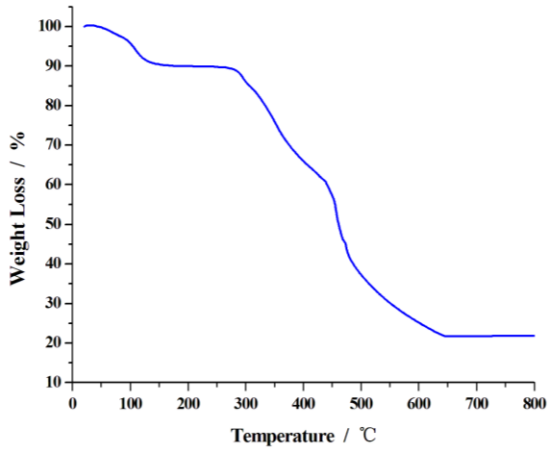


Figure S5. TG curve of **2**.

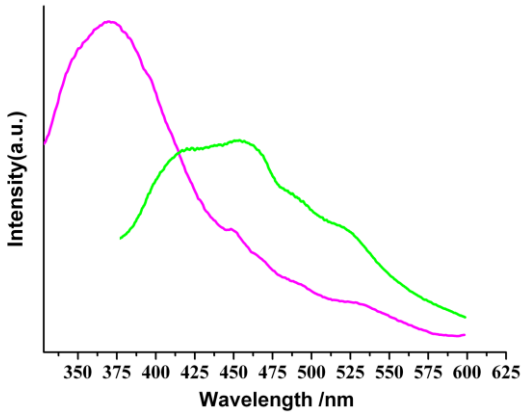


Figure S6. Emission spectra of **1** (pink) and **2** (green) in solid state at room temperature