Supplementary Material (ESI) for Chemical Communications

Electronic Supplementary Information

Spontaneous Asymmetrical Crystallization of a Three-dimensional Diamond-type Framework Material from Achiral Precursors

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Table S1 A summary of the 15 structure determinations of **1** with the *R* factors and Flack absolute structure parameters for each refinement.

	a	b	c	R_1	wR_2	Flack paramete
1	8.2676(8)	11.1516(11)	11.2300(11)	0.0299	0.0619	-0.001(17)
1-1	8.2569(6)	11.1344(8)	11.2113(9)	0.0283	0.0630	0.007(16)
1-2	8.2756(36)	11.1568(52)	11.2342(53)	0.0252	0.0568	0.008(13)
1-3	8.2664(12)	11.1527(16)	11.2213(10)	0.0258	0.0490	0.011(11)
1-4	8.2725(9)	11.1547(13)	11.2439(17)	0.0274	0.0529	-0.014(12)
1-5	8.2707(38)	11.1570(51)	11.2259(52)	0.0247	0.0485	-0.007(12)
1-6	8.2745(9)	11.1656(11)	11.2413(12)	0.0245	0.0521	-0.014(15)
1-7	8.2670(13)	11.2233(19)	11.1380(20)	0.0677	0.1256	0.02(5)
1-8	8.2639(7)	11.2145(10)	11.1520(11)	0.0352	0.0641	-0.002(17)
1-9	8.3116(11)	11.2851(15)	11.2055(15)	0.0438	0.0896	0.01(2)
1-10	8.2786(11)	11.1824(17)	11.2521(17)	0.0632	0.1373	1.01(3)
1-11	8.2682(32)	11.1509(41)	11.2289(44)	0.0249	0.0562	-0.001(13)
1-12	8.2642(26)	11.1573(36)	11.2244(36)	0.0230	0.0475	-0.003(11)
1-13	8.2594(8)	11.1233(11)	11.2100(11)	0.0392	0.0720	0.008(17)
1-14	8.2454(10)	11.1291(11)	11.1810(14)	0.0307	0.0609	0.016(14)

UV-Vis and luminescence spectra: The UV-Vis and luminescence spectra of the deprotonated ligand (AMTD) were measured by dissolving the HAMTD in the NaOH solution. The measurement were performed on a Perkin-Elmer Lambda 45 UV/VIS spectrophotometer and a HORIBA Jobin-Yvon FluoroMax-4 spectrometer, respectively.

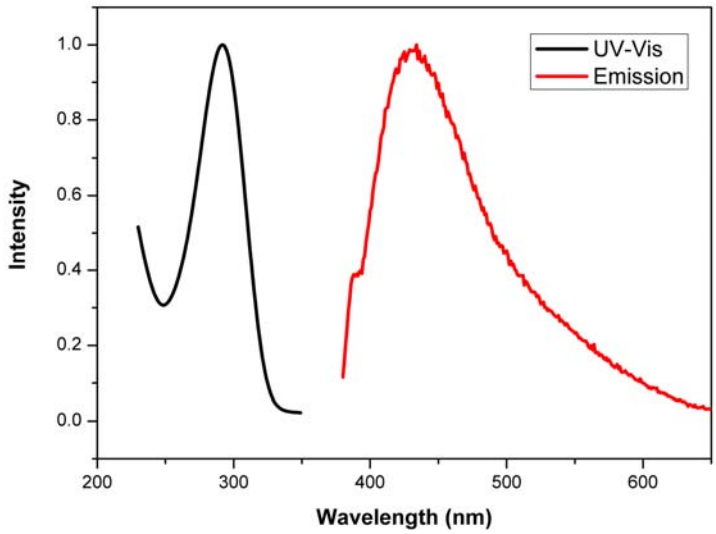

Figure S1. The UV-Vis (black) and luminescence (red) spectra of the deprotonated ligand at room temperature.

Thermal Analysis: The thermal analysis was performed on Netzsch STA449C under the flowing nitrogen atmosphere. A total of 5.831 mg of **1** was heated between room temperature and 1000 ºC at a heating rate of 10 ºC/min.

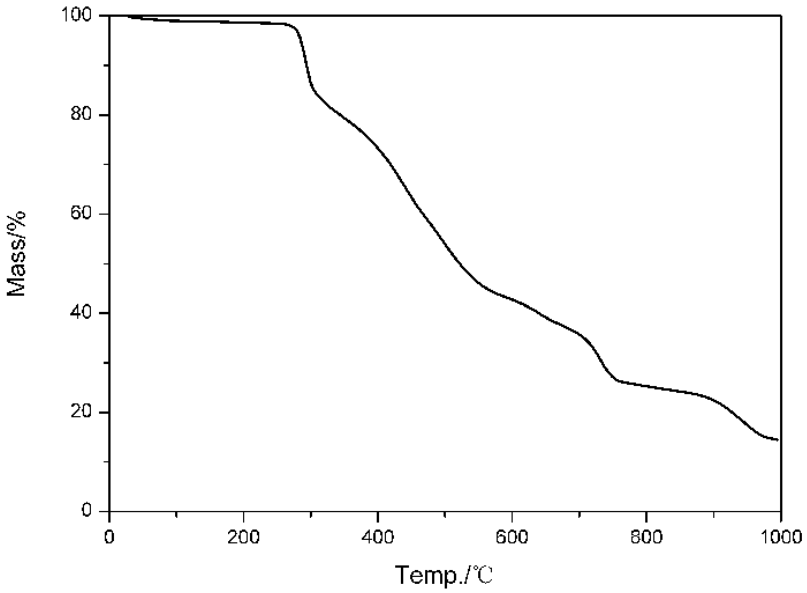

Figure S2. The TGA diagram of **1**. There is continuing weight loss from 260 to 980 °C. The remaining weight of 14.5% is likely from the decomposition product (Zn)

X-ray powder diffraction: X-ray powder diffraction experiments were performed on A PANalytical X'pert PRO diffractometer with Cu Ka radiation (40 kV, 40 mA) was used to identify the crystal structure of the sample. The measurement was conducted in the continuous scanning mode. The 2θ scanning range was from 10° to 75° in steps of 0.02° with a collection time of 12 s per step.

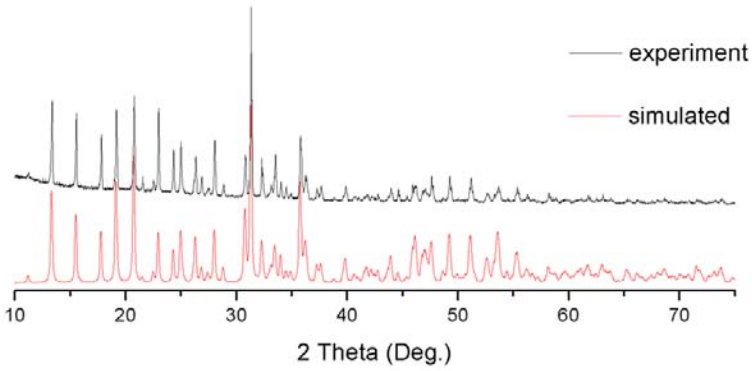

Figure S3. XPRD patterns for **1**. (top) Taken at room temperature; (bottom) calculated on the basis of the structure determined by single-crystal X-ray diffraction.