

## Supporting Information

# Configuration Determination of Flexible Tetracarboxylate

## Ligands in Two Supramolecular Structures

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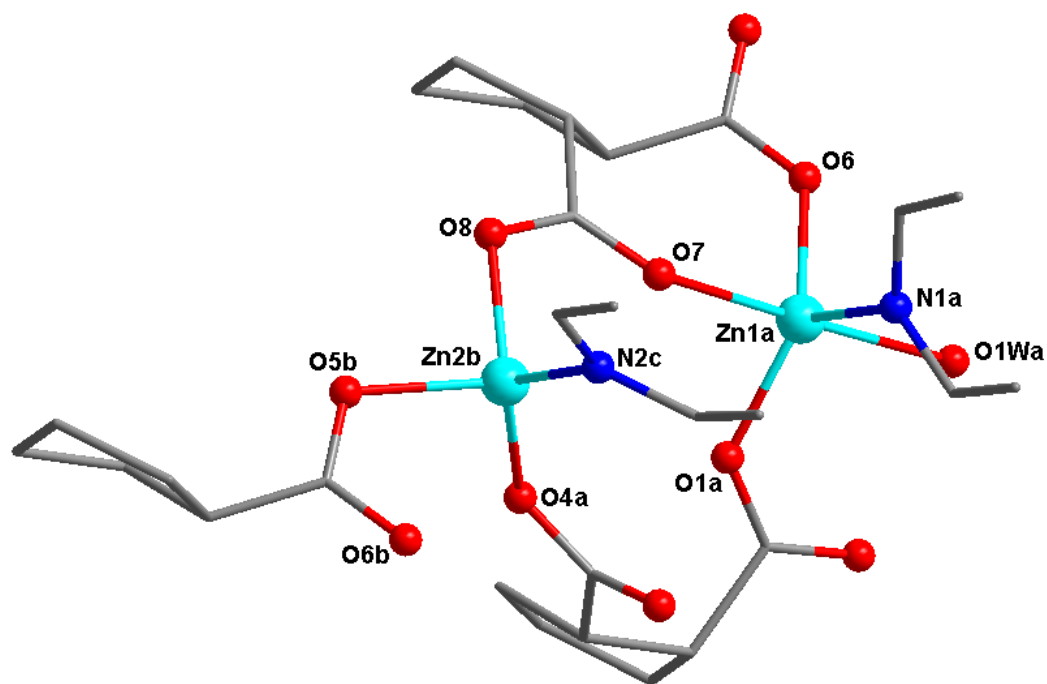
**X-ray Crystallography.** Suitable single crystals of the two complexes were carefully selected under an optical microscope and glued to thin glass fibers. Structural measurements were performed on a computer-controlled Rigaku Mercury CCD Diffractometer with

graphite-monochromated Mo K $\alpha$  radiation ( $\lambda_{\text{Mo K}\alpha} = 0.71073 \text{ \AA}$ ) at  $T = 293.2 \text{ K}$ . Absorption

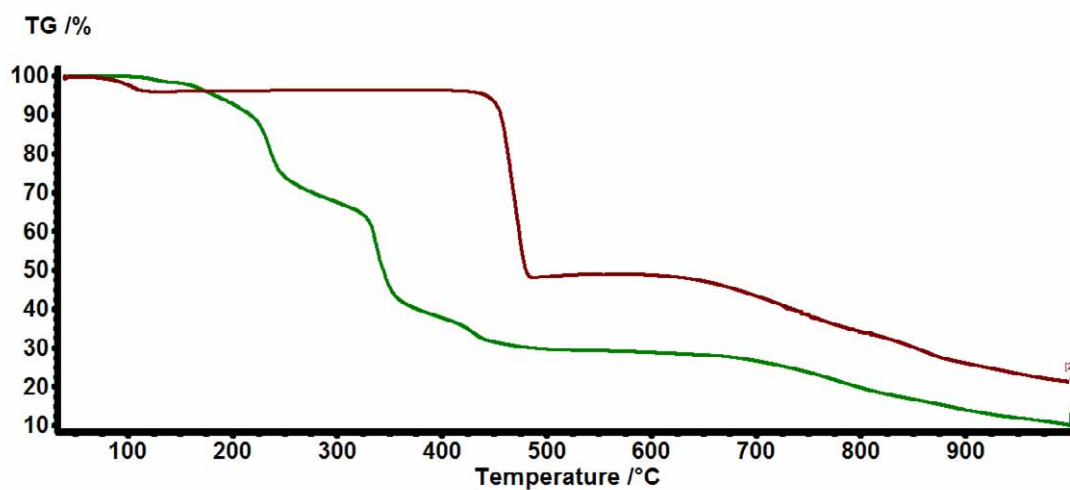
corrections were made using the SADABS program. The structures were solved using the direct method and refined by full-matrix least-squares methods on  $F^2$  by using the SHELX-97 program package. All non-hydrogen atoms were refined anisotropically, and hydrogen atoms attached to carbon atoms were fixed at their ideal positions. And the water hydrogen atoms were located from difference maps and refined with isotropic temperature factors.

**Table S1** Geometrical Parameters of Hydrogen bonds in **1** and **2**.

D-H...A	D-H [ $\text{\AA}$ ]	H...A [ $\text{\AA}$ ]	D...A [ $\text{\AA}$ ]	D-H...A [ $^\circ$ ]
<b>Complex 1</b>				
O1W-H1WA...O8 <sup>1</sup>	0.82	1.87	2.676(3)	169.3
O1W-H1WB...O9 <sup>2</sup>	0.82	1.98	2.780(3)	167.6
O2W-H2WA...O3 <sup>3</sup>	0.82	1.96	2.764(3)	167.0
O2W-H2WB...O2 <sup>2</sup>	0.82	1.94	2.701(3)	154.4
O4-H4...N2 <sup>4</sup>	0.83	1.80	2.629(4)	173.2
O6-H6...O3W	0.83	2.05	2.775(6)	144.4
O6-H6...O3W <sup>5</sup>	0.83	1.92	2.716(6)	157.8
symmetry codes: (1) -x+1, -y, -z; (2) x-1, y, z; (3) -x+1, -y+1, -z; (4) x-2, y, z+1; (5) -x, -y, -z+1.				
<b>Complex 2</b>				
O2W-H2WB...O3	0.85	2.24	3.093(13)	179.2
O2W-H2WA...O3 <sup>1</sup>	0.85	1.92	2.770(12)	179.1
O1W-H1WA...O2	0.82	1.90	2.625(6)	146.5
O1W-H1WB...O3 <sup>2</sup>	0.83	2.09	2.898(6)	164.4
symmetry codes: (1) -x+1, -y+1, -z+1; (2) x+1, y, z.				



**Fig. S1** The coordination environment of Zn centers in **2**. symmetry codes: a = 1-x, 1-y, -z; b = 1+x, y, z; c = x, 1+y, -1+z.



**Fig. S2** TGA curves of **1** (green) and **2** (red).

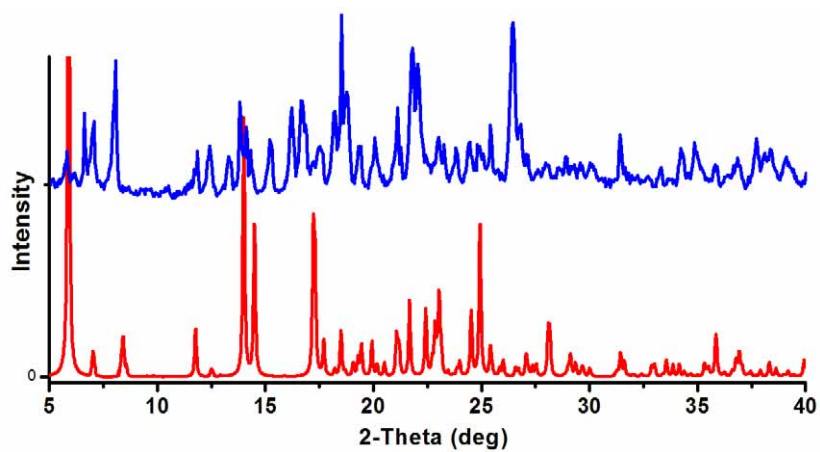


Fig. S3 Simulation (red) and experiment (blue) XPRD data for 1.

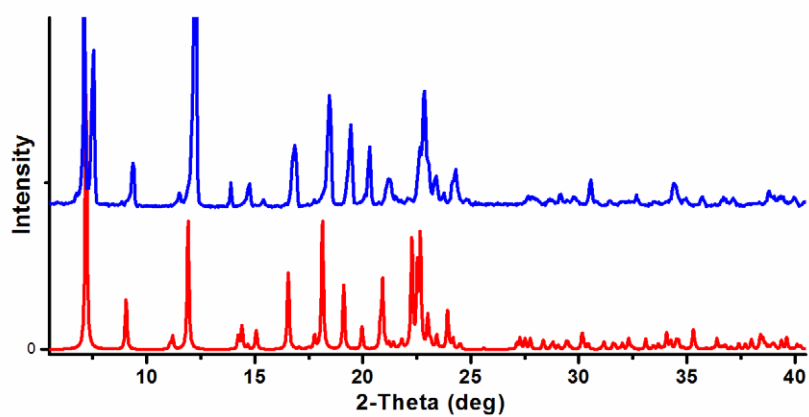


Fig. S4 Simulation (red) and experiment (blue) XPRD data for 2.