

Supporting Information for

Two New Polar Coordination Polymers with Diamond Networks: Interpenetration and Thermal Phase Transition

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Supplementary Index

Fig. S1. Simplifying illustration of the 4-connected node for **2**.

Fig. S2. TG curves of the as-synthesized **1** under N₂ atmosphere

Fig. S3 VTPXRD patterns of **1**

Fig. S4. DSC curves of the as-synthesized **1**

Fig. S5. TG curve of the as-synthesized **2** under N₂ atmosphere

Fig. S6. DSC curves of the as-synthesized **2**

Table S1 Summary of the Crystal Data and Structure Refinements for a crystal of **2** measured at different temperatures

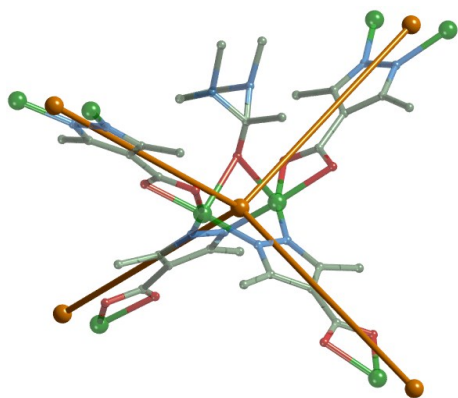


Fig. S1. Simplifying illustration of the 4-connected node for **2**.

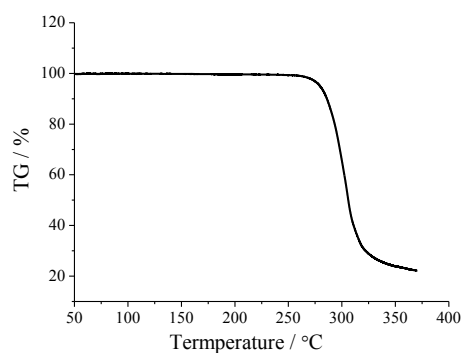


Fig. S2. TG curve of the as-synthesized **1** under N₂ atmosphere

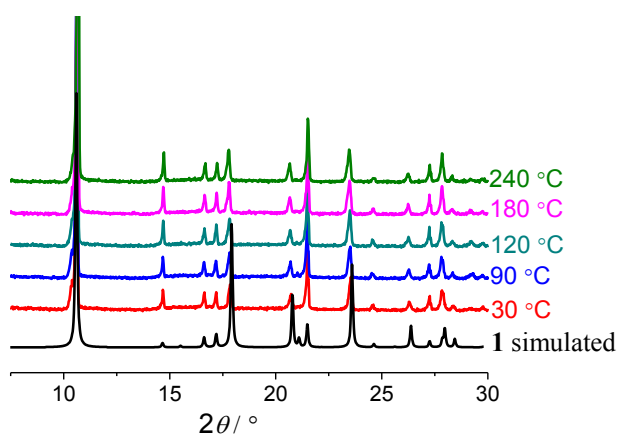


Fig. S3 VTPXRD patterns of **1**

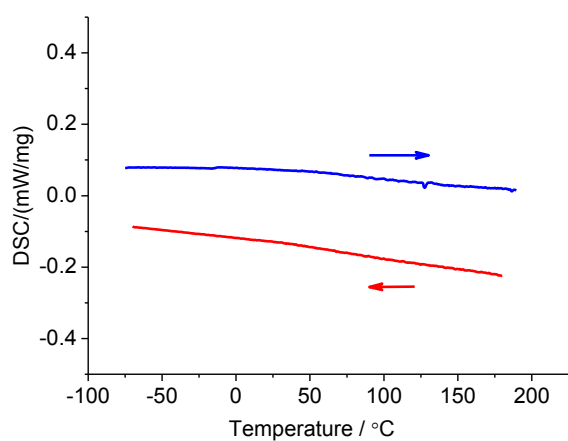


Fig. S4 DSC curves of the as-synthesized **1**

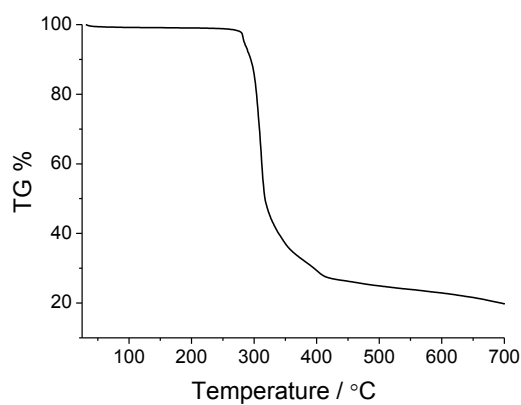


Fig. S5. TG curve of the as-synthesized **2** under N₂ atmosphere

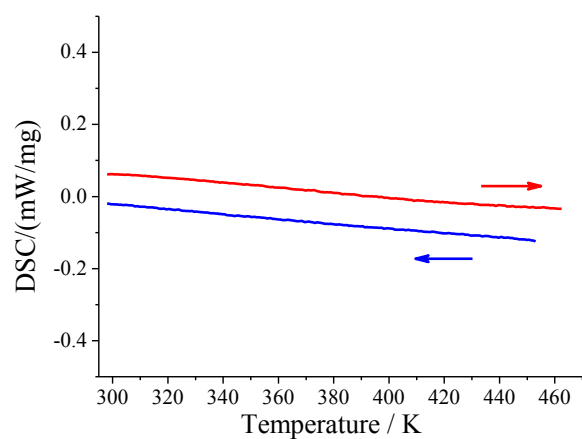


Fig. S6 DSC curves of the as-synthesized **2**

Table S1. Summary of the Crystal Data and Structure Refinements for a crystal of **2** measured at different temperatures

	300 K	440 K	300 K	440 K
phase	2α	2β	2α	2β
Formula	C ₁₆ H ₂₁ Cu ₂ N ₅ O ₅	C ₁₆ H ₂₁ Cu ₂ N ₅ O ₅	C ₁₆ H ₂₁ Cu ₂ N ₅ O ₅	C ₁₆ H ₂₁ Cu ₂ N ₅ O ₅
Formula weight	490.46	490.46	490.46	490.46
Crystal system	Tetragonal	Tetragonal	Tetragonal	Tetragonal
Space Group	<i>P</i> 4 ₃	<i>P</i> 4 ₂ <i>nm</i>	<i>P</i> 4 ₁	<i>P</i> 4 ₂ <i>nm</i>
<i>a</i> /Å	10.9932(1)	10.9780(3)	10.9902(1)	10.9855(3)
<i>b</i> /Å	10.9932(1)	10.9780(3)	10.9902(1)	10.9855(3)
<i>c</i> /Å	18.0928(3)	9.1059(4)	18.094 (3)	9.1106(4)
<i>V</i> /Å ³	2186.52(5)	1097.41(6)	2185.5(4)	1099.48(6)
<i>Z</i>	4	2	4	2
<i>D</i> _c (g·cm ⁻³)	1.490	1.484	1.491	1.481
μ (mm ⁻¹)	2.703	2.693	2.705	2.688
<i>R</i> ₁	0.0421/0.0423	0.0229/0.0231	0.0292/0.0294	0.0214/0.0216
<i>wR</i> ₂	0.1028/0.1031	0.0615/0.0617	0.0807/0.0807	0.0601/0.0602
GOF	1.054/1.069	1.018/1.065	1.023/1.052	1.020/1.059
$\Delta\rho/e\cdot\text{\AA}^3$	0.503/-0.506	0.153/-0.231	0.259/-0.432	0.149/-0.190
BASF	0.498	—	0.504	—
Flack	—	0.09(6)	—	0.04(5)