

Electronic Supplementary Information

The Self-Assembly of Single-Walled Metal-Organic Nanotubes Constructed from CuCl₂ Chains and Ditetrazoles

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Synthesis of 1,3-di(1H-tetrazol-1-yl)benzene

Fig. S1. The Coordination environment of the Cu^{II} ion in **1**.

Fig. S2. The ligand of DTB in **1**.

Fig. S3. (4,4) topological diagram of **1**.

Fig. S4. The temperature evolution of the inverse magnetic susceptibility χ_m^{-1} for **1** between 2.6 and 300 K, and the solid line was generated from the best fit by the Curie-Weiss expression in the range of 2.6 and 300 K with the Curie constant $C = 0.385 \text{ emu mol}^{-1} \text{ K}$ and the Weiss constant $\theta = 2.44 \text{ K}$.

Fig. S5. Field dependence of the magnetization for complex **1** at 1.8 K.

Fig. S6. Temperature dependences of in-phase (χ'_m) (a) and out-of-phase (χ''_m) (b) signals of the AC magnetic susceptibility measurements at 1–1500 Hz in field of 0 G.

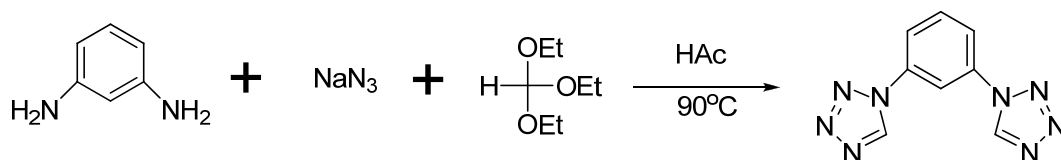
Fig. S7. Thermogravimetric (TG) curve of **1** measured in the range of 30–800 °C under air atmosphere with the heating rate of 10 °C/min.

Fig. S8. PXRD patterns of the bulk product and the calculated pattern based on the single-crystal solution of **1**.

Fig. S9. IR spectra of **1** and DTB.

Synthesis of 1,3-di(1H-tetrazol-1-yl)benzene

m-Phenylenediamine of 8.0 g (73.8 mmol), 30.6 g triethyl orthoformate (206.7 mmol) and 12.6 g sodium azide (192 mmol) were dissolved in 130 ml glacial acetic acid and stirred at 90 °C for 10 h. The suspension was then poured into 1 L of water and the resulting precipitate was collected by filtration, washed with cold water^[1].



Scheme 1. synthesis of 1,3-di(1H-tetrazol-1-yl)benzene

- 1 P. L. Franke, J. G. Haasnoot, A. P. Zuur. *Inorg. Chim. Acta.*, 1982,5,59.

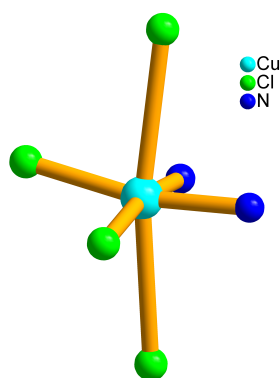


Fig. S1. The Coordination environment of the Cu^{II} ion in 1.

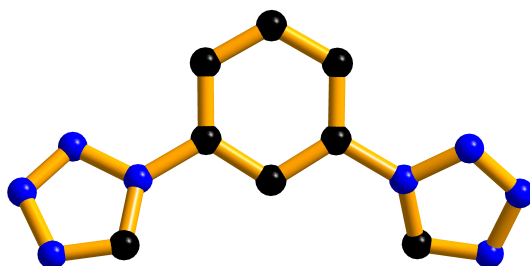


Fig. S2. The ligand of DTB in 1.

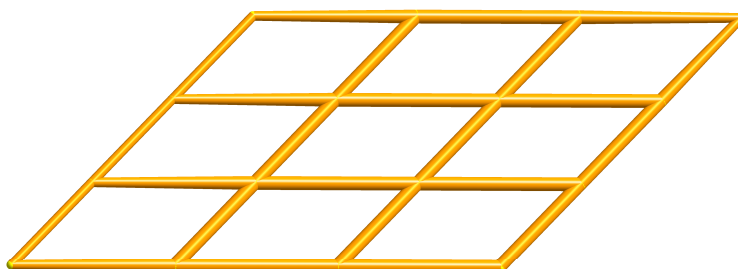


Fig. S3. (4,4) topological diagram of 1.

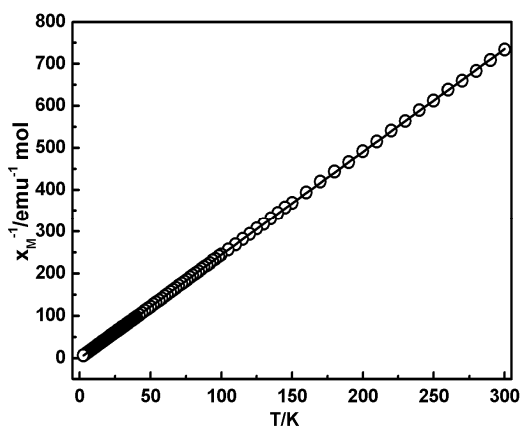


Fig. S4. The temperature evolution of the inverse magnetic susceptibility χ_m^{-1} for **1** between 2.6 and 300 K, and the solid line was generated from the best fit by the Curie-Weiss expression in the range of 2.6 and 300 K with the Curie constant $C = 0.367 \text{ emu mol}^{-1} \text{ K}$ and the Weiss constant $\theta = 0.407 \text{ K}$.

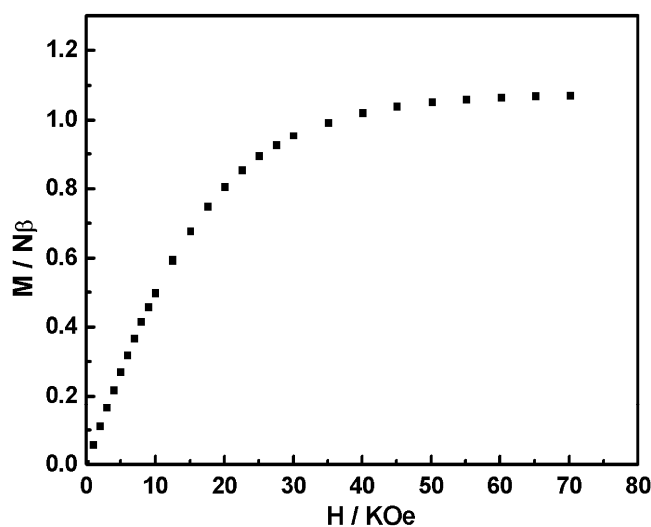


Fig. S5. Field dependence of the magnetization for complex **1** at 1.8 K.

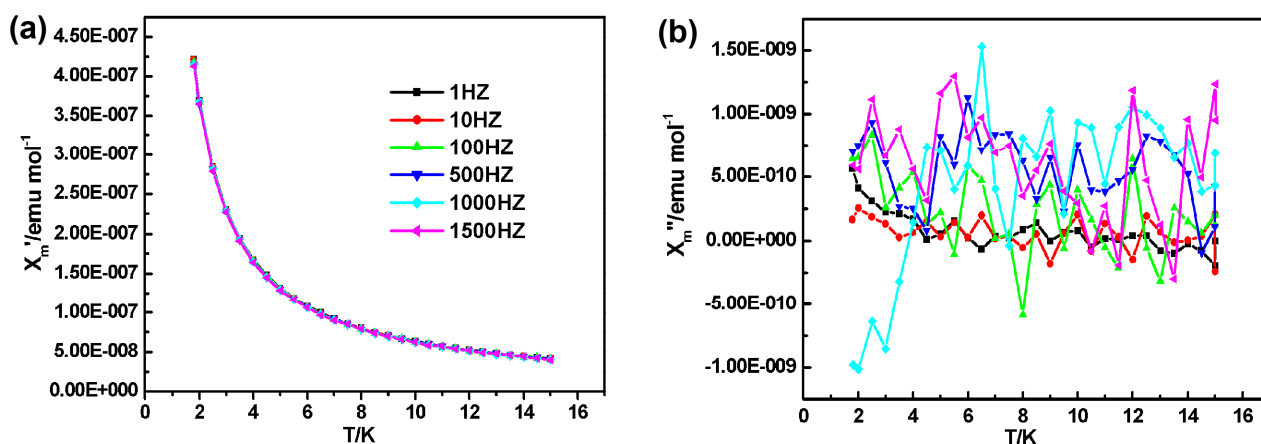


Fig. S6. Temperature dependences of in-phase (χ'_m) (a) and out-of-phase (χ''_m) (b) signals of the AC magnetic susceptibility measurements at 1–1500 Hz in field of 0 G.

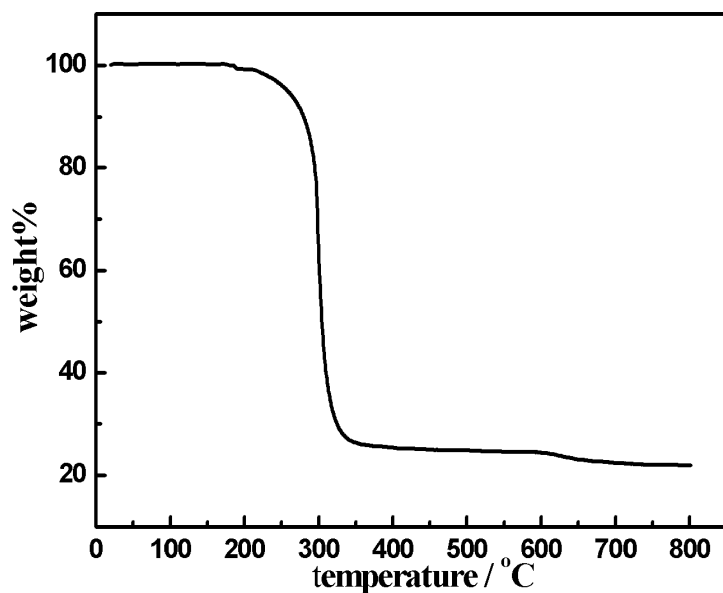


Fig. S7. Thermogravimetric (TG) curve of **1** measured in the range of 30–800 °C under air atmosphere with the heating rate of 10 °C/min.

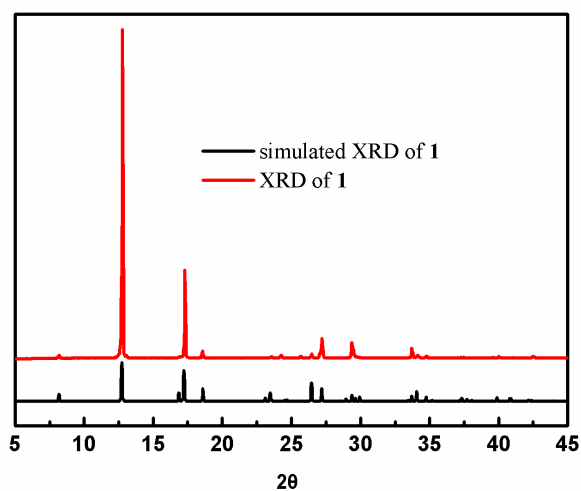


Fig. S8. PXRD patterns of the bulk product and the calculated pattern based on the single-crystal solution of **1**.

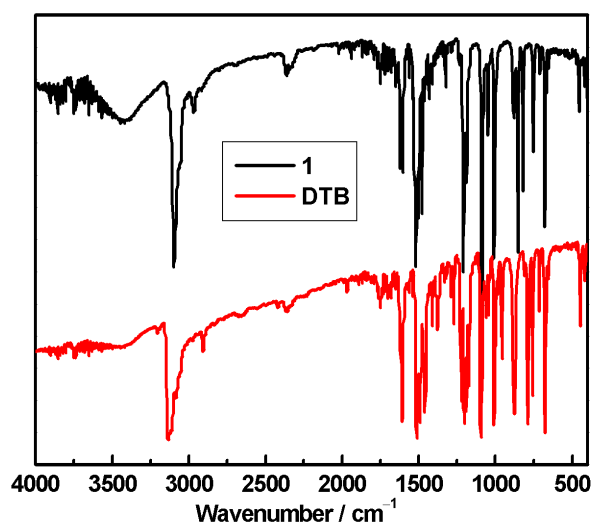


Figure S9. IR spectra of **1** and DTB.