Supplementary Material (ESI) for Chemical Communications

An Azido-Cu^{II}-triazolate Complex with utp-Type Topological Network, Showing Spin-canted Antiferromagnetism

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Materials, Methods, and Characterizations

All the reagents for synthesis were obtained commercially and used as received.

Elemental analyses were performed on a Perkin-Elmer 240C analyzer. IR spectrum was measured on a TENSOR 27 (Bruker) FT-IR spectrometer with KBr pellets. The X-ray powder diffraction (XRPD) was recorded on a Rigaku D/Max-2500 diffractometer at 40 kV, 100 mA for a Cu-target tube and a graphite monochromator. Simulation of the XRPD spectra was carried out by the single-crystal data and diffraction-crystal module of the commercially available *Cerius2* program (*Cerius2*, Molecular Simulation Incorporated, San Diego, CA, 2001.).

Complex **1** was obtained as crystals by low-temperature hydrothermal reaction. Several experiments in which the ratio of reactants was scanned showed that the formation of **1** is almost independent on the ratio. The material is stable in air at ambient temperature and almost insoluble in common solvents such as water, alcohol, acetonitrile, chloroform, acetone and toluene. XRPD pattern (Fig. 1S) and IR spectrum (Figure 2S) are shown below. Due to the potential explosive nature, the thermal analysis of **1** was not carried out.

Single-crystal X-ray diffraction measurement for **1** was carried out on a Rigaku R-AXIS RAPID IP diffractometer equipped with a graphite crystal monochromator situated in the incident beam for data collection at 293(2) K. Data collections and cell refinement were performed with RAPID-AUTO (Rigaku. *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan, 2004). Data reduction was carried out using CrystalStructure (Rigaku/MSC. *CrystalStructure.* Rigaku/MSC Inc. The Woodlands, Texas, USA, 2004). The structure was solved by direct methods using the SHELXS program of the SHELXTL package and refined with SHELXL (Sheldrick, G. M., *SHELXTL Version 6.1. Program for Solution and Refinement of Crystal Structures*, University of Göttingen, Germany, 1998). The final refinement was performed by full matrix least-squares methods with anisotropic thermal parameters

for non-hydrogen atoms on F^2. H atoms of trz were added theoretically, riding on the concerned atoms and refined with fixed thermal factors. The terminal N atom of N_3^- group is disordered, and was refined in two sites with the occupancies being fixed at 0.5.

Crystallographic data for the structure of **1** have also been deposited with the Cambridge Crystallographic Data Centre as supplementary publication, no. CCDC-635768. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (.44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

Magnetic data were collected at the Unitat de Mesures Magnètiques (Universitat de Barcelona) using crushed crystals of the sample on a Quantum Design MPMS-XL SQUID magnetometer equipped with a 5T magnet. Diamagnetic corrections were calculated using Pascal's constants and an experimental correction for the sample holder was applied.

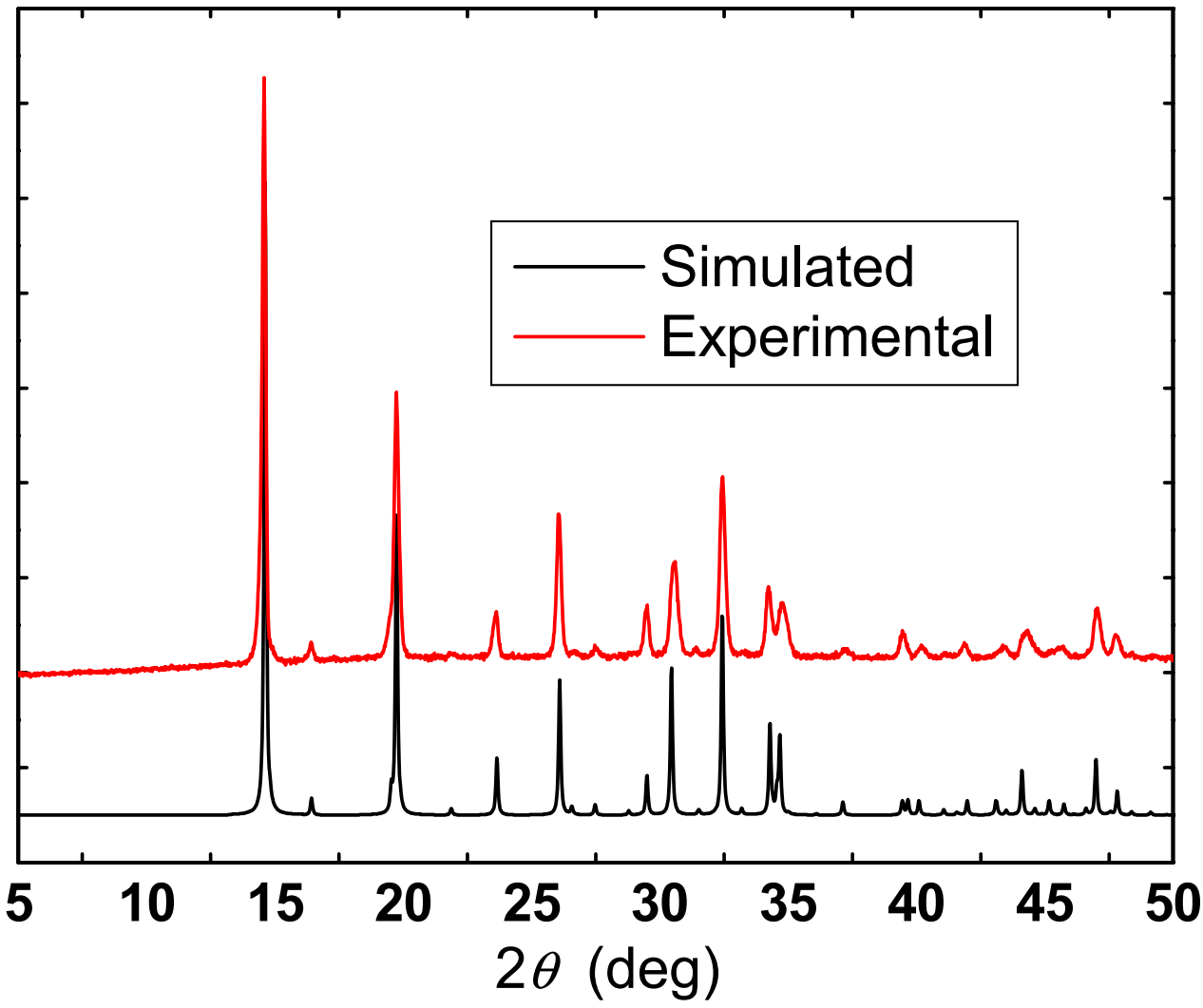


Fig. 1S. XRPD patterns for **1**.

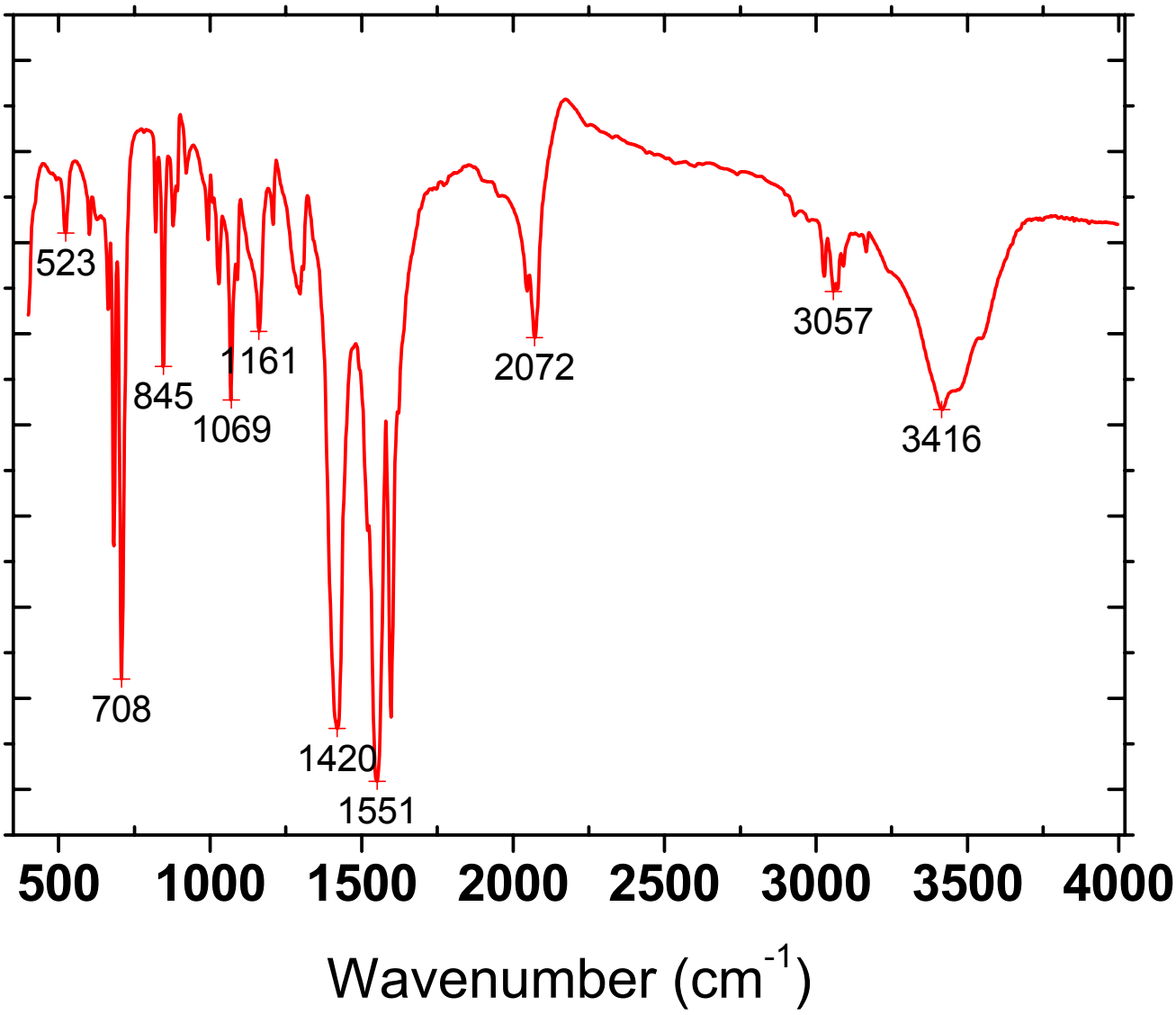
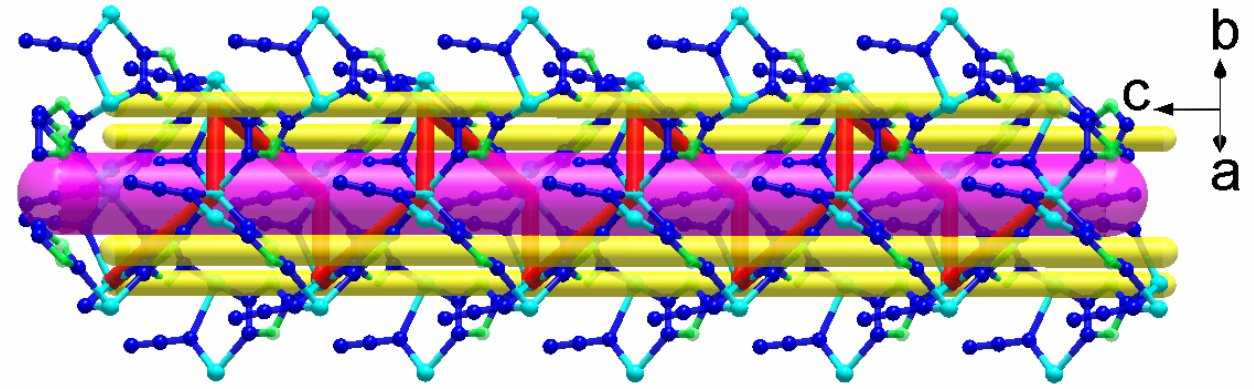
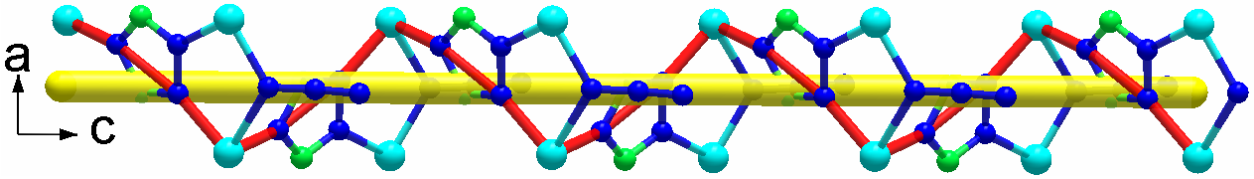


Fig. 2S. FT-IR spectrum of **1**.

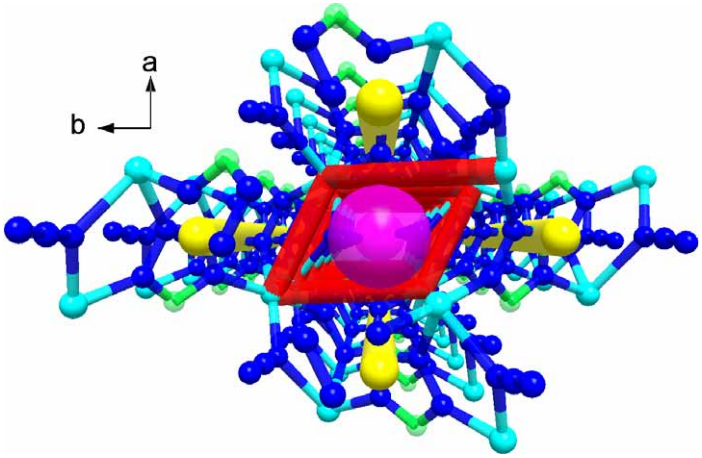
Additional Structural Figures



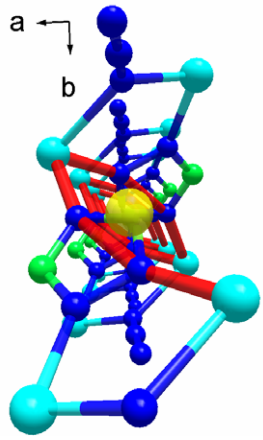
(a)



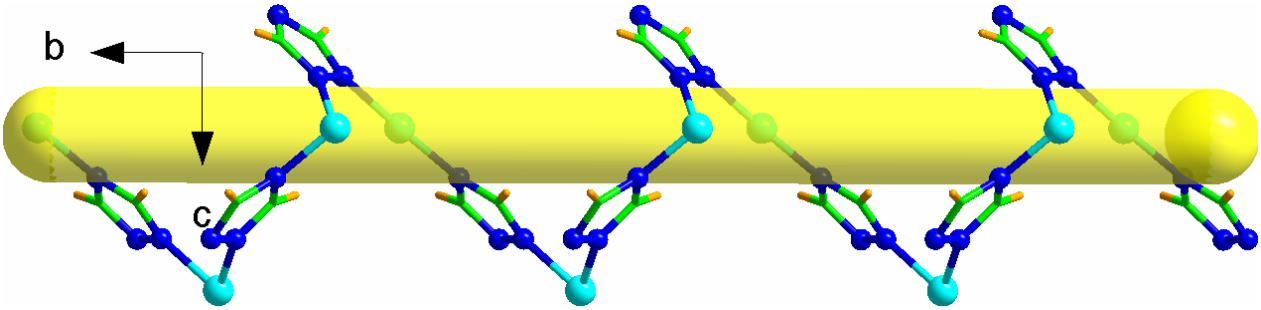
(b)



(c)



(d)



(e)

Fig. 3S. Several helixes in the structure of **1**: (a)~(d) along the *c* direction, side view and top view; (e) along the *b* direction, side view. H atoms were omitted in (a)~(d) for clarity.

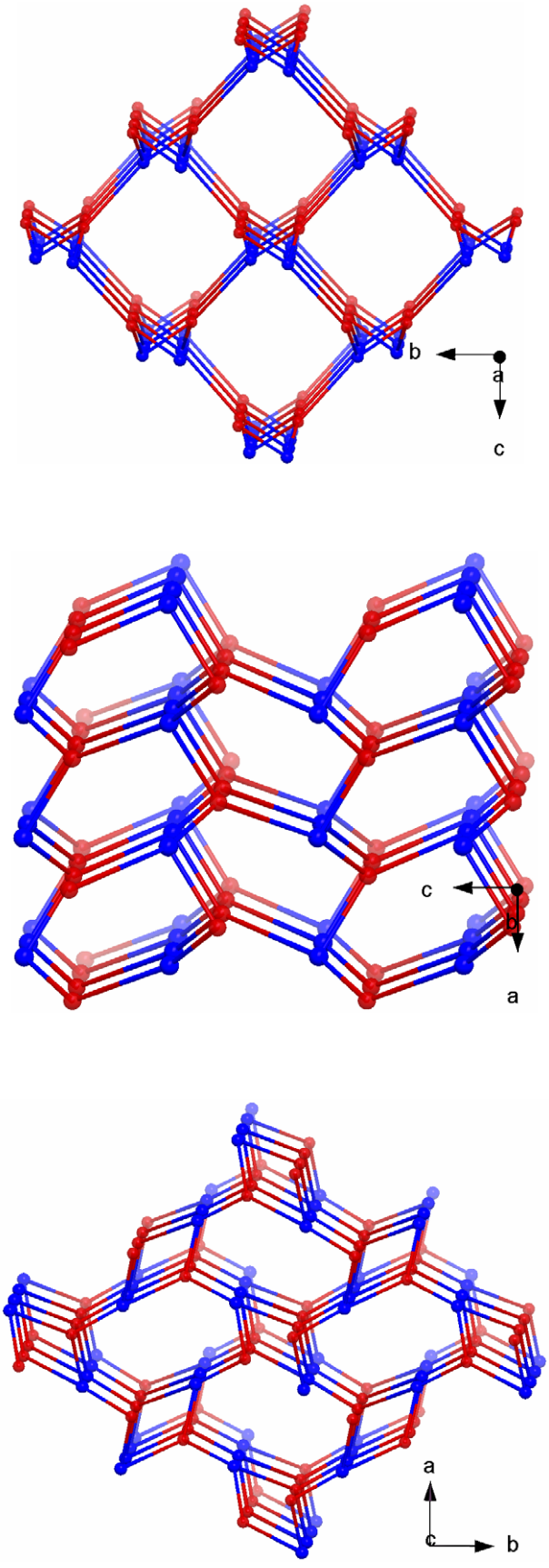


Fig. 4S. Schematic representations the overall 3-connected **utp** [(10,3)-d] type topological network of **1** viewed along the different directions. The ligand nodes represented as red and Cu^{II} as blue spheres.