Four Cu$^{1}$(ett) Coordination polymorphs and Changes in XRD Upon Hydrothermal Condition Optimization

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Supporting Information

Fig. S1. The crystal photograph for 1-α, 1-β, 1-γ and 1-δ
Fig. S2 (a) The asymmetric unit of 1-α; (b) The 1D infinite chain in $ab$ plane of 1-α; (c) The 2D inorganic-organic network structure by two coordination mode ($\mu_5$-$\eta^1 \cdot \eta^1 \cdot \eta^1 \cdot \eta^1 \cdot \eta^1 \cdot \eta_S^1$ and $\mu_3$-$\eta^1 \cdot \eta^1 \cdot \eta^1$ coordination mode)
Fig. S3 (a) The asymmetric unit of 1-β and 1-γ; (b) The 1D infinite chain in $ab$ plane of 1-β; (c) The 2D inorganic-organic network structure by $\mu_4$-$\eta^1$,$\eta^1$,$\eta^1$,$\eta^1$ coordination mode
Fig. S4. (a) The asymmetric unit of 1-δ; (b) The 3D structure along the a axis; (c) The 2D inorganic-organic network structure by two coordination mode ($\mu_4-\eta^1,\eta^1,\eta^1,\eta^1_S$ and $\mu_4-\eta^1,\eta^1,\eta^1,\eta^1$ coordination mode)
Fig. S5. XPRD patterns for 1-α and 1-δ: (top) measured at room temperature; (bottom) calculated on the basis of the structure determined by single-crystal X-ray diffraction.

Fig S6. The simulated PXRD patterns for 1-α, 1-β, 1-γ and 1-δ
Thermal Stability of the Polymorphs.

Thermogravimetric experiments were carried out from room temperature to 800 °C under a nitrogen atmosphere for 1-α, 1-β, 1-γ and 1-δ, and the results are shown in Fig S7. Four coordination polymorphs start to decompose around 295 °C. The total weight loss of about 57% (calculated 58.4%) corresponds to the decomposition of organic ligand and leftover Cu₂S. From the TG/DTG analysis, 1-α have more sharply decompose behavior than 1-β, 1-γ and 1-δ, which may arise from the different coordination mode of ett in these four coordination polymorphs.