Electronic Supplementary Material (ESI) for Dalton Transactions.


# Supporting Information

## Syntheses, structures, and magnetic properties of two unique Cu(II)-based coordination polymers involving crystal-to-crystal structural transformations from 1D chain to 3D network

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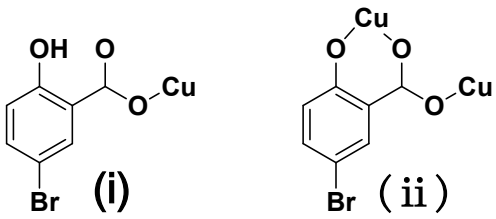


**Scheme S1** The different coordination modes of **$H_2$bsal** ligand in **1** (i) and **2** (ii) [(i) $\mu_1$-$\eta^1$ monodentate mode, (ii) $\mu_2$-$\eta^1$:$\eta^1$:$\eta^1$ chelating/bridging coordination mode)]

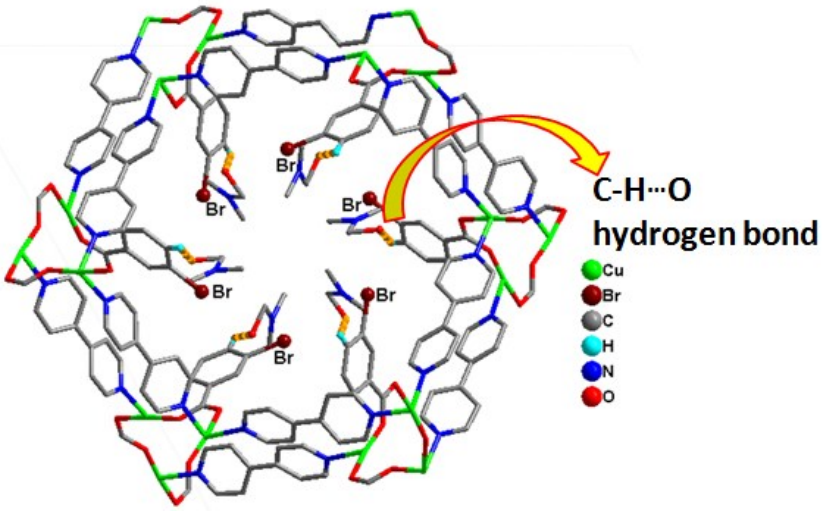


**Fig. S1** The internal environment of 1-D channel of **2**.

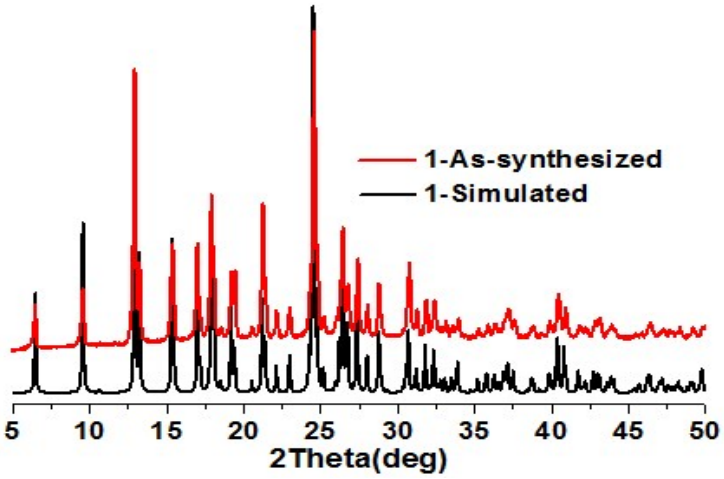


**Fig. S2** PXRD patterns of as-synthesized **1.**

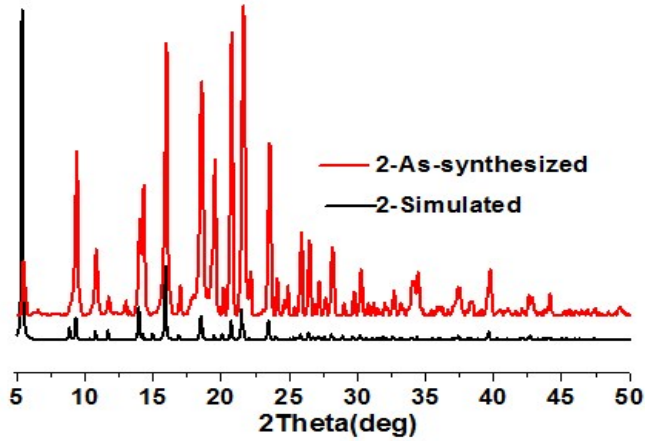


**Fig. S3** PXRD patterns of as-synthesized **2.**

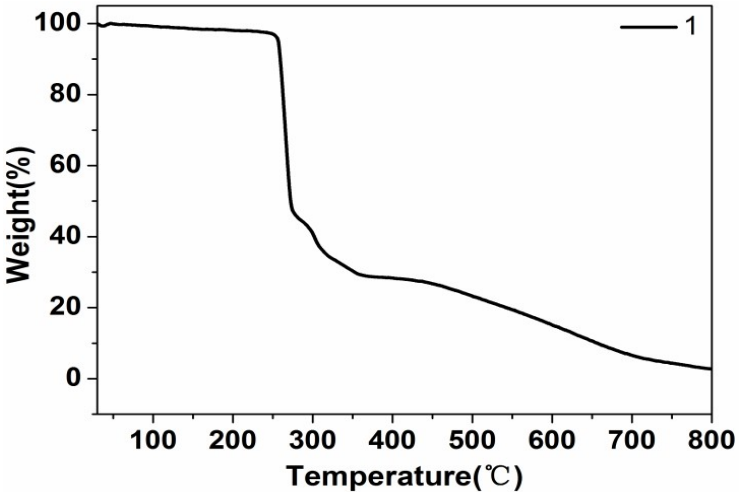


**Fig. S4** TGA curve of as-synthesized **1.**

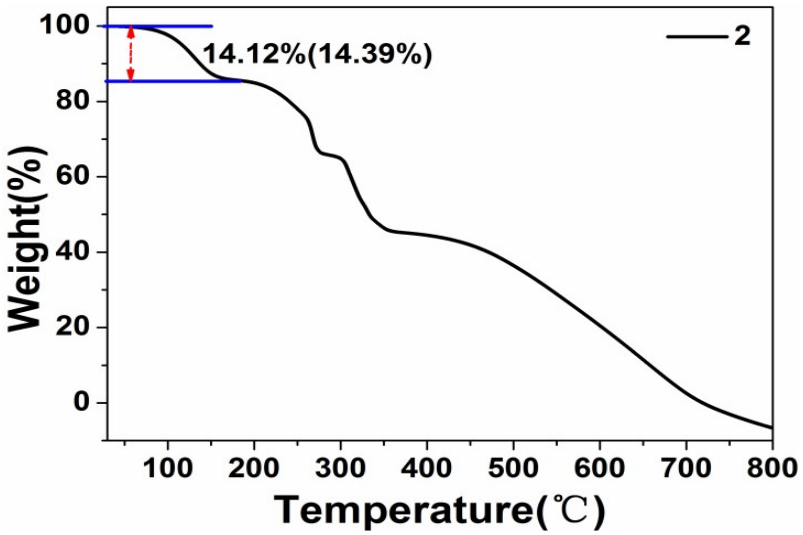


**Fig. S5** TGA curve of as-synthesized **2.**

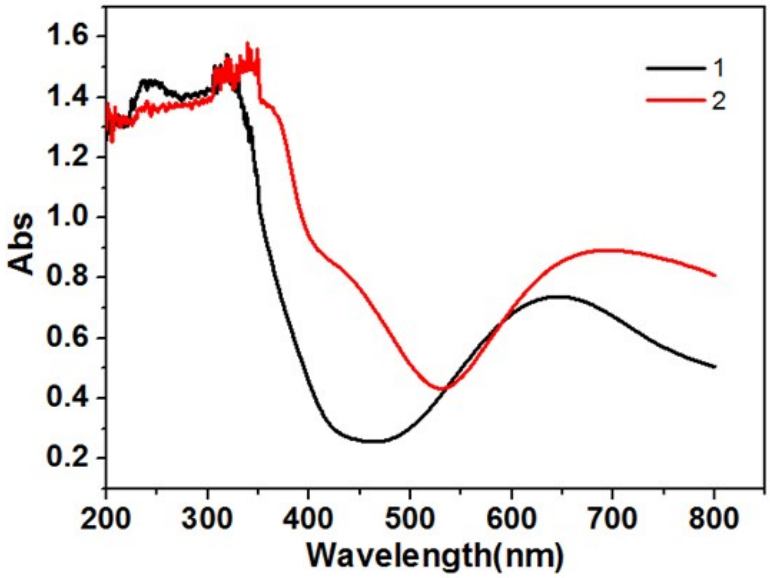


**Fig. S6** The UV-visible absorption of **1** and **2** in solid state

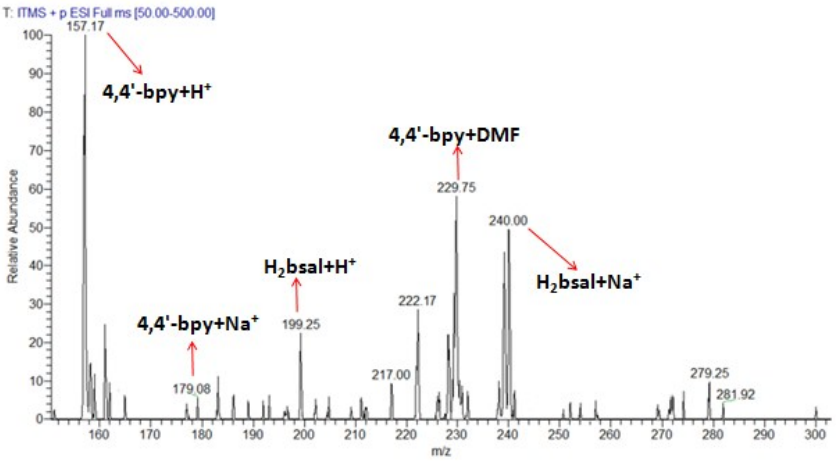


**Fig. S7** The MS of the DMF solution after soaking sample **1.**

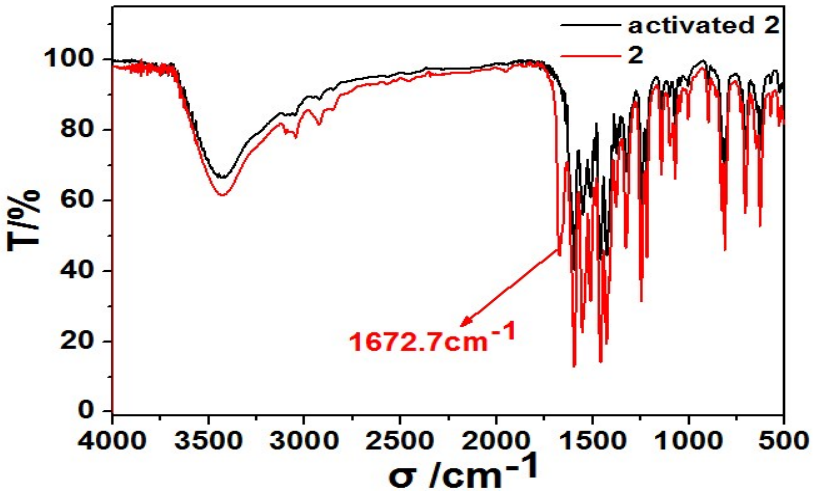


**Fig. S8** IR spectra of **2** and activated **2**.

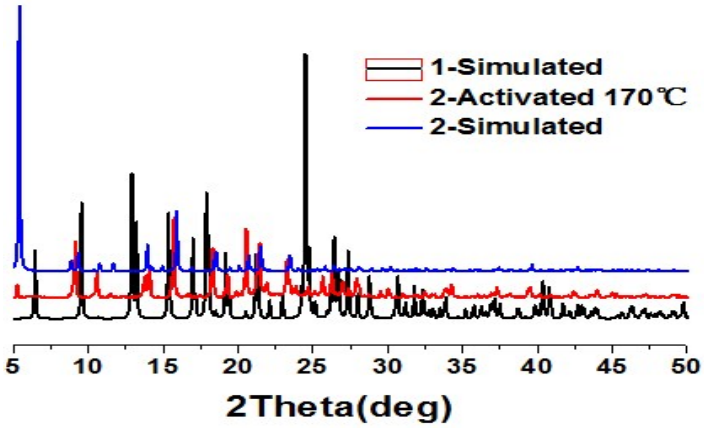


**Fig. 9** PXRD patterns of activated **2.**


**Fig. S10** The syn-anti carboxylate bridged 1D spiral chain of **2**

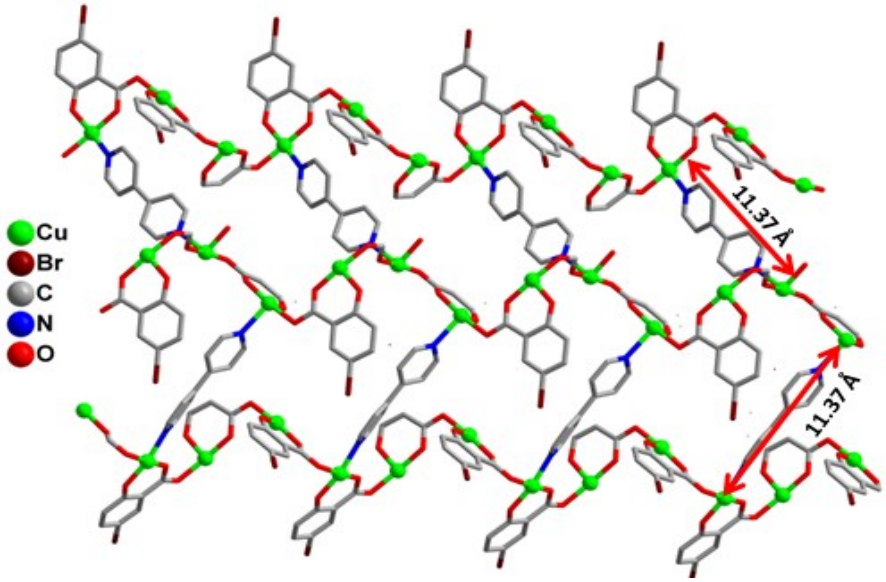


**Fig. S11** Perspective views of the **4,4'-bpy**-bridged layer in the *bc* plane of **2**

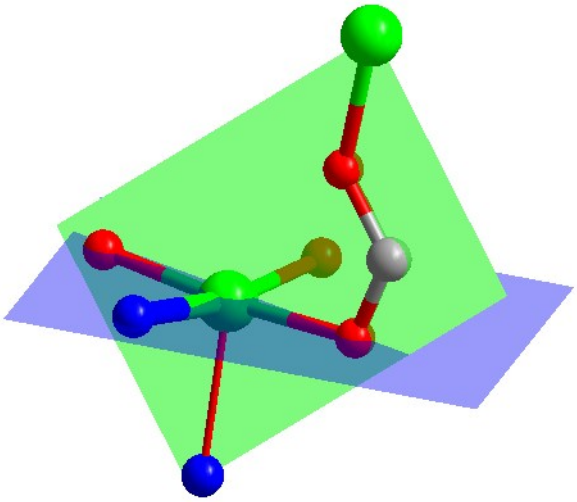

**Fig. S12** A graphical representation of the dihedral angle defined by the equatorial plane of $CuO_3N_2$ distorted square-pyramid (light purple), and the plane of O–C–O group (light green) for the Cu(II) center of **2**.

**Table S1** Selected distance (Å) and angles(°) of complex **1**

| | | | | | |
|---|---|---|---|---|---|
| Cu1-O2 | 1.963 (3) | Cu1-N3 | 2.318 (5) | Cu1-N1 | 1.902 (2) |
| Cu1-O2$^{i}$ | 1.963 (3) | | | | |
| O2-Cu1-O2$^{i}$ | 179.69 (3) | O2-Cu1-N1$^{i}$ | 89.31 (14) | O2$^{i}$-Cu1- N1$^{i}$ | 90.67 (14) |
| O2-Cu1- N1 | 90.67 (14) | O2$^{i}$-Cu1- N1 | 89.31 (14) | N1$^{i}$-Cu1-N1 | 172.1 (2) |
| O2-Cu1-N3 | 90.15 (10) | O2$^{i}$-Cu1-N3 | 90.15 (10) | N1$^{i}$- Cu1-N3 | 93.94 (11) |
| N1- Cu1-N3 | 93.94 (11) | | | | |

Symmetry codes: (i) -*x*+1, *y*, -*z*+3/2; (ii) -*x*, *y*, -*z*+3/2.

**Table S2** Selected distance (Å) and angles(°) of complex **2**

| | | | | | |
|---|---|---|---|---|---|
| Cu1-O1 | 1.910 (3) | Cu1-O2 | 1.940 (3) | Cu1-O3$^{i}$ | 1.990 (3) |
| Cu1-N2 | 2.041 (4) | Cu1-N1$^{v}$ | 2.292 (4) | | |
| O1-Cu1-O2 | 91.92 (14) | O1-Cu1-O3$^{i}$ | 88.70 (14) | O2-Cu1-O3$^{i}$ | 173.41 (14) |
| O1-Cu1-N2 | 167.82 (15) | O2-Cu1-N2 | 88.44 (14) | O3$^{i}$ -Cu1-N2 | 89.58 (14) |
| O1-Cu1-N1 | 98.50 (15) | O2-Cu1-N1 | 93.72 (14) | O3$^{i}$-Cu1-N1 | 92.68 (14) |
| N2-Cu1-N1 | 93.62 (15) | | | | |

Symmetry codes: (i) -*y*+4/3, *x*-*y*+5/3, *z*-1/3; (ii) *x*-*y*+4/3, *x*+2/3, -*z*+5/3; (iii) *y*-2/3, -*x*+*y*+2/3, -*z*+5/3; (iv) -*x*+*y*-1/3, -*x*+4/3, *z*+1/3.