

Supporting information

Liquid/Vapor-Induced Reversible Dynamic Structural Transformation of a Three-Dimensional Cu-based MOF to a One-Dimensional MOF Showing Gate Adsorption

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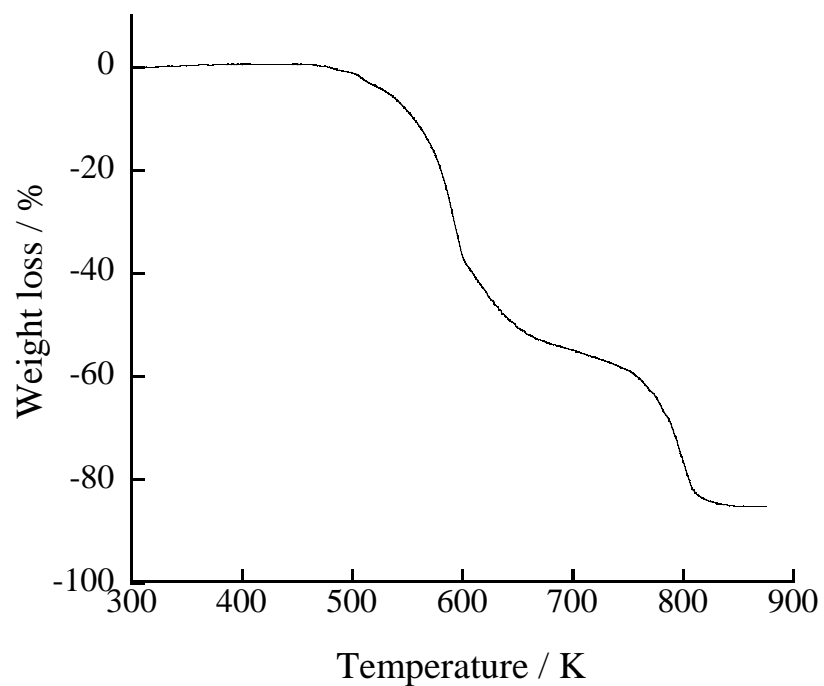


Figure S1. A TG curve of **1(3D)** at a heating rate of 10 K min^{-1} under air flow (150 ml/min).

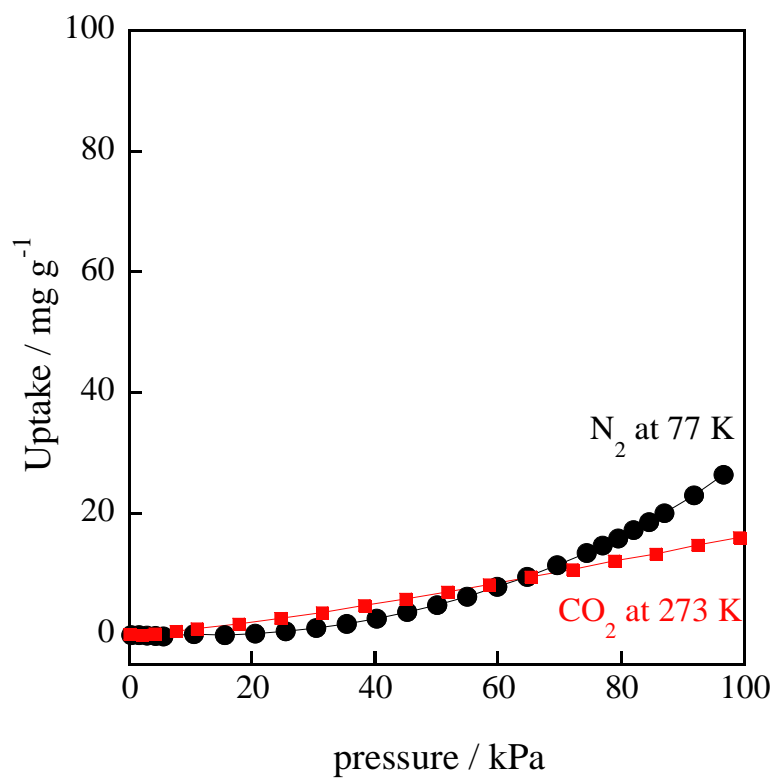


Figure S2. Nitrogen (black) and CO_2 (red) adsorption isotherm on **1(3D)**.

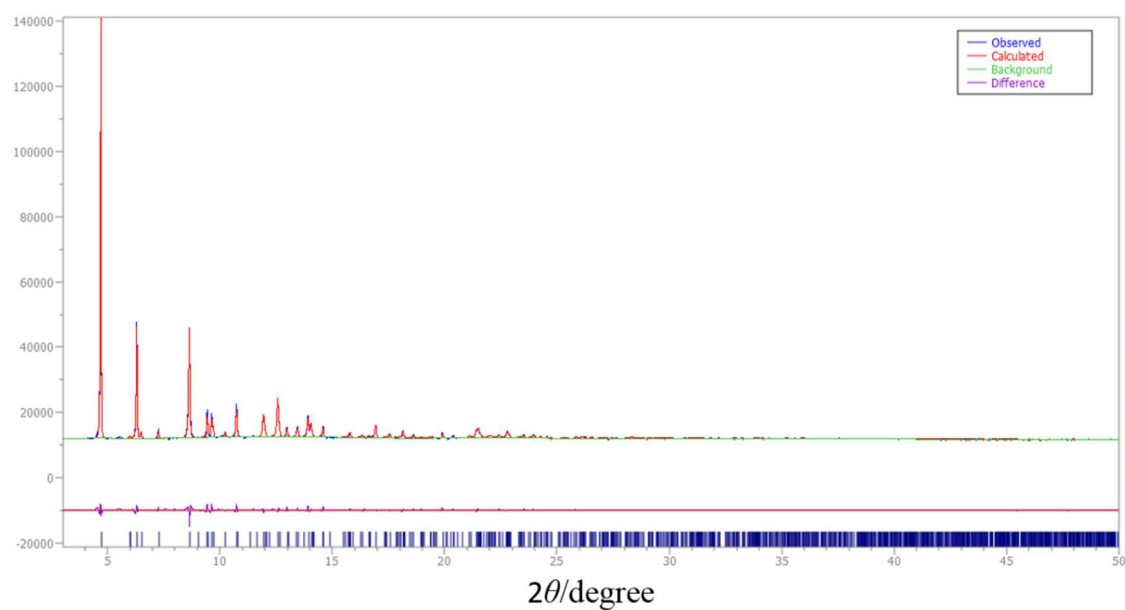


Figure S3. Le Bail pattern fit of a synchrotron X-ray diffraction pattern of **1(3D)** after immersion in ethanol/water mixture at a room temperature. Observed, calculated, background, and differential patterns are shown in blue, red, right green, and purple. ($\lambda = 0.79917(2) \text{ \AA}$)

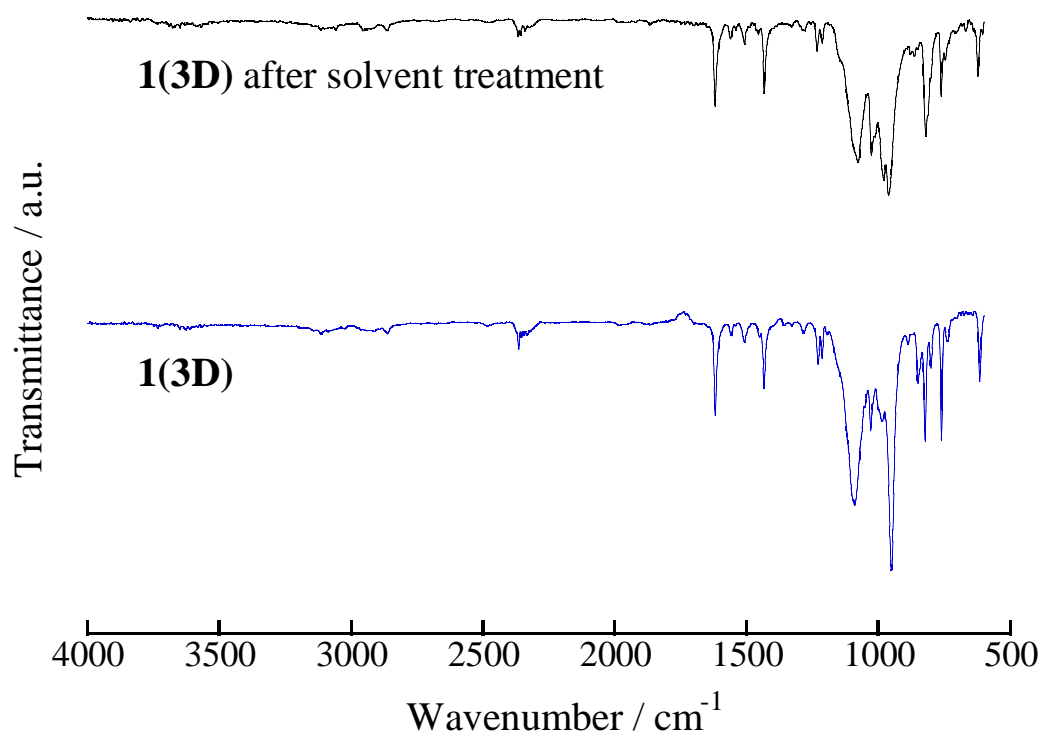


Figure S4. FT-IR spectra of **1(3D)** and **1(3D)** after solvent treatment, which correspond to **2(1D)**.

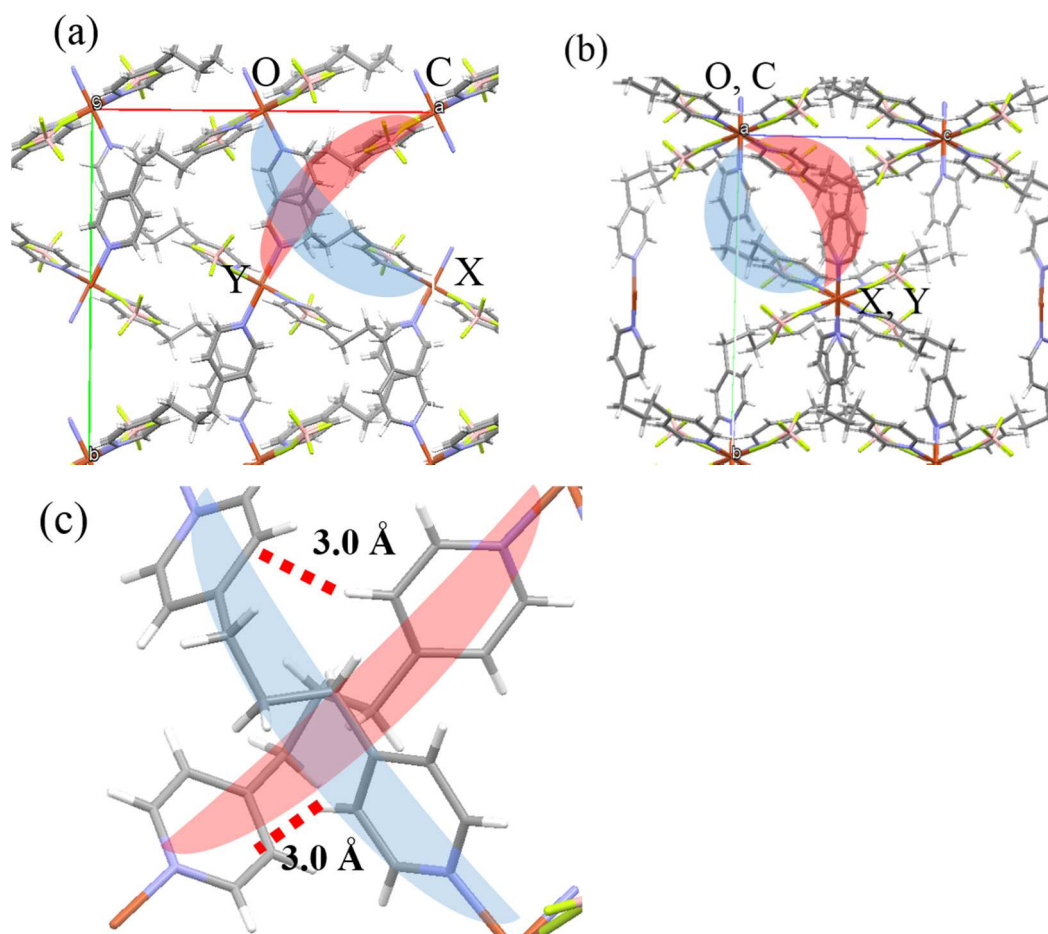


Figure S5. Crystal structure of **1(3D)** along (a) *c* axis and (b) *a* axis, and (c) schematic representation of C-H... π interaction between bpp ligands.

Table S1. CHN elemental analysis of **2(1D)** and **1(3D)** after the solvent treatment.

element	Calcd. ^a	2(1D) [2]	1(3D) after the solvent treatment
C/ %	49.30	49.09	49.15
H/ %	4.50	4.57	4.52
N/ %	8.80	8.75	8.83

a. The values were calculated based on the chemical formula of $[\text{Cu}(\text{BF}_4)_2(\text{bpp})_2]$.

Table S2. Full width at half maximum (FWHM) of selected diffraction lines in XRD patterns.

Sample	FWHM (°) of each diffraction line				
	Miller indices				
	110	111	111	401	221
Directly prepared one	0.167	0.192	0.234	0.307	0.241
Converted one	0.271	0.222	0.376	0.348	0.381

Table S3. Results of the mixed solution adsorption by gas chromatography.

Mixture (volume %)	Peak ratio (%)		Adsorbed amount per Cu atom
	Before adsorption	After adsorption	
Benzene (50%)	52.0	49.0	1.9
Cyclohexane (50%)	48.0	51.0	-

References

- [1] E. Nishibori, M. Takata, K. Kato, M. Sakata, Y. Kubota, S. Aoyagi, Y. Kuroiwa, M. Yamakata, N. Ikeda, *Nucl. Instrum. Methods A*, **2001**, *467-468*, 1045.
- [2] R. Kotani, A. Kondo, K. Maeda., *Chem. Commun.*, **2012**, *48*, 11316.