

Electronic Supplementary Information

For

Anion-dependent coordinative networking of macrocycle with copper(I) halides

In-Hyeok Park,[‡] Hyun Jee Kim[‡] and Shim Sung Lee^{*}

*Department of Chemistry and Research Institute of Natural Science,
Gyeongsang National University, Jinju 660-701, S. Korea*

[‡]These authors contributed equally.

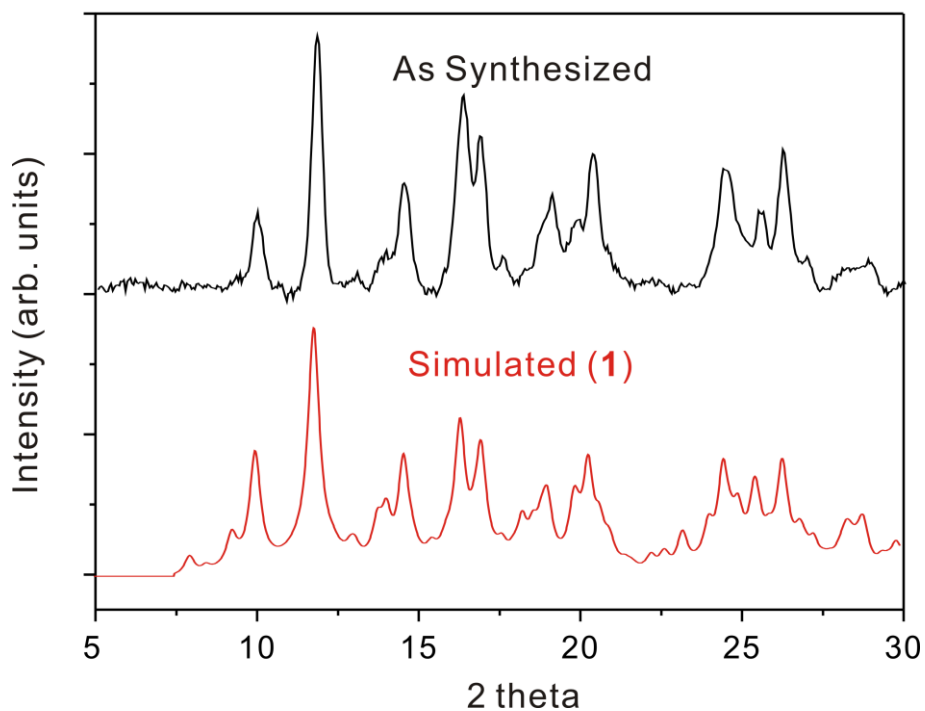


Fig. S1 Comparison of XRPD patterns: (top) as synthesized and (bottom) **1** simulated from the single crystal X-ray data.

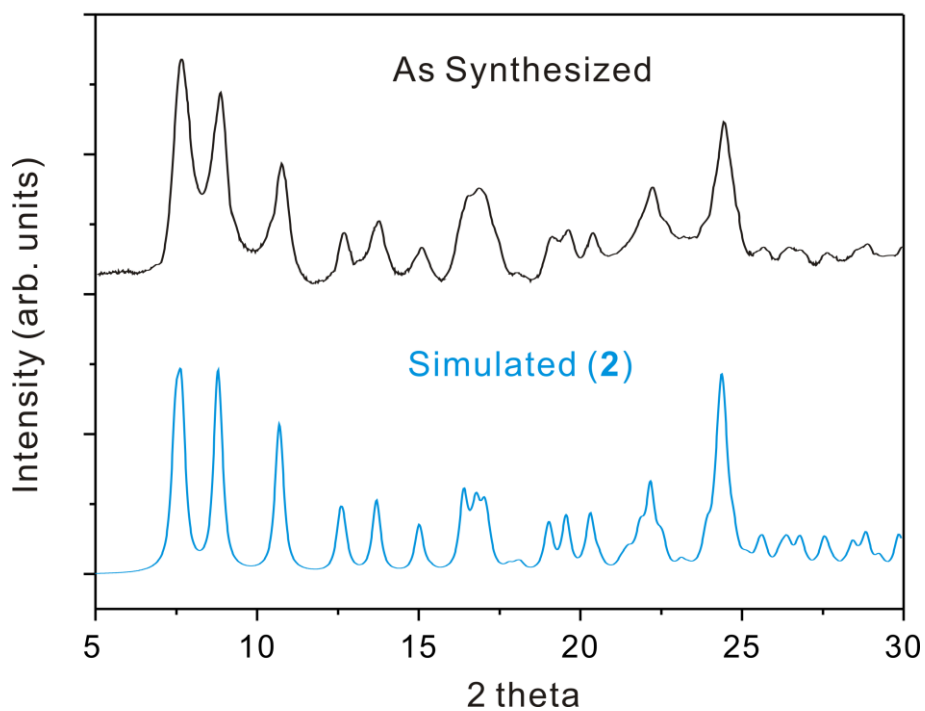


Fig. S2 Comparison of XRPD patterns: (top) as synthesized and (bottom) **2** simulated from the single crystal X-ray data.

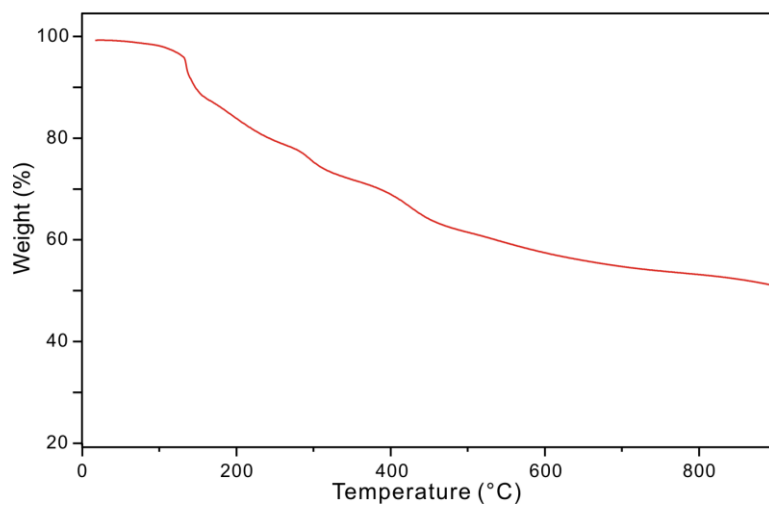


Fig. S3 TGA curve of **1**.

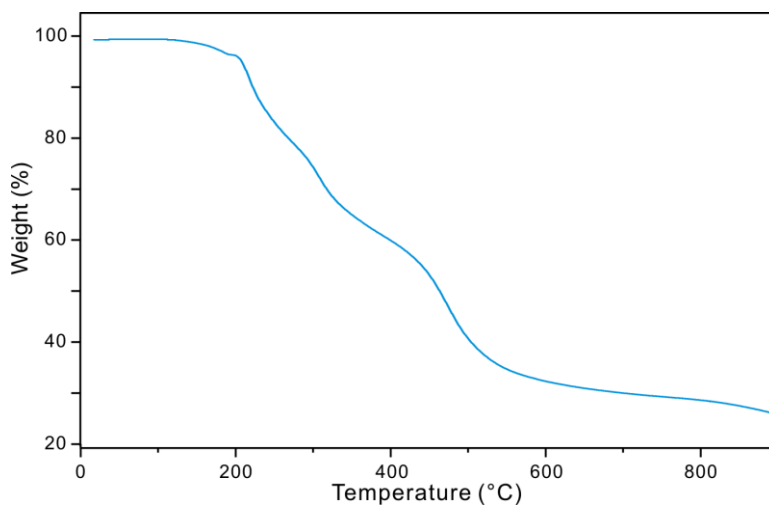


Fig. S4 TGA curve of **2**.

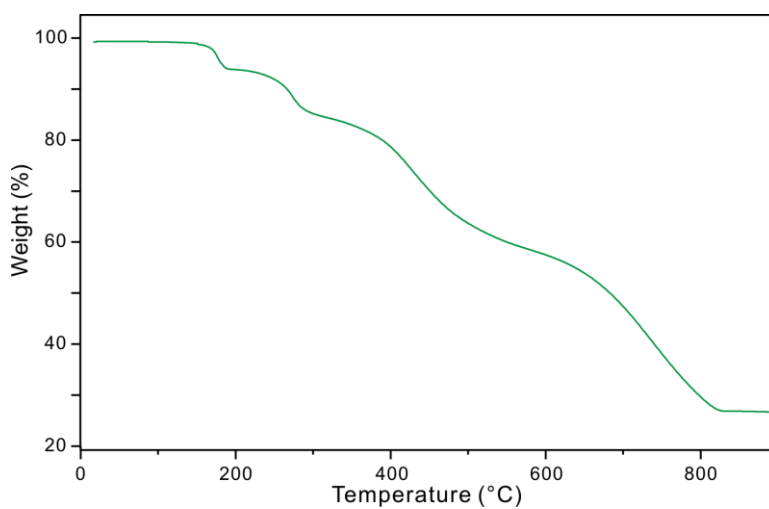


Fig. S5 TGA curve of **3**.

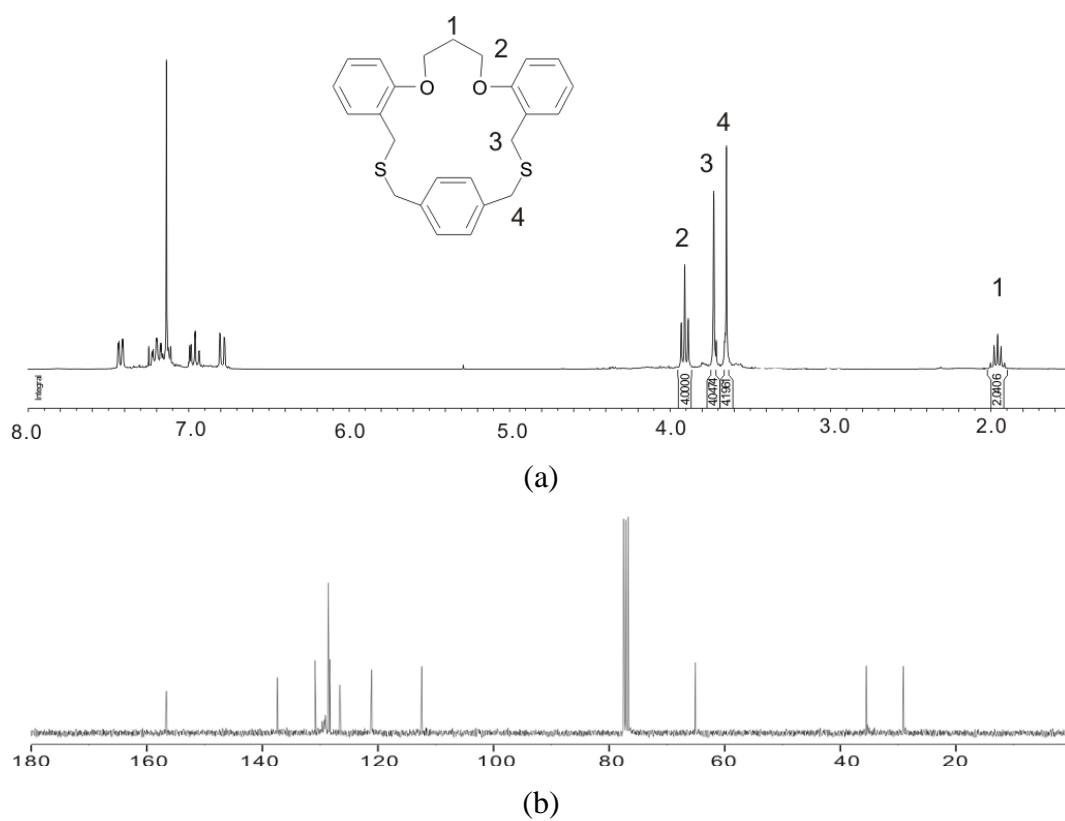


Fig. S6 (a) ¹H and (b) ¹³C NMR spectra of **L** in CDCl₃.

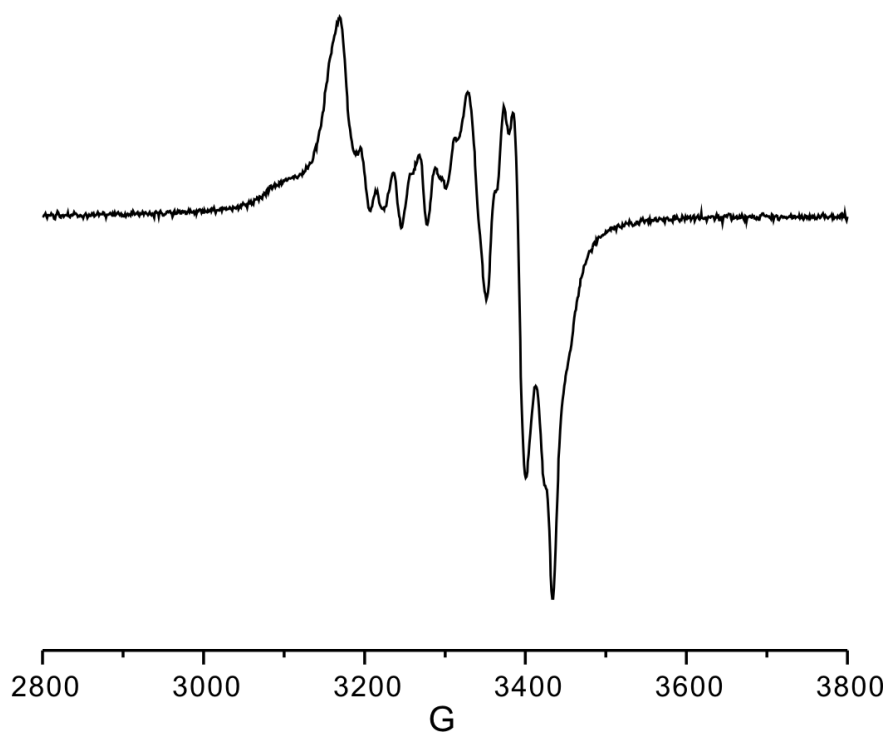


Fig. S7 EPR spectrum of **1** at room temperature.

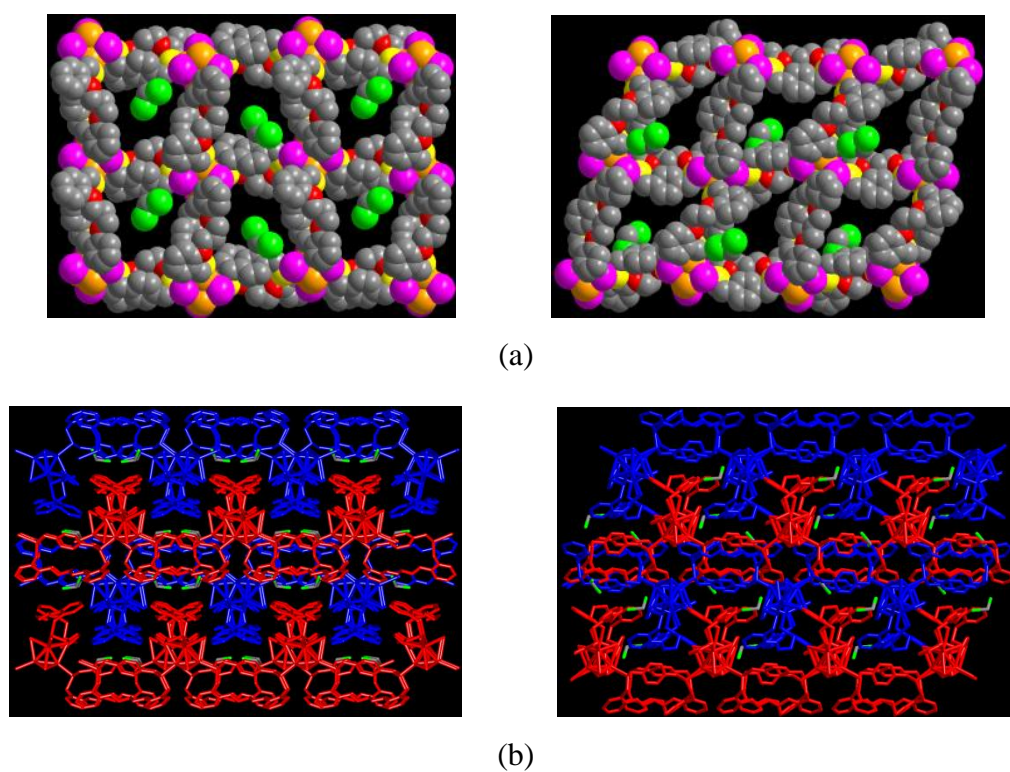


Fig. S8 Comparison of the 2D network structures of (*left*) **3a**, $\{[\text{Cu}_4\text{I}_4(\text{L})_2]\cdot\text{CH}_2\text{Cl}_2\}_n$ and (*right*) **3b**, $\{[\text{Cu}_4\text{I}_4(\text{L})_2]\cdot\text{CH}_2\text{Cl}_2\}_n$: (a) square grid structures (ball) and (b) layer-to-layer packing arrangements (stick).

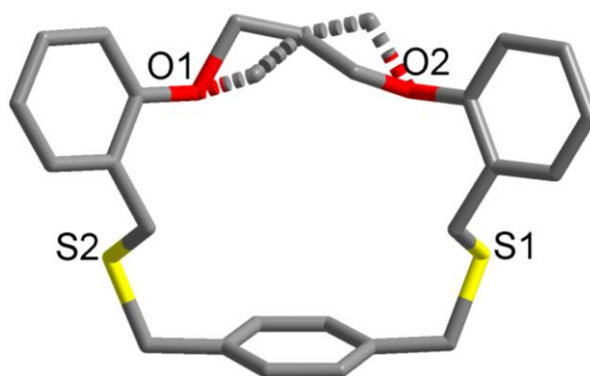


Fig. S9 Crystal structure of **L**, showing the disorder between two oxygen atoms (55:45).