Supporting Information

Phototriggered Mechanical Movement in A Bipyridinium-based Coordination Polymer Powered by Electron Transfer

Xiao-Dong Yang, Rui Zhu, Li Sun, Rui-Yun Guo and Jie Zhang*

MOE Key Laboratory of Cluster Science, Beijing Key Laboratory of Photoelectronic/Electrophotonic Conversion Materials, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 102488, P. R. China

**Corresponding author: zhangjie68@bit.edu.cn*

****

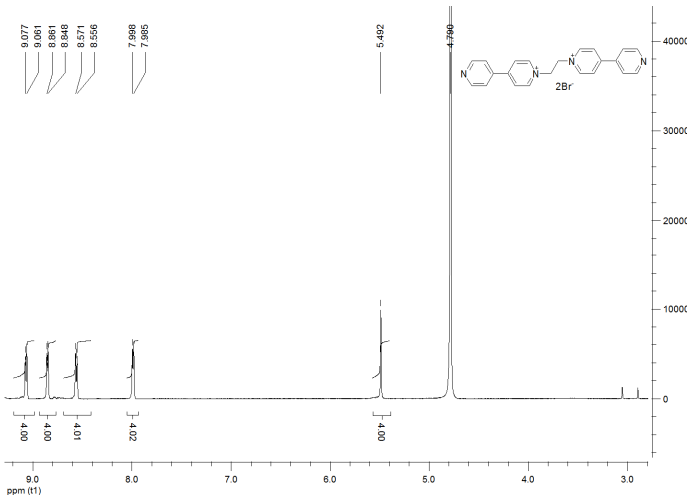


Figure S1. The ^{1}H NMR spectrum of $BpyenBr_2$ in D_2O (400 MHz).

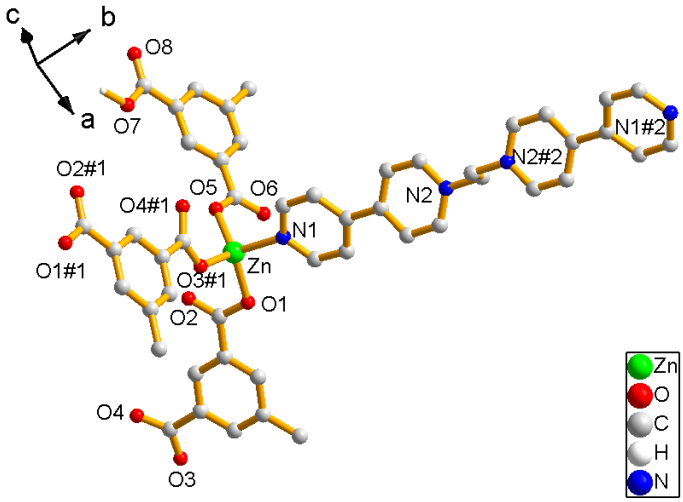


Figure S2. The coordination environment of Zn(II) ion in **1**. Symmetry codes: #1 x, -y, 0.5+z; #2 1-x, 1-y, 1-z. All hydrogen atoms and solvent molecules are omitted for clarity.

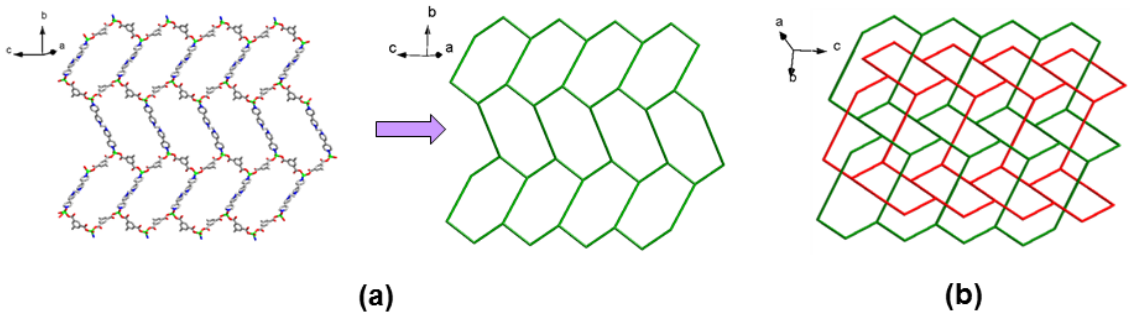
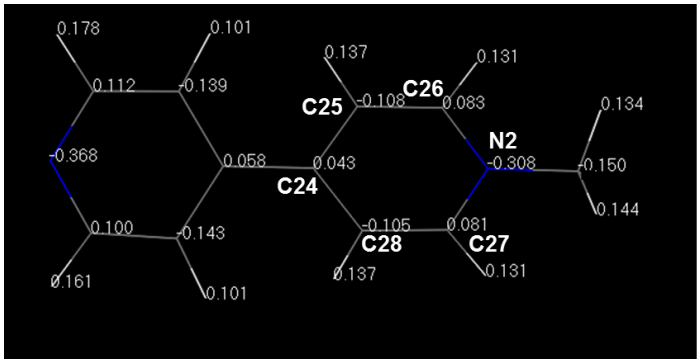
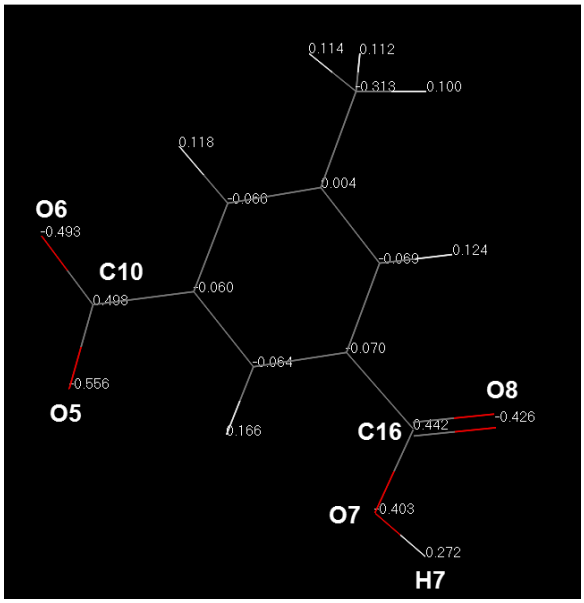


Figure S3. (a) The (6, 3)-connected network of **1**. (b) The 2-fold interpenetrated structure between adjacent networks in **1**.



(a)



(b)

Figure S4. The charge Mulliken population of $Bpyen^{2+}$ ligand (a) and $Hmip^{-}$ ligand (b).

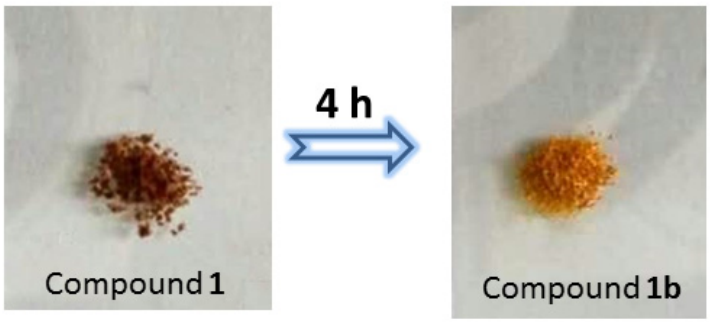


Figure S5. The photographs of piles of **1**, **1b**. The bulk phase exhibits more obvious color transformation after long time irradiation. .

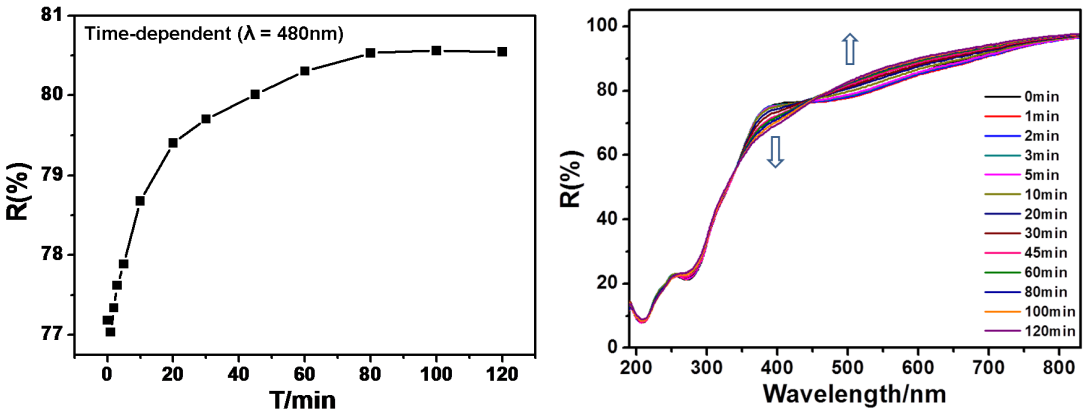


Figure S6. (a) Time-dependent reflectance at 480 nm of **1** under 365 nm light irradiation. (b) Time-dependent UV-vis diffuse reflectance spectral changes of **1** upon 365 nm light irradiation.

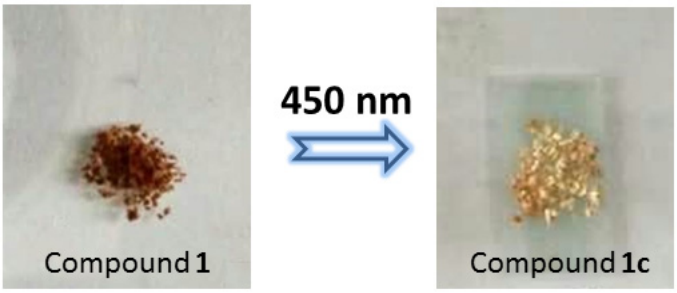
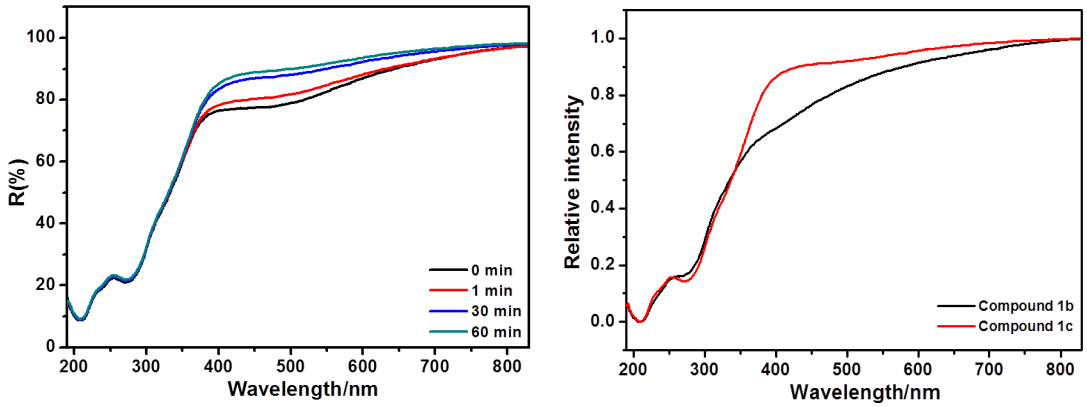


Figure S7. Color transformation of piles of **1** under the irradiation of 450 nm light within 60 min. The color discrepancy against Figure 3b is mainly due to the aggregation effect of single crystals.



(a) **(b)**

Figure S8. (a) UV-vis diffuse reflectance spectral changes of **1** under the irradiation of 450 nm light. (b) The normalized UV-vis diffuse reflectance spectra of **1b**, **1c**.

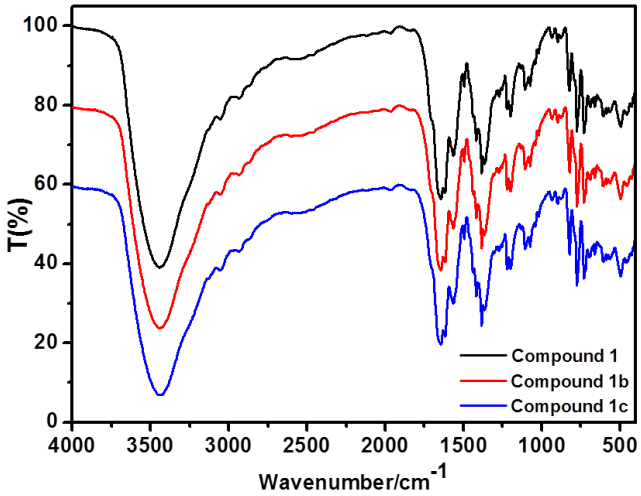


Figure S9. IR spectra of **1**, **1b**, **1c**.

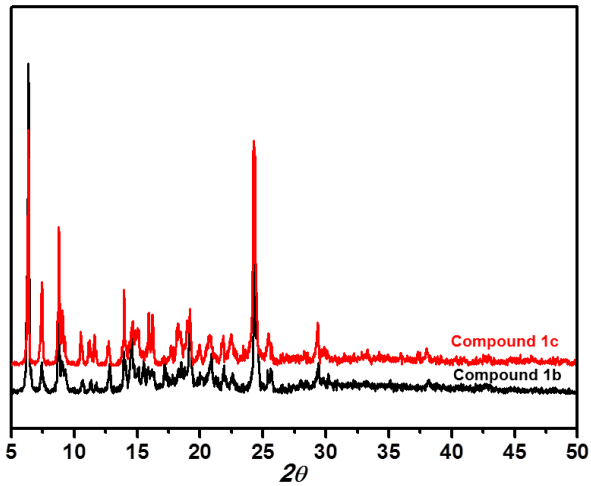


Figure S10. PXRD patterns of **1b**, **1c**.

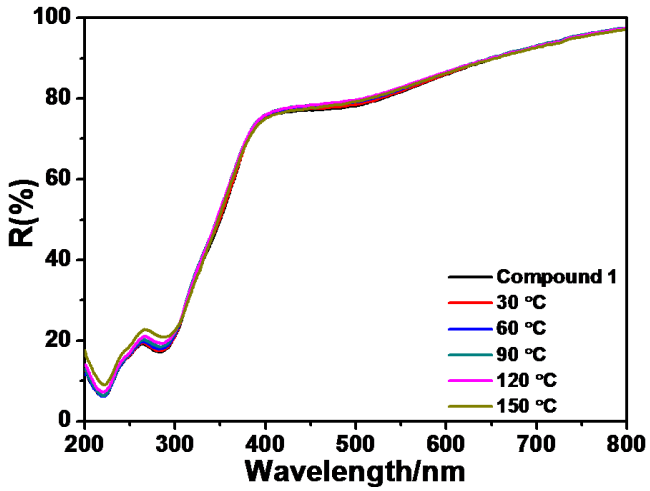


Figure S11. Variable-temperature UV-vis diffuse reflectance spectra of **1** measured from 30 °C to 150 °C.

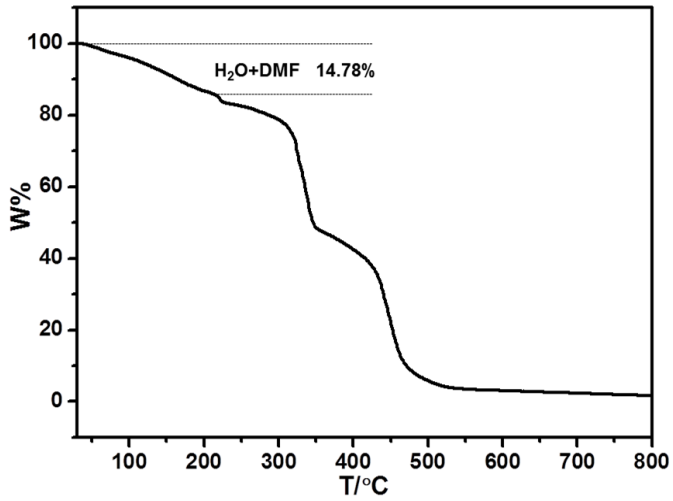


Figure S12. TGA curve of **1**. The TGA curve of **1** shows a weight loss of 14.78% from 30 to 220°C corresponding to the release of dissociative solvent molecules (DMF, H_2O) in the lattice (calcd: 14.38%).

Table S1. Selected Charges from the DFT Analysis

Group	Pyridinium ring	Carboxylate group	
Atom label	From N2 to C28	O5-C10-O6	O7-C16-O8
Total charge	+0.22	-0.55	-0.39