Supporting Materials

A photoactive porous metal-organic complex: synthesis, crystal morphology and the influence of photocycloaddition on fluorescence property and adsorption behavior

Li-Xuan Cai,^{ac} Cheng Chen,^a Bin Tan,^{ac} Ya-Jun Zhang,^{ac} Xiao-Dong Yang^{ac} and Jie Zhang*ab

^aState Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Fuzhou, Fujian 350002 P. R. China, Fax: (+86) 591-83710051, E-mail: <u>zhangjie@fjirsm.ac.cn</u>. ^bSchool of Chemistry, Beijing Institute of technology, Beijing, 100081, P. R. China. ^cUniversity of Chinese Academy of Sciences, Beijing 100049, P. R. China.



Fig.S1 ¹H NMR spectrum for *m*-HBCbpe Cl in d6-DMSO.





Fig.S3 IR spectra of 1 (a), desolventized sample 1' (b), and irradiated sample 1-i (c).



Fig.S4 PXRD patterns of simulated **1** (a), as-synthesized **1** (b), **1** exposed to UV light for 2 h (c), **1** exposed to UV light for 4 h (d), **1** exposed to UV light for 6 h (e), **1** is exposed to UV light for 38 h (f).



Fig.S5 ¹H NMR spectra of *m*-BCbpe in D₂O before and after 365 nm UV irradiation for 60 hours. The vinyl and cyclobutane protons are represented by (\bullet) and (\star), respectively. It shows that almost complete conversion has taken place.



Fig.S6 Emission profiles of *m*-BCbpe (black line) and its photodimer product obtained through exposing the sample to 365 nm UV light for 60 hours (red line) in H_2O ($\lambda_{ex} = 390$ nm).



Fig.S7 The TG Plots of compound 1 (black) and desolventized sample 1' (red).



Fig.S8 PXRD patterns of simulated 1 (black), desolventized sample 1' (red) and irradiated sample 1'-i after activation (blue).



Fig.S9 N_2 sorption isotherms for desolventized sample 1' (black) and irradiated sample 1'-i (red).



Fig.S10 H_2 sorption isotherms for desolventized sample 1' (black) and irradiated sample 1'-i (red).





Chart S1. Definitions of the Parameters Usually Considered To Be Geometric Criteria for [2+2] Photodimerization of Double Bonds (According to Ref: V.Ramamurthy, K.Venkatesan, *Chem. Rev.* **1987**, 87, 433–481; θ 3 is the Angle between the >C=C< and C=C-C=C Planes).