

## Electronic Supplementary Information (ESI)

### Photochromism of a pyrazolone derivative in crystalline state and in HPMC composite film

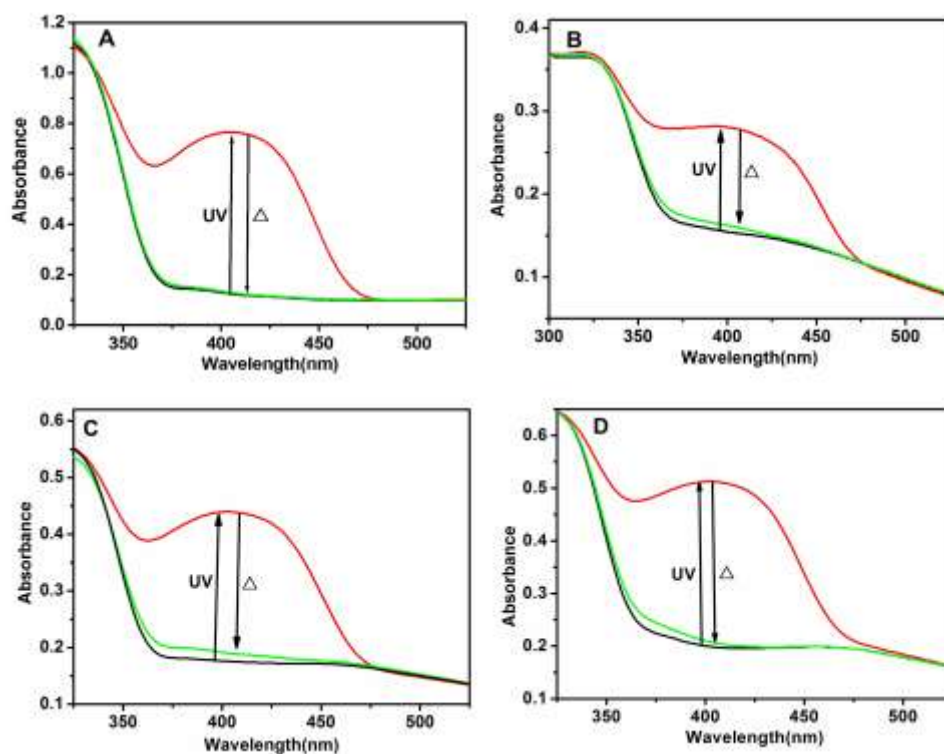
Hui Yuan,<sup>a</sup> Jixi Guo,<sup>a</sup> Dianzeng Jia,<sup>\*a</sup> Mingxi Guo,<sup>a</sup> Lang Liu,<sup>a</sup>  
Dongling Wu<sup>a</sup> and Feng Li<sup>b</sup>

*<sup>a</sup>Key laboratory of material and technology for clean energy, ministry of education; Key laboratory of advanced functional materials, autonomous region; Institute of Applied Chemistry, Xinjiang University, Urumqi 830046, Xinjiang, P. R. China.*

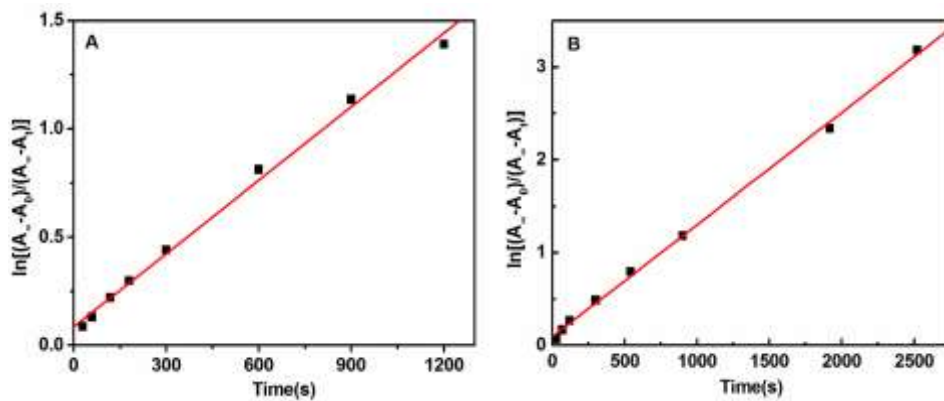
*<sup>b</sup>State Laboratory of Surface and Interface Science and Technology, School of Materials and Chemical Engineering, Zhengzhou University of Light Industry, Zhengzhou 450002, Henan, P. R. China.*

\*corresponding author: E-mail: [jdz0991@gmail.com](mailto:jdz0991@gmail.com)

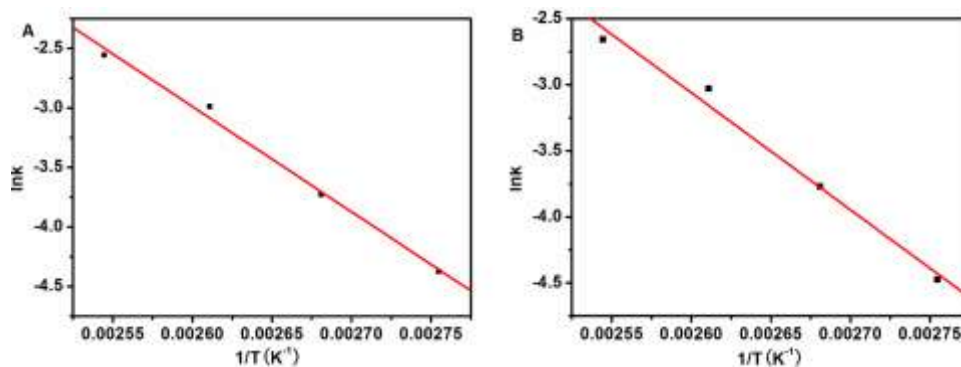
**Figure S1.** Absorption spectra changes of (A) **1a** in crystalline state and (B, C, D) **1a**/HPMC film (5 wt%, 10 wt%, 20 wt%) before (black) and after (red) irradiation with the UV light (365 nm) and after heating (green) at 120 °C.



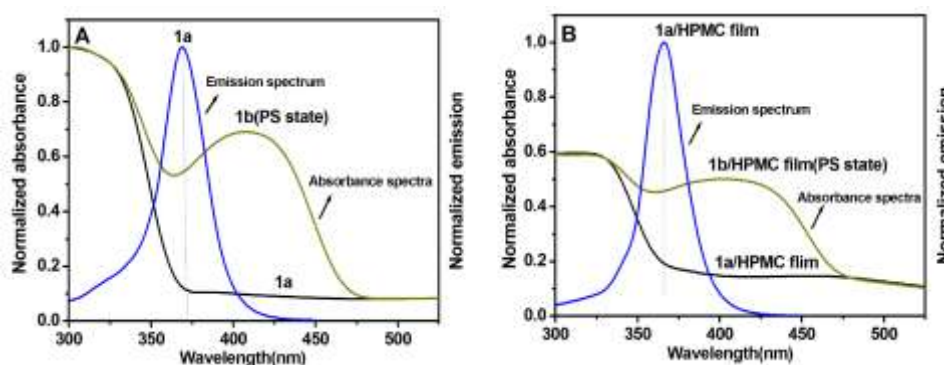
**Fig S2.** First-order kinetic plots of photoisomerization reaction of **1a** in (A) crystalline state and (B) HPMC composite film (20 wt%) induced by 365 nm light.



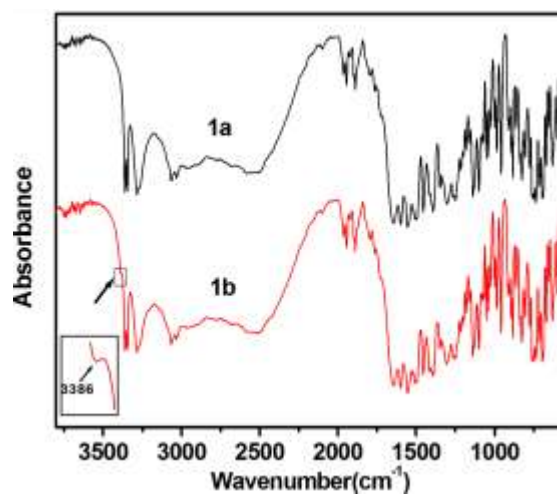
**Fig S3.** Arrhenius plots of the thermal bleaching rate constant of (A) **1b** in crystalline powders and (B) **1b**/HPMC composite film (20 wt%).



**Fig S4.** Normalized fluorescence emission spectra and absorbance spectra of (A) **1a** and **1b** in crystalline powders and (B) **1a**/HPMC composite film and **1b**/HPMC composite film (20 wt%).



**Fig S5.** FT-IR spectra of **1** in crystalline state, before UV irradiation (black), after UV irradiation (red).



We investigated the structural origin of their drastic color changes in crystalline state with IR spectra. Under irradiation of 365 nm light, a new sharp band attributed to the N–H stretching vibration appears at  $3386\text{ cm}^{-1}$  for the formation of *K*-form **1b**. The changes of structure are similar to the previous reports. This results support our suggested photochromic mechanism (scheme 1): Pyrazolones convert from *E*-form to *K*-form accompanied by proton transfer.

**Fig S5.** SEM images of the **1a** (A) in crystalline state and (B) HPMC composite film (20 wt%).

