Supporting Information

Achieving enhanced solid-state reversible photochromism and mechanochromism by introducing a rigid steric hindrance group

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Materials and Measurements

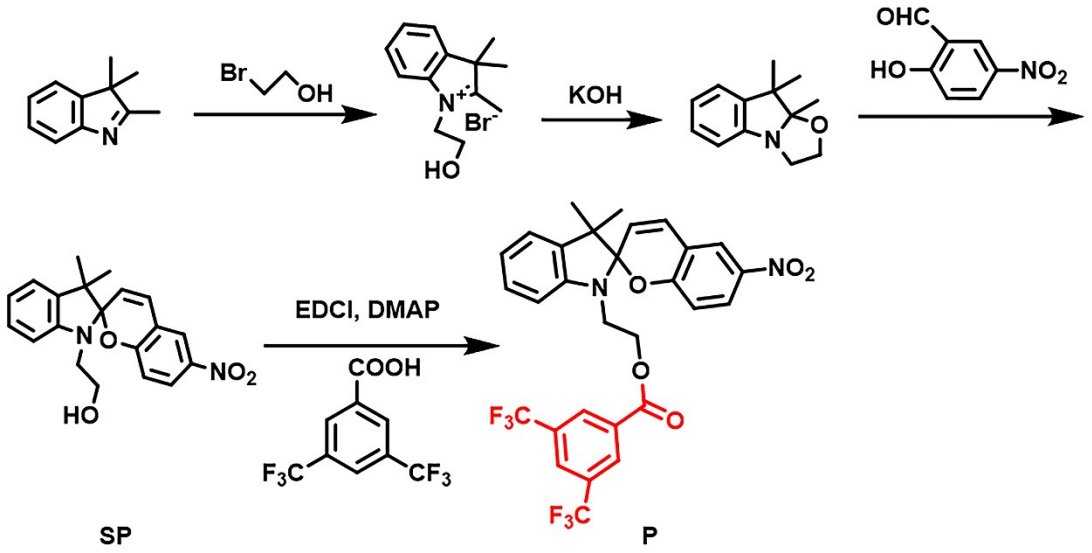
All the solvents and reactants were purchased from commercialized companies (J&K Chemicals and Aladdin. Analytical) and used as received without further purification except for specifying otherwise. Thin layer chromatography (TLC) was performed on Yantai chemical industry silica gel plates. Column chromatography was performed using silica gel 200-300 mesh.

^{1}H NMR and ^{13}C NMR spectra were with a BRUKER AVANCE AV400MHz (^{1}H: 400 MHz; ^{13}C: 100MHz) spectrometer at room temperature. Fluorescence spectra were conducted by using a fluorescence spectrophotometer (F-46001, HITACHI, Japan). UV-vis spectra were measured on a spectrometer (TU-1901, PERSEE, China). Thermogravimetric analyzer was performed with a PYRIS 1 (PerkinElmer, USA). Mass spectrometry (MS) was performed with a XEVO-G2STOF (ESI) (Waters, USA). The surface morphology was tested with a Carl Zeiss SMT Pte Ltd vltra55 (Germany) SEM at an accelerating voltage of 3 kV.

Computational methods

The ground state geometries were fully optimized by the density functional theory (DFT) method with the Becke three-parameter hybrid exchange and the Lee-Yang-Parr correlation functional (B3LYP) and 6-31G(d) basis set using the Gaussian 09 software package.

Synthesis



Scheme S1. Synthetic scheme for P.

Synthesis of compound SP. The compound SP was synthesized using modified procedures based on literature. [1] The PXRD spectra of SP (Figure S7) is same as the reported [2] and it prove that the structure of the molecule we synthesized is spiropyran form.

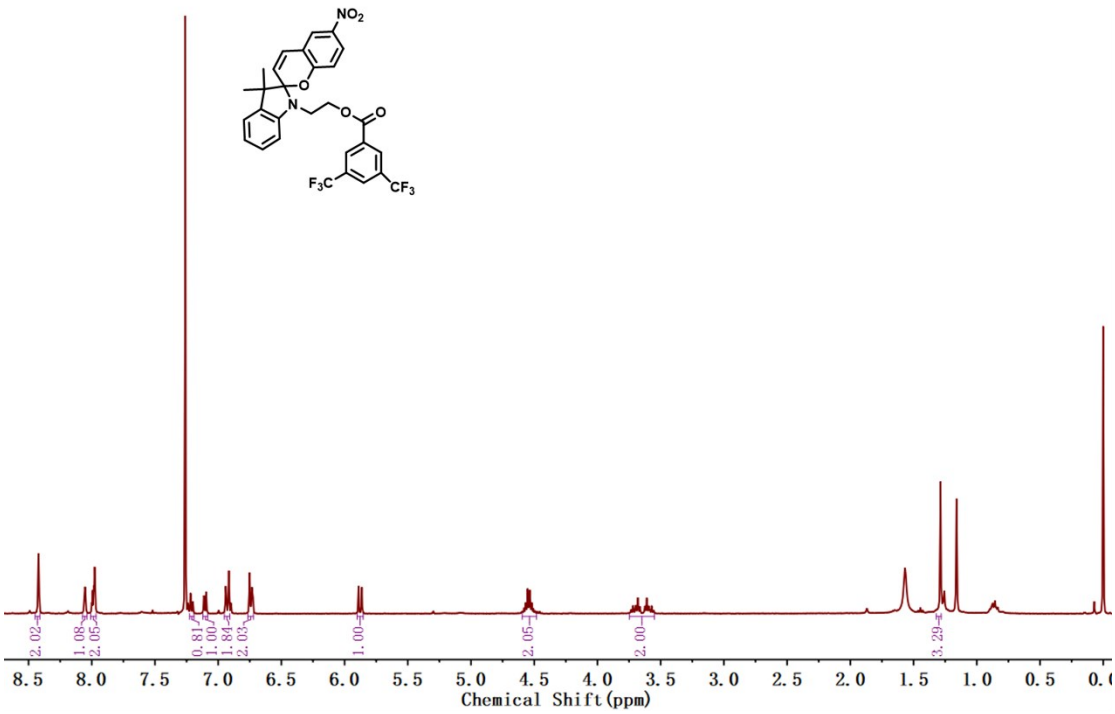


Figure S1. ^{1}H NMR spectrum of compound P in $CDCl_3$

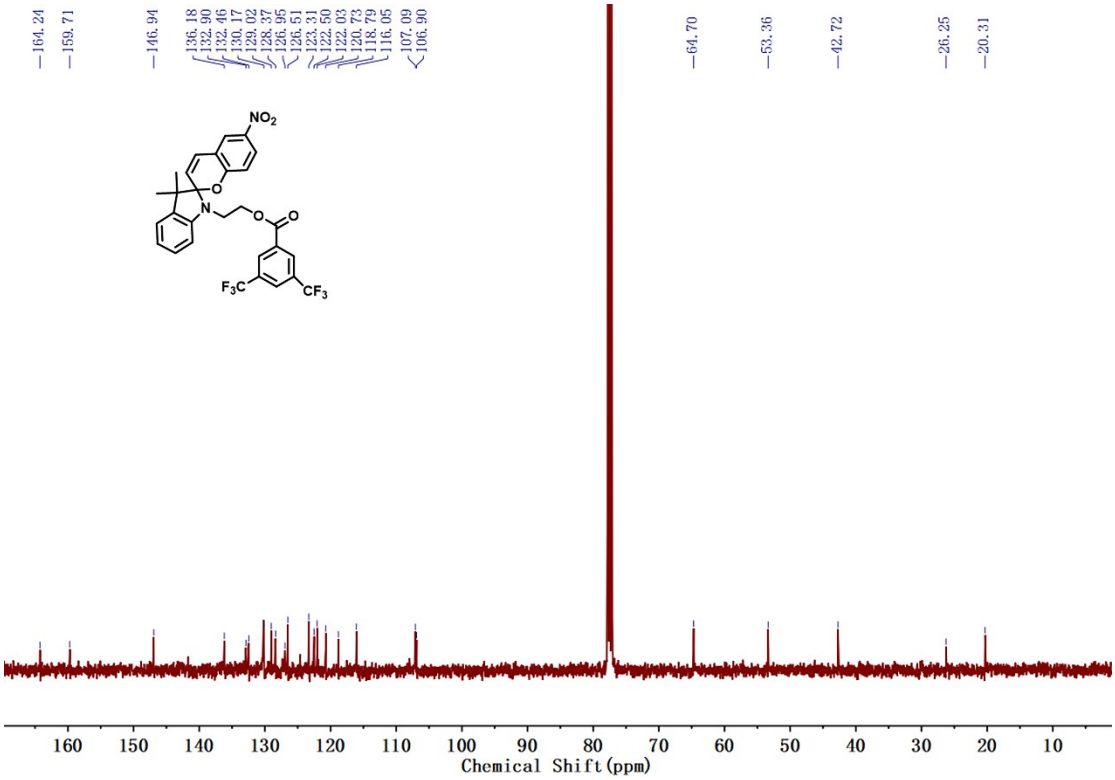


Figure S2. ^{13}C NMR spectrum of compound P in $CDCl_3$

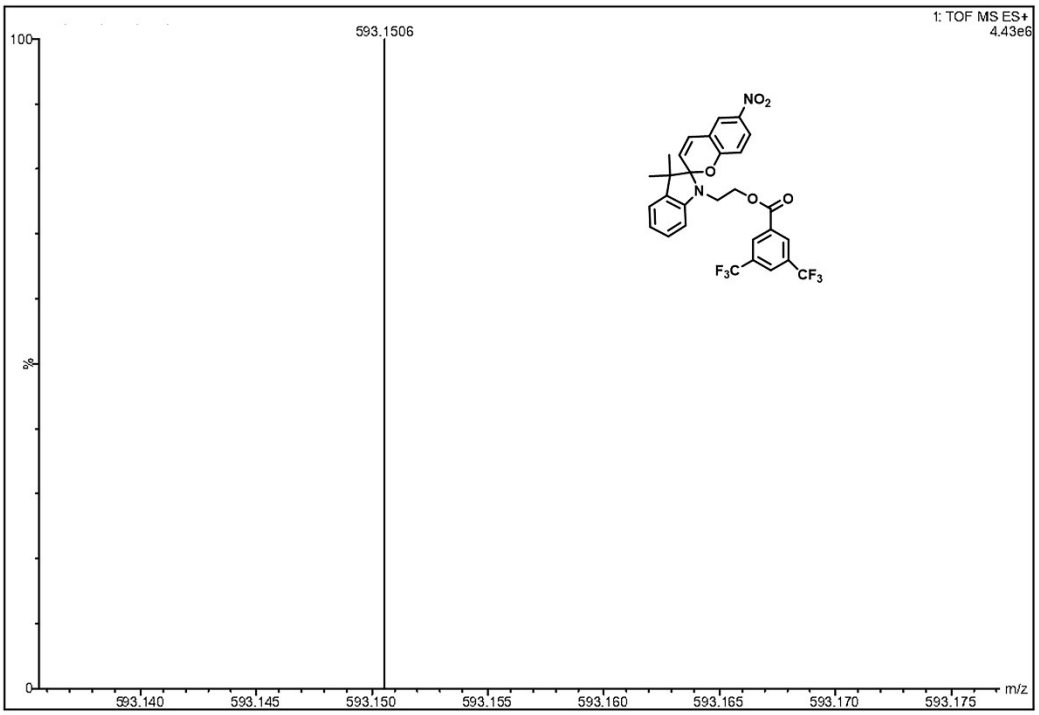


Figure S3. ESI-MS spectrum of compound P

Preparation of the PVP Film. P (**SP**) (10 mg) was dissolved in 0.5 mL of dibromoethane, followed

by the addition of PVP (40 mg). after stirring for 24 h at room temperature, a yellow transparent viscous solution was obtained. The resulting solution was filtered through a 0.2 μm PTFE filter and spin coated onto glass substrates to obtain the films. In order to remove the residual solvent, these obtained films were baked in a vacuum oven.

Table S1. Fluorescence quantum yield of P in powder and solution before and after 365 nm UV irradiation.

	Powder	Solution
Before UV irradiation	3.59%	9.68%
After UV irradiation	5.54%	/

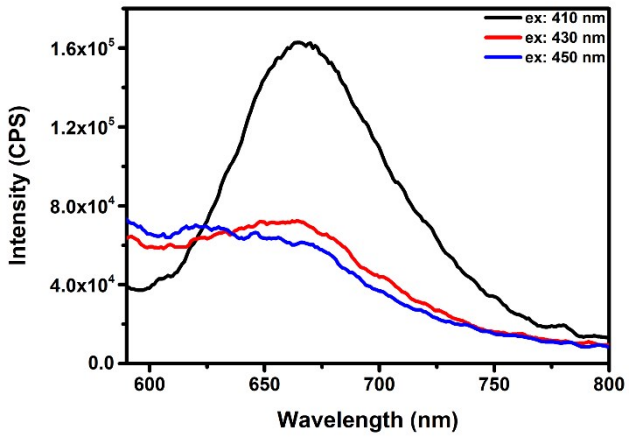


Figure S4. Fluorescence spectra of P by different excitation wavelength. Ex: 410 nm, 430 nm, 450 nm.

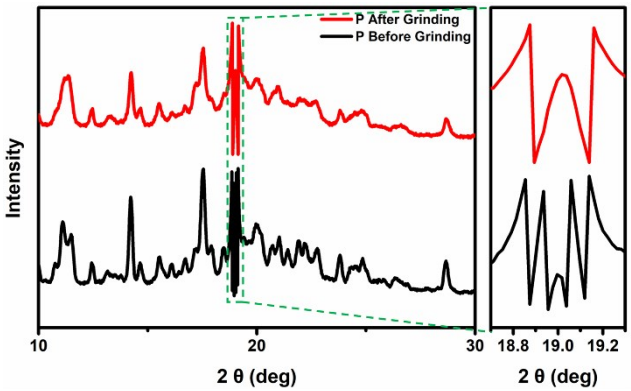


Figure S5. PXRD spectra of P powder before and after grinding.

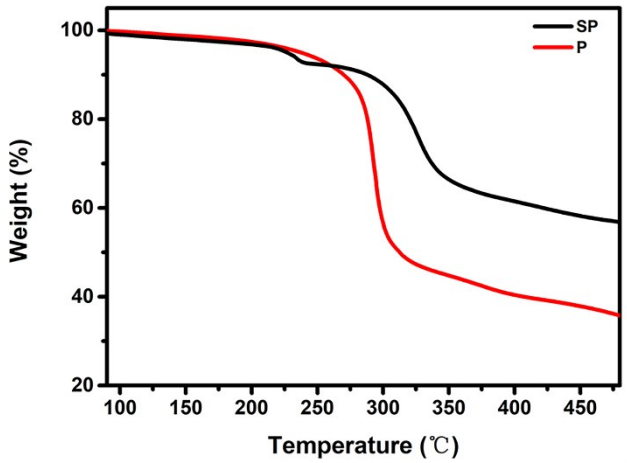


Figure S6. TGA curves of SP and P.

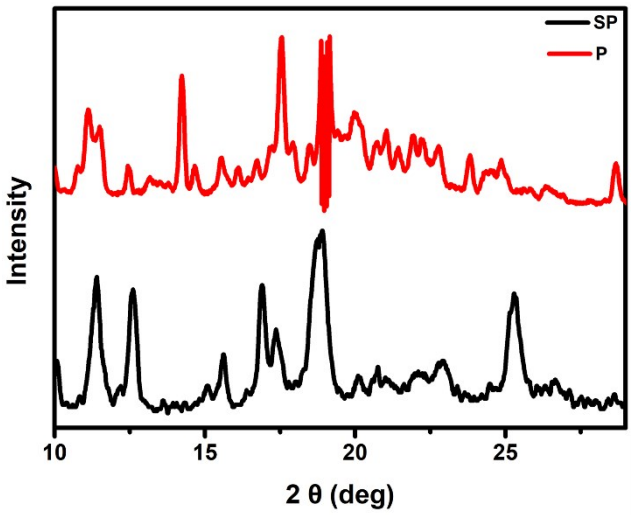


Figure S7. PXRD spectra of SP and P powder

References

1. G. O'Bryan, B. M. Wong and J. R. McElhanon, *ACS Appl. Mater. Interfaces*, 2010, **2**, 1594-1600.

2. V. M. Breslin and M. A. Garcia-Garibay, *Crystal Growth & Design*, 2017, **17**, 637-642.