Electronic Supplementary Information

CB[8] gated photochromism of a diarylethene derivative containing thiazole orange groups

Yueyuan Mao, Keyin Liu, Guanglei Lv, Ying Wen, Xingjun Zhu, Haichuang Lan, Tao Yi

Department of Chemistry, and Concerted Innovation Center of Chemistry for Energy Materials, Fudan University, 220 Handan Road, Shanghai, 200433, P.R. China

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1. Materials and general method
All starting materials were obtained from commercial suppliers and were used as received. CB[8] (25 mg, 99%+) was purchased from Strem Chemicals, Inc. 2-Methyl thiophene and methyl iodide were supplied from Sinopharm Chemical Reagent Co. Ltd., Shanghai. 2-Methyl benzothiazole and 4-cholorquinoline were obtained from TCI.

2. Physical measurements and instrumentation
1H NMR (400 MHz) and 13C NMR (100 MHz) spectra were recorded on a JEOL instrument (JEOL, Japan). Proton chemical shifts are reported in parts per million down field from tetramethylsilane (TMS). ESI-MS data were recorded on a Micro TOFII 10257 Instrument (Bruker Daltonics Inc., Germany). UV-visible absorption spectra were recorded on a Shimadzu UV-2250 spectrophotometer. Fluorescence spectra were recorded on an Edinburgh FLS5 spectrophotometer (Germany). The HPLC (High Performance Liquid Chromatography) was conducted on Autopurification LC-MS system (Waters, America). The photo cyclization process of 1 was performed by UV light, generated by a low pressure mercury lamp with 360 nm long wavelength pass filter. In the visible light induced ring open process, a 670 nm laser ($I = 0.8$ A) was used as light source. The optical filter was the band-pass from 530-543 nm.

3. The preparation of solution samples
The stock solution of 1O ($5.0 \times 10^{-4}$ M) was prepared in water with 2.5% DMSO. The stock solution of Cucurbit[8]uril (CB[8], $2.5 \times 10^{-4}$ M) was prepared in water. The solution samples for spectral testing were prepared by diluting the stock solution with water.

4. Binding constant calculating method
The following equations (E. 1 and E. 2) was used for the nonlinear least squares analysis of the absorption to determine the association constant($^{1-3}$) between 1O and CB[8] ($K_a$) (Fig. S4).

\begin{align}
K_a &= \frac{[1O\cdot CB[8]_2]}{[1O][CB[8]]^2} \quad (E. 1) \\
Y &= Y_0 + \frac{(Y_{lim} - Y_0)(1 + \frac{C_{1O}}{C_{CB[8]}} + \frac{1}{K_aC_{CB[8]}} - (1 + \frac{C_{1O}}{C_{CB[8]}} + \frac{1}{K_aC_{CB[8]}})^2}{4C_{1O}C_{CB[8]}}) \quad (E. 2)
\end{align}

$Y$ was the recorded absorbance, $Y_0$ was the initial absorbance without adding CB[8]; $Y_{lim}$ was the limiting value with sufficient CB[8]; $[1O\cdot CB[8]_2]$, $[1O]$ and $[CB[8]]$ were the realistic concentration of the guest molecule CB[8], host molecule 1O and the binding complex 1O-CB[8]$_2$ respectively, $C_{1O}$ and $C_{CB[8]}$ were the added
5. Calculation method of the conversion yield and cyclization quantum yield of 1O·CB[8]

(1) The photocyclization efficiency ($\alpha$) of 1O·CB[8]$_2$ was calculated according to the HPLC result, which was showed in Fig. S5. The efficiency was calculated according to the integration of the area of peaks at different retention time. The efficiency $\alpha_{O \to C}$ of 1O·CB[8]$_2$ with irradiation of 365 nm was estimated as 40.2% and the reversed efficiency $\alpha_{C \to O}$ was 96.9%.

(2) Cyclization quantum yield of 1O·CB[8]$_2$ was calculated according to the absorbance change at 385 nm before and after UV light irradiation. 4, 5

6. Additional data

Fig. S1 $^1$HNMR spectrum of 1O in d$_6$-DMSO/D$_2$O (10% of DMSO in volume).
**Fig. S2** The changes of absorbance at 476 and 413 nm of 1O (5μM) with addition of different concentration of CB[8].

**Fig. S3** The fluorescent spectra of 1O (5μM) with addition of different concentration of CB[8].
**Fig. S4** (a) The absorption and (b) fluorescent spectra of the mixture solution of 1O and CB[8] with different molar ratio. The total concentration of 1O + CB[8] = 15 μM, while The concentration of CB[8] ranged from 0 to 15 μM.

![Absorption and Fluorescent Spectra](image)

**Fig. S5** The change of the absorbance at 513 nm of 1O with different concentration of CB[8] which was used for determination of association constant. The nonlinear least squares analysis (red line) gives $K_a = 3.36 (\pm 0.75) \times 10^6$ L·mol$^{-2}$ ($R^2 = 0.97847$).

![Absorbance Change](image)

**Fig. S6** HPLC of 1O·CB[8]$_2$ (black line), at PSS after 365 nm irradiation (red line) and recovered state after 670 nm irradiation (blue line).

![HPLC](image)
**Fig. S7** The absorption spectra of $1\cdot$CB[8]$_2$ at PSS with irradiation of 670 nm from 0 - 10 min.

**Fig. S8** The absorption changes of $1O\cdot$CB[8]$_2$ (a) and $1C\cdot$CB[8]$_2$ (b) with irradiation of 515 nm light.
**Fig. S9** The absorption changes of 1O·CB[8]₂ (5 μM) at wavelengths of 476 and 513 nm with addition of different concentration of AD.

**Fig. S10** The fluorescent spectra of 1O·CB[8]₂ with addition of different concentration of AD.
Fig. S11  The absorbance changes at different wavelengths at different processes including 1O to 1O-CB[8]₂ to PSS, addition of AD from 0 – 10 eq, rest as room temperature from 0 to 72 h in dark.

7. References