Electronic Supplementary Information (ESI)

A fluorescent photochromic diarylethene based on naphthalic anhydride with strong solvatochromism

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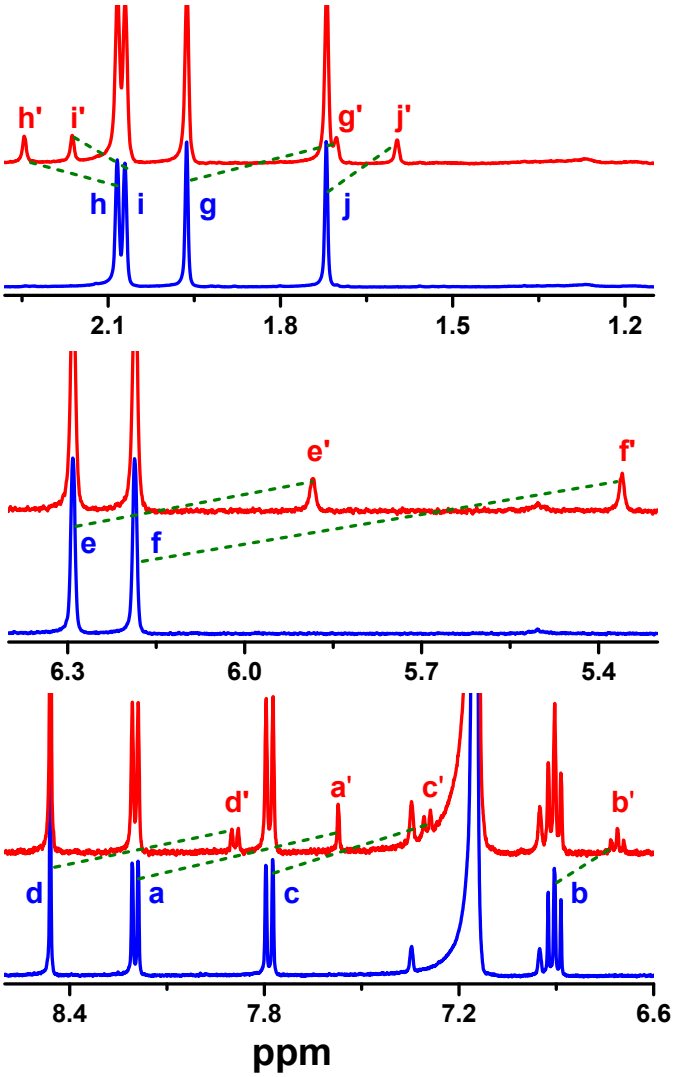


Fig. S1 ^{1}H NMR signal changes of **BTE-O** before and after 365 nm photo-irradiation in C_6D_6 (2.35×10^{-2} M).

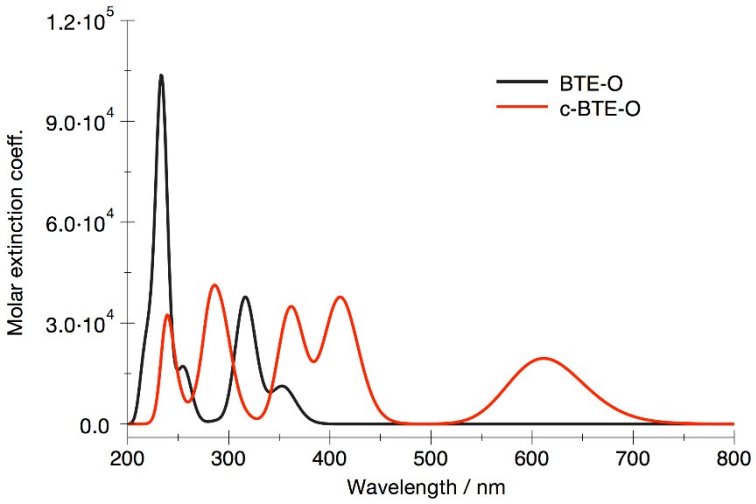


Fig. S2 Simulated absorption spectra of **BTE-O** and ***c*-BTE-O** in cyclohexane.

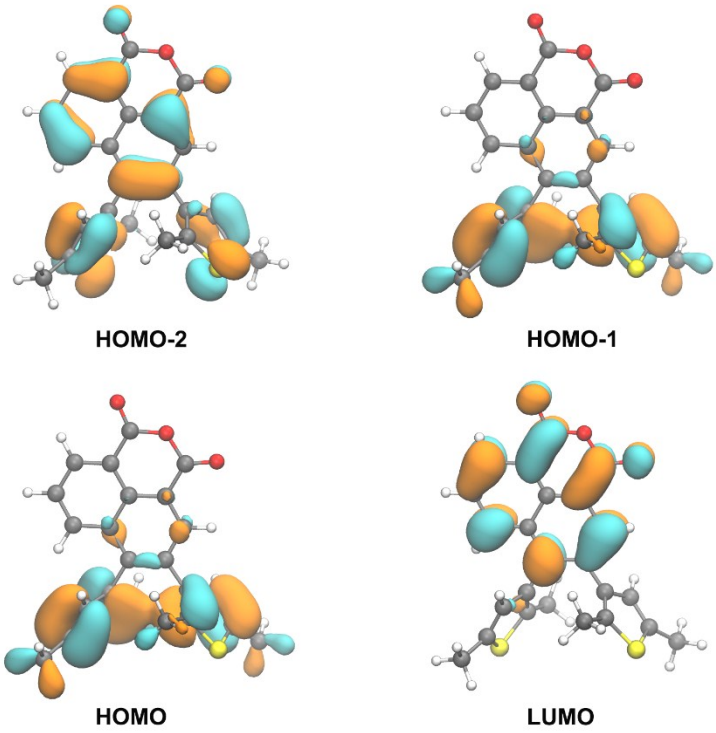


Fig. S3 Frontier molecular orbitals of **BTE-O** in cyclohexane.

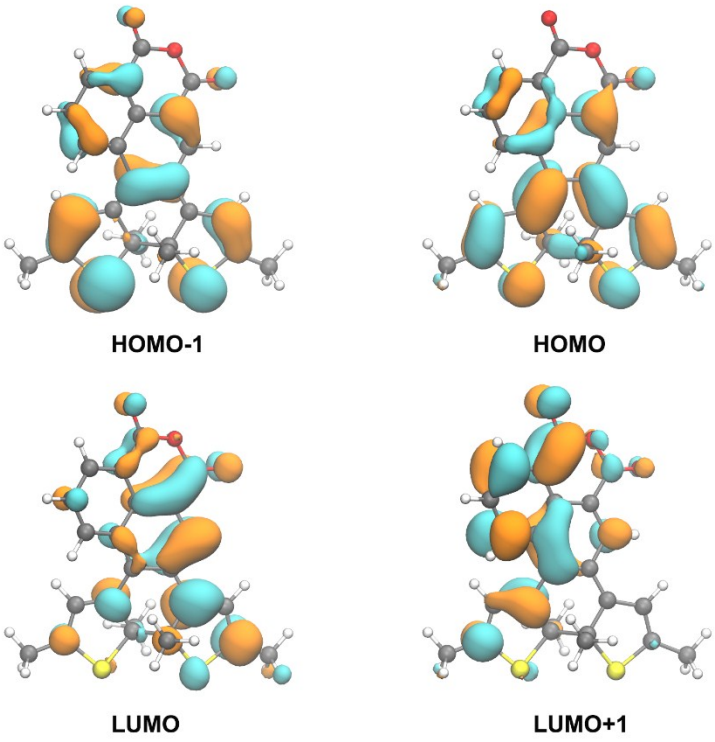


Fig. S4 Frontier molecular orbitals of ***c*-BTE-O** in cyclohexane.

Table S1. Computed excitation energy, absorption wavelength, oscillator strength and molecular orbital composition for the lowest excited states in cyclohexane

Compound	Excited state	Excitation energy	Oscillator strength	MO composition
BTE-O	S1	3.50 eV, 353 nm	0.1199	H –› L (85%)
	S2	3.91 eV, 317 nm	0.3445	H-2 –› L (45%) H-1 –› L (19%) H-3 –› L (18%)
	S3	3.96 eV, 313 nm	0.0681	H-1 –› L (48%) H-2 –› L (30%)
***c*-BTE-O**	S1	2.02 eV, 613 nm	0.2103	H –› L (96%)
	S2	3.02 eV, 411 nm	0.4061	H –› L+1 (91%)
	S3	3.42 eV, 362 nm	0.3758	H-1 –› L (90%)

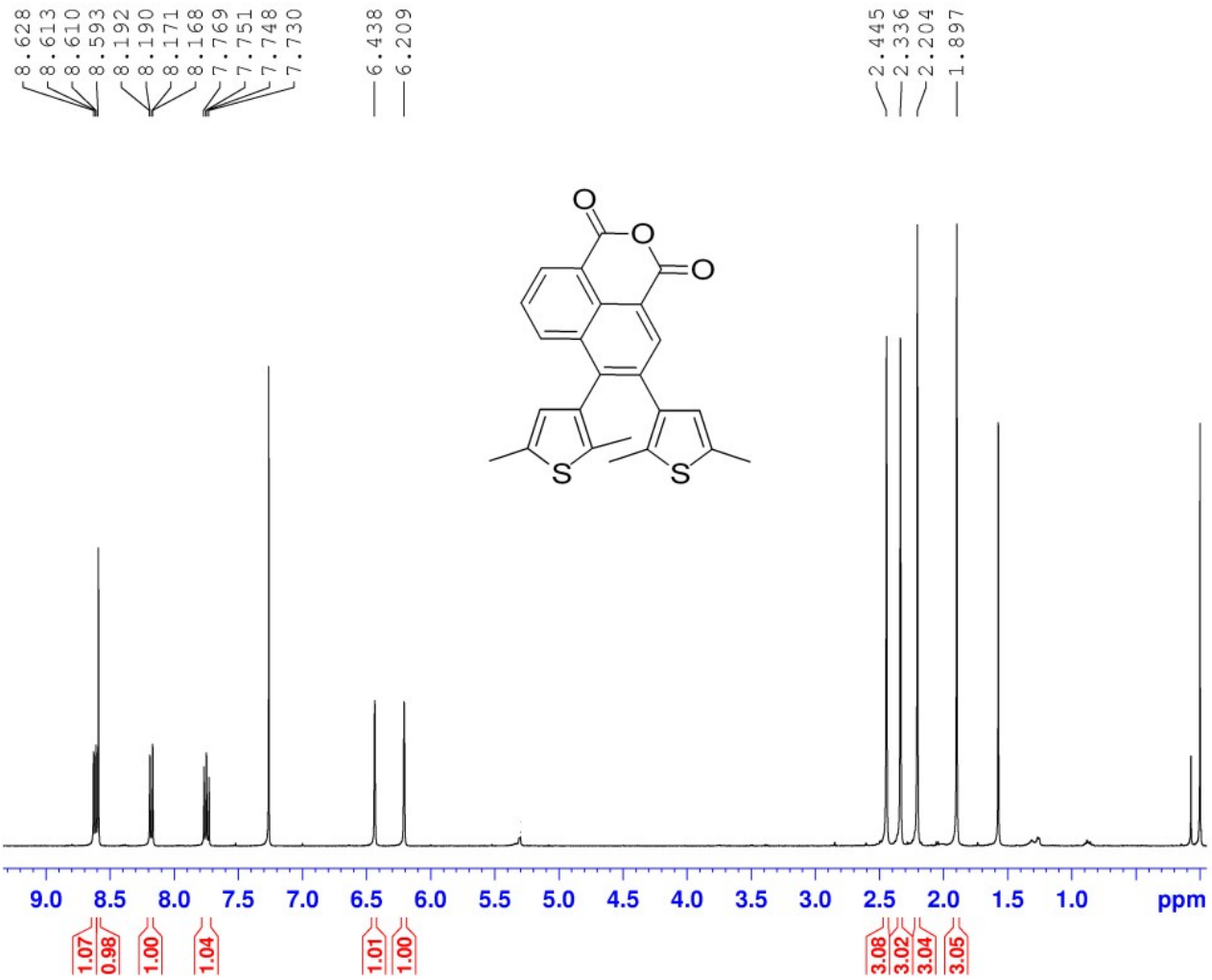


Fig. S5 ^{1}H NMR spectra of **BTE-O** (400 MHz, $CDCl_3$, ppm).

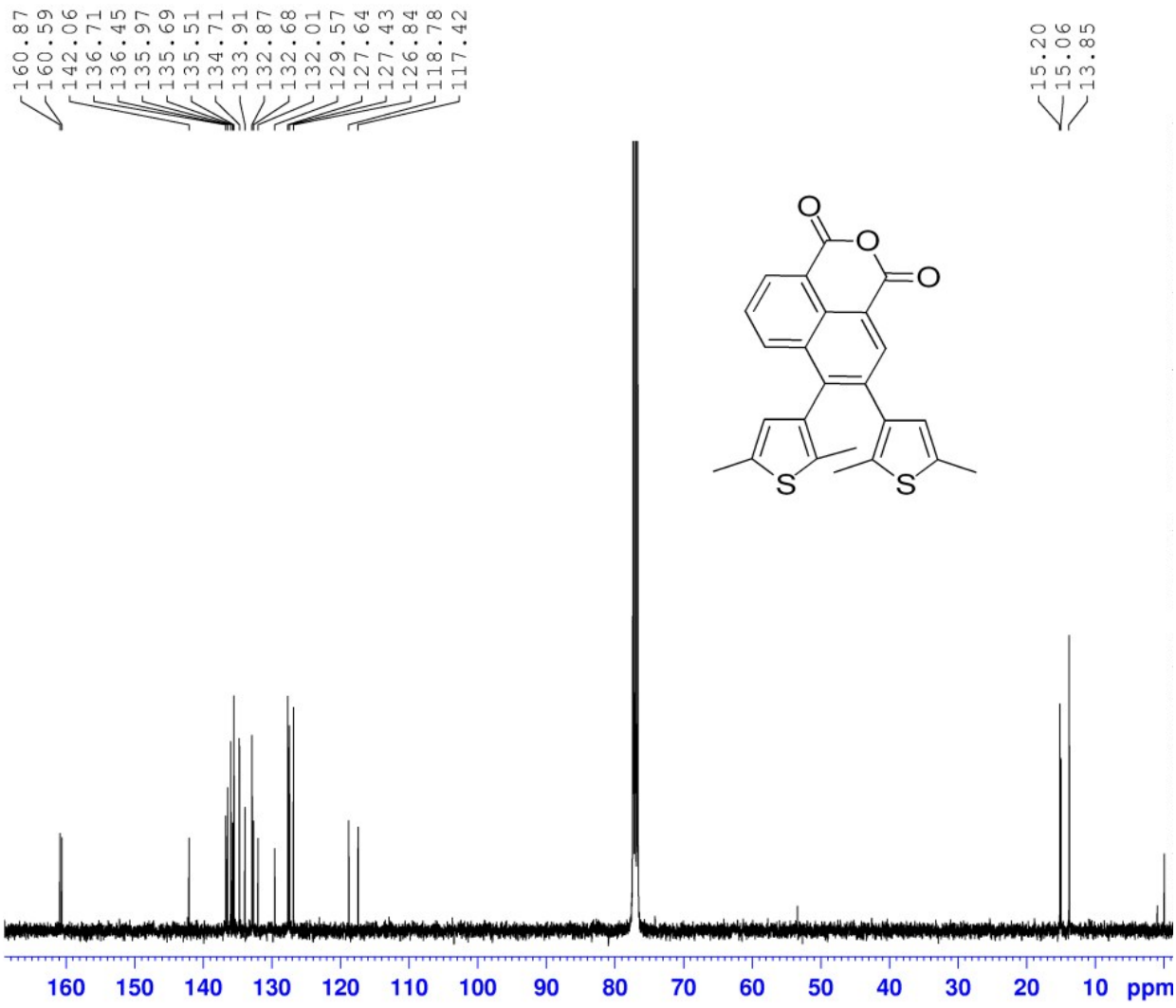
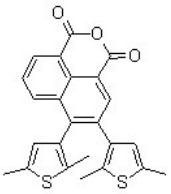


Fig. S6 ^{13}C NMR spectra of **BTE-O** (100 MHz, $CDCl_3$, ppm).

Elemental Composition Report **Page 1**

Single Mass Analysis

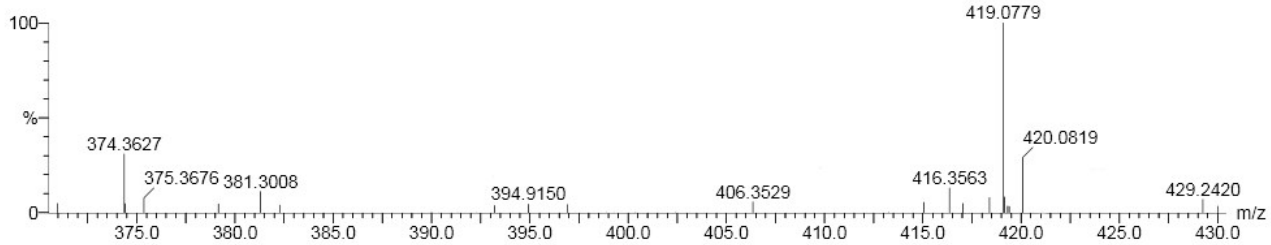
Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
400 formula(e) evaluated with 69 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-80 H: 0-150 O: 0-12 S: 0-8

ZHU-WH ECUST institute of Fine Chem 07-Dec-2011 19:33:29

ZWH-SLW-45 29 (0.987) Cm (25:32) 1: TOF MS ES+ 4.80e+003



Minimum:				-1.5			
Maximum:		50.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
419.0779	419.0776	0.3	0.7	15.5	39.3	0.0	C24 H19 O3 S2

Fig. S7 High resolution mass spectrum of **BTE-O.**