Supplementary material

Multicolor Photochromism of Two-Component Diarylethene Crystals Containing Oxidized and Unoxidized Benzothiophene Groups

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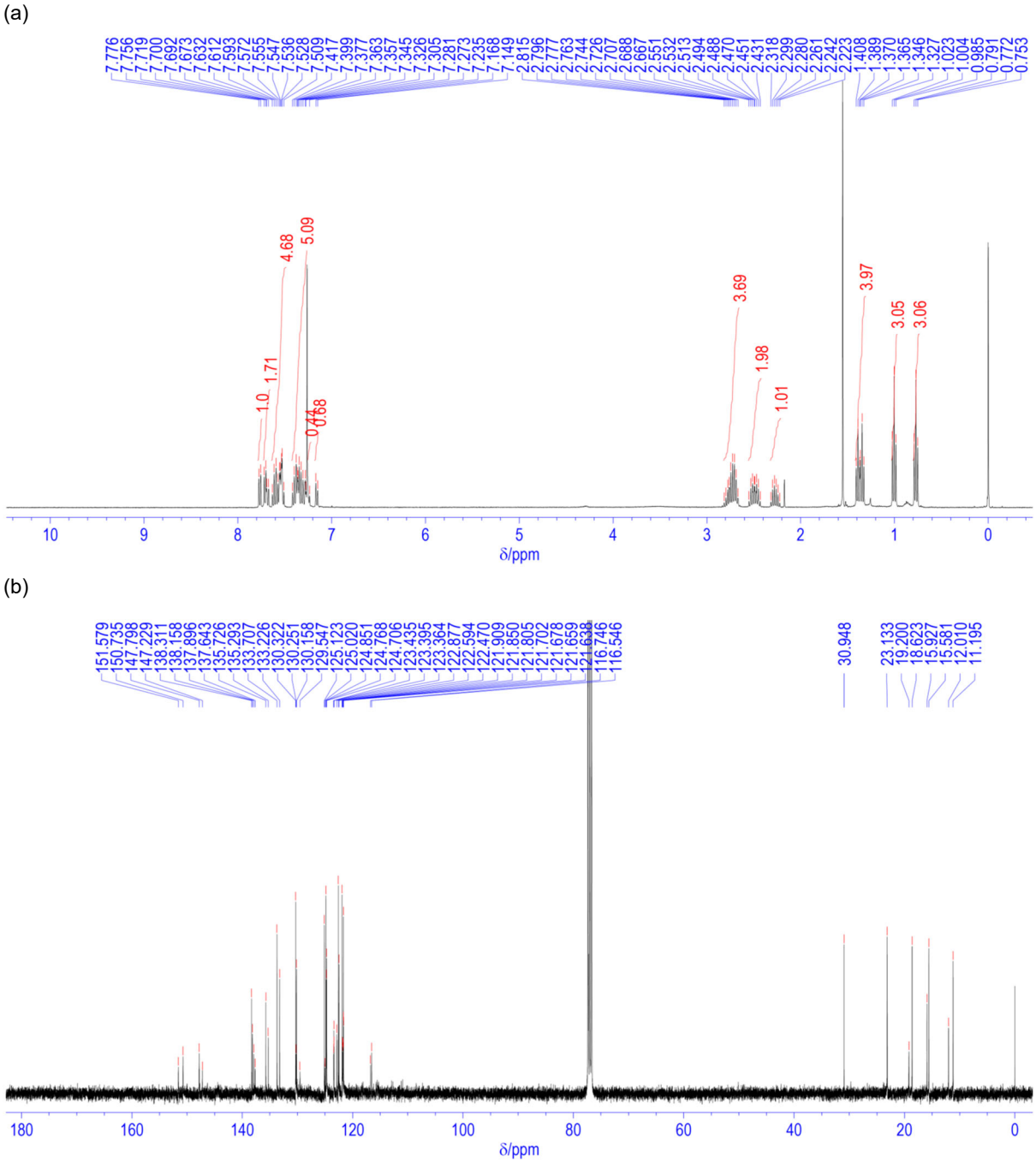


Figure S1. (a) 400MHz ^{1}H NMR spectrum of **2a** in $CDCl_3$. (b) 100 MHz ^{13}C NMR spectrum of **2a** in $CDCl_3$. The NMR spectra contain signals of anti-parallel and parallel conformers of the open-ring isomer **2a**.

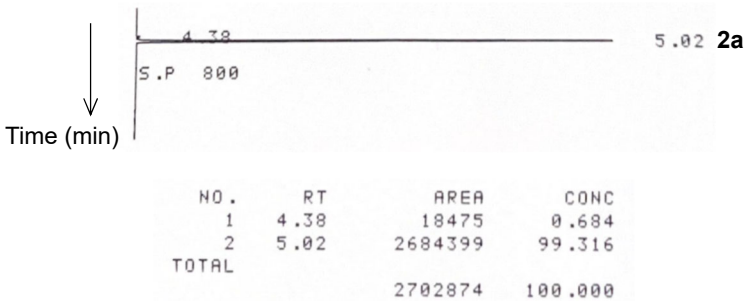


Figure S2. HPLC chromatogram of **2a** after recrystallization from diethyl ether. Pump: Hitachi L-2130, detector: Hitachi L-2420, column: Wakosil® 5SIL (ϕ4.6 mm × 250 mm), eluent: hexane/ethyl acetate = 70/30, 1 mL min^{-1}, detection: 313 nm. The purity (> 99%) of **2a** was confirmed.

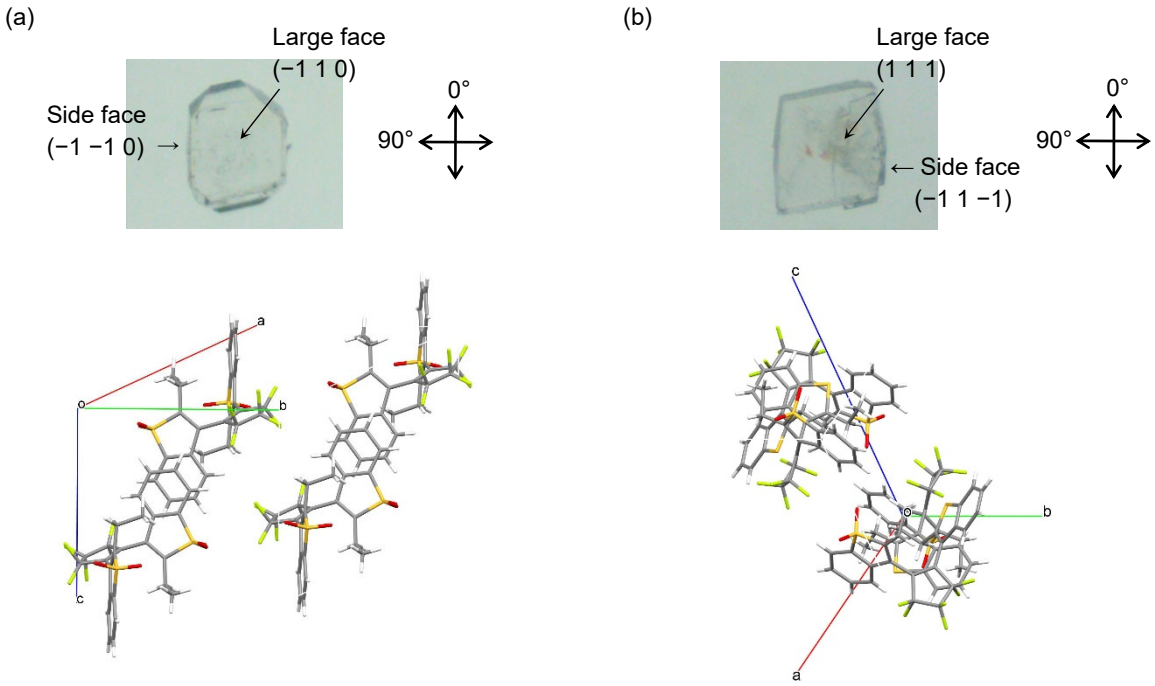
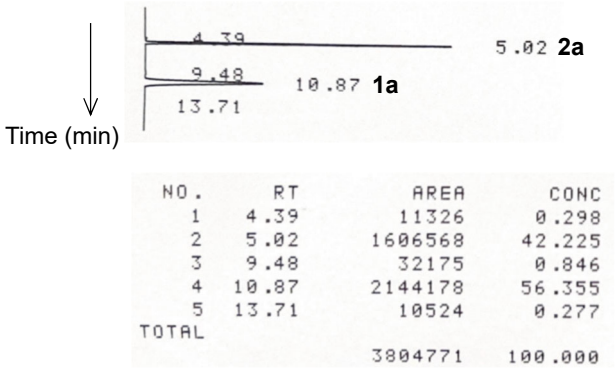


Figure S3. Molecular packing diagrams of single-component crystal of **1a** viewed from (−1 1 0) face (a) and single-component crystal of **2a** viewed from (1 1 1) face (b). The polarized absorption spectra were measured on (−1 1 0) and (1 1 1) faces for **1a** and **2a**, respectively. The arrows indicate the direction in the polarized absorption spectral measurement in Figure 3. The direction of 0° is parallel to (−1 −1 0) face for **1a** and (−1 1 −1) for **2a**.



NO.	RT	AREA	CONC
1	4.39	11326	0.298
2	5.02	1606568	42.225
3	9.48	32175	0.846
4	10.87	2144178	56.355
5	13.71	10524	0.277
TOTAL		3804771	100.000

Figure S4. HPLC chromatogram of two-component mixed crystal containing **1a** and **2a** (entry 3 in Table 2). Pump: Hitachi L-2130, detector: Hitachi L-2420, column: Wakosil® 5SIL (ϕ4.6 mm × 250 mm), eluent: hexane/ethyl acetate = 70/30, 1 mL min^{-1}, detection: 313 nm. The composition ratio of **1a** : **2a** was calculated to be 53 : 47 by correcting the peak areas in HPLC with molar absorption coefficients of **1a** and **2a** at 313 nm (**1a**: 5.01 $\times 10^3$ M^{-1} cm^{-1}, **2a**: 4.21 $\times 10^3$ M^{-1} cm^{-1}).

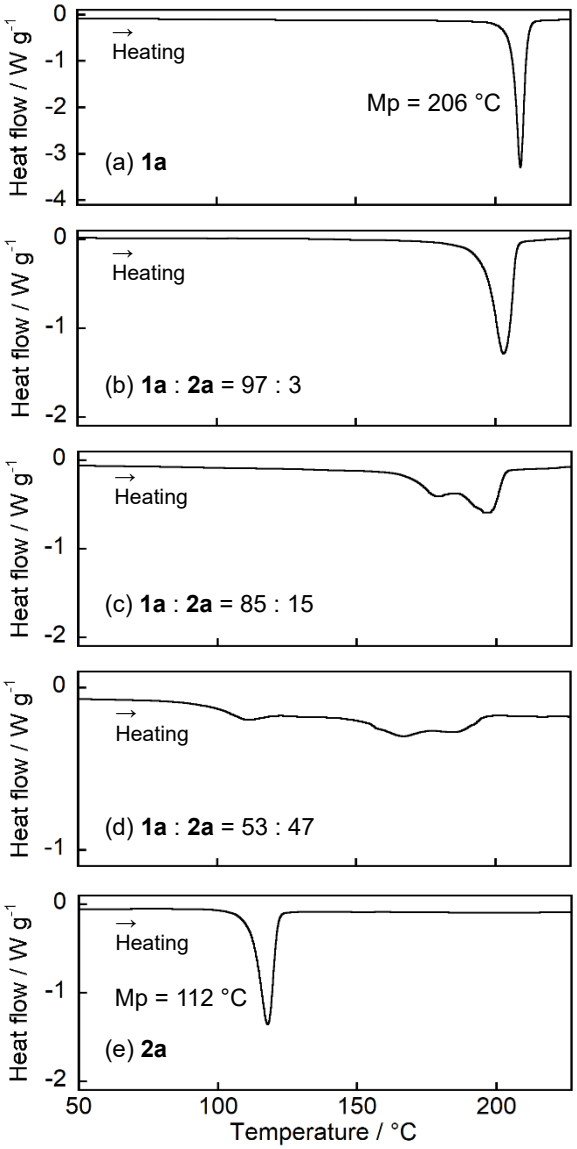


Figure S5. DSC curves for single-component crystals of **1a** and **2a** and two-component mixed crystals containing **1a** and **2a**. (a) **1a**, (b) **1a** : **2a** = 97 : 3 (entry 1 in Table 2), (c) **1a** : **2a** = 85 : 15 (entry 2), (d) **1a** : **2a** = 53 : 47 (entry 3), (e) **2a**. The scan rate was 10 °C min^{-1}.

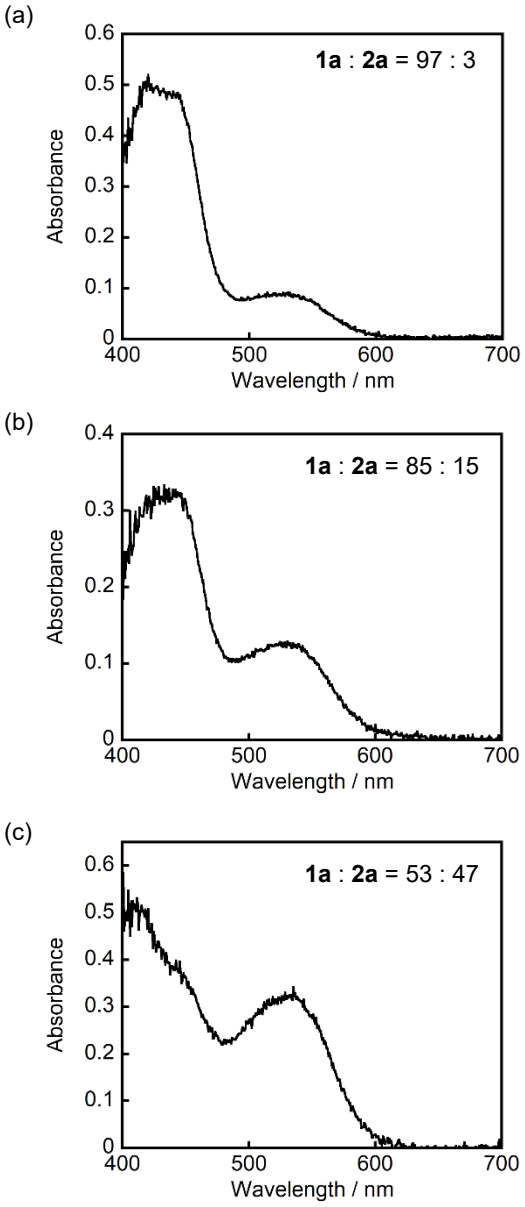


Figure S6. Absorption spectra of two-component mixed crystals containing **1a** and **2a** with different composition ratios after irradiation with 365 nm light. (a) **1a** : **2a** = 97 : 3 (entry 1 in Table 2), (b) **1a** : **2a** = 85 : 15 (entry 2), (c) **1a** : **2a** = 53 : 47 (entry 3).