Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

A photo- and halochromic multicolor switching system consisting of diarylethene and malachite green moieties

Yuto Tatsumi,[a] Noriko Fujinaga,[a] Megumi Kasuno,*[a] Masakazu Morimoto,[b]
Satoshi Yokojima,[c] Shinichiro Nakamura,[d] and Kingo Uchida*[a]

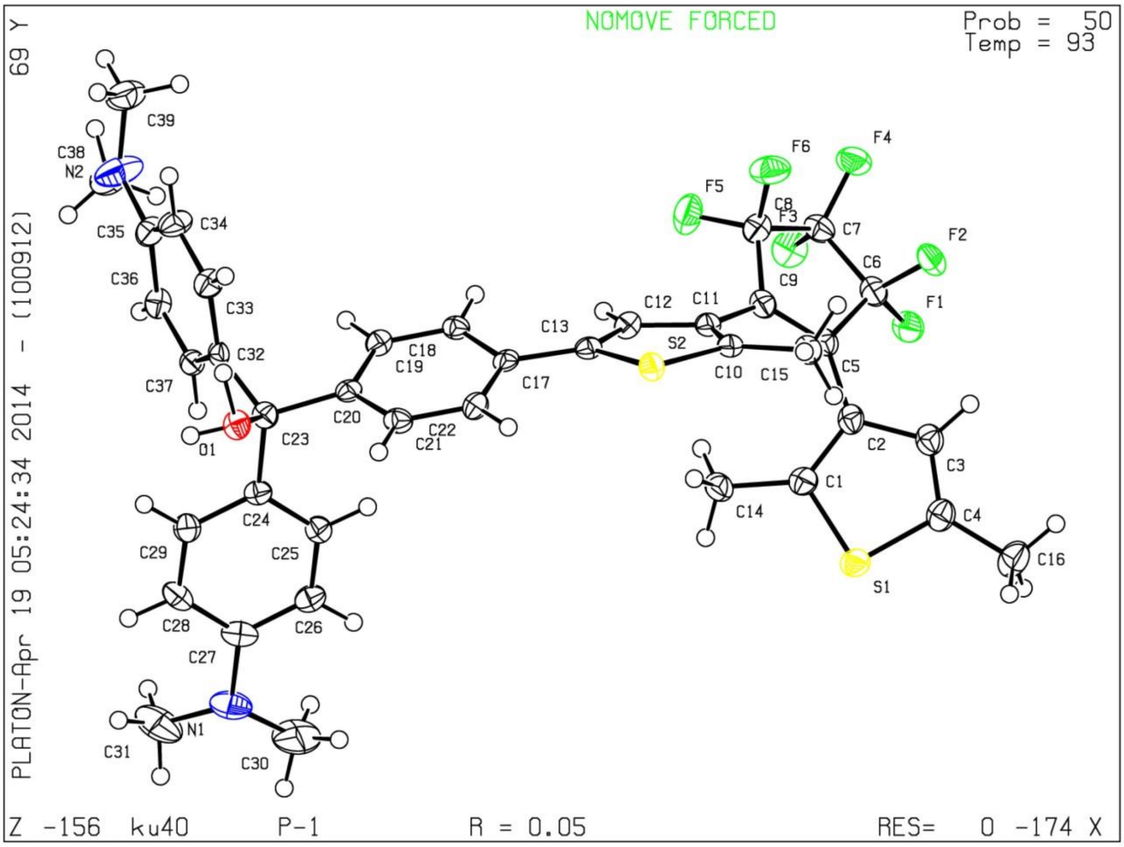


Figure S1. Ellipsoid Plot of **1**

Table S1. Crystal data for **1A**

formula	$C_{39}H_{36}F_6N_2OS_2$
formula weight	726.82
T / K	93(2)
crystal system	Triclinic
space group	P-1
a / Å	11.2558(7)
b / Å	11.4911(7)
c / Å	15.6438(9)
α / °	70.6330(10)
β / °	82.6990(10)
γ / °	64.0730(10)
V / Å^3	1716.39(18)
Z	2
ρ_{calc} / g cm^{-3}	1.406
reflections collected	16967
independent reflections	6058 [R(int) = 0.0307]
goodness-of-fit on F^2	1.108
R_1 ($I > 2\sigma(I)$)	0.0540
wR_2 ($I > 2\sigma(I)$)	0.1186
R_1 (all data)	0.0637
wR_2 (all data)	0.1239

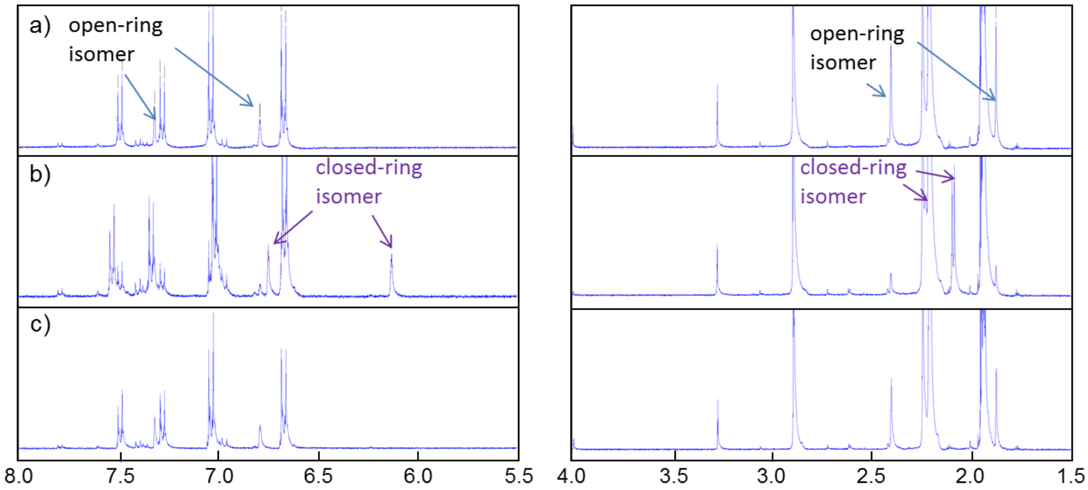


Figure S2. ^{1}H NMR Spectral changes of **1C** in acetonitrile-d_3 a) before UV irradiation; b) after UV irradiation; c) visible light (λ > 480 nm) irradiation.

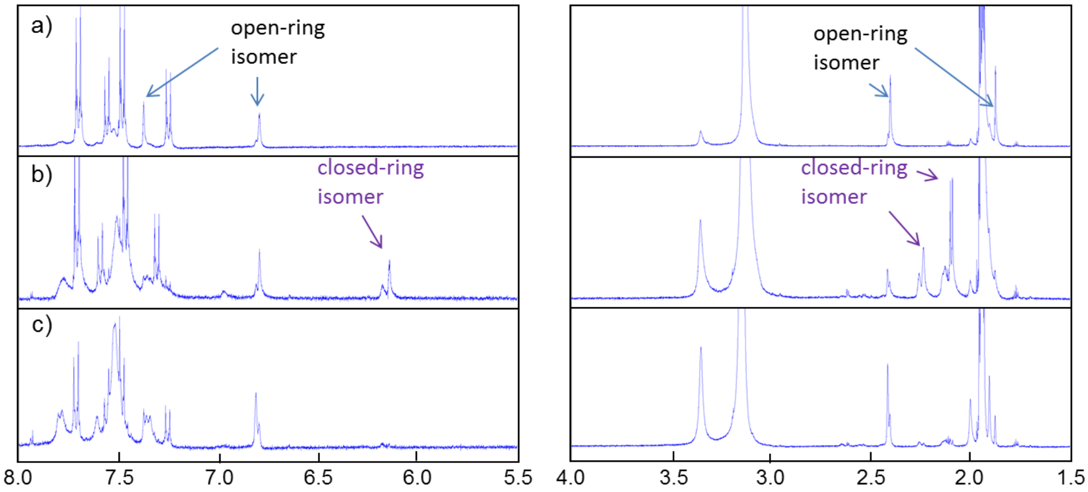
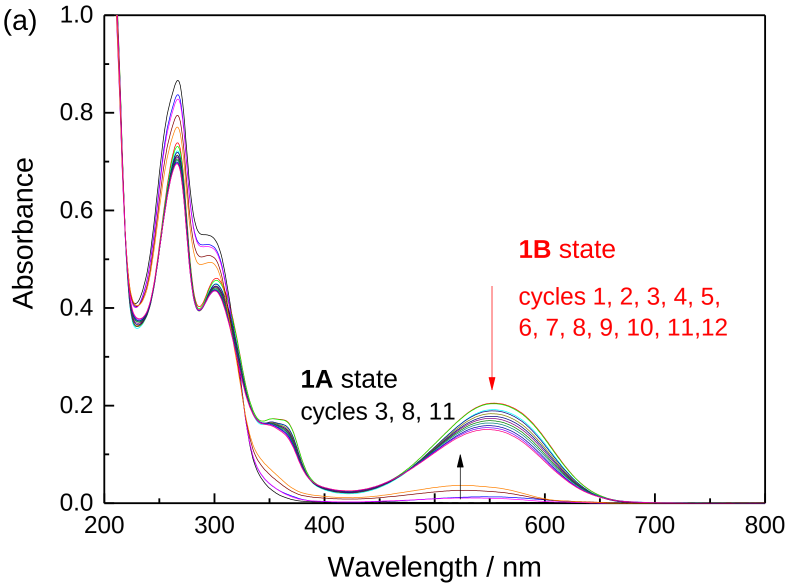


Figure S3. ^{1}H NMR Spectral changes of **1E** in acetonitrile-d_3: a) before UV irradiation; b) after UV irradiation; c) visible light (λ > 480 nm) irradiation.



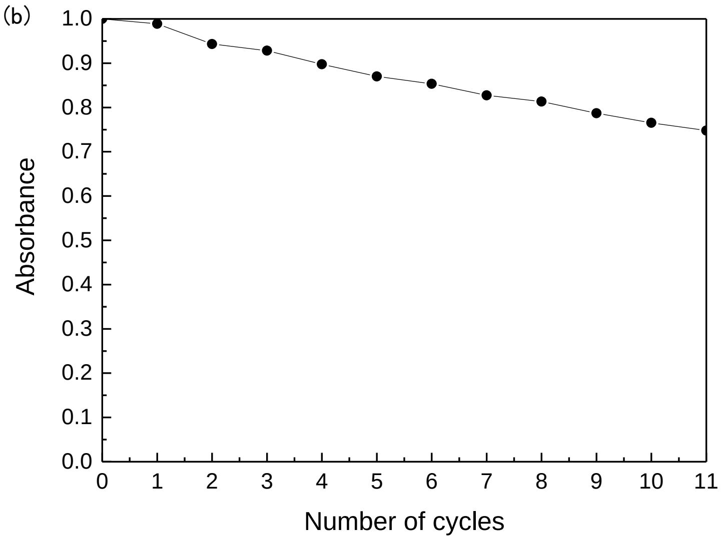


Figure S4. Fatigue resistant property between **1A** and **1B** states (a) absorption spectral changes between **1A** and **1B** upon alternate irradiation with UV (313 nm for 15 s) and visible (λ > 500 nm for 60 s) light; (b) reduction of the absorbance at 533 nm of the λ_{max} of **1B** with each coloration-decoloration cycles

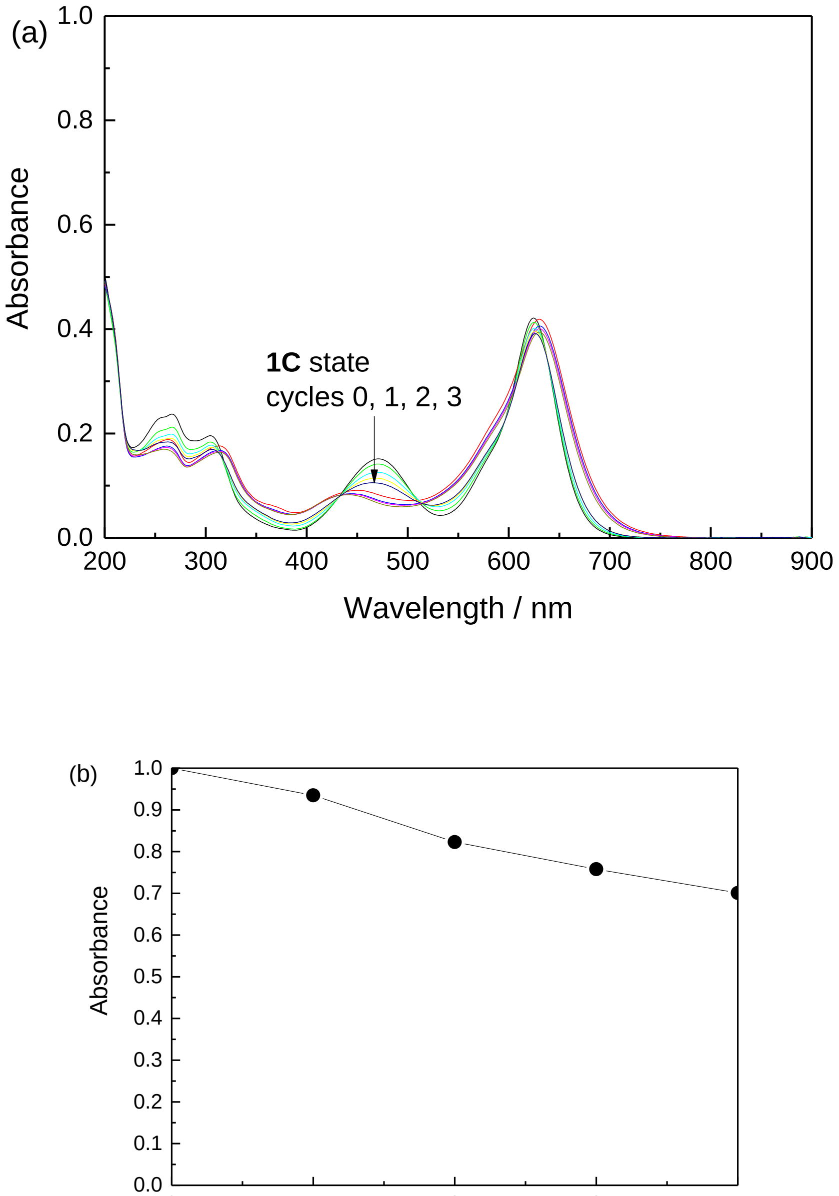
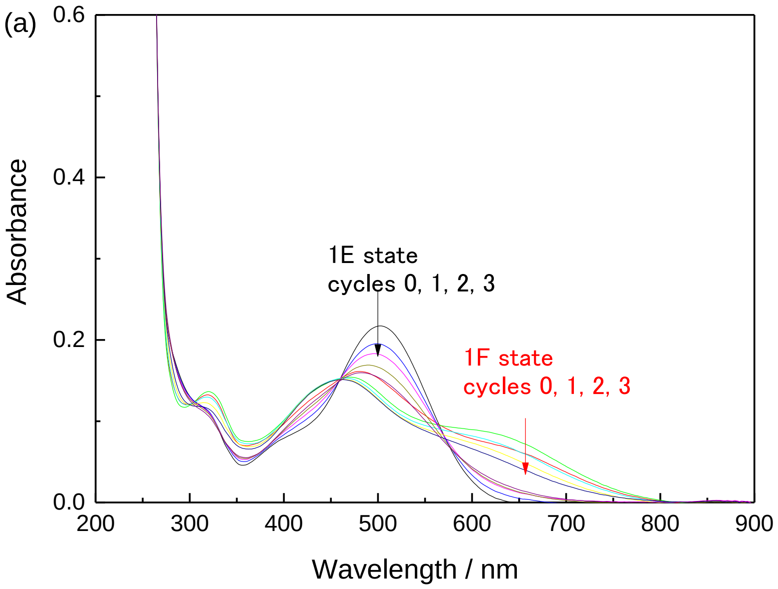


Figure S5. Fatigue resistant property between **1C** and **1D** states (a) absorption spectral changes between **1C** and **1D** upon alternate irradiation with UV (313 nm for 3 min) and visible light (λ > 430 nm for 3 min); (b) reduction of the absorbance at 471 nm of the λ_{max} of **1C** with each coloration-decoloration cycles.



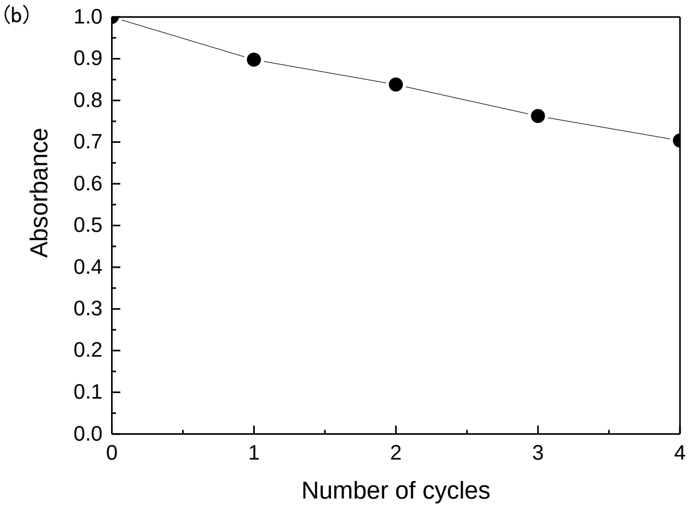


Figure S6. Fatigue resistant property between **1E** and **1F** states (a) absorption spectral changes between **1E** and **1F** upon alternate irradiation with UV (313 nm for 3 min) and visible light ($\lambda > 640$ nm for 20 min); (b) reduction of the absorbance at 502 nm of the λ_{max} of **1E** with each coloration-decoloration cycles.

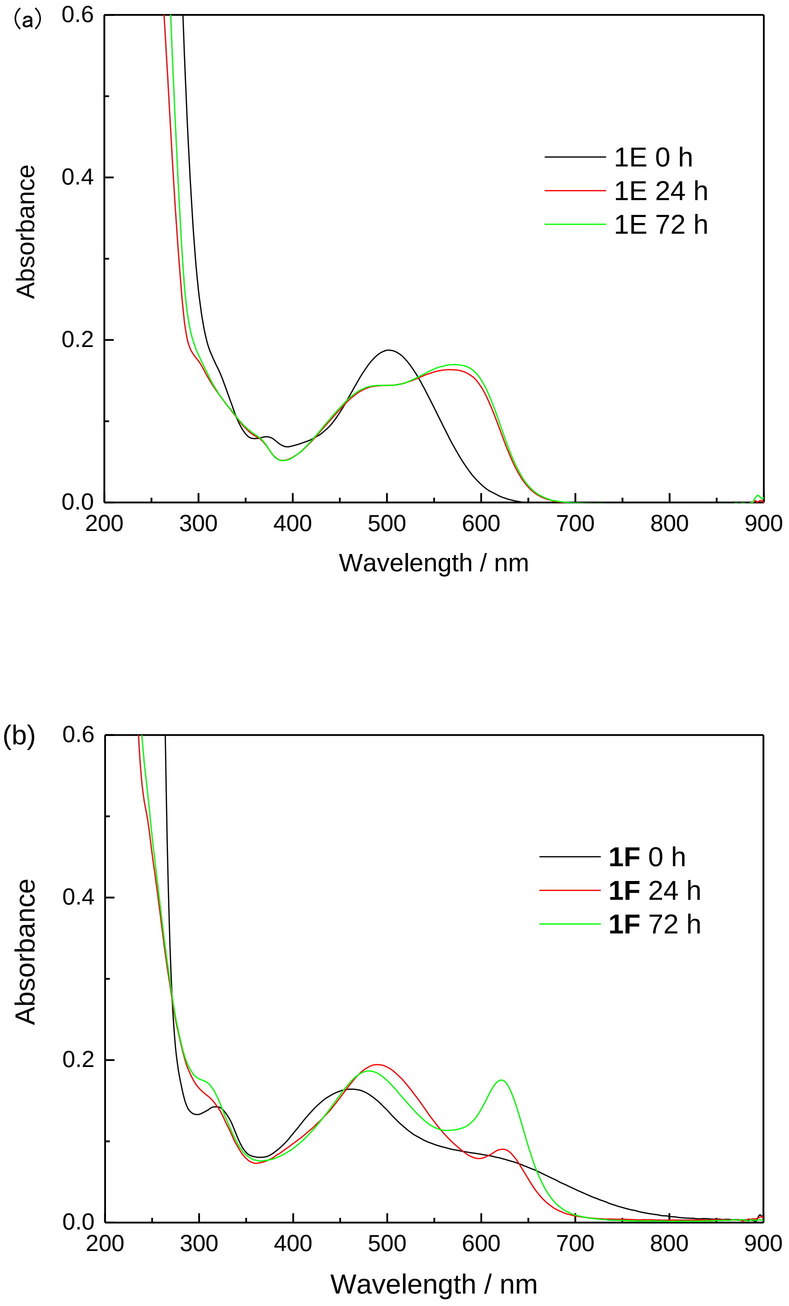


Figure S7. Absorption spectral changes of **1E** (a) and **1F** (b) states at 70 °C in the dark after 24 and 72 h.

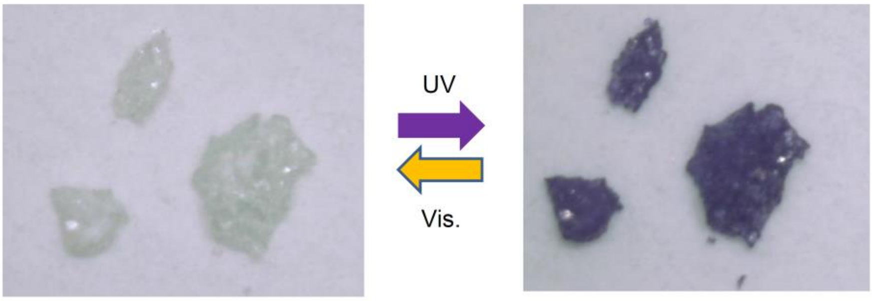


Figure S8. Photochromism between **1A** and **1B** states in the crystalline state

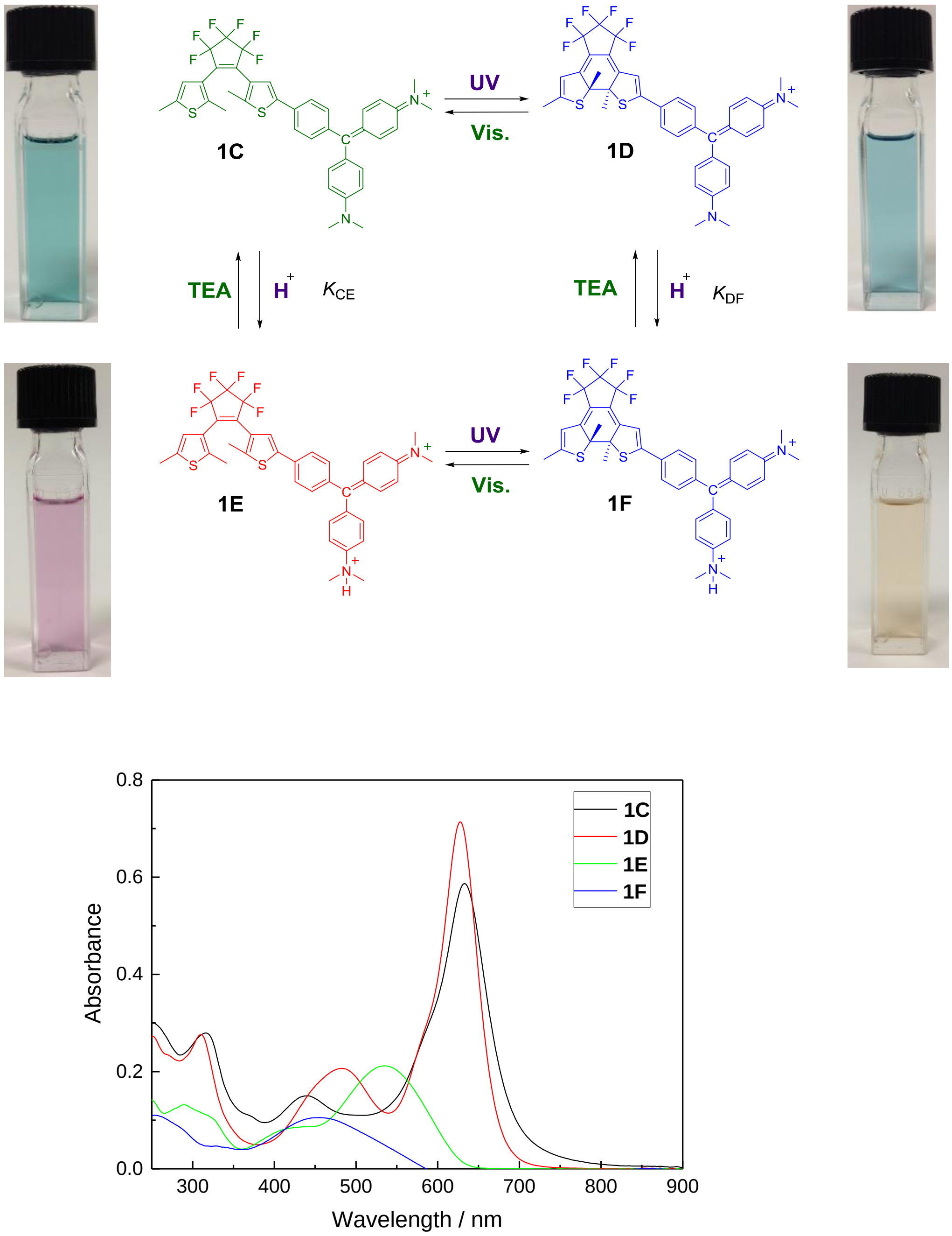


Figure S9. Multicolor switching of **1** in chloroform

Derivative **1** does not form **1A** and **1B** states and directly forms **1C** state in chloroform because of the trace of acid. Upon UV (313 nm) irradiation, **1C** forms **1D**. By addition of 50 μL of 1 M trifluoromethanesulfonic acid (TFMSA) **1C** was converted to **1E,** which is turned to be **1F** upon UV irradiation. By addition of triethylamine, **1E** and **1F** states were reverted to **1C** and **1D** states, respectively.

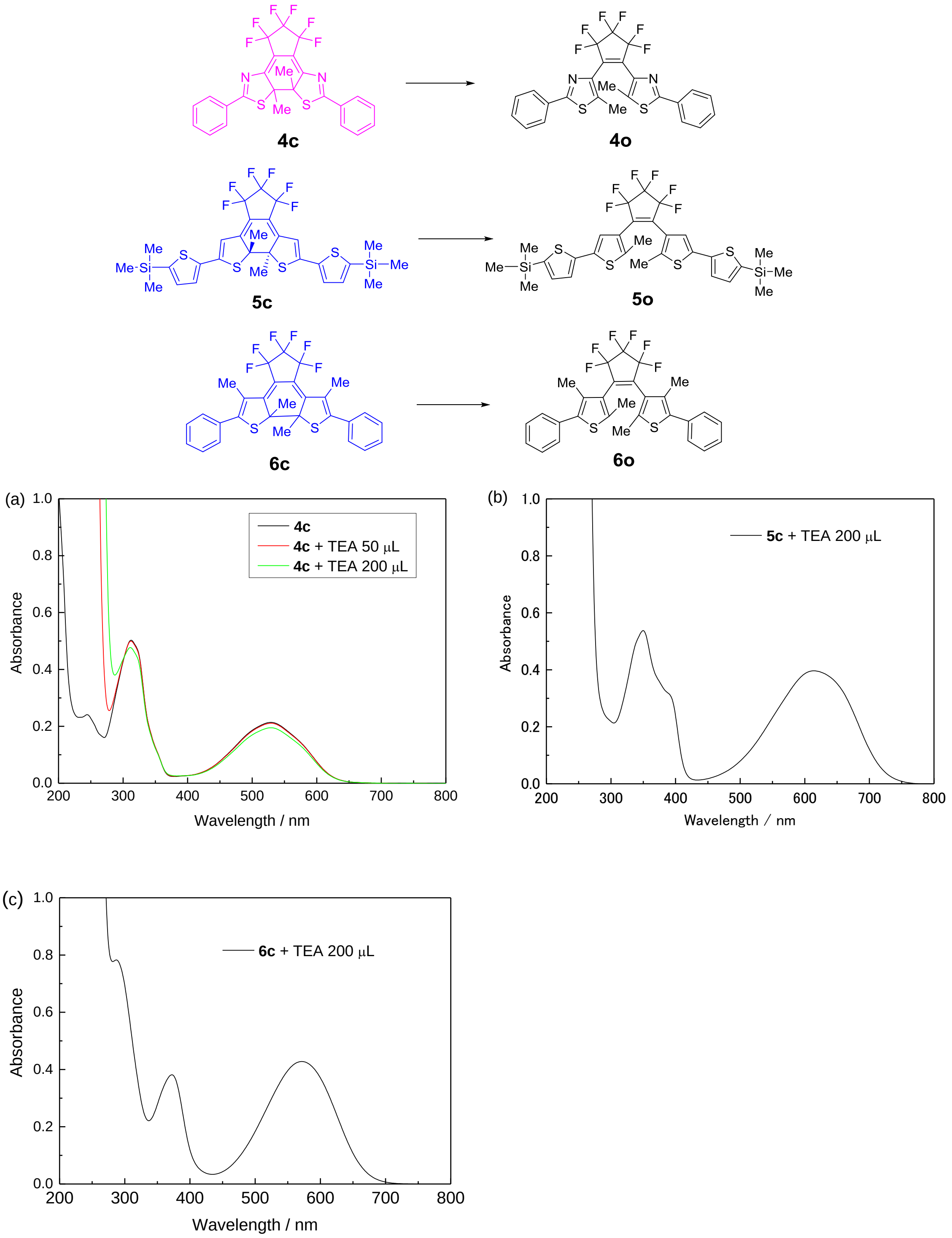


Figure S10 Observation of the spectral changes of the closed-ring isomers **4c, 5c,** and **6c** by addition of triethylamine (TEA) in acetonitrile. After addition of TEA, no spectral changes were observed for the acetonitrile solutions of (a) **4c**, (b) **5c**, (c) **6c.**

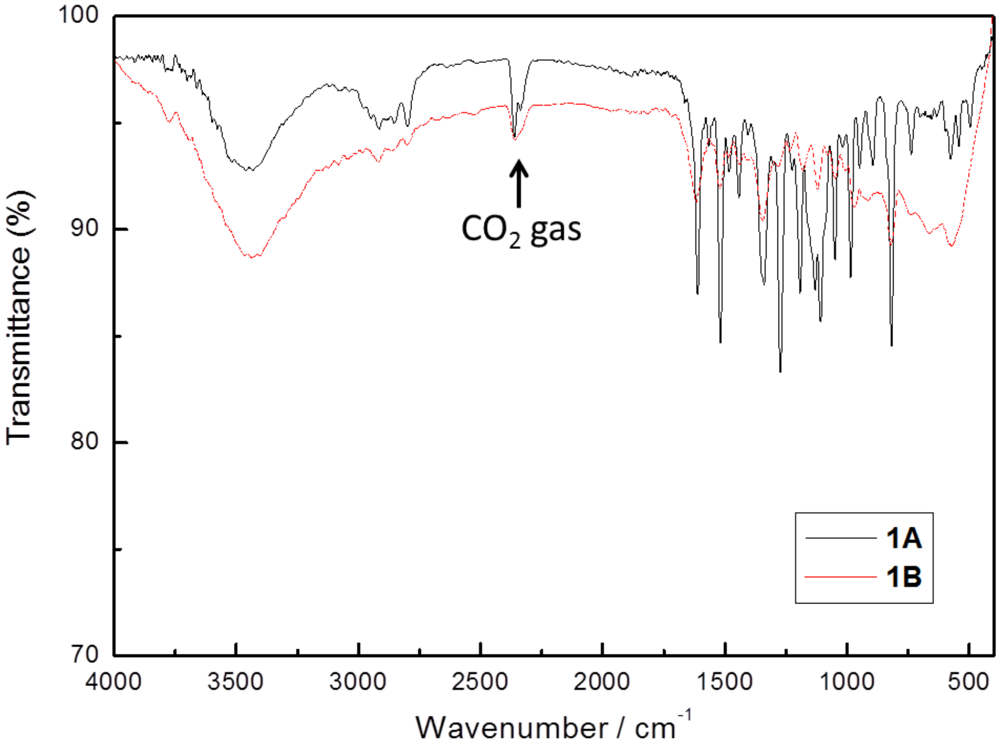


Figure S11. IR spectra of **1A** and **1B** states