Contents

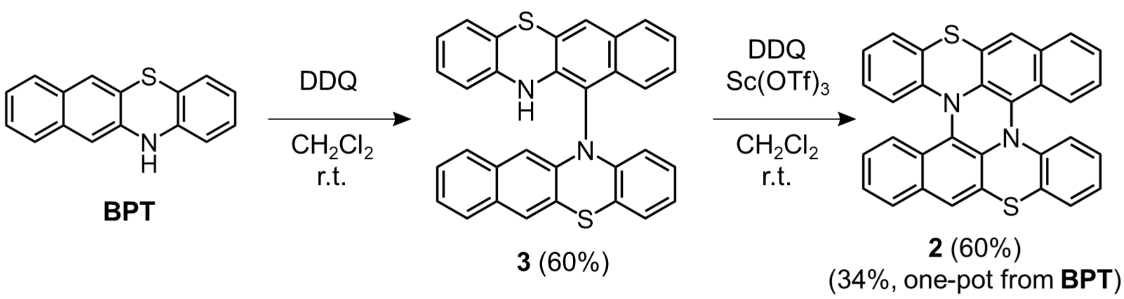
General Information

All the purchased reagents were of standard quality and used without further purification. Dichloromethane used as reaction solvent were purchased from Nacalai Tesque Co., Inc. Benzo[*b*]phenothiazine (**BPT**) was synthesized by solid-state condensation of *o*-aminothiophenol and 2,3-dihydroxynaphthalene by modifying the reported procedure.[S1] All the reactions were carried out under N_2 atmosphere. Flash chromatography was performed with a Biotage Isorela medium pressure liquid chromatography (MPLC) system and a SNAP Sfär flash silica gel cartridge (Biotage). ^{1}H and ^{13}C NMR spectra were recorded by a Varian 400-MR FT-NMR spectrometer. Low- and high-resolution fast atom bombardment (FAB+) mass spectra (MS) were obtained on a JEOL JMS-700 mass spectrometer. UV-Vis-NIR absorption spectra were obtained with a JASCO V-670 spectrometer. Emission spectra were measured with a Shimadzu RF-6000 spectrofluorometer with a UNISOKU CoolSpeK cryostat. Absolute emission quantum yields at room temperature were measured with a Shimadzu RF-6000 spectrofluorometer with an integrating sphere. Absolute photoluminescence quantum yields at 77 K were measured with a Hamamatsu Photonics Quantaurus-QY Plus C13534-01 and a sample holder for low temperature A11238-05. Fluorescence lifetimes were measured with a Horiba FluoroCube spectrofluorometer system. Phosphorescence lifetimes were measured with a Shimadzu RF-6000 spectrofluorometer. Cyclic voltammetry and differential pulse voltammetry were measured in BAS Electrochemical Analyzer ALS Model 612B. Circular dichroism (CD) spectra were recorded on a JASCO J-820 spectropolarimeter. Circularly polarized luminescence (CPL) spectra were recorded on a JASCO CPL-200S. Low-temperature CPL spectra were measured with a JASCO CPL-200S equipped with a UNISOKU CoolSpeK cryostat. Films of **1** and **2** doped in β-estradiol were prepared according to the literature.[S2] **1** and **2** were dissolved in melted β-estradiol (mass fraction of 0.3 %) at 200 °C, and the mixture was spread between two quartz substrates at 200 °C. The substrates were cooled to room-temperature to give transparent films.

[S1] X. Pan, C. Fang, M. Fantin, N. Malhotra, W. Y. So, L. A. Peteanu, A. A. Isse, A. Gennaro, P. Liu and K. Matyjaszewski, K. *J. Am. Chem. Soc.*, 2016, **138**, 2411–2425.

[S2] S. Hirata and M. Vacha, *J. Phys. Chem. Lett.* **2016**, *7*, 1539−1545.

Synthetic Details



Scheme S1. Synthesis of **2**.

3: To a solution of 12*H*-Benzo[*b*]phenothiazine (**BPT**) (1.24 g, 5 mmol) in CH_2Cl_2 (800 mL) was added DDQ (0.57 g, 2.5 mmol), and the solution was kept stirring for 18 h under N_2 atmosphere at rt. The reaction mixture was quenched by adding hydrazine hydrate (ca. 2 mL), and extracted with CH_2Cl_2. The organic layer was dried over Na_2SO_4, and the solvent was removed under reduced pressure. The crude product was chromatographed on silica gel (hexane/dichloromethane as eluent) to afford **3** (0.74 g, 60%) as yellow powder. ^{1}H NMR (400 MHz, dichloromethane-d_2): δ = 7.72–7.70 (m, 1H), 7.66–7.58 (m, 4H), 7.32–7.27 (m, 2H), 7.26–7.16 (m, 4H), 7.02 (dd, $J_1 = 7.8$ Hz, $J_2 = 1.6$ Hz, 1H), 6.93–6.78 (m, 5H), 6.54 (s, 1H), 6.48 (dd, $J_1 = 7.8$ Hz, $J_2 = 1.2$ Hz, 1H), 6.29 (dd, $J_1 = 7.8$ Hz, $J_2 = 1.6$ Hz, 1H); ^{13}C NMR spectrum was not recorded due to low solubility; HRMS FAB$^+$ (Matrix = 3-Nitrobenzyl alcohol) ($C_{32}H_{20}N_2S_2$): Found 496.1031; Calcd. 496.1068.

2 (from **3**): To a solution of **3** (99.3 mg, 0.2 mmol) in CH_2Cl_2 (450 ml), was added DDQ (23 mg, 0.1 mmol) and Sc(OTf)$_3$ (49 mg, 0.1 mmol), and the solution was kept stirring for 18 h under N_2 atmosphere. To the reaction solution, DDQ (23 mg, 0.1 mmol) and Sc(OTf)$_3$ (49 mg, 0.1 mmol) were added and kept stirring for 18 h. The reaction mixture was quenched by adding hydrazine hydrate (1 mL) and was extracted with CH_2Cl_2. The organic layer was dried over Na_2SO_4, and the solvent was removed under reduced pressure. The crude product was reprecipitated with CH_2Cl_2 as good solvent and hexane as poor solvent for several times until TLC showed only one spot to afford **2** (59.3 mg, 60%) as yellow powder: ^{1}H NMR (400 MHz, dichloromethane-d_2): $\delta = 7.74$ (d, $J = 8.2$ Hz, 2H), 7.67 (s, 2H), 7.44 (dd, $J_1 = 7.6$ Hz, $J_2 = 1.6$ Hz, 2H), 7.36–7.29 (m, 4H), 7.20 (t, $J = 8.0$ Hz 2H), 7.05 (t, $J = 7.8$ Hz, 2H), 6.95 (t, $J = 7.8$ Hz, 2H), 6.45 (dd, $J_1 = 8.2$ Hz, $J_2 = 1.4$ Hz, 2H); ^{13}C NMR (100 MHz, CH_2Cl_2): $\delta = 145.24$, 137.39, 132.09, 128.71, 127.99, 127.53, 127.34, 127.12, 125.93, 125.71, 125.36, 125.02, 123.64, 123.09, 122.78, 117.75; HRMS FAB$^+$ (Matrix = 3-Nitrobenzyl alcohol) ($C_{32}H_{18}N_2S_2$): Found 494.0912; Calcd. 494.0911.

2 (from **BPT**): To a solution of **BPT** (1.24 g, 5.0 mmol) in CH_2Cl_2 (700 ml) was added DDQ (0.57 g, 2.5 mmol), and the solution was kept stirring for 5 h under N_2 atmosphere. After checking the formation of **3** by TLC, DDQ (0.28 g, 1.25 mmol) and Sc(OTf)$_3$ (0.62

g, 1.25 mmol) were added to the reaction solution and kept stirring for 18 h. DDQ (0.28 g, 1.25 mmol) and $Sc(OTf)_3$ (0.62 g, 1.25 mmol) were added again to the reaction solution and kept stirring for another 18 h. The reaction mixture was quenched by adding hydrazine hydrate (3 mL) and was extracted with CH_2Cl_2. The crude product was reprecipitated with CH_2Cl_2 as good solvent and hexane as poor solvent for several times until TLC showed only one spot to afford **2** (0.42 g, 34%) as yellow powder.

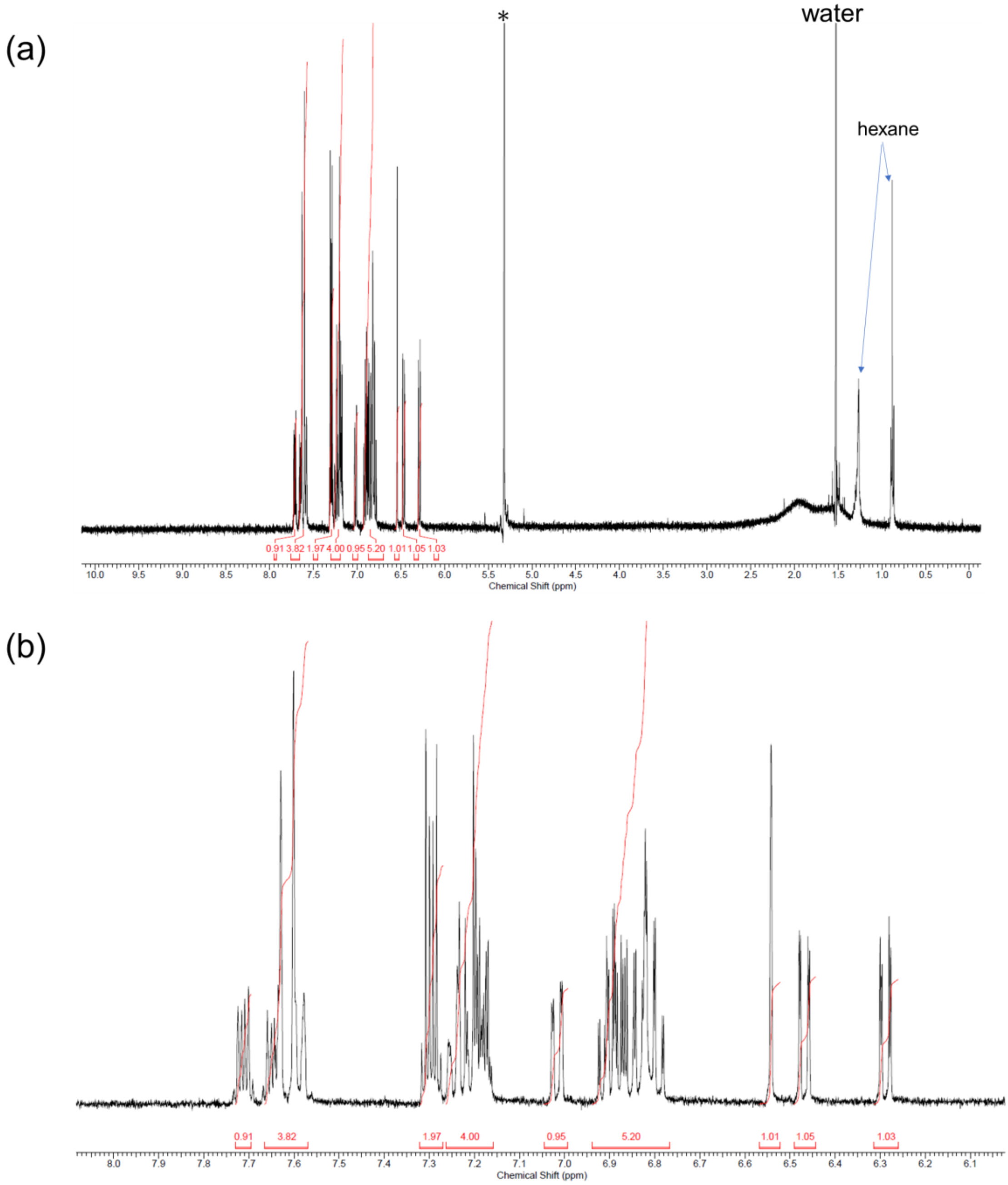


Fig. S1 ^{1}H NMR spectra of **3** in dichloromethane-d_2. a) 0–10 ppm and b) aromatic region. Asterisk denotes the solvent residual peak.

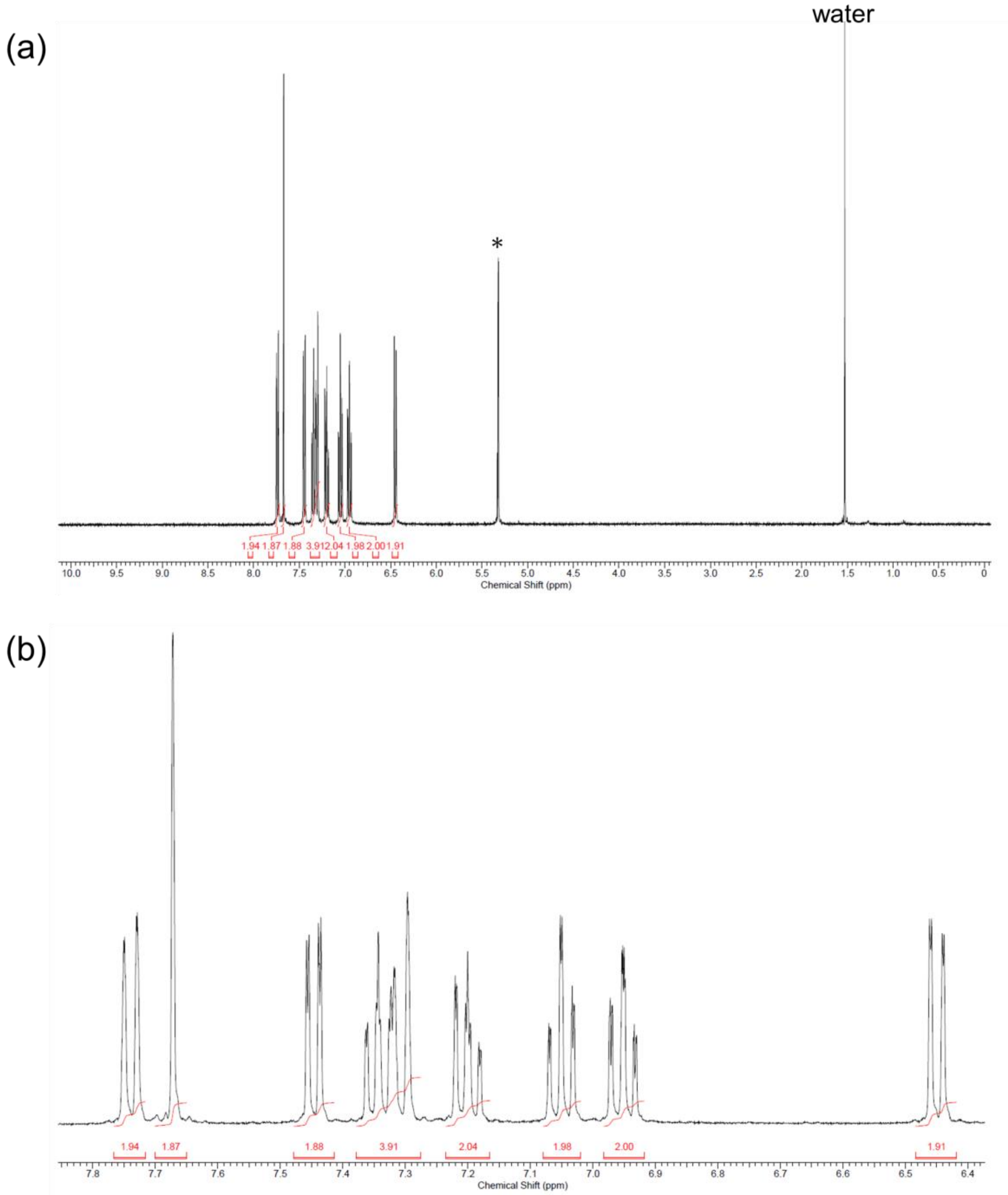


Fig. S2 ^{1}H NMR spectra of **2** in dichloromethane-d_2. a) 0–10 ppm and b) aromatic region. Asterisk denotes the solvent residual peak.

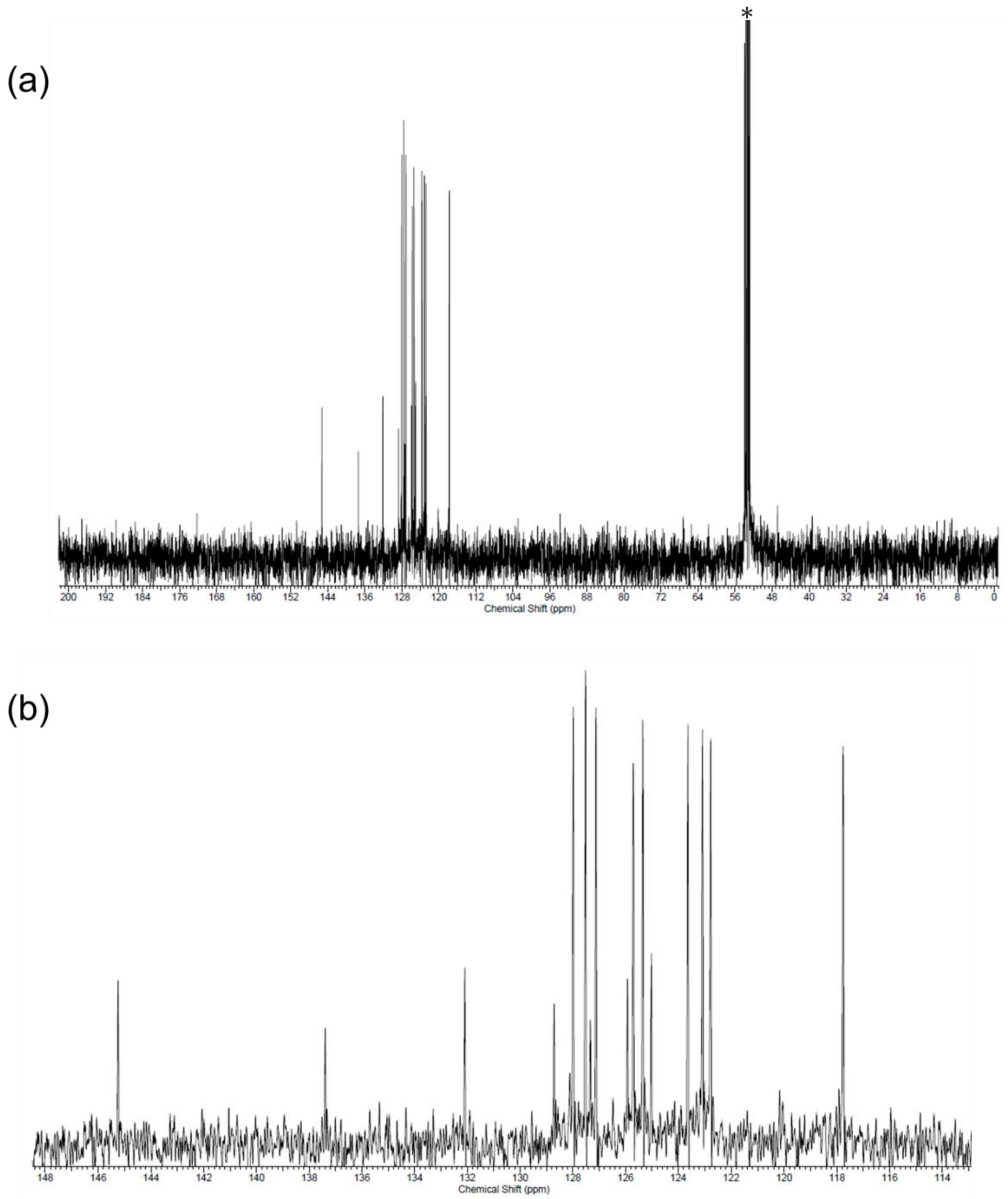


Fig. S3 ^{13}C NMR spectra of **2** in dichloromethane-d_2. a) 0–200 ppm and b) aromatic region. Asterisk denotes the solvent residual peak.

X-ray Crystallography

The single crystal of *rac*-**2** was obtained by the slow diffusion of hexane vapor into a toluene solution of racemic **2**. Data collections were performed on a Rigaku R-AXIS RAPID diffractometer with Mo-Kα radiation at 173 K. The hydrogen atoms were refined using the riding model. All the calculations were performed by using CrystalStructure crystallographic software package,[S2] except for refinement, which was performed by using SHELXL Version 2017/1.[S3] The CIF file has been deposited on the Cambridge Crystallographic Data Centre (CCDC), under deposition numbers CCDC 2103647.

[S2] CrystalStructure 4.3: Crystal Structure Analysis Package, Rigaku Corporation (2000-2018). Tokyo 196-8666, Japan.

[S3] G. M. Sheldrick, Acta Cryst. A **2008**, *64*, 112.

Table S1: X-ray crystallographic data for *rac*-**2**.

empirical formula	$C_{32}H_{18}N_2S_2$
formula weight	494.63
T [˚C]	–100
λ [Å]	0.71075
crystal system	tetragonal
space group	$I\,4_1/a$
Z	8
a [Å]	20.735(3)
c [Å]	10.5694(7)
V [Å^3]	4544.1(9)
ρ_{calcd} [g cm^{-3}]	1.446
collected data	20753
unique data / R_{int}	2580/0.0420
no. of parameters	163
goodness-of-fit[a]	1.044
$R1$ ($I > 2\sigma$), $wR2$ (all reflections)[b]	0.0338, 0.0829
residual density [e Å^{-3}]	0.31/–0.25

[a] GOF = $\left\{\sum\left[w\left(F_0^2 - F_c^2\right)^2\right]\big/(n-p)\right\}^{1/2}$, where n and p denote the number of data and parameters.

[b] $\mathrm{R1} = \sum\left(\|F_0\| - \|F_c\|\right)\big/\sum\|F_0\|$ and $\mathrm{wR2} = \left\{\sum\left[w\left(F_0^2 - F_c^2\right)^2\right]\big/\sum\left[w\left(F_0^2\right)^2\right]\right\}^{1/2}$ where $w = 1\big/\left[\sigma^2\left(F_0^2\right) + (a\cdot P)^2 + b\cdot P\right]$ and $P = \left[\left(\mathrm{Max};0,F_0^2\right) + 2\cdot F_c^2\right]\big/3$.

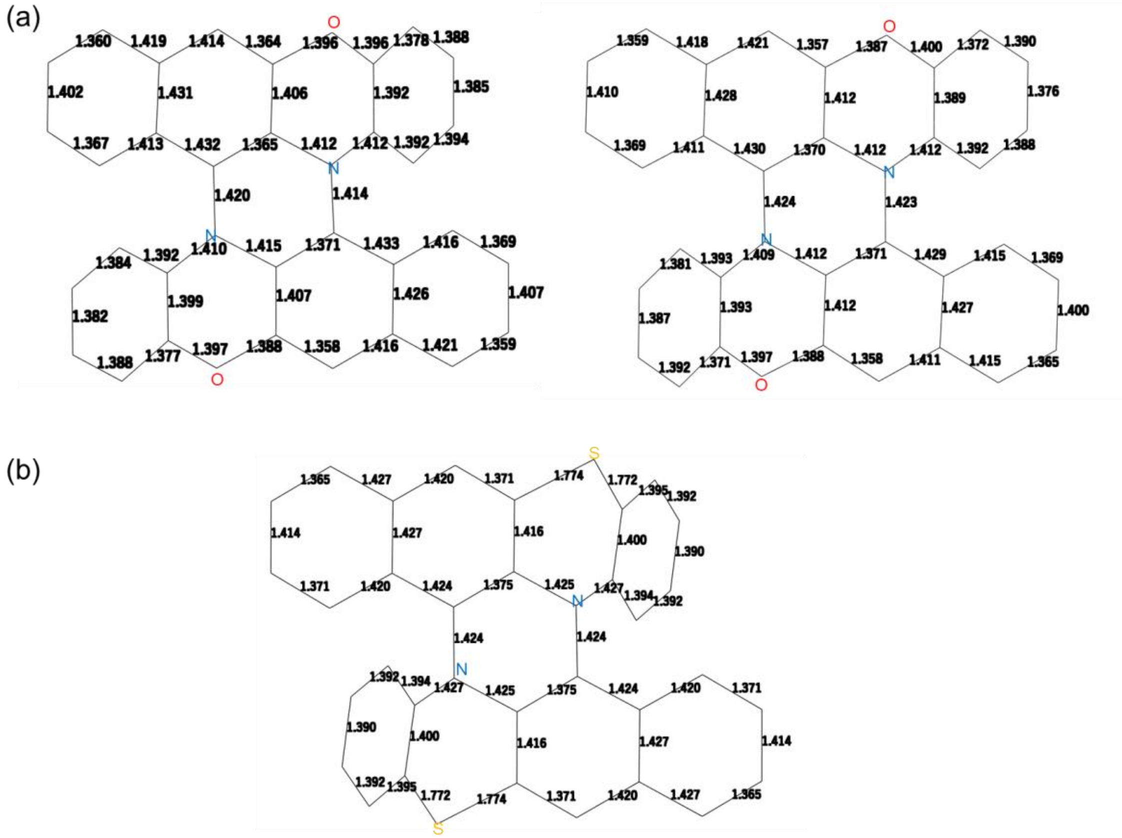


Fig. S4 Bond lengths of (a) **1** (two crystallographically independent molecules) and (b) **2** in their racemic crystals.

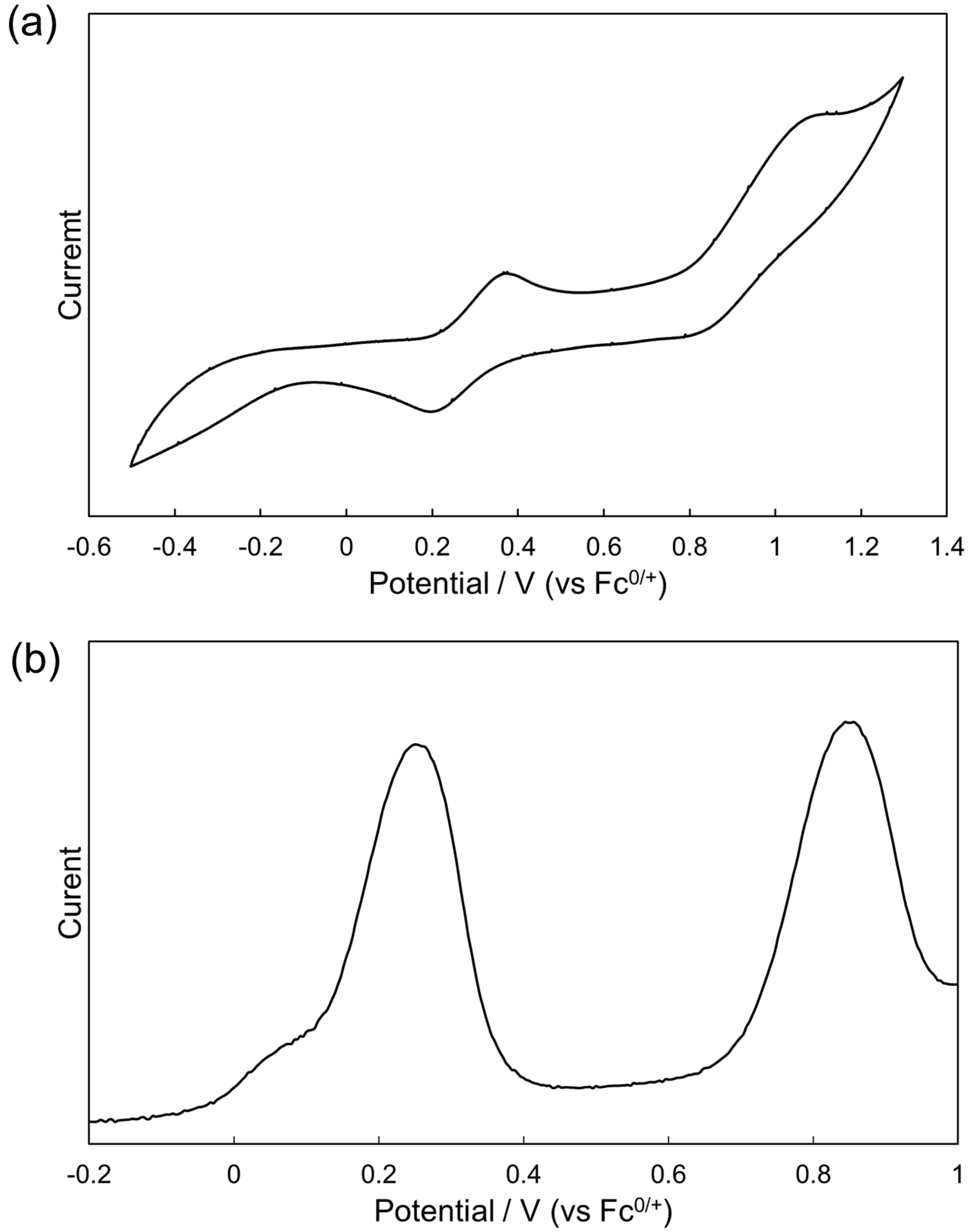


Fig. S5 Cyclic voltammogram of **2** in dichloromethane (1×10^{-3} M) containing 0.1 M $n\mathrm{Bu_4NBF_4}$ at 298 K.

Table S2. Oxidation potentials (V vs. Fc^0/Fc^{1+}) of **1** and **2** in CH_2Cl_2 (0.1 M $n$$Bu_4NBF_4$). Scan rate = 100 mVs^{-1}.

	E_1	E_2	$E_2 - E_1$
1	0.05	0.68	0.53
2	0.25	0.85	0.60

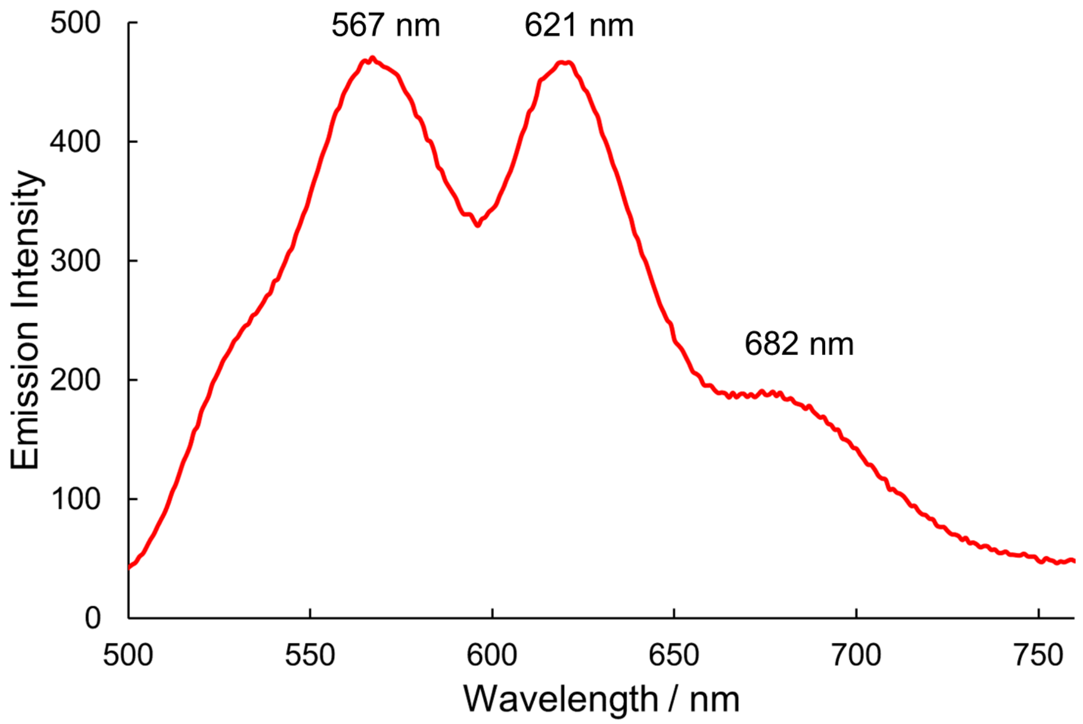


Fig. S6 Emission spectrum (λ_{ex} = 400 nm) of **1** in 2-MTHF at 78 K.

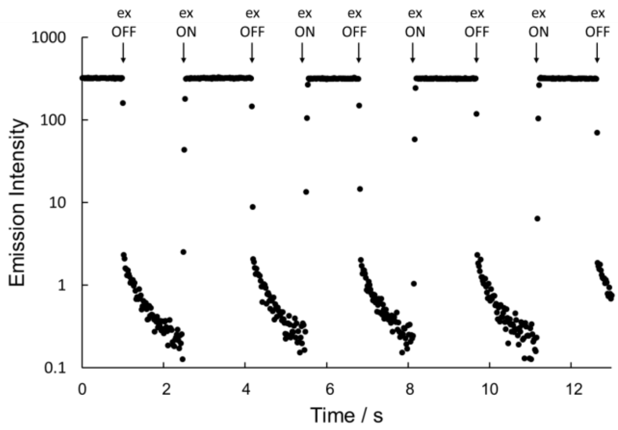


Fig. S7 Emission decay curves of **1** at 567 nm in 2-MTHF at 78 K (λ_{ex} = 400 nm). Emission intensity was measured every 20 ms.

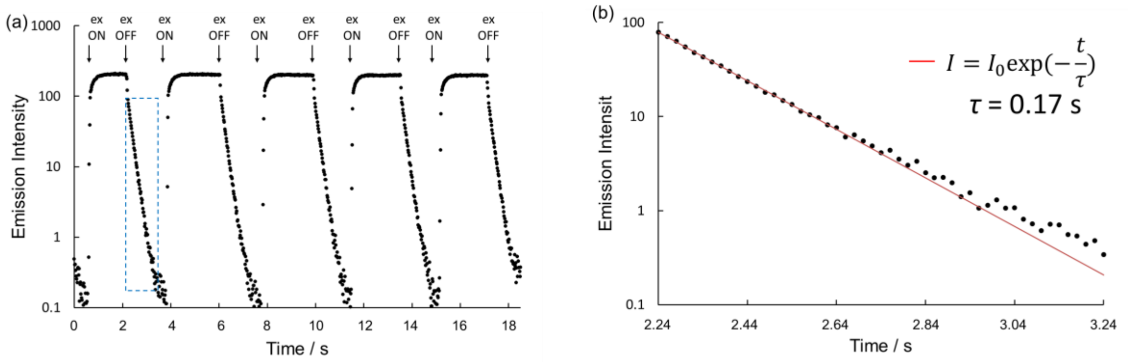


Fig. S8 (a) Emission decay curves of **1** at 621 nm in 2-MTHF at 78 K (λ_{ex} = 400 nm) and (b) fitting of a decay curve. Emission intensity was measured every 20 ms.

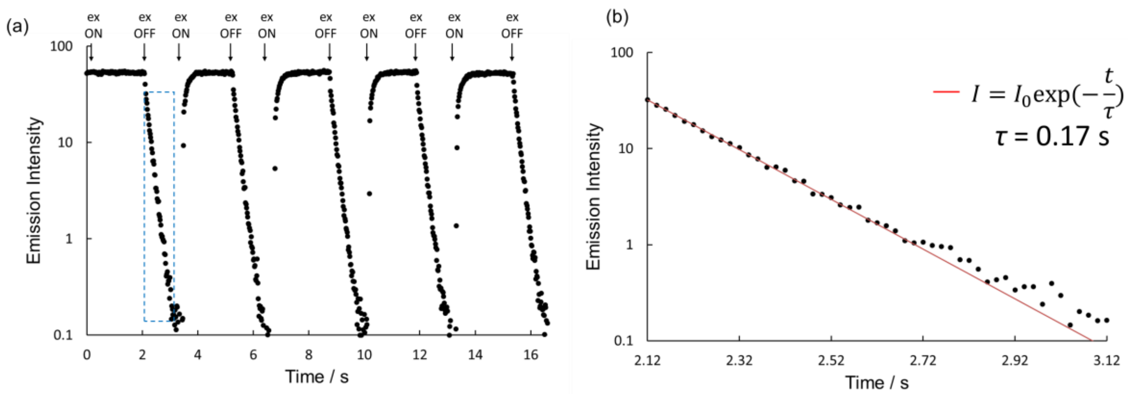


Fig. S9 Emission decay curves of **1** at 682 nm in 2-MTHF at 78 K (λ_{ex} = 400 nm) and (b) fitting of a decay curve. Emission intensity was measured every 20 ms.

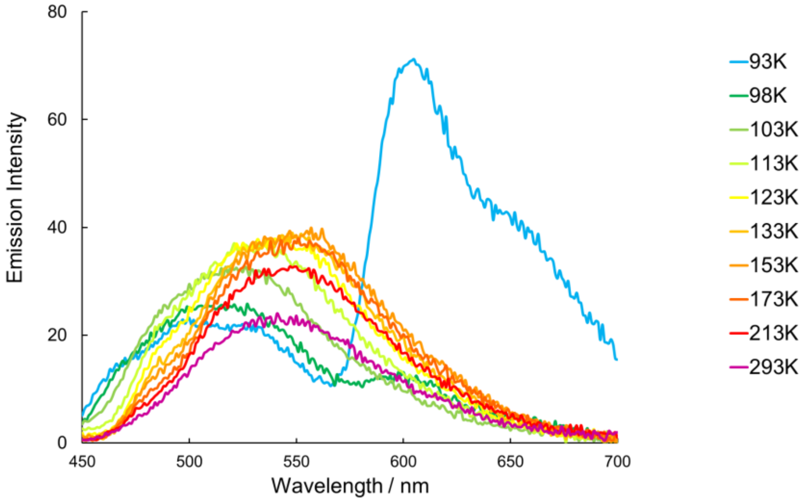


Fig. S10 Temperature dependence of the emission spectra (λ_{ex} = 365 nm) of **2** in 2-MTHF from 293 K to 93 K.

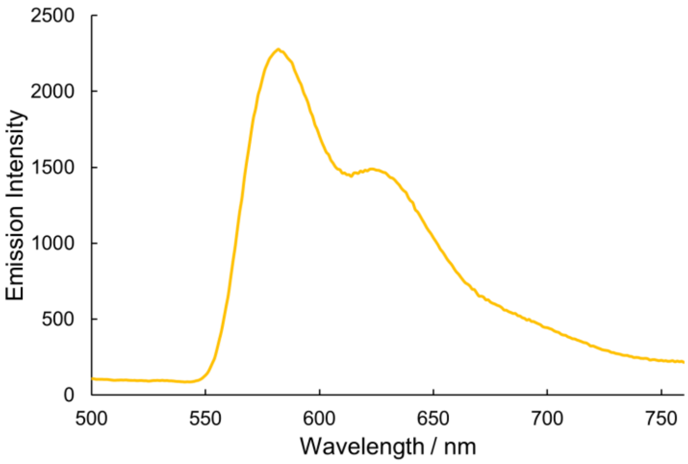


Fig. S11 Emission spectrum (λ_{ex} = 400 nm) of **2** in 2-MTHF at 78 K.

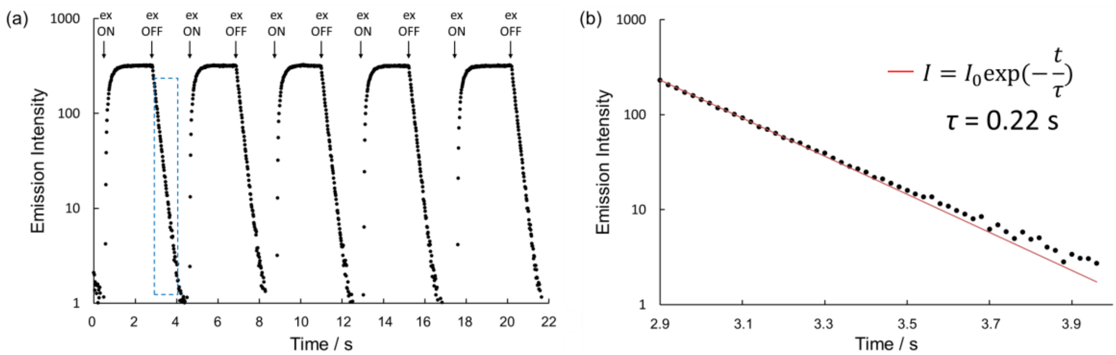


Fig. S12 Emission decay curves of **2** at 594 nm in 2-MTHF at 78 K (λ_{ex} = 400 nm) and (b) fitting of a decay curve. Emission intensity was measured every 20 ms.

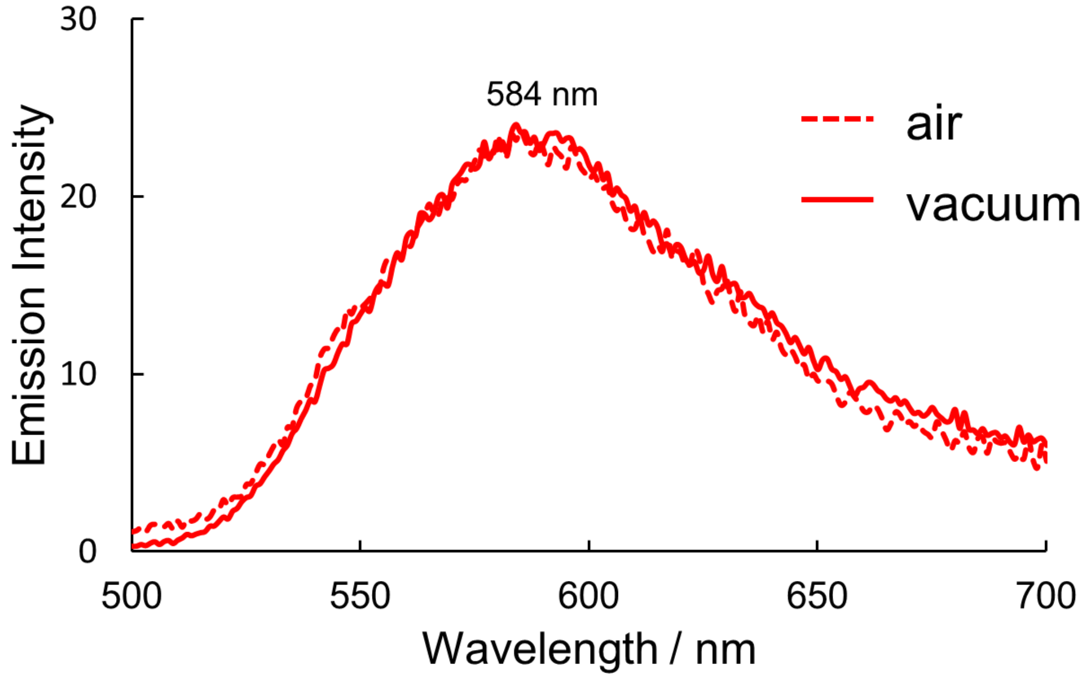


Fig. S13 Emission spectra (λ_{ex} = 365 nm) of polycrystalline **1** measured in air (dashed line) and under vacuum (solid line) at room temperature.

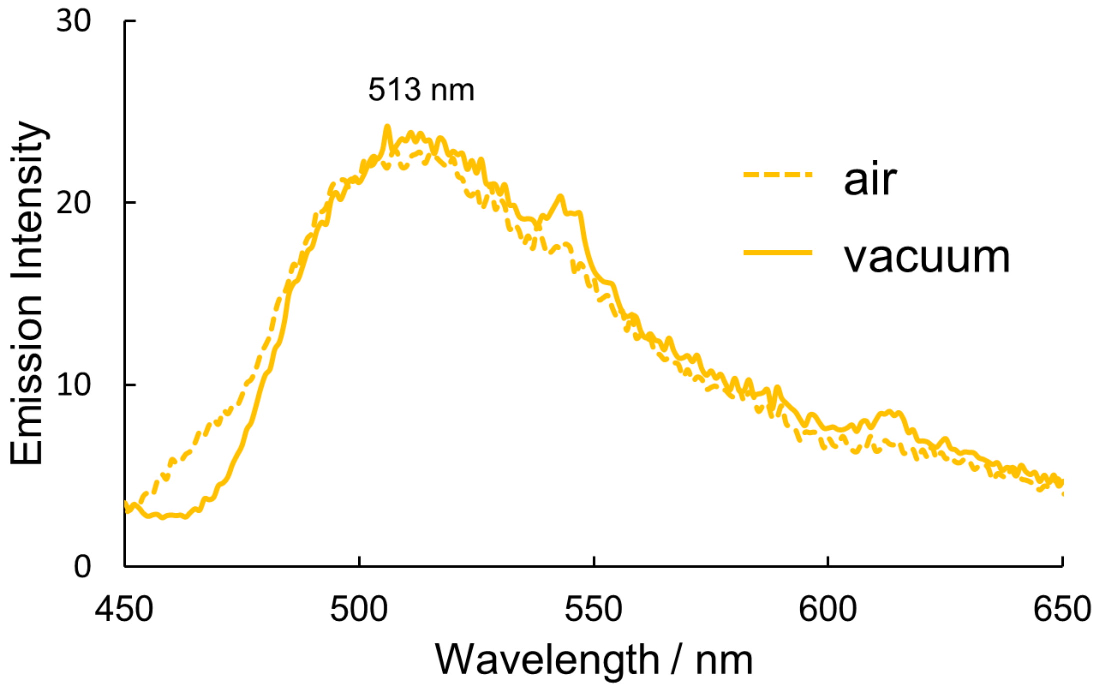


Fig. S14 Emission spectra (λ_{ex} = 365 nm) of polycrystalline **2** measured in air (dashed line) and under vacuum (solid line) at room temperature.

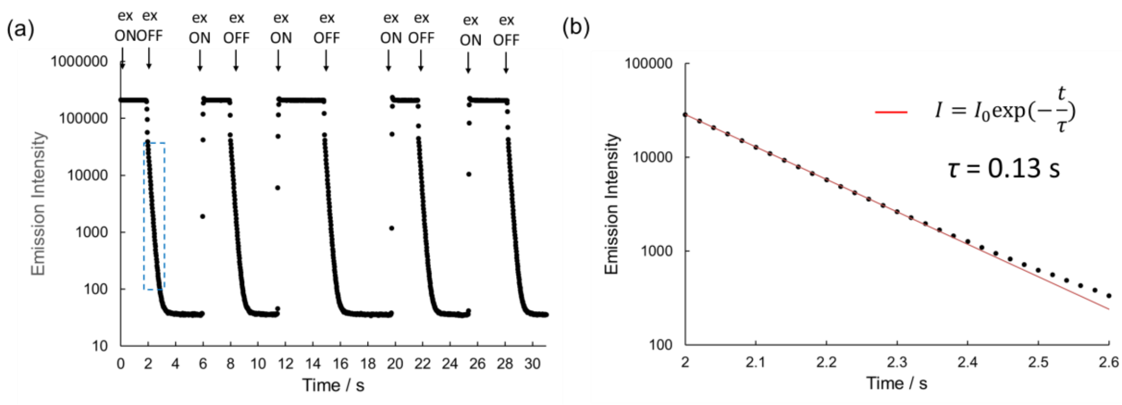


Fig. S15 Emission decay curves of **1** at 621 nm in β-estradiol (0.3wt%) at room temperature (λ_{ex} = 365 nm) and (b) fitting of a decay curve. Emission intensity was measured every 20 ms.

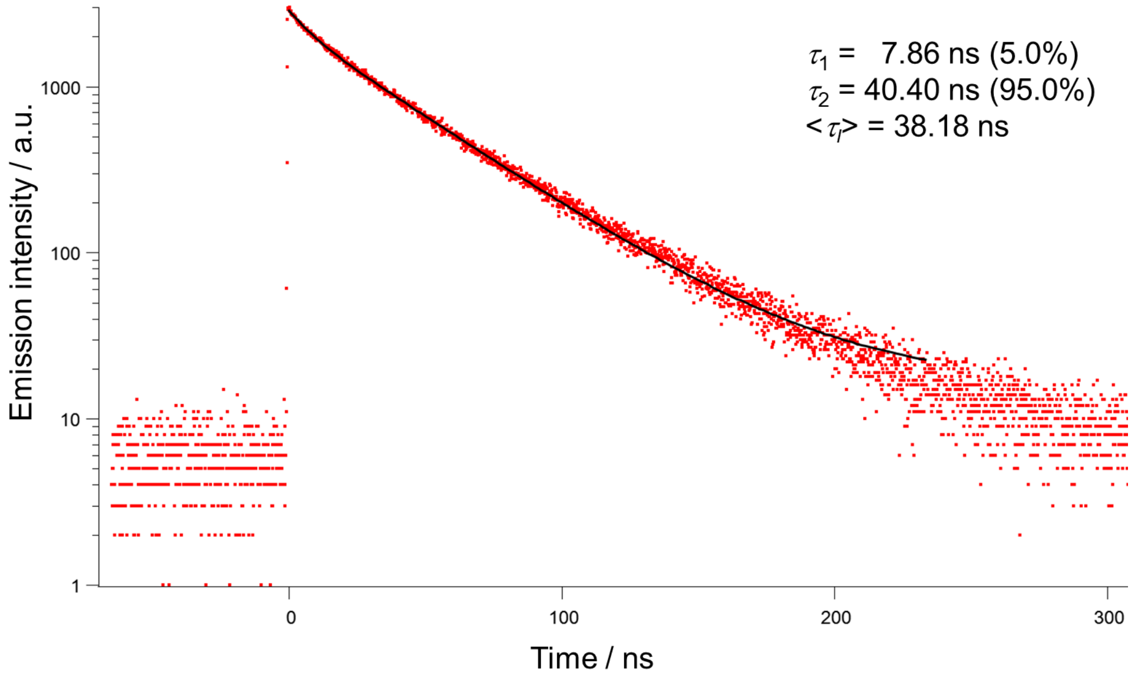


Fig. S16 Emission decay curves of **1** at 500 nm in β-estradiol (0.3wt%) at room temperature (λ_{ex} = 375 nm). Black line denotes the curve of best fit by a biexponential functions. The area-weighted ratio ($A_n\tau_n$) are shown in parentheses. The intensity-weighted mean emission lifetime $<\tau_I>$ was calculated as follows: $<\tau_I> = \Sigma(A_n\tau_n^2)/\Sigma(A_n\tau_n)$ where A_n is the coefficient of exponential function of the n-th component.

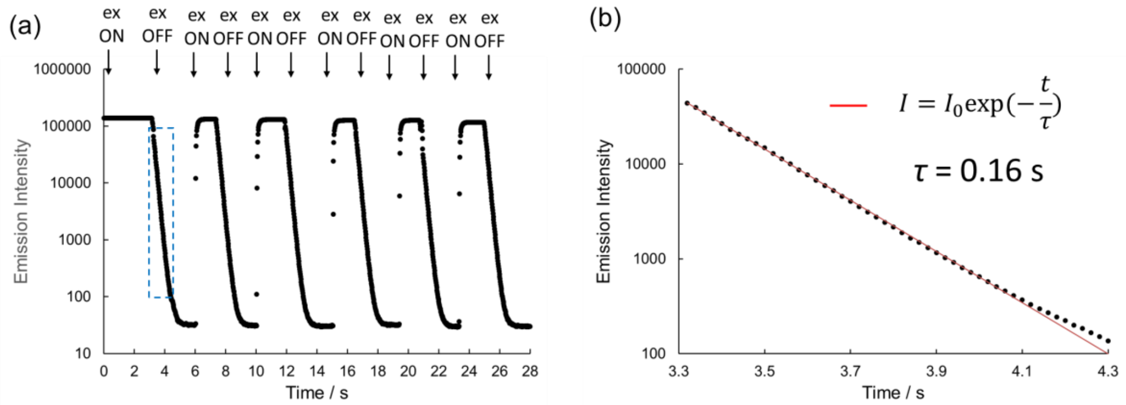


Fig. S17 Emission decay curves of **2** at 594 nm in β-estradiol (0.3wt%) at room temperature (λ_{ex} = 365 nm) and (b) fitting of a decay curve. Emission intensity was measured every 20 ms.

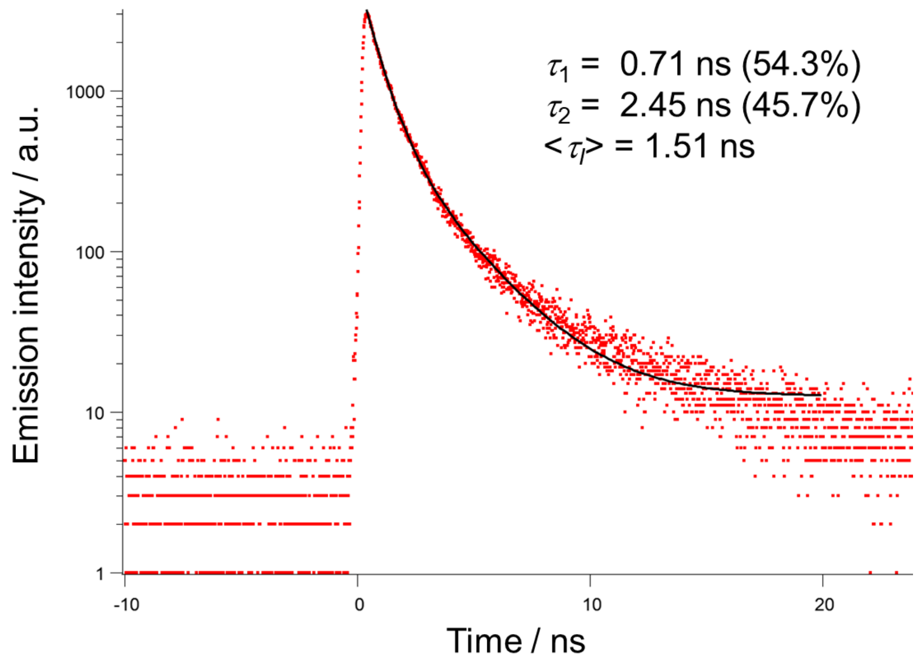


Fig. S18 Emission decay curves of **2** at 480 nm in β-estradiol (0.3wt%) at room temperature (λ_{ex} = 375 nm). Black line denotes the curve of best fit by a biexponential functions. The area-weighted ratio ($A_n\tau_n$) are shown in parentheses. The intensity-weighted mean emission lifetime $<\tau_I>$ was calculated as follows: $<\tau_I> = \Sigma(A_n\tau_n^2)/\Sigma(A_n\tau_n)$ where A_n is the coefficient of exponential function of the n-th component.

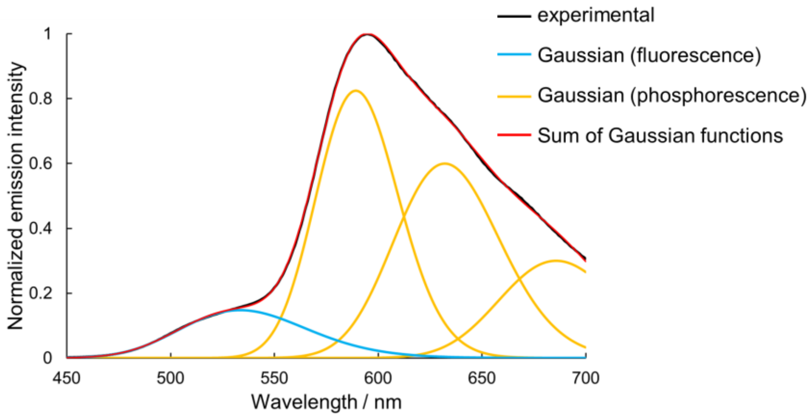


Fig. S19 Fitting of the emission spectrum of **2** doped in β-estradiol measured under ambient conditions with four Gaussian functions. The ratio of the area of fluorescence (cyan) to phosphorescence (yellow) was 13:87.

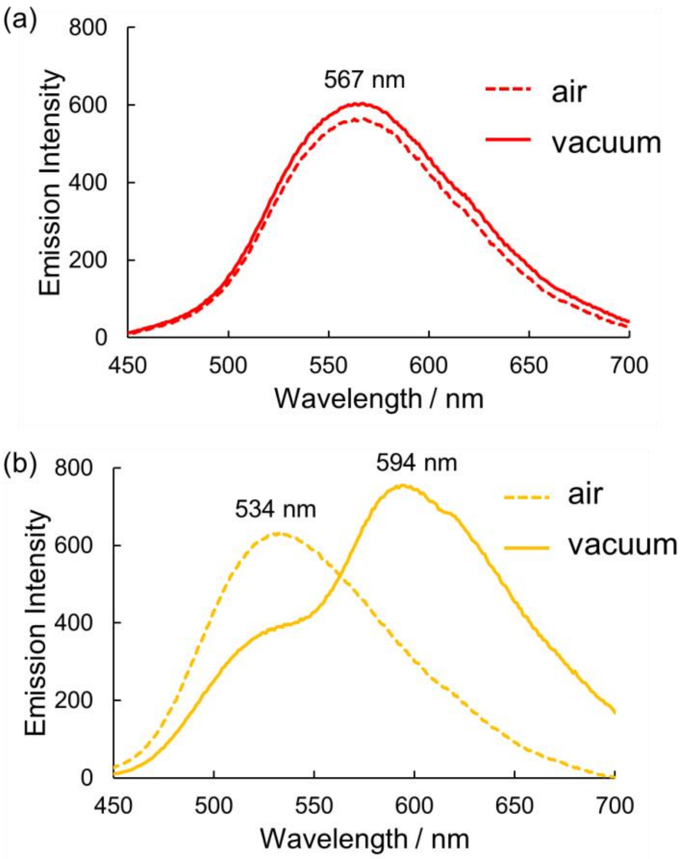


Fig. S20 Emission spectra (λ_{ex} = 365 nm) of (a) **1** and (b) **2** dispersed in PMMA (1wt%) measured at room temperature in air (dashed line) and under vacuum (solid line) and photographs of the films of (c) **1** and (d) **2** taken under irradiation with UV light at 365 nm.

DFT Calculations

All the DFT calculations were carried out by using Gaussian 16 program package (Revision C.01) at the B3LYP-GD3BJ/6-311G(2d,p) level of theory.

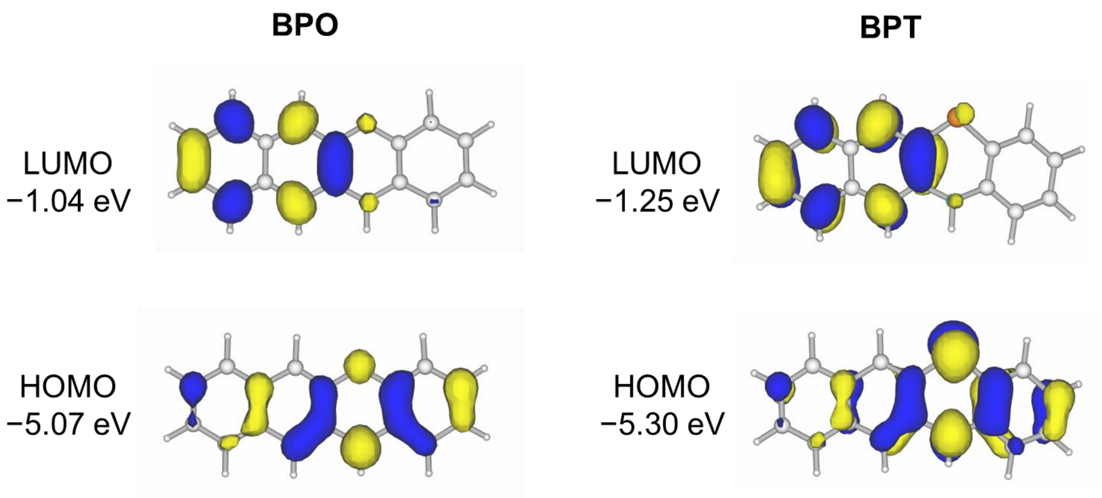


Fig. S21 Frontier Kohn-Sham molecular orbitals of **BPO** and **BPT** calculated at the B3LYP-GD3BJ/6-311G(2d,p) level.

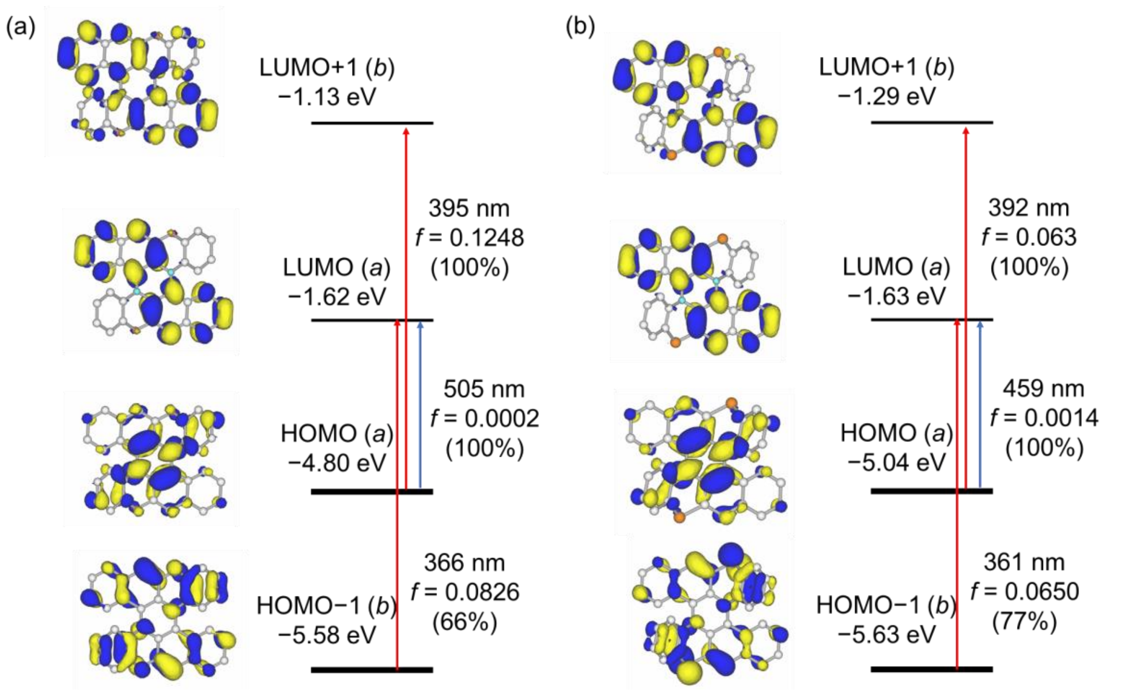


Fig. S22 TD-DFT calculated electronic transitions of (a) **1** and (b) **2** calculated at the B3LYP-GD3BJ/6-311G(2d,p) level.

Table S3: Exited states of **1** calculated at the B3LYP-GD3BJ/6-311G(2d,p) level.

state	symmetry	energy	configurations	
$S_1@S_1$	A	1.9536 eV (634.63 nm)	HOMO → LUMO	0.70411 (99.2%)
$T_1@T_1$	A	1.4521 eV (853.83 nm)	HOMO → LUMO	0.68519 (93.9%)
$T_2@T_2$	B	2.1261 eV (583.16 nm)	HOMO−3 → LUMO	-0.22342 (10.0%)
			HOMO−2→ LUMO+1	-0.15724 (4.9%)
			HOMO−1→LUMO	-0.32892 (21.6%)
			HOMO→LUMO+1	0.53012 (56.2%)

Table S4: Exited states of **2** calculated at the B3LYP-GD3BJ/6-311G(2d,p) level.

state	symmetry	energy	configurations	
$S_1@S_1$	A	2.1499 eV (576.70 nm)	HOMO → LUMO	0.70370 (99.0%)
$T_1@T_1$	A	1.6560 eV (748.70 nm)	HOMO−3 → LUMO+1	-0.11589 (2.7%)
			HOMO−2→ LUMO	-0.11028 (2.4%)
			HOMO−1→LUMO+1	0.10600 (2.2%)
			HOMO→LUMO	0.66872 (89.4%)
$T_2@T_2$	B	2.1457 eV (577.82 nm)	HOMO−3 → LUMO	-0.24068 (11.8%)
			HOMO−2→ LUMO+1	-0.17010 (7.1%)
			HOMO−1→LUMO	0.27650 (21.2%)
			HOMO→LUMO+1	0.53687 (52.6%)

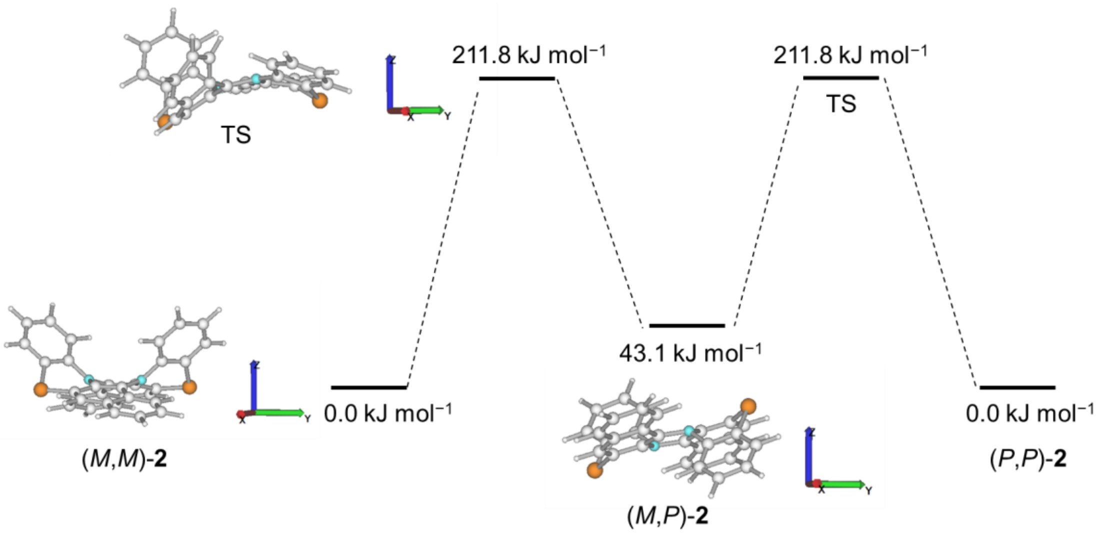


Fig. S23 Energy diagrams for the racemization of **2** calculated at B3LYP/6-31G(d) level.

Table S5. Summary of the results of TD-DFT calculations of **2** at the B3LYP-GD3BJ/6-311G(2d,p) level.

compound[a)] (transition)	Energy / nm	$\|\boldsymbol{\mu}\|$ / 10^{-20} esu·cm	$\|\boldsymbol{m}\|$ / 10^{-20} erg·G^{-1}	$\cos\theta_{\mu,m}$	D / 10^{-40} esu^2·cm^2	G / 10^{-40} erg^2·G^{-2}	R[b)] / 10^{-40} esu·esu·cm·G^{-1}	f	g_{CD} or g_{CPL} (theoretical)
2 ($S_0 \rightarrow S_1$)	459	37.3	1.25	1.0	1394	1.55	46.5	1.5×10^{-3}	0.133
2 ($S_1 \rightarrow S_0$)	577	18.1	1.43	1.0	328	2.04	25.9	3.1×10^{-4}	0.313

a) (M, M)-isomer, b) $|\boldsymbol{\mu}|\,|\boldsymbol{m}|\cos\theta_{\mu,m}$

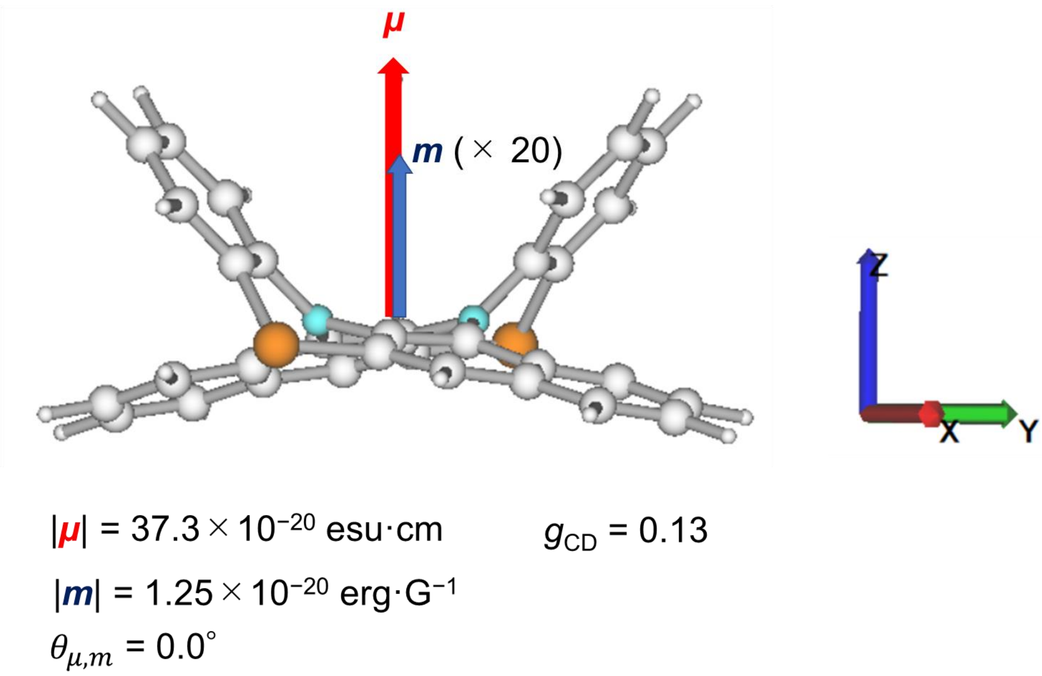
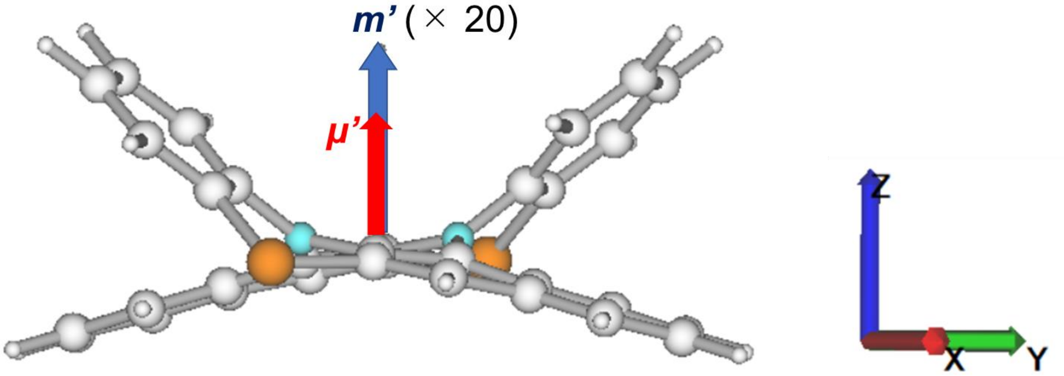


Fig. S24 TEDM and TMDM of (M, M)-**2** in the S_0 state calculated at the B3LYP-GD3BJ/6-311G(2d,p) level.



$|\boldsymbol{\mu'}| = 18.1 \times 10^{-20}$ esu·cm $\quad g_{CPL} = 0.31$

$|\boldsymbol{m'}| = 1.43 \times 10^{-20}$ erg·G^{-1}

$\theta_{\mu',m'} = 0.0^{\circ}$

Fig. S25 TEDM and TMDM of (*M*, *M*)-**2** in the S_1 state calculated at the B3LYP-GD3BJ/6-311G(2d,p) level.

Optical resolution of 2

Optical resolution of **2** was carried out under the following two conditions.

HPLC (JAI LaboACE LC-5060) equipped with a DAICEL CHIRALPAK-IE column (1 cm (i.d.) × 25 cm), eluent: *n*-hexane/toluene (2/1, v/v), flow rate: 1.4 mL/min, amount of sample: 0.5 mg)

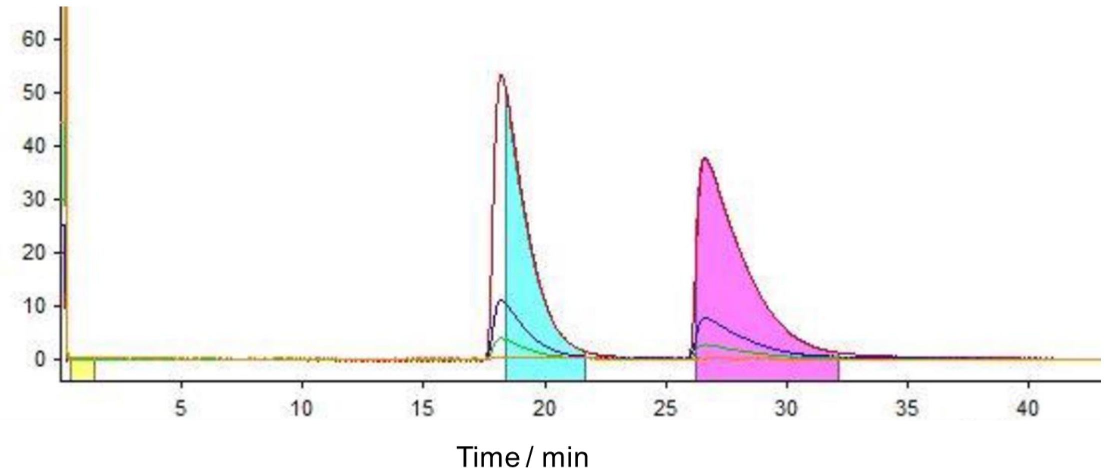


Fig. S26 Chromatograms for the enantiomers of **2** with HPLC.

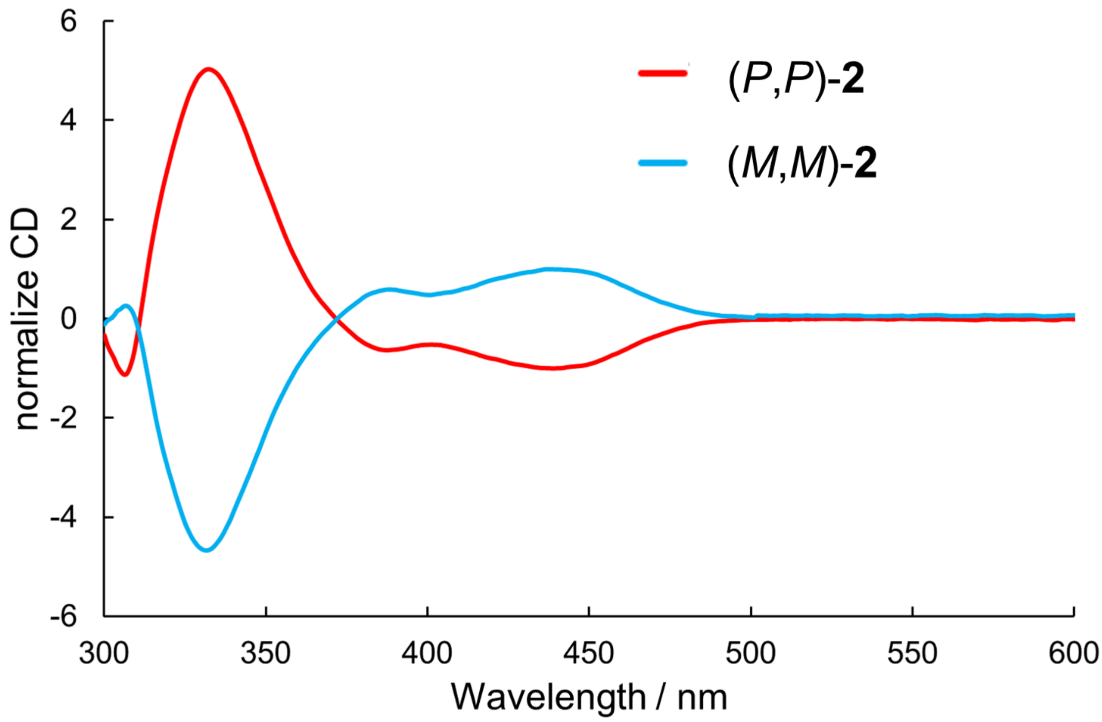


Fig. S27 (a) CD spectra of **2** doped in β-estradiol at room temperature.

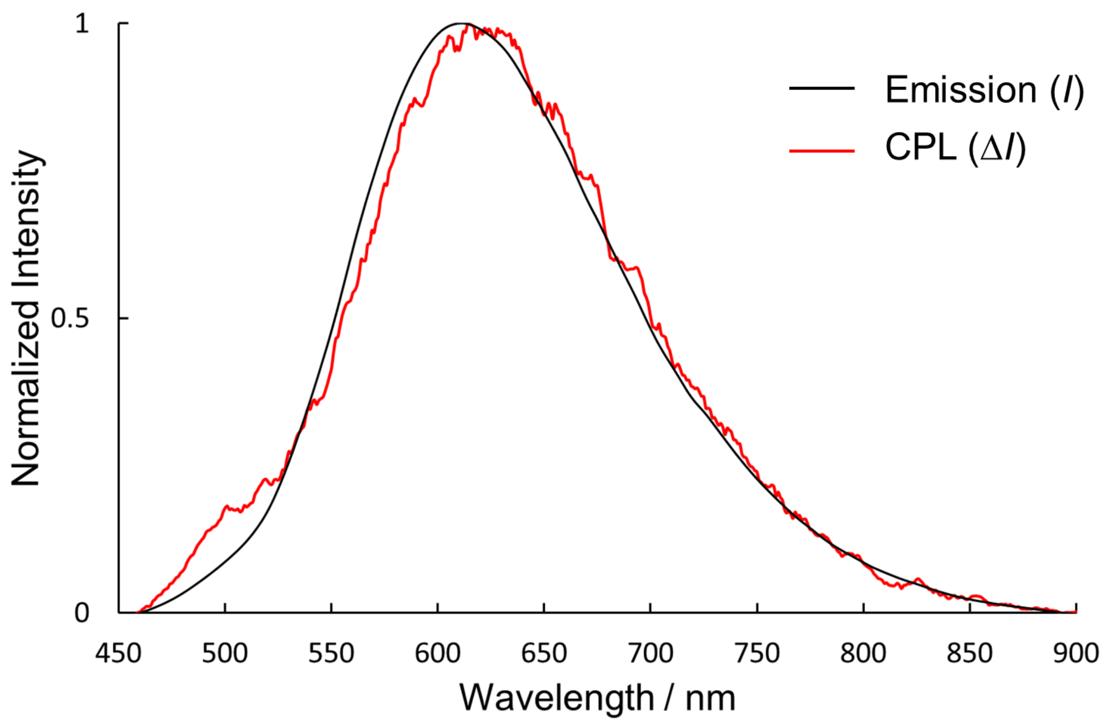


Fig. S28 Emission (black) and CPL (red) spectra of (*M*,*M*)-**2** doped in β-estradiol simultaneously measured with a CPL spectrometer at room temperature.

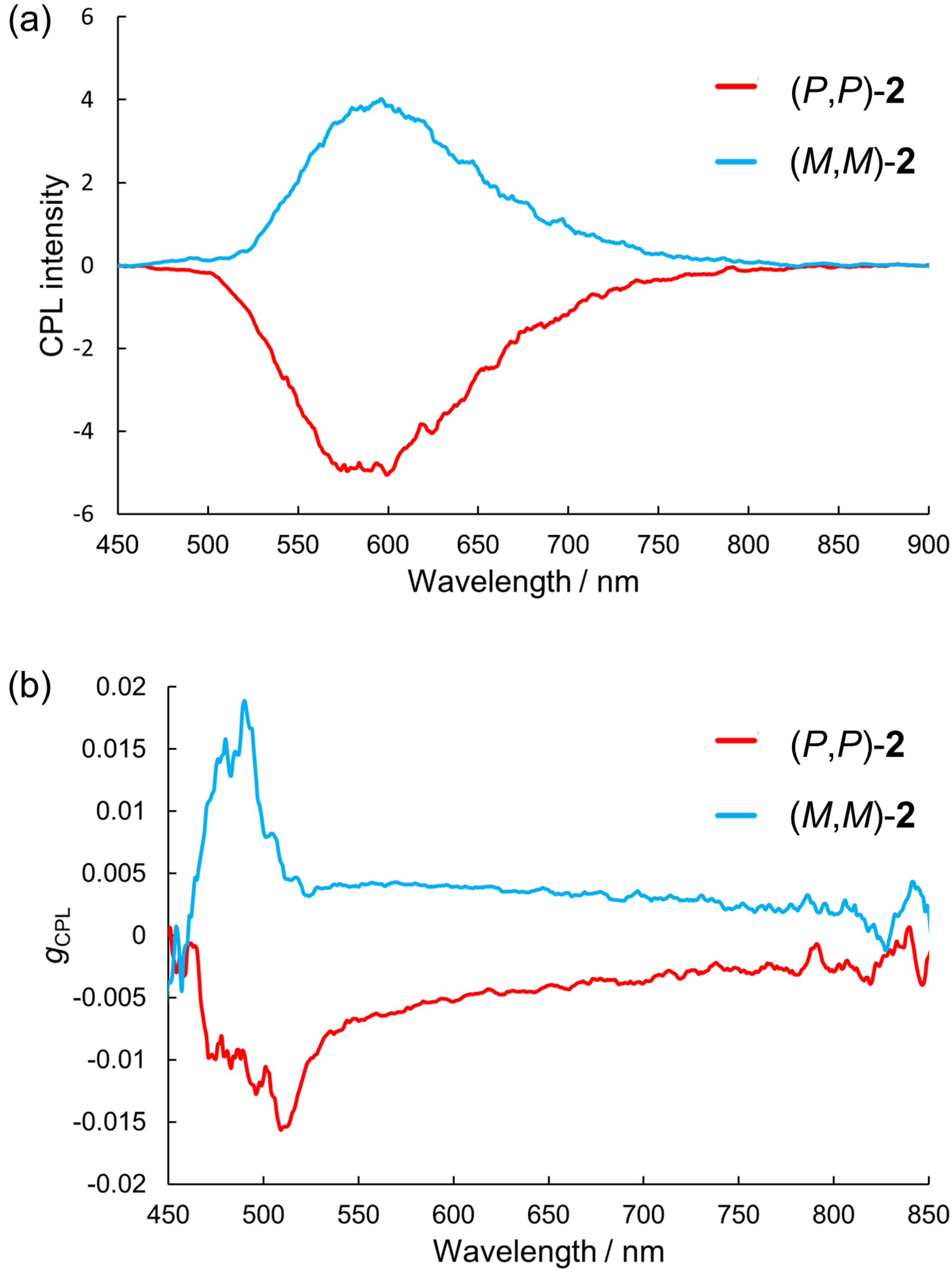


Fig. S29 (a) CPL spectra and (b) g_{CPL} of **2** in 2-MTHF at 83 K (λ_{ex} = 365 nm).

(M,M)-**1** (S_0@S_0), C_2 symmetry, B3LYP-GD3BJ/6-311G(2d,p)

O	-1.102286	3.456372	-0.813700
N	0.524313	1.274042	-0.623349
N	-0.524313	-1.274042	-0.623349
O	1.102286	-3.456372	-0.813700
C	0.000470	3.523311	0.019364
C	0.248851	4.687138	0.682114
C	1.390370	4.809117	1.511859
C	1.696970	6.003755	2.201077
C	2.804351	6.085040	3.007167
C	3.656231	4.971852	3.157957
C	3.386272	3.798736	2.500595
C	2.251875	3.681386	1.663920
C	1.951346	2.481354	0.977870
C	0.864228	2.400194	0.144985
C	-0.850824	1.074050	-0.841906
C	-1.390370	-0.189944	-0.909620
C	-2.735761	-0.359848	-1.351453
C	-3.297638	-1.618921	-1.670568
C	-4.604949	-1.725115	-2.071665
C	-5.418242	-0.579916	-2.172770
C	-4.894379	0.657743	-1.904175
C	-3.545358	0.810421	-1.508185
C	-2.991626	2.093906	-1.283147
C	-1.665620	2.213555	-0.988674
C	0.850824	-1.074050	-0.841906
C	1.390370	0.189944	-0.909620
C	2.735761	0.359848	-1.351453
C	3.297638	1.618921	-1.670568
C	4.604949	1.725115	-2.071665
C	5.418242	0.579916	-2.172770
C	4.894379	-0.657743	-1.904175
C	3.545358	-0.810421	-1.508185
C	2.991626	-2.093906	-1.283147
C	1.665620	-2.213555	-0.988674

C	-0.000470	-3.523311	0.019364
C	-0.248851	-4.687138	0.682114
C	-1.390370	-4.809117	1.511859
C	-1.696970	-6.003755	2.201077
C	-2.804351	-6.085040	3.007167
C	-3.656231	-4.971852	3.157957
C	-3.386272	-3.798736	2.500595
C	-2.251875	-3.681386	1.663920
C	-1.951346	-2.481354	0.977870
C	-0.864228	-2.400194	0.144985
H	-3.603549	2.981982	-1.370317
H	-5.505513	1.546946	-2.006161
H	-6.452239	-0.678267	-2.479375
H	-5.012188	-2.697789	-2.318038
H	-2.684426	-2.504796	-1.610120
H	2.607204	1.629342	1.090249
H	4.041636	2.942633	2.612147
H	4.528415	5.047197	3.795801
H	3.028009	7.006486	3.530563
H	1.040011	6.857898	2.082844
H	-0.433021	5.518738	0.556993
H	2.684426	2.504796	-1.610120
H	5.012188	2.697789	-2.318038
H	6.452239	0.678267	-2.479375
H	5.505513	-1.546946	-2.006161
H	3.603549	-2.981982	-1.370317
H	0.433021	-5.518738	0.556993
H	-1.040011	-6.857898	2.082844
H	-3.028009	-7.006486	3.530563
H	-4.528415	-5.047197	3.795801
H	-4.041636	-2.942633	2.612147
H	-2.607204	-1.629342	1.090249

(M,M)-**1** (S_1@S_1), C_2 symmetry, B3LYP-GD3BJ/6-311G(2d,p)

O	-1.210919	3.453815	-0.590159
N	0.507405	1.276924	-0.521808
N	-0.507405	-1.276924	-0.521808
O	1.210919	-3.453815	-0.590159
C	-0.015124	3.569422	0.067002
C	0.297894	4.767659	0.642539
C	1.514222	4.932024	1.344175
C	1.881472	6.157712	1.944310
C	3.058802	6.272466	2.638918
C	3.926129	5.166351	2.766963
C	3.599279	3.963913	2.197656
C	2.391756	3.811513	1.473673
C	2.040792	2.587916	0.870037
C	0.879008	2.467529	0.142629
C	-0.857335	1.078987	-0.690123
C	-1.378029	-0.234881	-0.823541
C	-2.735967	-0.416406	-1.252525
C	-3.257324	-1.646012	-1.698777
C	-4.584120	-1.768177	-2.072827
C	-5.432552	-0.659952	-2.023925
C	-4.936488	0.572314	-1.644787
C	-3.586172	0.737050	-1.277271
C	-3.058802	2.022477	-0.971810
C	-1.718876	2.178003	-0.729241
C	0.857335	-1.078987	-0.690123
C	1.378029	0.234881	-0.823541
C	2.735967	0.416406	-1.252525
C	3.257324	1.646012	-1.698777
C	4.584120	1.768177	-2.072827
C	5.432552	0.659952	-2.023925
C	4.936488	-0.572314	-1.644787
C	3.586172	-0.737050	-1.277271
C	3.058802	-2.022477	-0.971810
C	1.718876	-2.178003	-0.729241

C	0.015124	-3.569422	0.067002
C	-0.297894	-4.767659	0.642539
C	-1.514222	-4.932024	1.344175
C	-1.881472	-6.157712	1.944310
C	-3.058802	-6.272466	2.638918
C	-3.926129	-5.166351	2.766963
C	-3.599279	-3.963913	2.197656
C	-2.391756	-3.811513	1.473673
C	-2.040792	-2.587916	0.870037
C	-0.879008	-2.467529	0.142629
H	-3.693887	2.896994	-1.007075
H	-5.581781	1.442878	-1.640296
H	-6.474189	-0.761077	-2.303174
H	-4.959012	-2.727025	-2.407833
H	-2.612577	-2.510082	-1.757699
H	2.704504	1.741885	0.963983
H	4.263134	3.112094	2.286500
H	4.853111	5.273414	3.316368
H	3.328168	7.217877	3.093584
H	1.215710	7.007356	1.847605
H	-0.408732	5.583754	0.563526
H	2.612577	2.510082	-1.757699
H	4.959012	2.727025	-2.407833
H	6.474189	0.761077	-2.303174
H	5.581781	-1.442878	-1.640296
H	3.693887	-2.896994	-1.007075
H	0.408732	-5.583754	0.563526
H	-1.215710	-7.007356	1.847605
H	-3.328168	-7.217877	3.093584
H	-4.853111	-5.273414	3.316368
H	-4.263134	-3.112094	2.286500
H	-2.704504	-1.741885	0.963983

(M,M)-**1** (T_1@T_1), C_2 symmetry, B3LYP-GD3BJ/6-311G(2d,p)

O	-2.403794	2.760883	-0.062366
N	-0.000807	1.376733	-0.010173
N	0.000807	-1.376733	-0.010173
O	2.403794	-2.760883	-0.062366
C	-1.329432	3.29771	0.600493
C	-1.494945	4.526533	1.218411
C	-0.440372	5.086487	1.927355
H	-0.566927	6.049245	2.405536
C	0.762411	4.397865	2.043033
C	0.927759	3.168081	1.422728
C	-0.105393	2.625502	0.662579
C	-1.197023	0.687754	-0.166248
C	-1.197023	-0.734429	-0.295331
C	-2.390601	-1.403275	-0.726775
C	-2.416055	-2.736583	-1.176874
C	-3.602477	-3.341085	-1.559525
C	-4.79835	-2.626662	-1.517447
C	-4.793867	-1.295473	-1.131113
C	-3.607219	-0.648794	-0.752896
C	-3.593281	0.746586	-0.439792
C	-2.406251	1.385918	-0.20286
C	1.197023	-0.687754	-0.166248
C	1.197023	0.734429	-0.295331
C	2.390601	1.403275	-0.726775
C	2.416055	2.736583	-1.176874
C	3.602477	3.341085	-1.559525
C	4.79835	2.626662	-1.517447
C	4.793867	1.295473	-1.131113
C	3.607219	0.648794	-0.752896
C	3.593281	-0.746586	-0.439792
C	2.406251	-1.385918	-0.20286
C	1.329432	-3.29771	0.600493
C	1.494945	-4.526533	1.218411
C	0.440372	-5.086487	1.927355

H	0.566927	-6.049245	2.405536
C	-0.762411	-4.397865	2.043033
C	-0.927759	-3.168081	1.422728
C	0.105393	-2.625502	0.662579
H	-4.507368	1.323076	-0.475259
H	-5.715709	-0.725698	-1.132411
H	-5.727369	-3.102772	-1.805953
H	-3.593467	-4.370173	-1.896222
H	-1.495734	-3.2991	-1.231403
H	1.859555	2.630948	1.511476
H	-2.456775	5.015875	1.140913
H	1.495734	3.2991	-1.231403
H	3.593467	4.370173	-1.896222
H	5.727369	3.102772	-1.805953
H	5.715709	0.725698	-1.132411
H	4.507368	-1.323076	-0.475259
H	2.456775	-5.015875	1.140913
H	-1.859555	-2.630948	1.511476
H	1.577821	4.815268	2.619026
H	-1.577821	-4.815268	2.619026

(M,M)-**1** (T_2@T_2), C_2 symmetry, B3LYP-GD3BJ/6-311G(2d,p)

O	-2.369048	2.761261	-0.157173
N	-0.000611	1.368968	0.07683
N	0.000611	-1.368968	0.07683
O	2.369048	-2.761261	-0.157173
C	-1.347649	3.276851	0.617984
C	-1.552425	4.4935	1.240358
C	-0.536408	5.051929	2.011779
H	-0.690803	6.010552	2.489631
C	0.663786	4.370126	2.175319
C	0.865778	3.141761	1.560199
C	-0.131037	2.594473	0.753412
C	-1.197737	0.674927	-0.177718
C	-1.203421	-0.737687	-0.261671
C	-2.369048	-1.414447	-0.727097
C	-2.395602	-2.780575	-1.078903
C	-3.572707	-3.387312	-1.508193
C	-4.751085	-2.65572	-1.598886
C	-4.749286	-1.297763	-1.291051
C	-3.575459	-0.646444	-0.871661
C	-3.56404	0.750367	-0.617221
C	-2.375134	1.390616	-0.315713
C	1.197737	-0.674927	-0.177718
C	1.203421	0.737687	-0.261671
C	2.369048	1.414447	-0.727097
C	2.395602	2.780575	-1.078903
C	3.572707	3.387312	-1.508193
C	4.751085	2.65572	-1.598886
C	4.749286	1.297763	-1.291051
C	3.575459	0.646444	-0.871661
C	3.56404	-0.750367	-0.617221
C	2.375134	-1.390616	-0.315713
C	1.347649	-3.276851	0.617984
C	1.552425	-4.4935	1.240358
C	0.536408	-5.051929	2.011779

H	0.690803	-6.010552	2.489631
C	-0.663786	-4.370126	2.175319
C	-0.865778	-3.141761	1.560199
C	0.131037	-2.594473	0.753412
H	-4.471321	1.332604	-0.705433
H	-5.657673	-0.715528	-1.389408
H	-5.66703	-3.135009	-1.921227
H	-3.562982	-4.437971	-1.77014
H	-1.489462	-3.364142	-1.027974
H	1.79714	2.608886	1.685186
H	-2.504981	4.988951	1.105936
H	1.489462	3.364142	-1.027974
H	3.562982	4.437971	-1.77014
H	5.66703	3.135009	-1.921227
H	5.657673	0.715528	-1.389408
H	4.471321	-1.332604	-0.705433
H	2.504981	-4.988951	1.105936
H	-1.79714	-2.608886	1.685186
H	1.450558	4.791977	2.787378
H	-1.450558	-4.791977	2.787378

(M,M)-**2** (S_0@S_0), C_2 symmetry, B3LYP-GD3BJ/6-311G(2d,p)

S	-2.315282	3.182931	-0.492904
N	-0.000350	1.374454	-0.104862
N	0.000350	-1.374454	-0.104862
S	2.315282	-3.182931	-0.492904
C	-1.103010	3.324180	0.804122
C	-1.181882	4.357237	1.730315
C	-0.184399	4.516460	2.683976
H	-0.240801	5.333442	3.391766
C	0.873389	3.615404	2.731288
C	0.939171	2.560056	1.832352
C	-0.038733	2.415679	0.850149
C	-1.203896	0.682551	-0.374376
C	-1.203896	-0.692739	-0.415980
C	-2.366118	-1.397310	-0.842654
C	-2.382778	-2.794205	-1.065634
C	-3.536980	-3.427672	-1.448447
C	-4.731797	-2.700212	-1.622313
C	-4.741539	-1.343142	-1.435168
C	-3.566317	-0.652212	-1.055802
C	-3.558173	0.753096	-0.893357
C	-2.393234	1.410050	-0.599177
C	1.203896	-0.682551	-0.374376
C	1.203896	0.692739	-0.415980
C	2.366118	1.397310	-0.842654
C	2.382778	2.794205	-1.065634
C	3.536980	3.427672	-1.448447
C	4.731797	2.700212	-1.622313
C	4.741539	1.343142	-1.435168
C	3.566317	0.652212	-1.055802
C	3.558173	-0.753096	-0.893357
C	2.393234	-1.410050	-0.599177
C	1.103010	-3.324180	0.804122
C	1.181882	-4.357237	1.730315
C	0.184399	-4.516460	2.683976
H	-1.647860	-3.724223	3.480082

C	-0.873389	-3.615404	2.731288
C	-0.939171	-2.560056	1.832352
C	0.038733	-2.415679	0.850149
H	-4.478121	1.308927	-1.024689
H	-5.650983	-0.773079	-1.585627
H	-5.637905	-3.215784	-1.915664
H	-3.529517	-4.496372	-1.623641
H	-1.470857	-3.360373	-0.945443
H	1.755451	1.852103	1.875035
H	-2.021941	5.039433	1.692919
H	1.470857	3.360373	-0.945443
H	3.529517	4.496372	-1.623641
H	5.637905	3.215784	-1.915664
H	5.650983	0.773079	-1.585627
H	4.478121	-1.308927	-1.024689
H	2.021941	-5.039433	1.692919
H	-1.755451	-1.852103	1.875035
H	0.240801	-5.333442	3.391766
H	1.647860	3.724223	3.480082

(*M*,*M*)-**2** (S_1@S_1), C_2 symmetry, B3LYP-GD3BJ/6-311G(2d,p)

S	-2.405767	3.176678	-0.390639
N	0.000456	1.365079	-0.041348
N	-0.000456	-1.365079	-0.041348
S	2.405767	-3.176678	-0.390639
C	-1.046009	3.452979	0.700636
C	-1.007798	4.607857	1.478002
C	0.062901	4.847220	2.325360
H	0.086089	5.750703	2.921076
C	1.088933	3.910977	2.426797
C	1.058136	2.758657	1.662194
C	0.004660	2.530957	0.773231
C	-1.203318	0.705424	-0.267411
C	-1.186834	-0.706262	-0.374823
C	-2.365986	-1.413309	-0.786340
C	-2.372279	-2.775348	-1.137506
C	-3.546614	-3.413056	-1.501462
C	-4.751019	-2.706904	-1.529217
C	-4.768875	-1.358639	-1.228076
C	-3.588514	-0.675182	-0.870727
C	-3.588514	0.723195	-0.622655
C	-2.413352	1.403013	-0.377157
C	1.203318	-0.705424	-0.267411
C	1.186834	0.706262	-0.374823
C	2.365986	1.413309	-0.786340
C	2.372279	2.775348	-1.137506
C	3.546614	3.413056	-1.501462
C	4.751019	2.706904	-1.529217
C	4.768875	1.358639	-1.228076
C	3.588514	0.675182	-0.870727
C	3.588514	-0.723195	-0.622655
C	2.413352	-1.403013	-0.377157
C	1.046009	-3.452979	0.700636
C	1.007798	-4.607857	1.478002
C	-0.062901	-4.847220	2.325360
H	-1.913973	-4.076129	3.107428

C	-1.088933	-3.910977	2.426797
C	-1.058136	-2.758657	1.662194
C	-0.004660	-2.530957	0.773231
H	-4.519592	1.270142	-0.695847
H	-5.696008	-0.799581	-1.274725
H	-5.669560	-3.212257	-1.801665
H	-3.525269	-4.462626	-1.766308
H	-1.447640	-3.333899	-1.132531
H	1.851038	2.029093	1.736699
H	-1.831406	5.308178	1.420453
H	1.447640	3.333899	-1.132531
H	3.525269	4.462626	-1.766308
H	5.669560	3.212257	-1.801665
H	5.696008	0.799581	-1.274725
H	4.519592	-1.270142	-0.695847
H	1.831406	-5.308178	1.420453
H	-1.851038	-2.029093	1.736699
H	-0.086089	-5.750703	2.921076
H	1.913973	4.076129	3.107428

(M,M)-**2** (T_1@T_1), C_2 symmetry, B3LYP-GD3BJ/6-311G(2d,p)

S	-2.389685	3.173722	-0.471310
N	-0.001439	1.370126	-0.090439
N	0.001439	-1.370126	-0.090439
S	2.389685	-3.173722	-0.471310
C	-1.070111	3.435769	0.682264
C	-1.076129	4.556600	1.507014
C	-0.037328	4.773987	2.400634
H	-0.043262	5.655054	3.029506
C	0.991111	3.843254	2.502752
C	0.994292	2.716041	1.696885
C	-0.018385	2.519926	0.758701
C	-1.206460	0.703732	-0.314870
C	-1.192868	-0.719406	-0.394490
C	-2.378372	-1.429978	-0.778582
C	-2.389685	-2.798761	-1.100159
C	-3.570690	-3.443342	-1.438806
C	-4.770771	-2.737182	-1.475561
C	-4.780361	-1.376598	-1.205802
C	-3.599965	-0.693278	-0.871701
C	-3.592949	0.717600	-0.660588
C	-2.410942	1.396593	-0.439048
C	1.206460	-0.703732	-0.314870
C	1.192868	0.719406	-0.394490
C	2.378372	1.429978	-0.778582
C	2.389685	2.798761	-1.100159
C	3.570690	3.443342	-1.438806
C	4.770771	2.737182	-1.475561
C	4.780361	1.376598	-1.205802
C	3.599965	0.693278	-0.871701
C	3.592949	-0.717600	-0.660588
C	2.410942	-1.396593	-0.439048
C	1.070111	-3.435769	0.682264
C	1.076129	-4.556600	1.507014
C	0.037328	-4.773987	2.400634
H	-1.791625	-3.988839	3.216523

C	-0.991111	-3.843254	2.502752
C	-0.994292	-2.716041	1.696885
C	0.018385	-2.519926	0.758701
H	-4.521329	1.267163	-0.744979
H	-5.705955	-0.815912	-1.263048
H	-5.693063	-3.244439	-1.730549
H	-3.552749	-4.499387	-1.677225
H	-1.465435	-3.357796	-1.091463
H	1.789053	1.988542	1.776428
H	-1.905270	5.250154	1.446975
H	1.465435	3.357796	-1.091463
H	3.552749	4.499387	-1.677225
H	5.693063	3.244439	-1.730549
H	5.705955	0.815912	-1.263048
H	4.521329	-1.267163	-0.744979
H	1.905270	-5.250154	1.446975
H	-1.789053	-1.988542	1.776428
H	0.043262	-5.655054	3.029506
H	1.791625	3.988839	3.216523

(*M*,*M*)-**2** (T_2@T_2), C_2 symmetry, B3LYP-GD3BJ/6-311G(2d,p)

S	-2.333331	3.176876	-0.49735
N	0.001604	1.3669	-0.060102
N	-0.001604	-1.3669	-0.060102
S	2.333331	-3.176876	-0.49735
C	-1.101188	3.361966	0.774809
C	-1.164675	4.429803	1.662025
C	-0.156723	4.620562	2.599007
H	-0.201934	5.465312	3.274265
C	0.897144	3.716095	2.672738
C	0.949219	2.628921	1.813231
C	-0.038759	2.454175	0.845405
C	-1.202434	0.695494	-0.360618
C	-1.199647	-0.716167	-0.39869
C	-2.36307	-1.429562	-0.820226
C	-2.375999	-2.815522	-1.059062
C	-3.549265	-3.464463	-1.444295
C	-4.730453	-2.749149	-1.59842
C	-4.74183	-1.372368	-1.39177
C	-3.571988	-0.683447	-1.015127
C	-3.563978	0.722281	-0.846665
C	-2.375999	1.403225	-0.569173
C	1.202434	-0.695494	-0.360618
C	1.199647	0.716167	-0.39869
C	2.36307	1.429562	-0.820226
C	2.375999	2.815522	-1.059062
C	3.549265	3.464463	-1.444295
C	4.730453	2.749149	-1.59842
C	4.74183	1.372368	-1.39177
C	3.571988	0.683447	-1.015127
C	3.563978	-0.722281	-0.846665
C	2.375999	-1.403225	-0.569173
C	1.101188	-3.361966	0.774809
C	1.164675	-4.429803	1.662025
C	0.156723	-4.620562	2.599007
H	-1.678447	-3.848727	3.410324

C	-0.897144	-3.716095	2.672738
C	-0.949219	-2.628921	1.813231
C	0.038759	-2.454175	0.845405
H	-4.484298	1.278036	-0.971386
H	-5.654978	-0.806679	-1.533247
H	-5.641315	-3.258205	-1.888186
H	-3.532724	-4.532664	-1.620237
H	-1.463831	-3.384028	-0.95418
H	1.760607	1.916826	1.874196
H	-2.002138	5.113956	1.60775
H	1.463831	3.384028	-0.95418
H	3.532724	4.532664	-1.620237
H	5.641315	3.258205	-1.888186
H	5.654978	0.806679	-1.533247
H	4.484298	-1.278036	-0.971386
H	2.002138	-5.113956	1.60775
H	-1.760607	-1.916826	1.874196
H	0.201934	-5.465312	3.274265
H	1.678447	3.848727	3.410324