Electronic Supplementary Information

Multiply aryl-substituted dipyrrolyldiketone boron complexes exhibiting anion-responsive emissive properties

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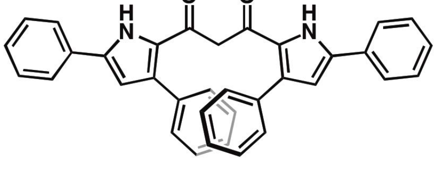
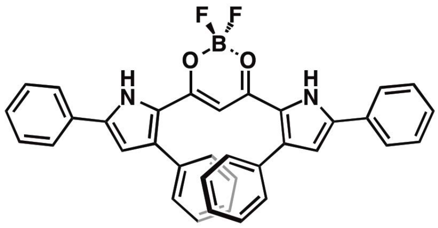
1. Synthetic procedures and spectroscopic data

General Procedures. Starting materials were purchased from FUJIFILM Wako Pure Chemical Corp, Nacalai Tesque Inc., and Sigma-Aldrich Co. and used without further purification unless otherwise stated. NMR spectra used in the characterization of products were recorded on a JEOL ECA-600 600 MHz spectrometer. All NMR spectra were referenced to solvent. UV-visible absorption spectra were recorded on a Hitachi U-3500 spectrometer. Fluorescence spectra and quantum yields were recorded on a Hitachi F-4500 fluorescence spectrometer and a Hamamatsu Quantum Yields Measurements System for Organic LED Materials C9920-02, respectively. High-resolution (HR) electrospray ionization mass spectrometries (ESI-MS) were recorded on a BRUKER microTOF using ESI-TOF method. TLC analyses were carried out on aluminum sheets coated with silica gel 60 (Merck 5554). Column chromatography was performed on Wakogel C-300.

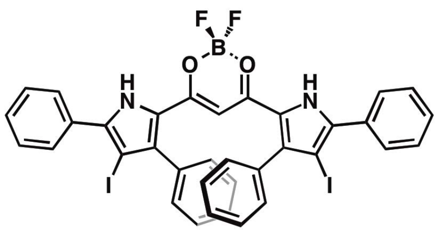
1,3-Bis(3,5-diphenylpyrrol-2-yl)-1,3-propanedione, 2a′. According to the literature procedure,[S1] to a solution of 2,4-diphenylpyrrole[S2] (878.0 mg, 4.00 mmol) in CH_2Cl_2 (100 mL) under N_2 was added malonyl chloride (193.0 µL, 2.00 mmol) at r.t. The mixture was stirred at r.t. for 1 h and added to saturated Na_2CO_3 aq. The suspension was extracted with CH_2Cl_2 and washed with water. Organic phase was dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (eluent: CH_2Cl_2) to give **2a′** (632.3 mg, 1.24 mmol, 64%) as a yellow solid. R_f = 0.25 (EtOAc:CH_2Cl_2 = 1:5). ^{1}H NMR (600 MHz, DMSO-d_6, 20 °C: diketone **2a′** was obtained as a mixture of keto and enol tautomers in the ratio of 0.87:1): keto form δ (ppm) 11.90 (s, 2H, NH), 7.91 (d, J = 7.8 Hz, 4H, Ph-H), 7.43–7.24 (m, 16H, Ph-H), 6.66 (d, J = 2.4 Hz, 2H, pyrrole-H), 3.60 (s, 2H, CH_2); enol form δ (ppm) 11.78 (s, 2H, NH), 7.87 (d, J = 7.8 Hz, 4H, Ph-H), 7.43–7.24 (m, 16H, Ph-H), 6.71 (d, J = 2.4 Hz, 2H, pyrrole-H), 6.08 (s, 1H, CH). ^{13}C NMR (151 MHz, DMSO-d_6, 20 °C): δ (ppm) 185.46, 176.96, 137.58, 137.01, 136.62, 136.05, 134.44, 132.29, 131.83, 131.61, 130.15, 129.97, 129.67, 129.62, 129.04, 128.87, 128.76, 128.42, 128.21, 127.74, 126.58, 126.16, 126.02, 111.78, 111.74, 96.51, 51.98. ESI-TOF-MS (HR): 505.1915. Calcd for $C_{35}H_{25}N_2O_2$ ([M – H]$^-$): 505.1922.



BF$_2$ complex of 1,3-bis(3,5-diphenylpyrrol-2-yl)-1,3-propanedione, 2a. According to the literature procedure,[S2] to a solution of **2a′** (507.3 mg, 1.00 mmol) in CH_2Cl_2 (800 mL) under N_2 was added $BF_3\cdot OEt_2$ (378 µL, 3.0 mmol) at r.t. The mixture was stirred for 30 min and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2) to give **2a** (487.5 mg, 0.86 mmol, 86%) as a red solid. R_f = 0.11 (CH_2Cl_2). ^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C): δ (ppm) 9.63 (s, 2H, NH), 7.66 (d, J = 7.8 Hz, 4H, Ph-H), 7.48 (t, J = 6.6 Hz, 4H, Ph-H), 7.41 (t, J = 7.2 Hz, 2H, Ph-H), 7.27 (d, J = 7.2 Hz, 4H, Ph-H), 7.18 (d, J = 6.6 Hz, 6H, Ph-H), 6.63 (d, J = 2.4 Hz, 2H, pyrrole-H), 6.40 (s, 1H, CH). ^{13}C NMR (151 MHz, CD_2Cl_2, 20 °C): δ (ppm) 168.31, 139.68, 137.87, 134.23, 130.25, 129.62, 129.45, 129.06, 128.98, 128.85, 125.66, 123.51, 113.41, 93.23. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 525 (0.90). ESI-TOF-MS (HR): 553.1905. Calcd for $C_{35}H_{24}BF_2N_2O_2$ ([M – H]$^-$): 553.1904. This compound was further characterized by single-crystal X-ray diffraction analysis.

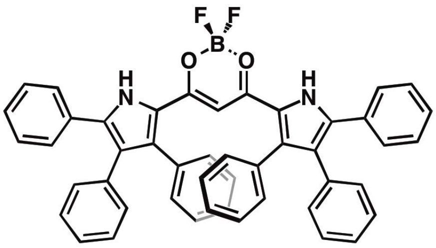


BF$_2$ complex of 1,3-bis(4-iodo-3,5-diphenylpyrrol-2-yl)-1,3-propanedione, 2b. According to the literature procedure,[S3] to a solution of **2a** (40.2 mg, 0.073 mmol) in pyridine (5 mL) under N_2 was added *N*-iodosuccinimide (42.4 mg, 0.19 mmol) at r.t. The mixture was stirred for 12 h and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2) to give **2b** (53.2 mg, 0.066 mmol, 90%) as an orange solid. R_f = 0.20 (CH_2Cl_2). ^{1}H NMR (600 MHz, DMSO-d_6, 20 °C): δ (ppm) 12.83 (s, 2H, NH), 7.69 (d, J = 7.2 Hz, 4H, Ph-H), 7.53 (t, J = 7.2 Hz, 4H, Ph-H), 7.48 (t, J = 7.2 Hz, 2H, Ph-H), 7.43–7.40 (m, 6H, Ph-H), 7.50 (d, J = 6.0 Hz, 4H, Ph-H), 5.70 (s, 1H, CH). ^{13}C NMR (151 MHz, DMSO-d_6, 20 °C): δ (ppm) 168.64, 141.62, 138.46, 134.20, 130.58, 129.87, 129.45, 129.16, 128.64, 128.24, 127.88, 124.40, 94.98, 74.58. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 504 (0.92). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 548 (504). ESI-TOF-MS (HR): 804.9836. Calcd for $C_{35}H_{22}BF_2I_2N_2O_2$ ([M – H]$^-$): 804.9837. This compound was further characterized by single-crystal X-ray diffraction analysis.

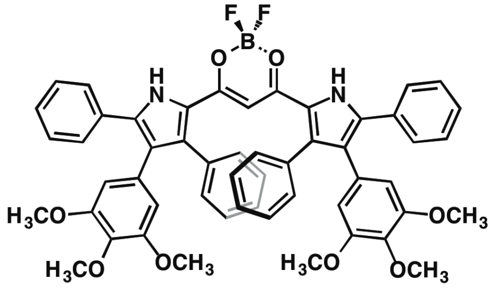


General produce of BF_2 complexes of 1,3-bis(4-aryl-3,5-diphenylpyrrol-2-yl)-1,3-propanedione, 3a–c. According to the literature procedure,[S4] a round-bottomed flask placed with **2b** (80.0 mg, 0.099 mmol), 2-aryl-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (0.300 mmol), $Pd(OAc)_2$ (3.37 mg, 15.0 μmol), 2-dicyclohexylphosphino-2′,6′-dimethoxybiphenyl (Sphos) (24.6 mg, 180 μmol), K_2CO_3 (82.9 mg, 0.60 mmol), and tetrabutylammonium chloride (TBACl) was flushed with N_2 and charged with a mixture of degassed THF (1.6 mL) and water (0.2 mL). The mixture was heated at 80 °C for 12 h, cooled, then partitioned between water and CH_2Cl_2. The combined organic extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column to give **3a**–**c**.

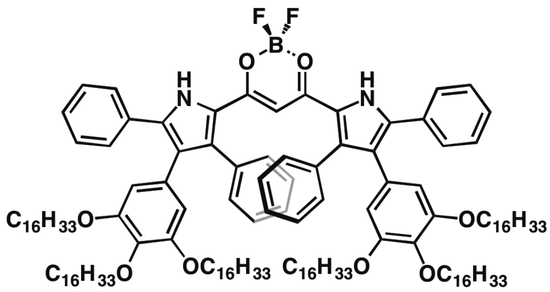
BF_2 complex of 1,3-bis(3,4,5-triphenylpyrrol-2-yl)-1,3-propanedione, 3a. From **2b** (40.2 mg, 49.9 μmol) and 4,4,5,5-tetramethyl-2-phenyl-1,3,2-dioxaborolane (30.6 mg, 150.0 μmol). Yield: 23.6 mg (33.4 μmol, 67%), orange solid. R_f = 0.17 (CH_2Cl_2). ^1H NMR (600 MHz, CD_2Cl_2, 20 °C): δ (ppm) 9.42 (s, 2H, NH), 7.34–7.27 (m, 10H, Ph-H), 7.18–7.09 (m, 12H, Ph-H), 6.97–6.92 (m, 8H, Ph-H), 5.75 (s, 1H, CH). ^{13}C NMR (151 MHz, CD_2Cl_2, 20 °C): δ (ppm) 168.92, 137.53, 135.54, 133.89, 133.29 131.20, 130.91, 130.52, 129.13, 129.10, 128.68, 128.37, 128.22, 128.08, 127.46, 127.23, 123.41, 93.86. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 512 (0.94). ESI-TOF-MS (HR): 705.2531. Calcd for $C_{47}H_{32}BF_2N_2O_2$ ([M – H]$^-$): 705.2531. This compound was further characterized by single-crystal X-ray diffraction analysis.



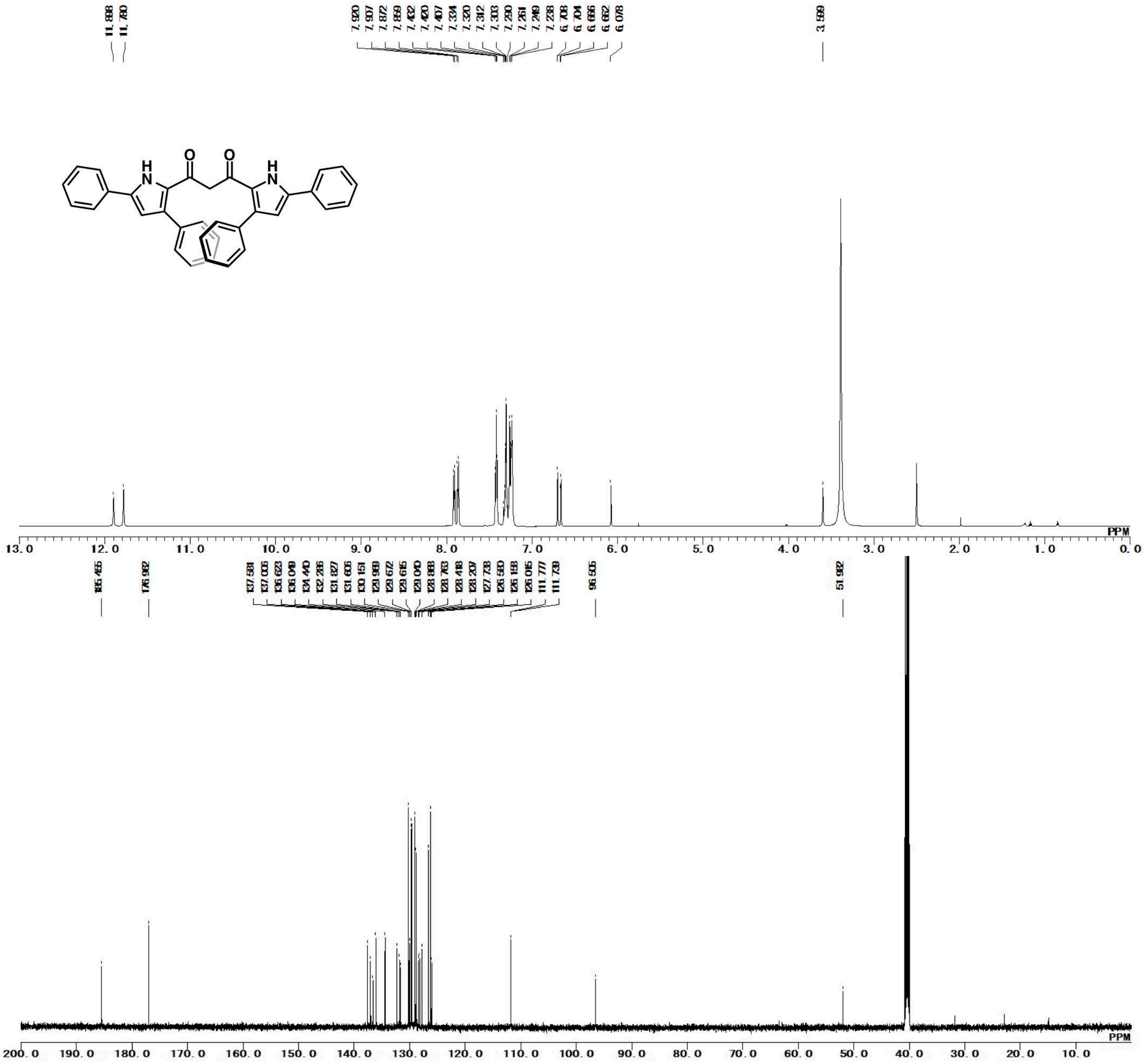
BF_2 complex of 1,3-bis(4-(3,4,5-trimethoxyphenyl)-3,5-diphenylpyrrol-2-yl)-1,3-propanedione, 3b. From **2b** (80.6 mg, 0.10 mmol) and 2-(3,4,5-trimethoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (91.2 mg, 0.31 μmol). Yield: 55.8 mg (0.063 mmol, 63%), orange solid. R_f = 0.10 (EtOAc:*n*-hexane = 1:5). ^1H NMR (600 MHz, DMSO-d_6, 20 °C): δ (ppm) 9.41 (s, 2H, NH), 7.38–7.34 (m, 10H, Ph-H), 7.20–7.13 (m, 6H, Ph-H), 6.99 (d, J = 6.6 Hz, 4H, Ph-H), 6.05 (s, 4H, Ar-H), 5.79 (s, 1H, CH), 3.70 (s, 6H, OCH_3), 3.40 (s, 12H, OCH_3). ^{13}C NMR (151 MHz, DMSO-d_6, 20 °C): δ (ppm) 168.84, 153.19, 137.49, 137.32, 135.24, 133.46, 130.90, 130.50, 129.23, 129.10, 128.87, 128.74, 128.40, 128.17, 127.15, 123.32, 108.41, 93.91, 60.81, 56.07. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 516 (1.02). ESI-TOF-MS (HR): 885.3164. Calcd for $C_{53}H_{44}BF_2N_2O_8$ ([M – H]$^-$): 885.3164.



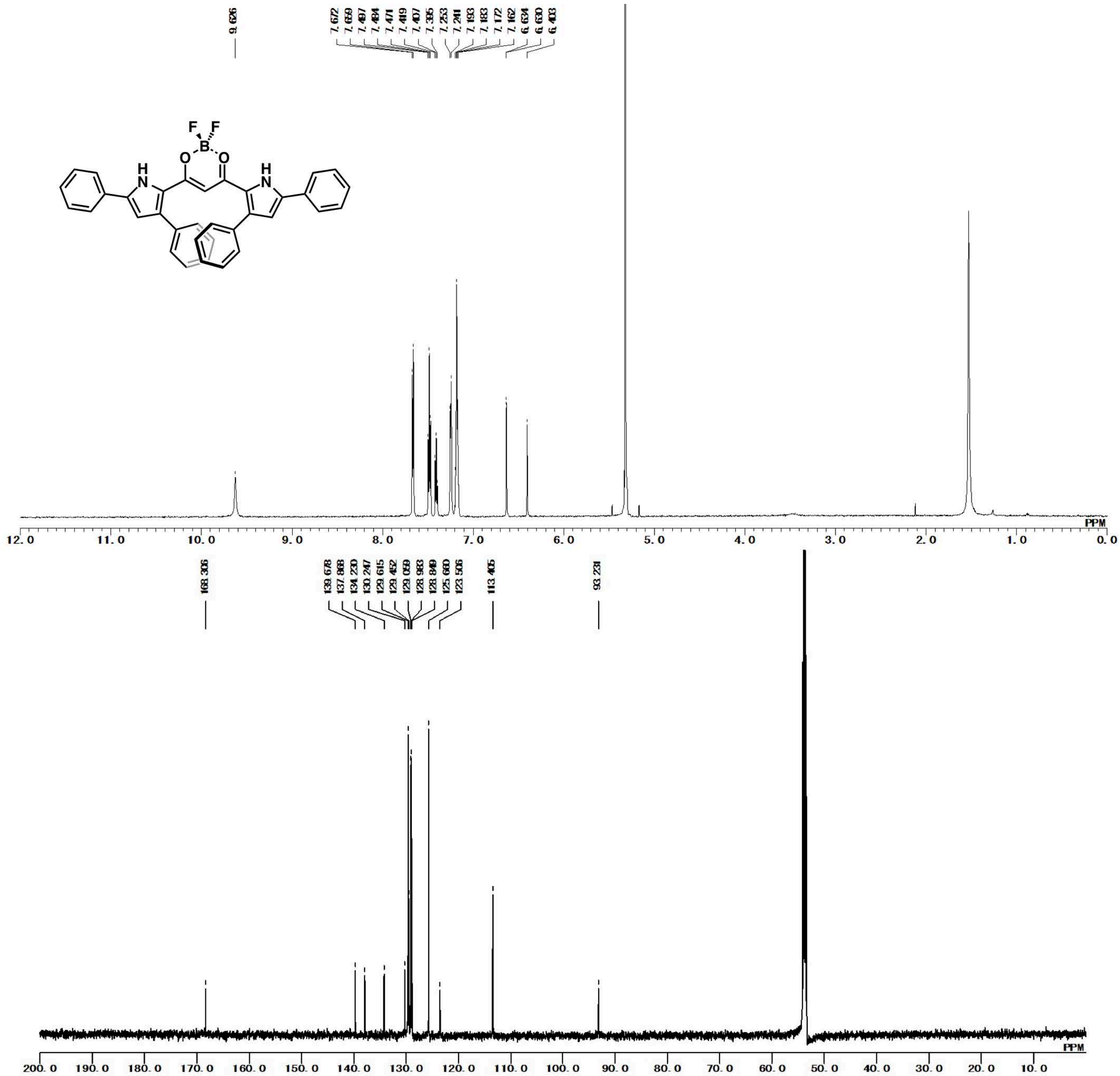
BF_2 complex of 1,3-bis(4-(3,4,5-trihexadecyloxyphenyl)-3,5-diphenylpyrrol-2-yl)-1,3-propanedione, 3c. From **2b** (81.4 mg, 0.10 mmol) and 2-(3,4,5-trihexadecyloxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (277.6 mg, 0.30 mmol). Yield: 133.2 mg (0.62 mmol, 62%), orange solid. R_f = 0.67 (CH_2Cl_2). ^1H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.41 (s, 2H, NH), 7.36–7.31 (m, 10H, Ph-H), 7.17–7.12 (m, 6H, Ph-H), 6.98 (d, J = 7.2 Hz, 4H, Ph-H), 6.02 (s, 4H, Ar-H), 5.79 (s, 1H, CH), 3.84 (t, J = 6.6 Hz, 4H, OCH_2), 3.50 (t, J = 6.6 Hz, 8H, OCH_2), 1.67–1.27 (m, 168H, $OCH_2(CH_2)_{14}$), 0.89–0.87 (m, 18H, $O(CH_2)_{15}CH_3$). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) δ (ppm) 168.79, 152.97, 137.43, 137.35, 135.27, 133.55, 130.97, 130.52, 129.17, 129.08, 128.80, 128.35, 128.27, 128.12, 127.46, 123.31, 109.59, 93.86, 73.55, 69.08, 32.35, 30.69, 30.15, 30.09, 30.02, 29.80, 29.75, 29.53, 26.51, 26.41, 23.12, 14.30 (some of the hexadecyl signals were overlapped with other signals). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 518 (0.99). ESI-TOF-MS (upon the addition of TBAF): *m/z* (% intensity): 2146.7240. Calcd for $C_{143}H_{224}BF_2N_2O_8$ ([M – H]$^-$): 2146.7249.



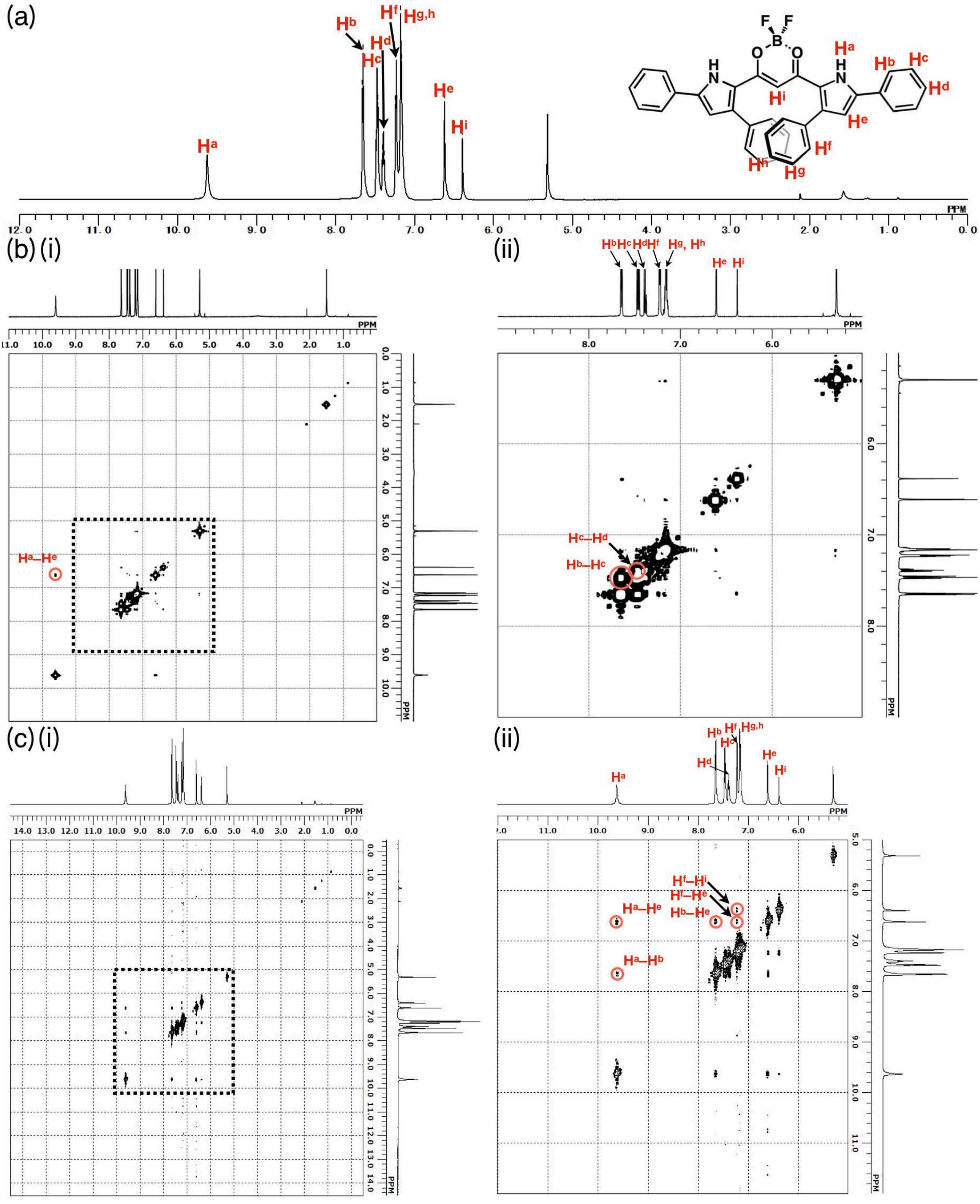
[S1] H. Maeda, Y. Haketa and T. Nakanishi, *J. Am. Chem. Soc.*, 2007, **129**, 13661–13674.
[S2] D. Imbri, N. Netz, M. Kucukdisli, L. M. Kammer, P. Jung, A. Kretzschmann and T. Opatz, *J. Org. Chem.*, 2014, **79**, 11750–11758.
[S3] N. Netz, C. Díez-Poza, A. Barbero and T. Opatz, *Eur. J. Org. Chem.*, 2017, 4580–4599.
[S4] S. Sugiura, W. Matsuda, W. Zhang, S. Seki, N. Yasuda and H. Maeda, *J. Org. Chem.*, 2019, **84**, in press (DOI: 10.1021/acs.joc.9b00754).



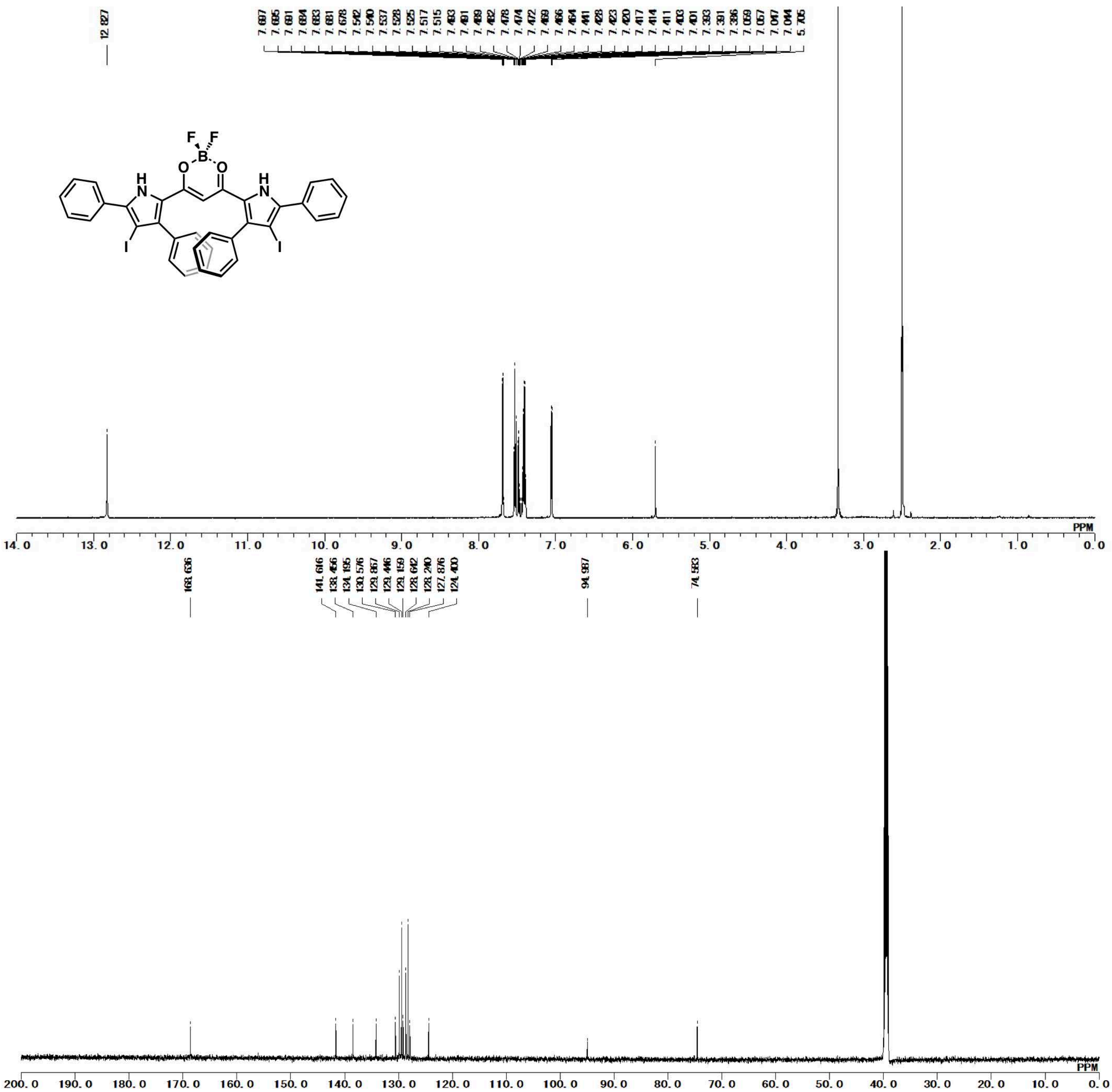
Supporting Figure 1 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **2a´** in DMSO-d_6.



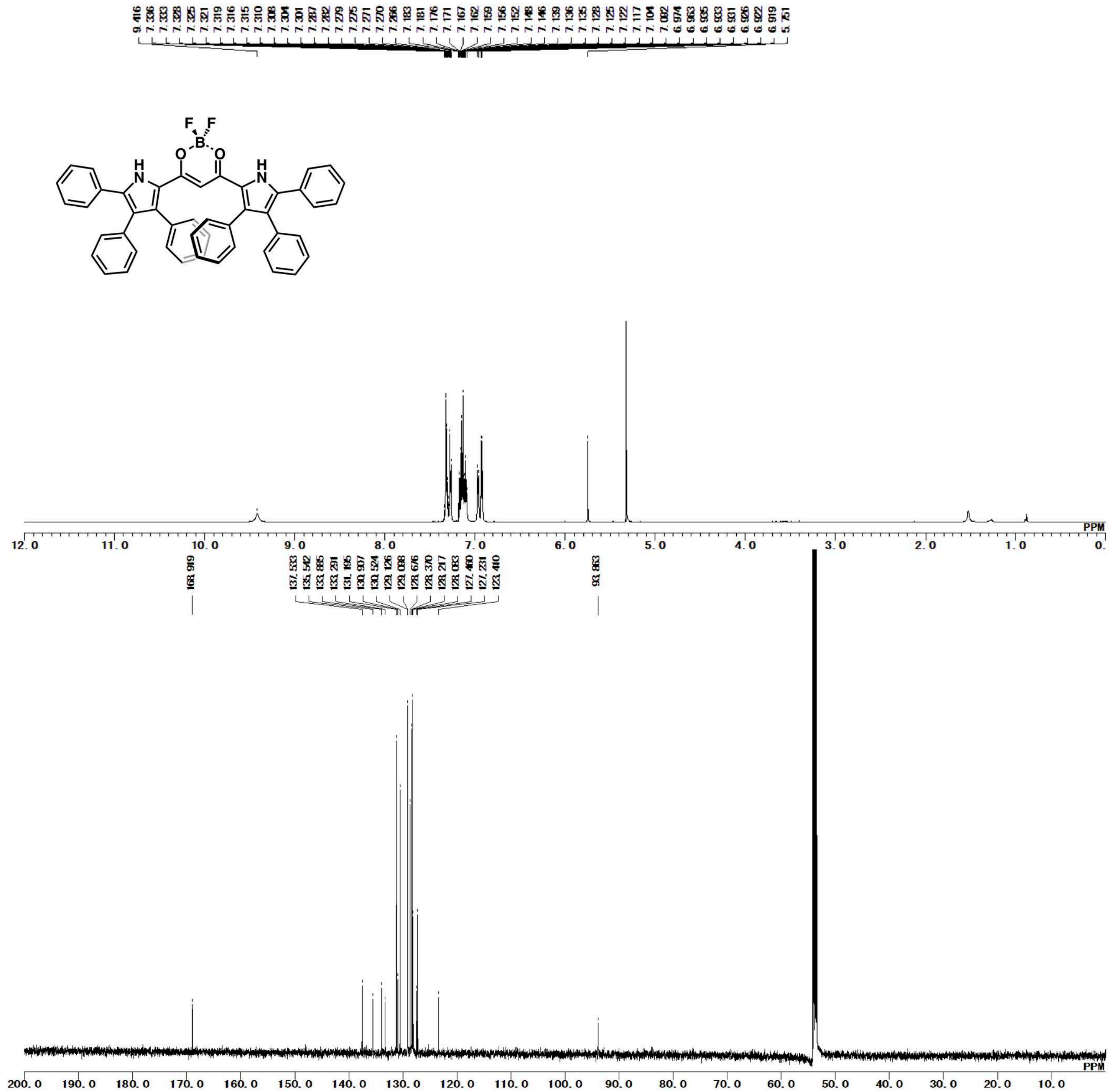
Supporting Figure 2 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **2a** in CD_2Cl_2.



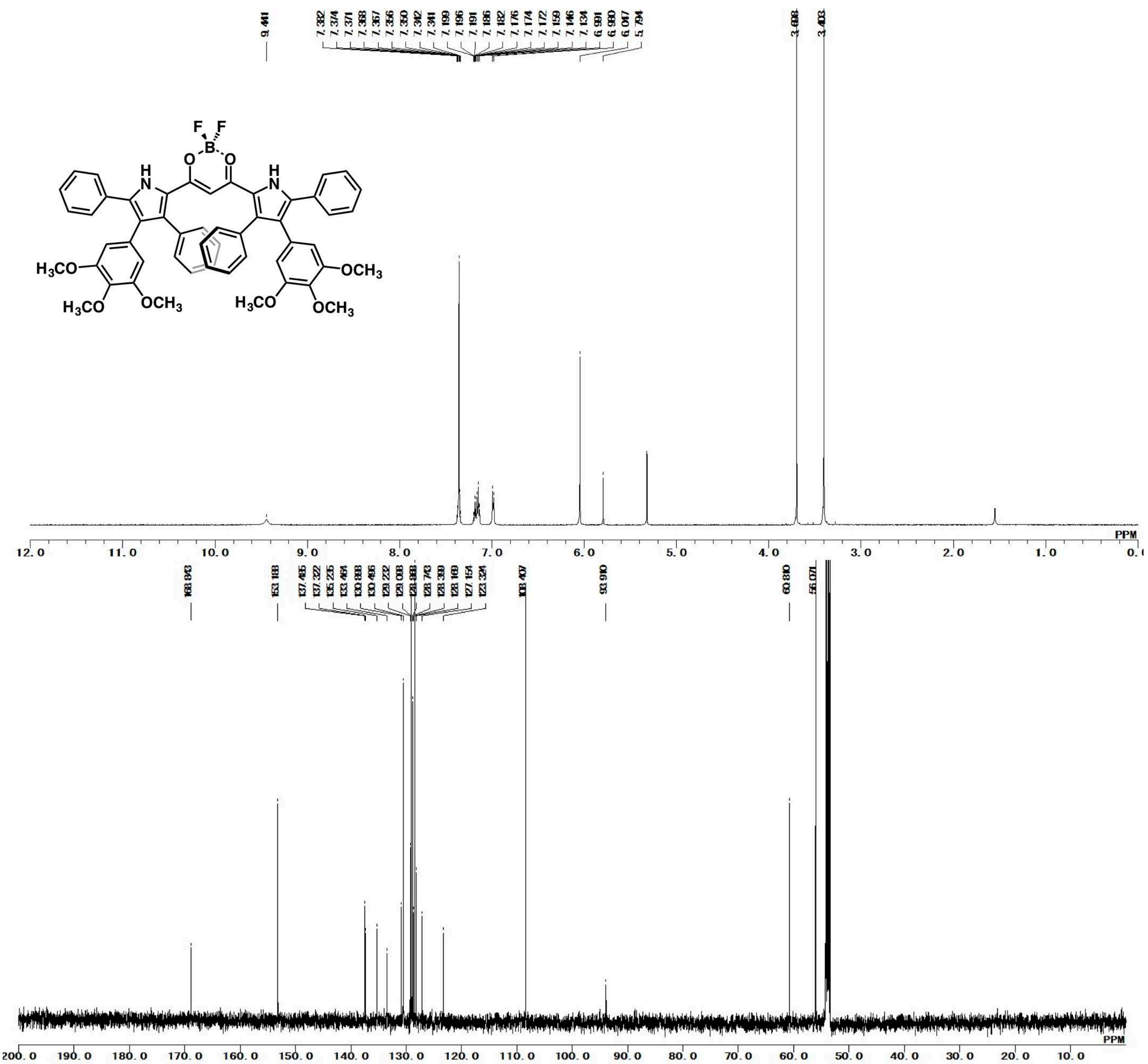
Supporting Figure 3 (a) 1D ^{1}H NMR (as the selected part in Supporting Figure 2), (b) COSY ((i) overview chart and (ii) enlarged version), and (c) NOESY ((i) overview chart and (ii) enlarged version) of **2a** in CD_2Cl_2 at 20 °C.



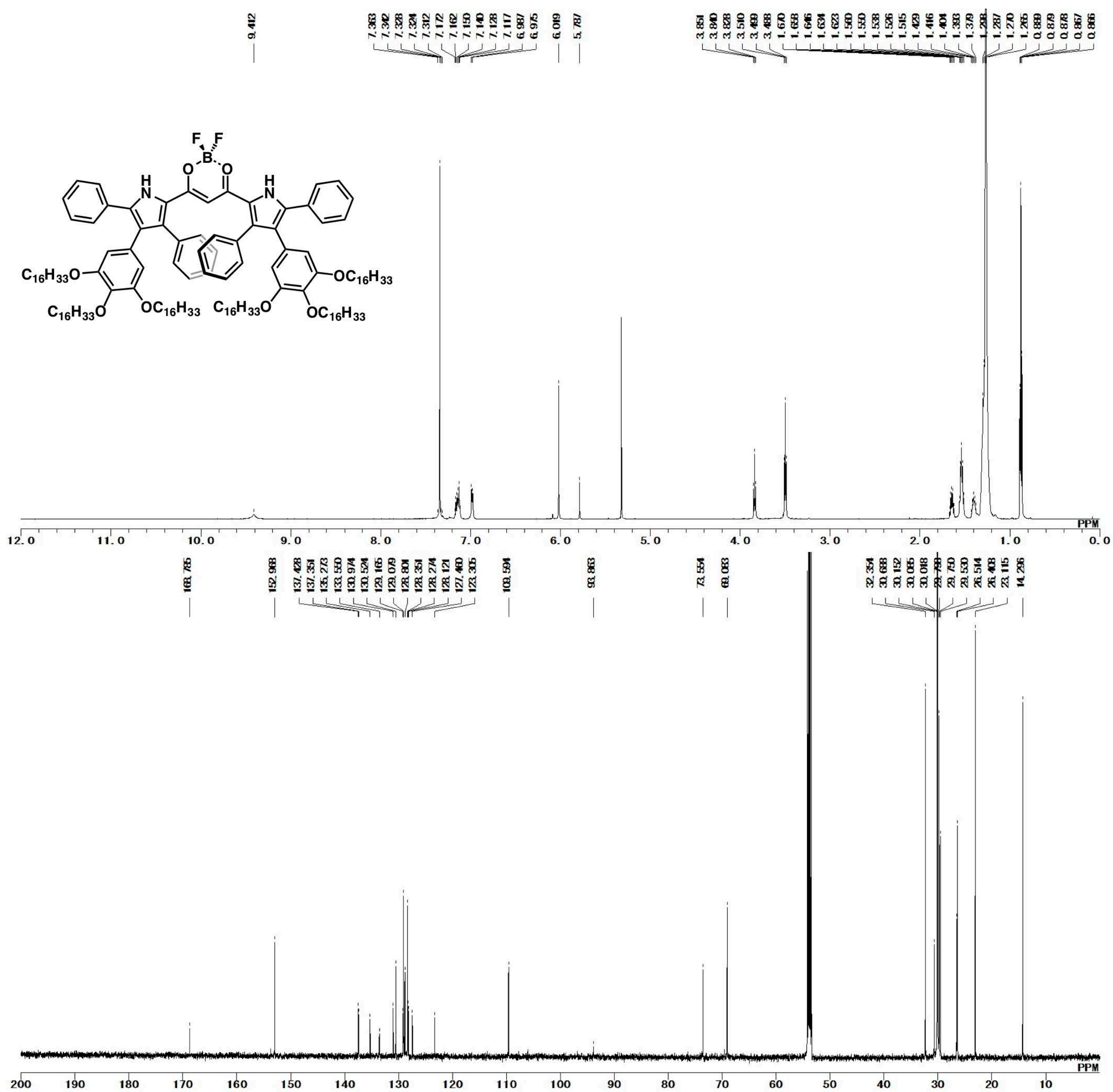
Supporting Figure 4 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **2b** in DMSO-d_6.



Supporting Figure 5 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **3a** in CD_2Cl_2.

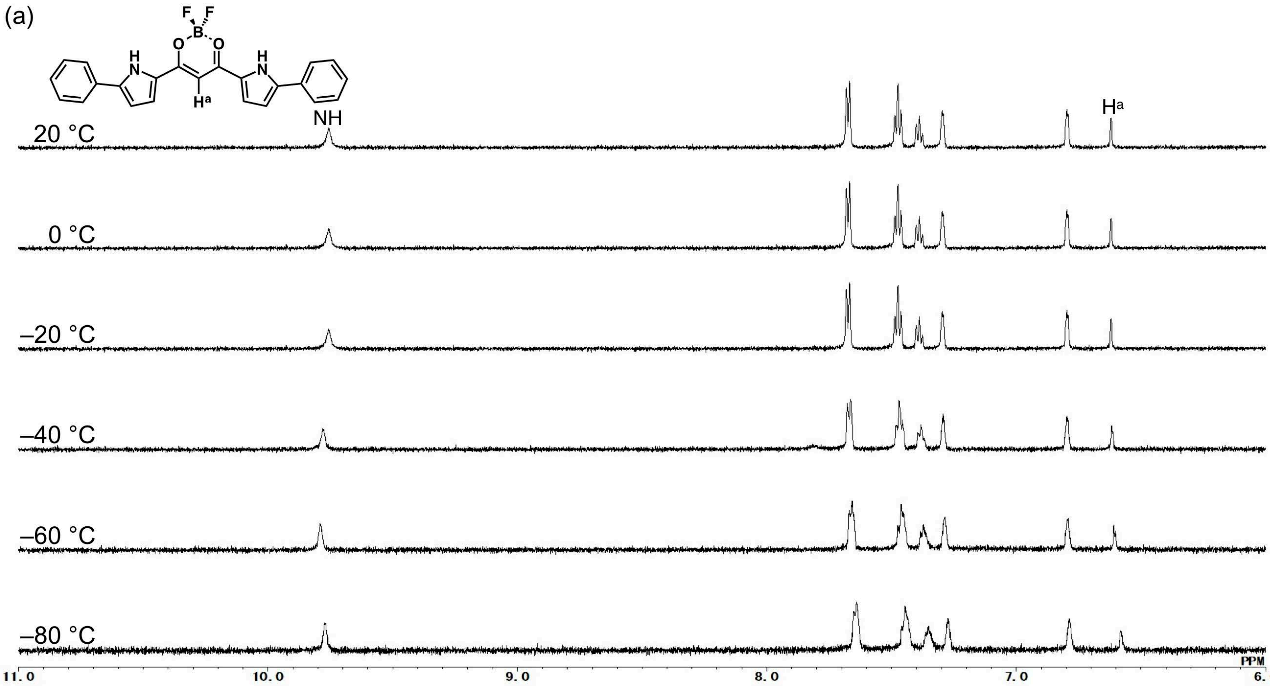


Supporting Figure 6 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **3b** in CD_2Cl_2.

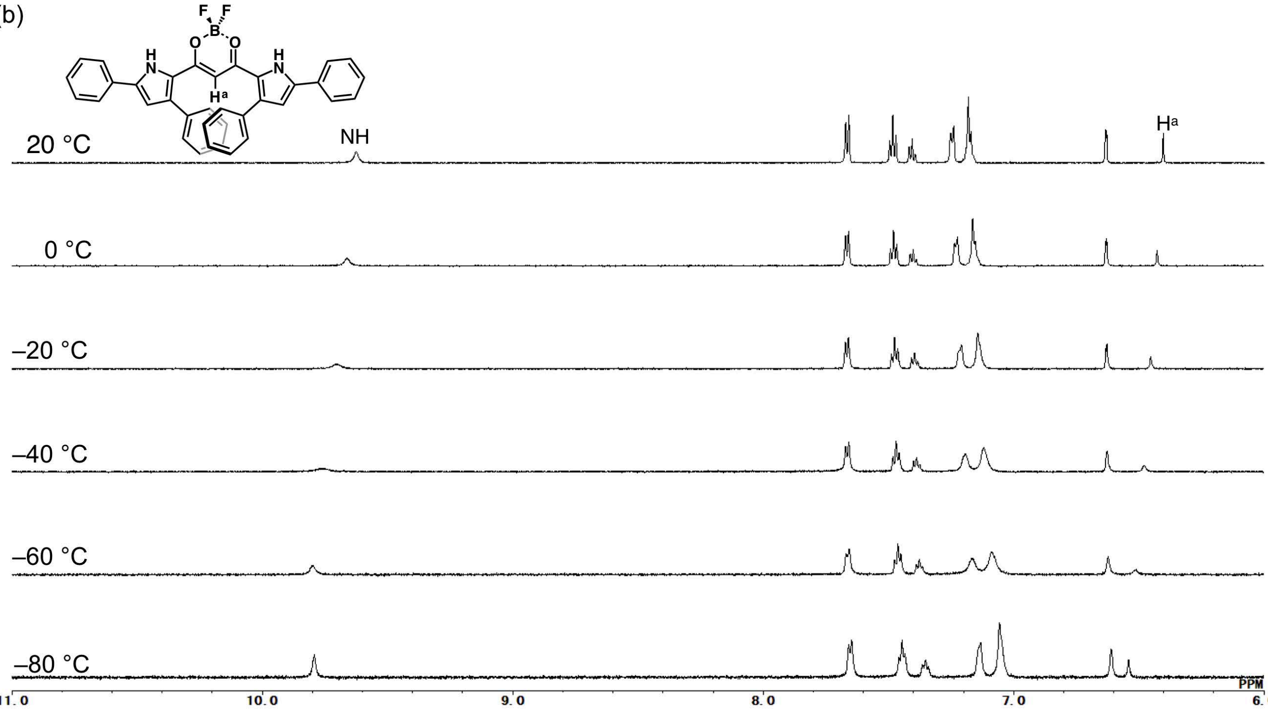


Supporting Figure 7 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **3c** in CD_2Cl_2.

(a)

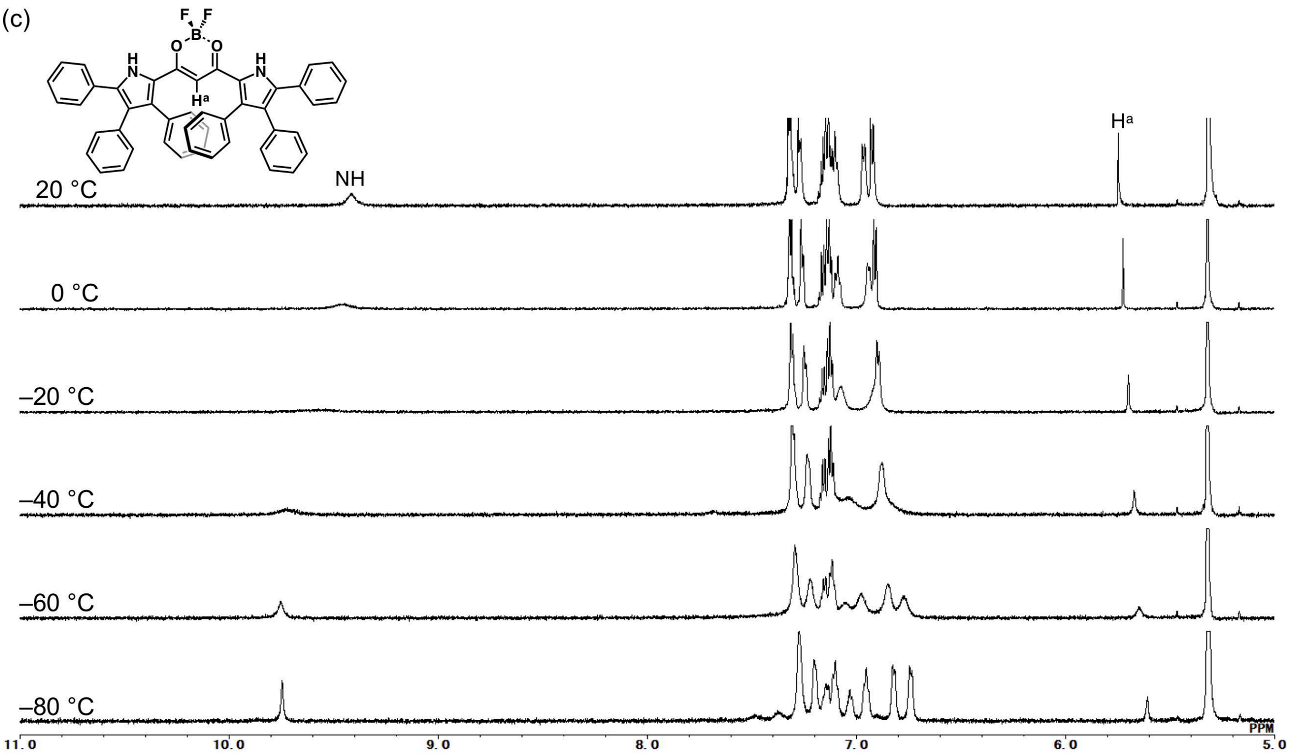


(b)

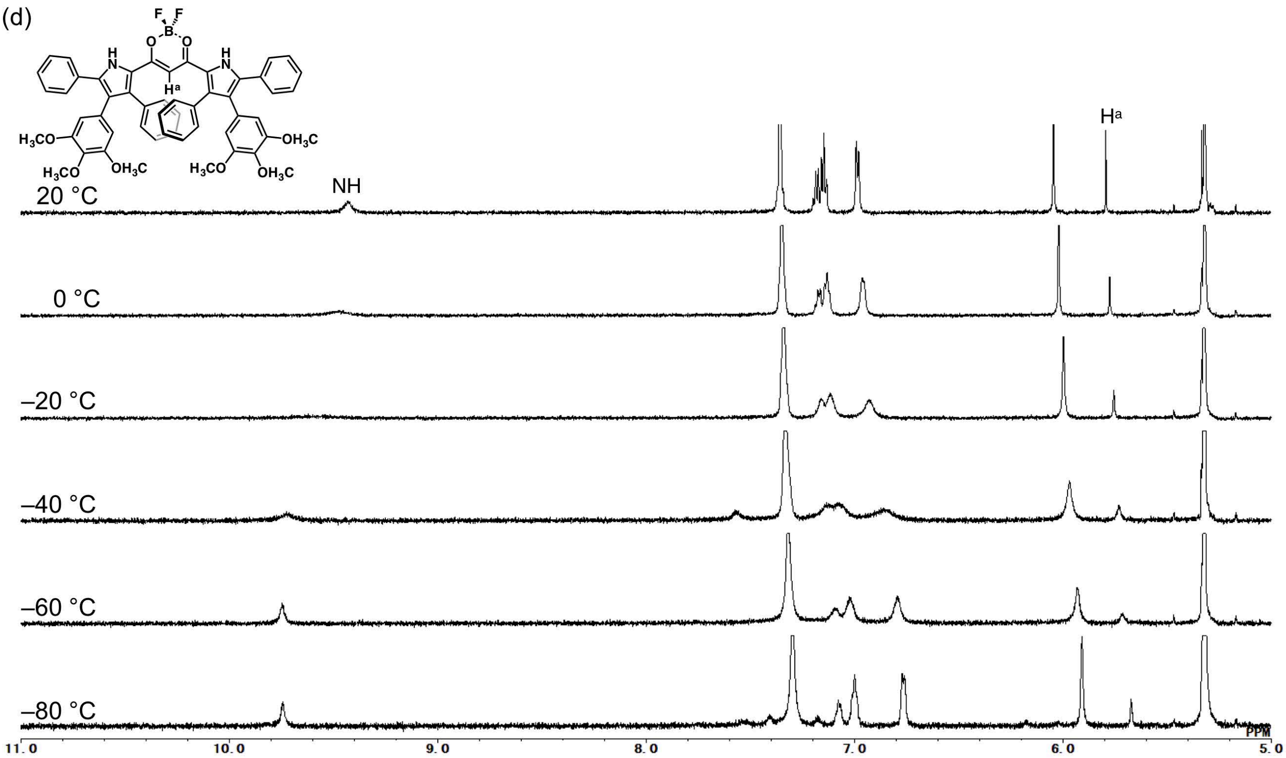


Supporting Figure 8 NMR spectral changes of (a) **1a**, (b) **2a**, (c) **3a**, and (d) **3b** in CD_2Cl_2 (1×10^{-3} M) at variable temperatures. Temperature-depending signal shifts with broadening for **2a** and **3a**,**b** suggested the transitions between two states probably due to the orientations of substituted aryl rings.

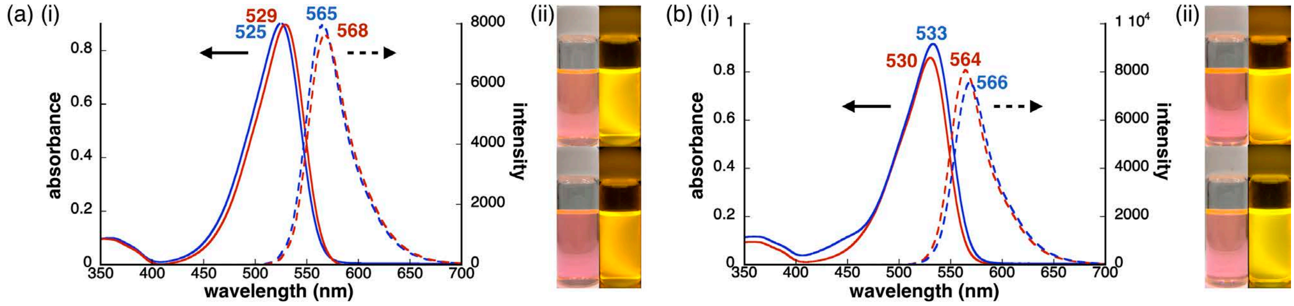
(c)



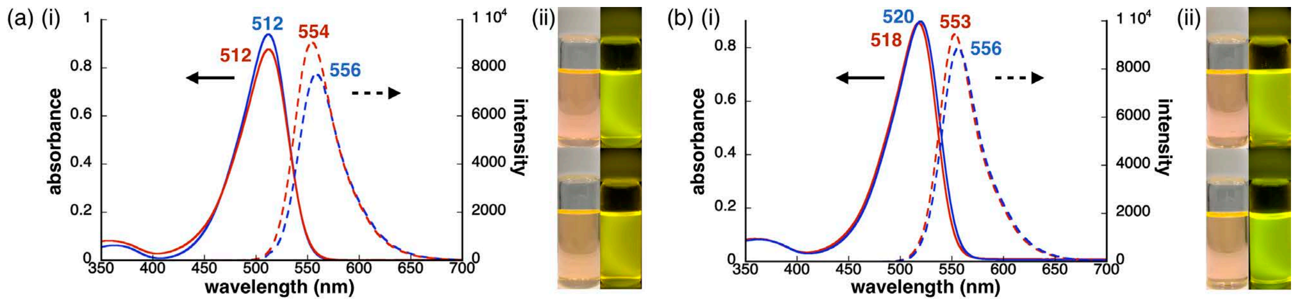
(d)



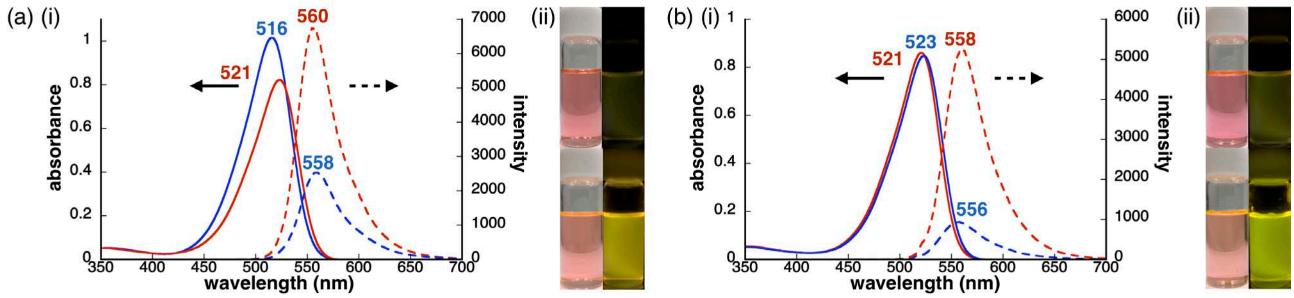
Supporting Figure 8 (Continued)



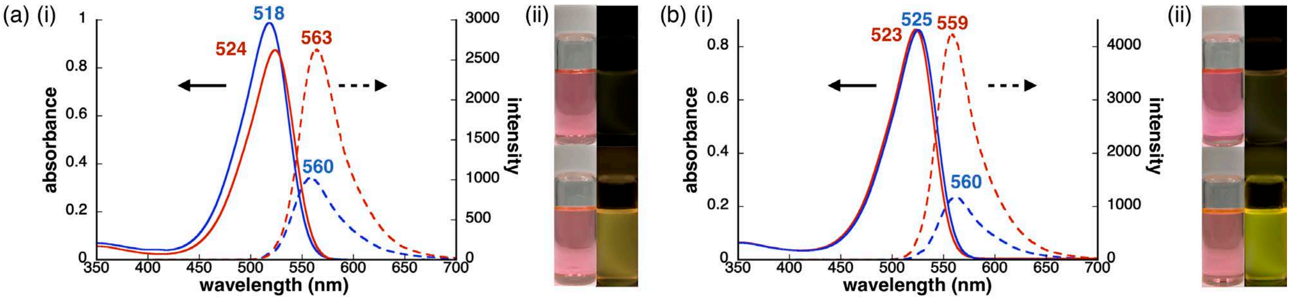
Supporting Figure 9 (i) UV/vis absorption (solid line) and fluorescence spectra (broken line) (1.0×10^{-5} M) of **2a** and (ii) photographs under visible light (left) and 365-nm UV light (right): (a) those in CH_2Cl_2 (blue for (i) and top for (ii)) and $CHCl_3$ (red for (i) and bottom for (ii)); (b) those in 1,2-dichlorobenzene (blue for (i) and top for (ii)) and chlorobenzene (red for (i) and bottom for (ii)). The fluorescence spectra were obtained by the excitation at the absorption maxima. Fluorescence quantum yields are 0.88 (CH_2Cl_2), 0.81 ($CHCl_3$), 0.90 (1,2-dichlorobenzene), and 0.90 (chlorobenzene).



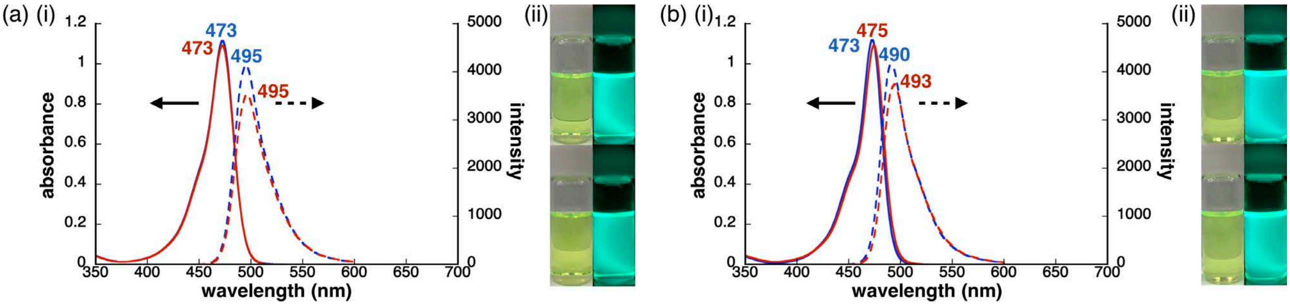
Supporting Figure 10 (i) UV/vis absorption (solid line) and fluorescence spectra (broken line) (1.0×10^{-5} M) of **3a** and (ii) photographs under visible light (left) and 365-nm UV light (right): (a) those in CH_2Cl_2 (blue for (i) and top for (ii)) and $CHCl_3$ (red for (i) and bottom for (ii)); (b) those in 1,2-dichlorobenzene (blue for (i) and top for (ii)) and chlorobenzene (red for (i) and bottom for (ii)). The fluorescence spectra were obtained by the excitation at the absorption maxima. Fluorescence quantum yields are 0.89 (CH_2Cl_2), 0.86 ($CHCl_3$), 0.92 (1,2-dichlorobenzene), and 0.92 (chlorobenzene).



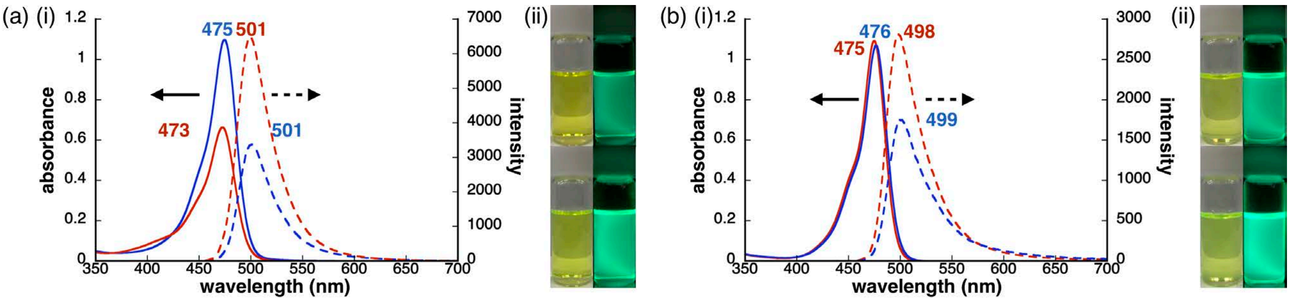
Supporting Figure 11 (i) UV/vis absorption (solid line) and fluorescence spectra (broken line) (1.0×10^{-5} M) of **3b** and (ii) photographs under visible light (left) and 365-nm UV light (right): (a) those in CH_2Cl_2 (blue for (i) and top for (ii)) and $CHCl_3$ (red for (i) and bottom for (ii)); (b) those in 1,2-dichlorobenzene (blue for (i) and top for (ii)) and chlorobenzene (red for (i) and bottom for (ii)). The fluorescence spectra were obtained by the excitation at the absorption maxima. Fluorescence quantum yields are 0.084 (CH_2Cl_2), 0.53 ($CHCl_3$), 0.26 (1,2-dichlorobenzene), and 0.63 (chlorobenzene).



Supporting Figure 12 (i) UV/vis absorption (solid line) and fluorescence spectra (broken line) (1.0×10^{-5} M) of **3c** and (ii) photographs under visible light (left) and 365-nm UV light (right): (a) those in CH_2Cl_2 (blue for (i) and top for (ii)) and $CHCl_3$ (red for (i) and bottom for (ii)); (b) those in 1,2-dichlorobenzene (blue for (i) and top for (ii)) and chlorobenzene (red for (i) and bottom for (ii)). The fluorescence spectra were obtained by the excitation at the absorption maxima. Fluorescence quantum yields are 0.027 (CH_2Cl_2), 0.28 ($CHCl_3$), 0.11 (1,2-dichlorobenzene), and 0.40 (chlorobenzene).

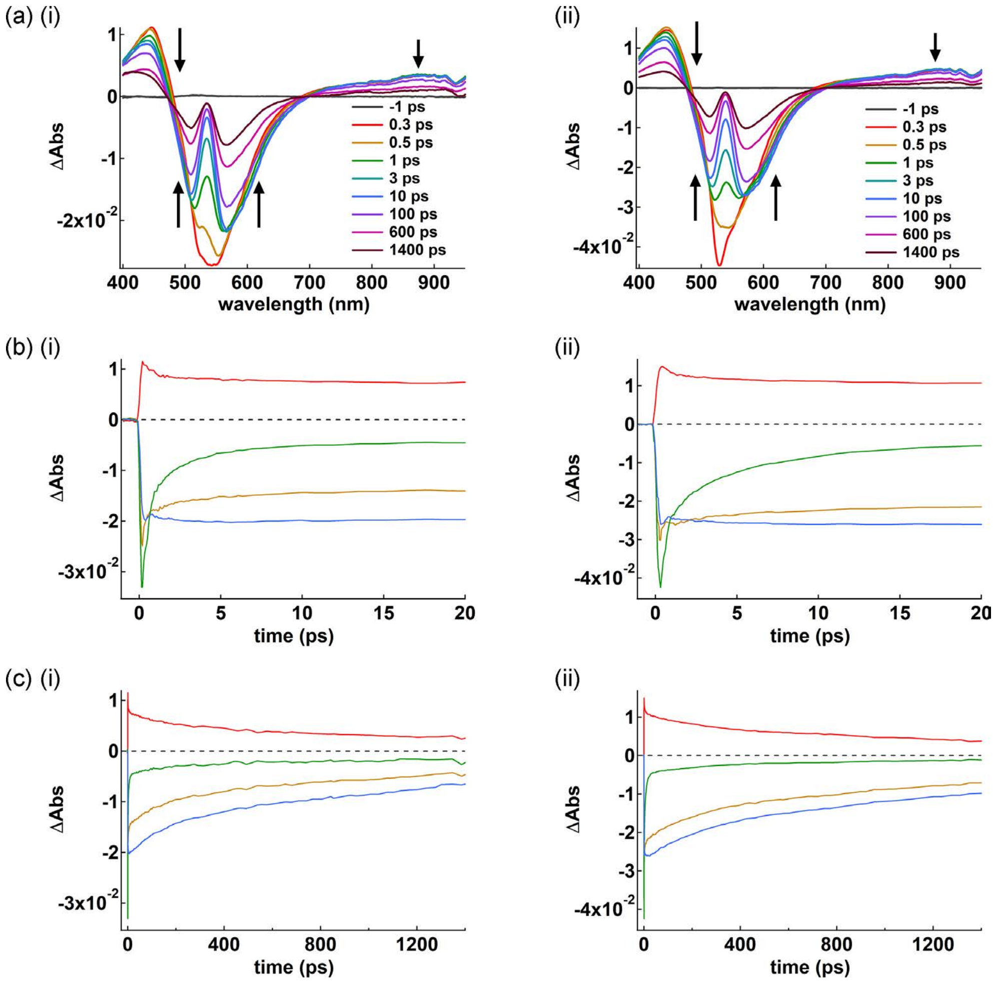


Supporting Figure 13 (i) UV/vis absorption (solid line) and fluorescence spectra (broken line) (1.0×10^{-5} M) of **1c** and (ii) photographs under visible light (left) and 365-nm UV light (right): (a) those in CH_2Cl_2 (blue for (i) and top for (ii)) and $CHCl_3$ (red for (i) and bottom for (ii)); (b) those in 1,2-dichlorobenzene (blue for (i) and top for (ii)) and chlorobenzene (red for (i) and bottom for (ii)). The fluorescence spectra were obtained by the excitation at the absorption maxima. Fluorescence quantum yields are 0.85 (CH_2Cl_2), 0.71 ($CHCl_3$), 0.87 (1,2-dichlorobenzene), and 0.87 (chlorobenzene).

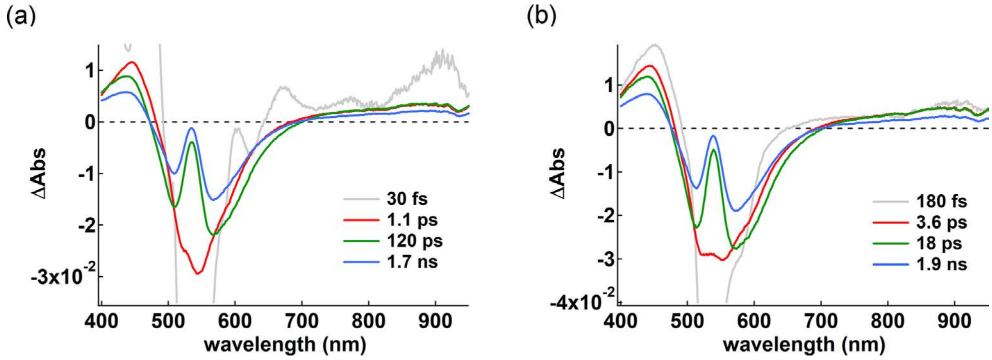


Supporting Figure 14 (i) UV/vis absorption (solid line) and fluorescence spectra (broken line) (1.0×10^{-5} M) of **1d** and (ii) photographs under visible light (left) and 365-nm UV light (right): (a) those in CH_2Cl_2 (blue for (i) and top for (ii)) and $CHCl_3$ (red for (i) and bottom for (ii)); (b) those in 1,2-dichlorobenzene (blue for (i) and top for (ii)) and chlorobenzene (red for (i) and bottom for (ii)). The fluorescence spectra were obtained by the excitation at the absorption maxima. Fluorescence quantum yields are 0.23 (CH_2Cl_2), 0.46 ($CHCl_3$), 0.53 (1,2-dichlorobenzene), and 0.78 (chlorobenzene).

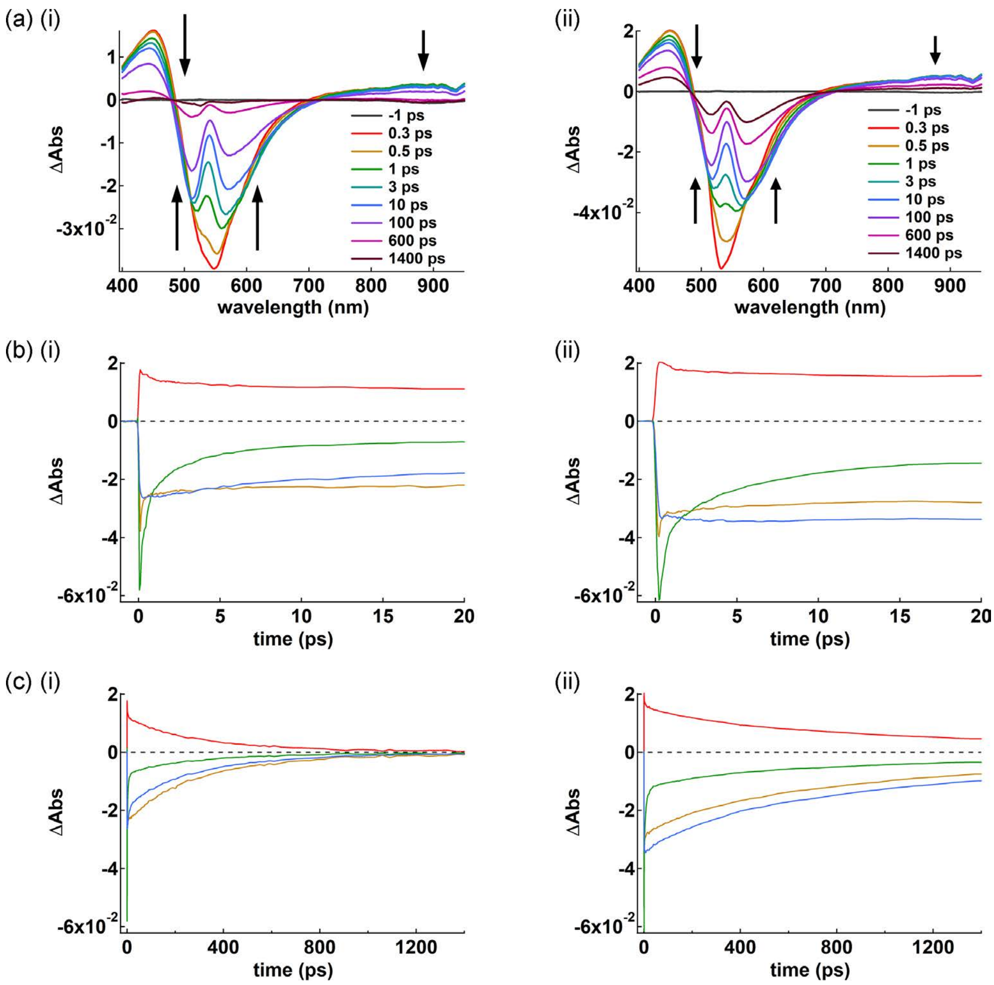
Method for femtosecond transient absorption measurements. Transient absorption measurements on the sub-picosecond to nanosecond time scale were conducted by a homemade pump-probe system. An amplified femtosecond laser, Spirit One 1040-8 (Spectra-Physics, 1040 nm, the pulse width: ~270 fs), was split into two beams with a ratio of 1:9. The stronger beam was directed to a noncollinear optical parametric amplifier (NOPA), Spirit-NOPA-3H (Spectra-Physics), to generate the 525-nm femtosecond laser pulse for the pump beam. The pump beam was chopped prior to the sample at 500 Hz for signal differencing. The other weaker beam was focused to a deuterated water placed in a 10-mm quartz cuvette to generate the white light continuum for the probe beam. Both pump and probe beams were focused to the sample solution placed in the 2-mm quartz cuvette. The polarization between the pump and probe pulses was set at magic angle. The intensity of the pump pulse was set to 105 μJ cm^{-2} (the pulse energy and the full-width of the half maximum of the beam spot were 60 nJ $pulse^{-1}$ and 270 μm, respectively). The transmitted probe beam was detected with multichannel detection system, PK120-C-RK (UNISOKU), composed of a CMOS linear image sensor and a polychromator. The obtained spectra were calibrated for group velocity dispersion using the data obtained by the optical Kerr signal of CH_2Cl_2 between the pump pulse and the white-light continuum. The instrumental response function was shorter than approximately 60 fs. The sample solution was stirred with a stirrer during the experiments and the measurements were performed at room temperature.



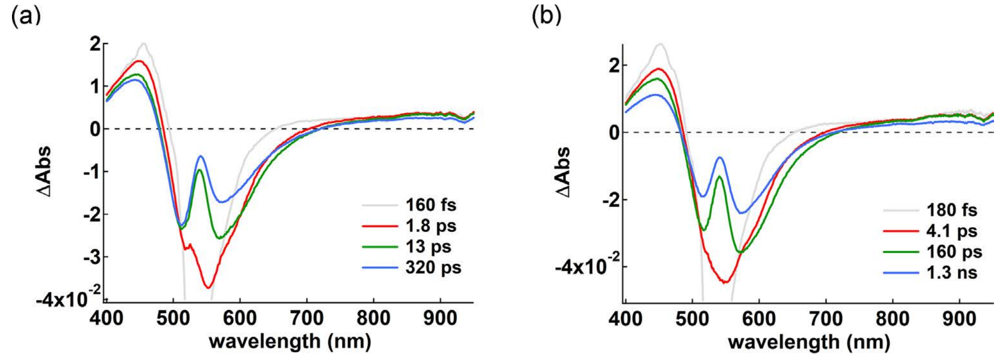
Supporting Figure 15 (a) Sub-picosecond to nanosecond transient absorption spectra of (i) **3a** in degassed CH_2Cl_2 (0.40 mM) and (ii) **3a** (0.44 mM) in degassed $CHCl_3$ excited at 525 nm with delay time spanning from –1 ps (gray) to 1400 ps (purple). Arrows indicate the spectral changes in transient absorptions. Transient absorption decay profiles in the ranges (b) from –1 ps to 20 ps and (c) from –20 ps to 1400 ps of **3a** (i) in degassed CH_2Cl_2 and (b) in degassed $CHCl_3$ excited at 525 nm and monitored at 450 nm (red), 515 nm (yellow), 540 nm (green), and 580 nm (blue). The transient absorption spectra and dynamics show that the relaxation pathways of **3a** are almost the same in CH_2Cl_2 and in $CHCl_3$.



Supporting Figure 16 Evolution-associated spectra obtained through singular value decomposition analysis of sub-picosecond to nanosecond transient time scale transient absorption spectra of **3a** (a) in degassed CH_2Cl_2 and (b) in degassed $CHCl_3$. Curves are labeled with the respective time constants (τ) of **3a** in degassed CH_2Cl_2 (30 fs: gray; 1.1 ps: red; 120 ps: green; 1.7 ns: blue) and **3a** in degassed $CHCl_3$ (180 fs: gray; 3.6 ps: red; 18 ps: green; 1.9 ns: blue). The spectra of fastest decay-time components (30 and 180 fs) were derived from the superposition of impulsive solvent responses and the Franck-Condon state of **3a**. It is noted that the ratio of the ground-state bleaching signal at 514 nm and the stimulated emission signal at 572 nm does not change with time in both solvents.



Supporting Figure 17 (a) Sub-picosecond to nanosecond transient absorption spectra of (i) **3b** in degassed CH_2Cl_2 (0.52 mM) and (ii) **3b** (0.69 mM) in degassed $CHCl_3$ excited at 525 nm with delay time spanning from –1 ps (gray) to 1400 ps (purple). Arrows indicate the spectral changes in transient absorptions. Transient absorption decay profiles in the ranges (b) from –1 ps to 20 ps and (c) from –20 ps to 1400 ps of **3b** (i) in degassed CH_2Cl_2 and (ii) in degassed $CHCl_3$ excited at 525 nm and monitored at 450 nm (red), 515 nm (yellow), 540 nm (green), and 580 nm (blue). The transient absorption spectra and dynamics show that the relaxation pathway of **3b** in CH_2Cl_2 is clearly different from that in $CHCl_3$. The spectral change is discussed in the caption of Supporting Figure 18.



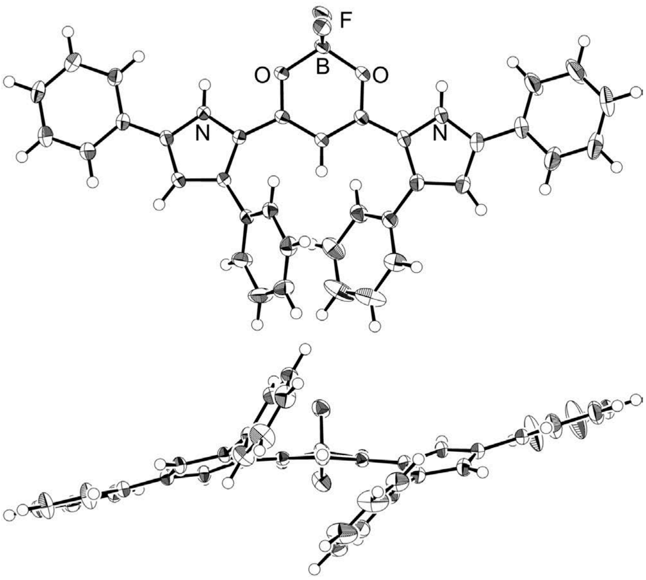
Supporting Figure 18 Evolution-associated spectra obtained through singular value decomposition analysis of sub-picosecond to nanosecond transient time scale transient absorption spectra of **3b** (a) in degassed CH_2Cl_2 and (b) in degassed $CHCl_3$. Curves are labeled with the respective time constants of **3b** in degassed CH_2Cl_2 (160 fs: gray; 1.8 ps: red; 13 ps: green; 320 ps: blue) and **3b** in degassed $CHCl_3$ (180 fs: gray; 4.1 ps: red; 160 ps: green; 1.3 ns: blue). The spectra of fastest decay-time components (160 and 180 fs, respectively) were derived from the superposition of impulsive solvent responses and the Franck-Condon state of **3b**. Evolution-associated spectra show that the stimulated emission signal at 573 nm in **3b** in degassed CH_2Cl_2 decreases relatively faster than the ground-state bleaching signal at 517 nm. On the other hand, the ratio of the ground-state bleaching signal at 514 nm and the stimulated emission signal at 572 nm does not change with time in degassed $CHCl_3$. This suggests that the HOMO level of the core π-electronic systems is occupied by the electron transfer from the HOMO level of the electron-rich 4-aryl units in CH_2Cl_2. Therefore, the time constant of 13 ps could be assigned to the photoinduced electron transfer (PET). The stimulated emission signal is still observed after the PET probably because the system reaches the quasi-equilibrium state by both forward and back electron transfers due to the close energy levels between the HOMO level of the core π-electronic systems and that of the trialkoxyphenyl unit. The acceleration of the longer decay species from 1.3 ns to 320 ps is most probably due to the increased nonradiative relaxation by the forward and back electron transfers.

2. X-ray crystallographic data

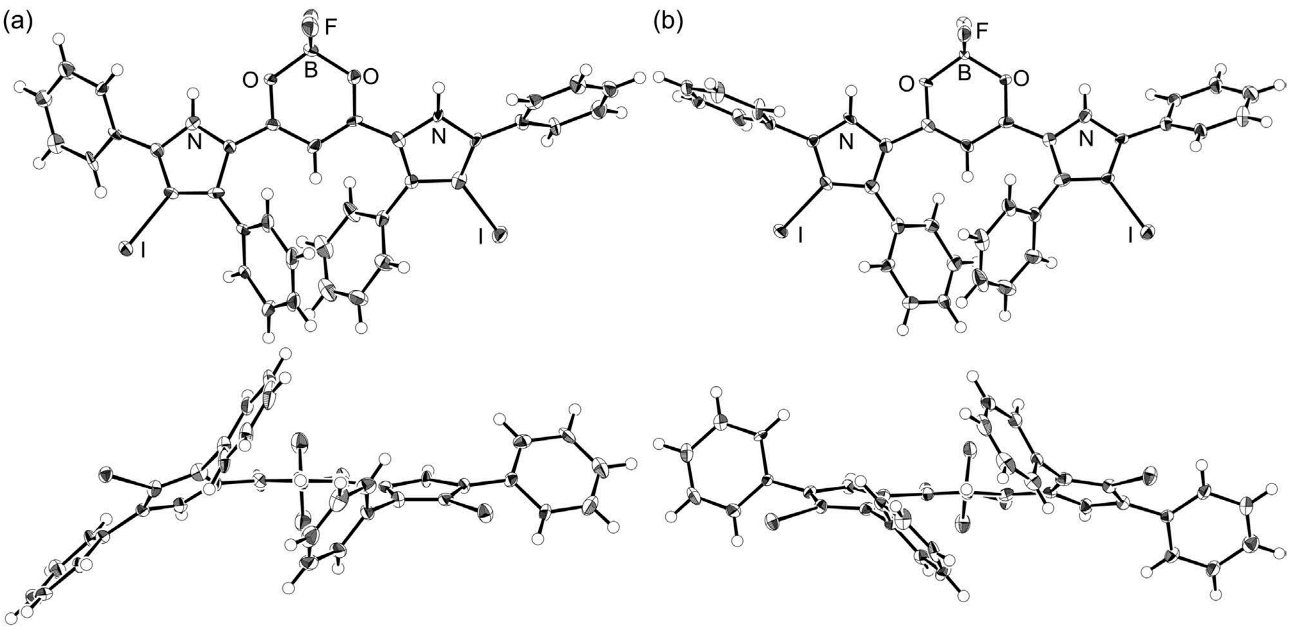
Method for single-crystal X-ray analysis. Crystallographic data are summarized in Supporting Table 1. A single crystal of **2a** was obtained by vapor diffusion of *n*-hexane into a $CHCl_3$ solution of **2a**. The data crystal was an orange block of approximate dimensions 0.100 mm × 0.100 mm × 0.050 mm. A single crystal of **2b** was obtained by vapor diffusion of *n*-hexane into a pyridine solution of **2b**. The data crystal was a red prism of approximate dimensions 0.020 mm × 0.020 mm × 0.020 mm. A single crystal of **3a** was obtained by vapor diffusion of D-limonene ((*R*)-1-methyl-4-(1-methylethenyl)cyclohexene) into a CH_2Cl_2 solution of **3a**. The same crystals were also obtained from *n*-hexane/CH_2Cl_2. The data crystal was a red prism of approximate dimensions 0.100 mm × 0.060 mm × 0.020 mm. A single crystal of $\mathbf{2a}_2{\cdot}Cl^-$-TBA$^+$ was obtained by vapor diffusion of *n*-hexane into a CH_2Cl_2 solution of the 2:1 mixture of **2a** and TBACl. The data crystal was an orange prism of approximate dimensions 0.100 mm × 0.070 mm × 0.050 mm. The data of **2a** and **3a** were collected at 100 K on a Pilatus3 CdTe 1M with Si (311) monochromated synchrotron radiation (λ = 0.4307 and 0.4403 Å, respectively) at BL02B1 (SPring-8), and those of **2b** and $\mathbf{2a}_2{\cdot}Cl^-$-TBA$^+$ were collected at 95 and 90 K, respectively, on a DECTRIS EIGER X 1M diffractometer with Si (111) monochromated synchrotron radiation (λ = 0.8104 and 0.81128 Å, respectively) at BL40XU (SPring-8).[S5] All the structures were solved by dual-space method. The calculations were performed using Yadokari-XG.[S6] CIF files (CCDC-1908871–1908874) can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Supporting Table 1 Crystallographic details.

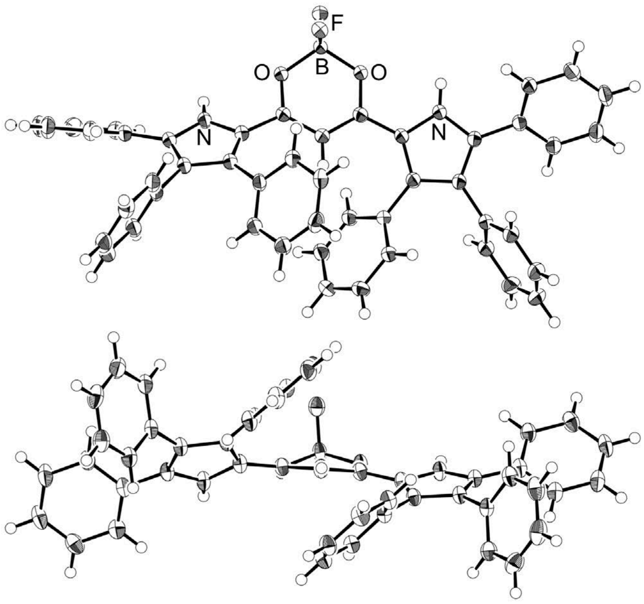
	2a	**2b**	**3a**	$\mathbf{2a}_2{\cdot}Cl^-$-TBA$^+$
formula	$C_{35}H_{25}BF_2N_2O_2$	$C_{35}H_{23}BF_2I_2N_2O_2{\cdot}2C_5H_5N$	$C_{47}H_{33}BF_2N_2O_2$	$2C_{35}H_{25}BF_2N_2O_2Cl{\cdot}C_{16}H_{36}N{\cdot}2CH_2Cl_2$
fw	554.38	964.36	706.56	1556.51
crystal size, mm	0.100 × 0.100 × 0.050	0.020 × 0.020 × 0.020	0.100 × 0.060 × 0.020	0.100 × 0.070 × 0.050
crystal system	triclinic	orthorhombic	triclinic	triclinic
space group	*P*-1 (no. 2)	$P2_12_12_1$ (no. 19)	*P*-1 (no. 2)	*P*-1 (no. 2)
a, Å	8.8174(8)	9.1316(2)	6.046(2)	13.3755(4)
b, Å	11.1450(10)	22.7041(4)	16.965(6)	14.9439(5)
c, Å	14.6195(13)	37.6937(7)	17.347(6)	21.2804(7)
α, °	105.387(7)	90	92.138(7)	74.334(2)
β, °	91.946(7)	90	94.827(7)	78.710(2)
γ, °	100.712(7)	90	90.828(6)	78.821(2)
V, Å^3	1355.8(2)	7814.8(3)	1771.5(11)	3971.3(2)
ρ_{calcd}, gcm^{-3}	1.358	1.639	1.325	1.302
Z	2	8	2	2
T, K	100(2)	95(2)	100(2)	90(2)
μ, mm^{-1}	0.041	2.334	0.040	0.348
no. of reflns	41130	79959	40777	42693
no. of unique reflns	6225	14283	8110	14488
variables	379	1009	487	988
λ, Å	0.4307	0.8104	0.4403	0.81128
R_1 ($I > 2\sigma(I)$)	0.0502	0.0569	0.0485	0.1293
wR_2 ($I > 2\sigma(I)$)	0.1174	0.1471	0.1391	0.3632
GOF	1.034	1.208	1.025	1.491



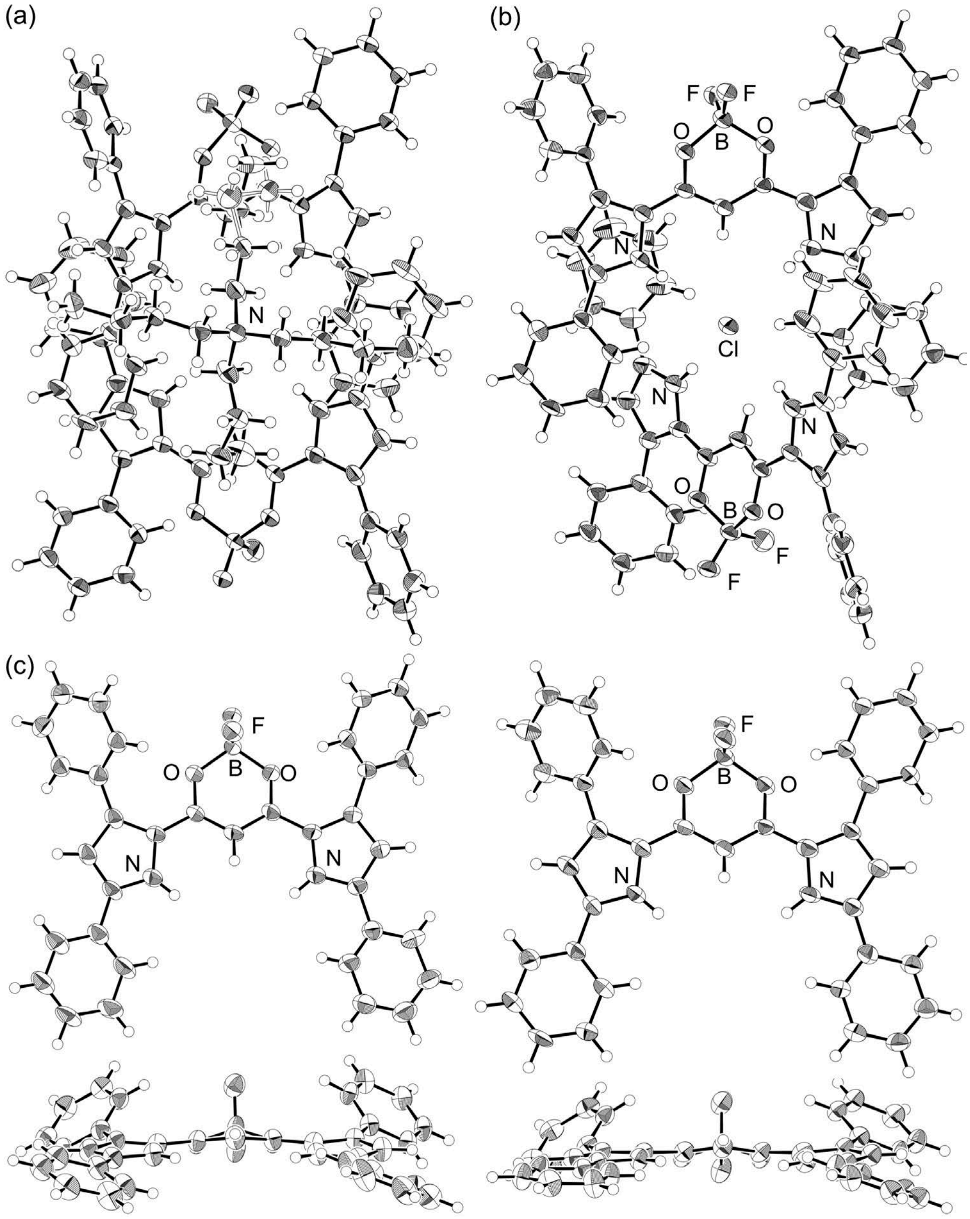
Supporting Figure 19 Ortep drawing of single-crystal X-ray structure (top and side views) of **2a**. Thermal ellipsoids are scaled to the 50% probability level.



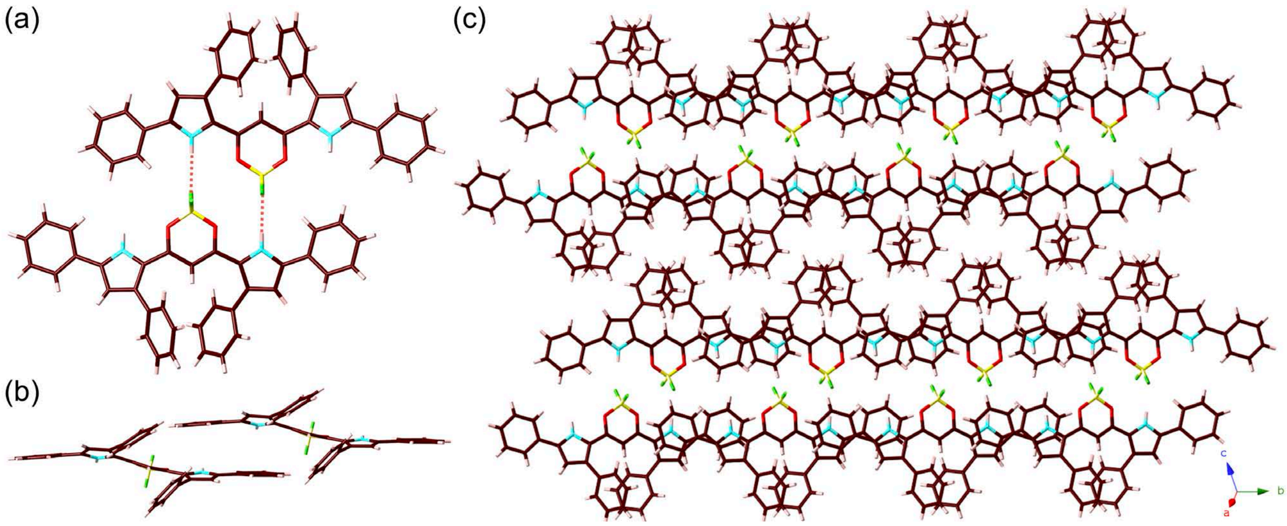
Supporting Figure 20 Ortep drawing of single-crystal X-ray structure (top and side views) of **2b**, which shows two independent structures (a,b) with different chirality. Thermal ellipsoids are scaled to the 50% probability level. Solvent molecules are omitted for clarity.



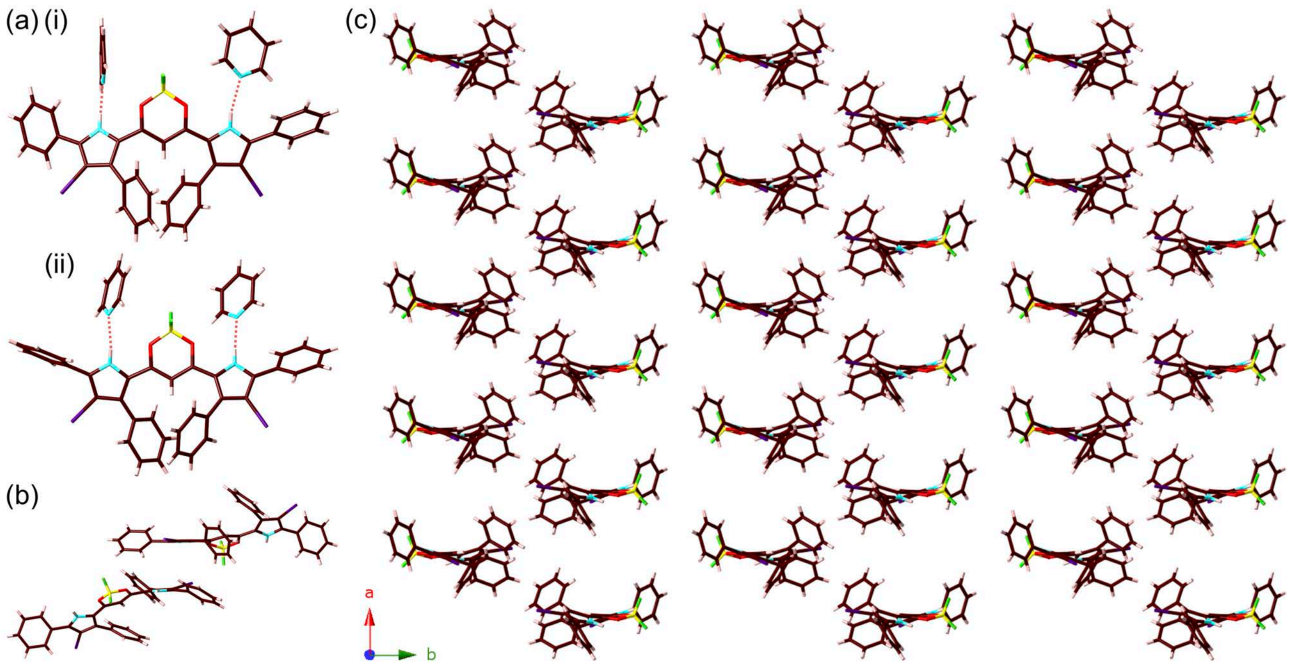
Supporting Figure 21 Ortep drawing of single-crystal X-ray structure (top and side views) of **3a**. Thermal ellipsoids are scaled to the 50% probability level.



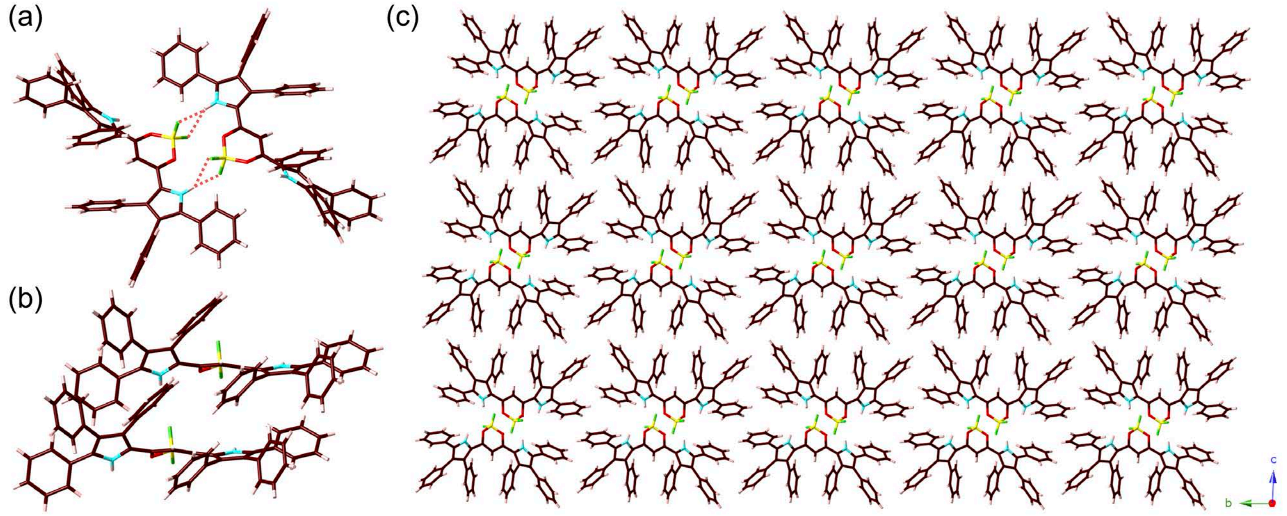
Supporting Figure 22 Ortep drawing of single-crystal X-ray structure (top and side views) of **2a**$_2$·Cl^--TBA^+, a [2+1]-type complex, as (a) ion-pairing form, (b) receptor–anion complex part, and (c) two receptor units. TBA^+ has disordered structures in the ratio of 71:29, and the disordered structures are represented by black and white bonds for major and minor structures, respectively. Thermal ellipsoids are scaled to the 50% probability level. Solvent molecules are omitted for clarity.



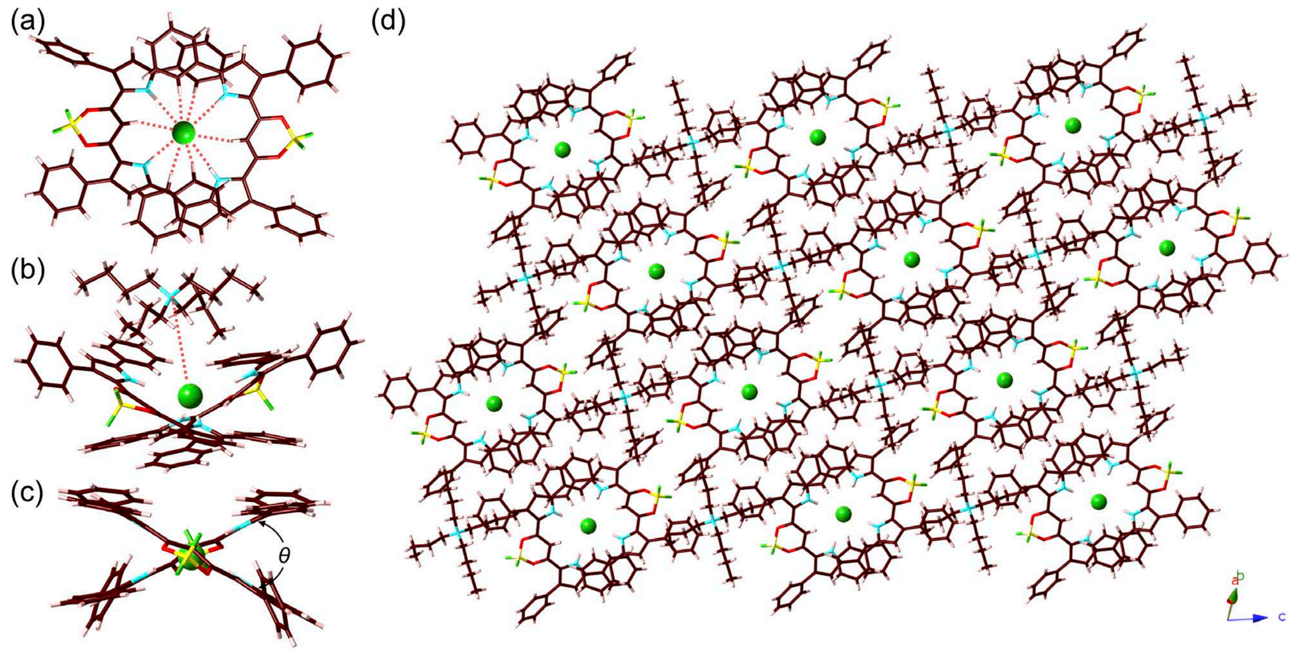
Supporting Figure 23 Packing diagrams of **2a**: (a) a hydrogen-bonding dimer with N(–H)···F distances of 2.953 and 3.586 Å, (b) a stacking dimer with a π–π distance of 3.567 Å, which was estimated by using the average distance between mean planes of pyrrole and 5-phenyl units (11 atoms), and (c) packing diagram. Atom color code: brown, pink, yellow, blue, red, and green refer to carbon, hydrogen, boron, nitrogen, oxygen, and fluorine, respectively.



Supporting Figure 24 Packing diagrams of **2b**: (a) two independent structures (i) and (ii) with intermolecular interaction with N(–H)···N distances of 2.839/2.923 and 2.832/2.884 Å, respectively, (b) a stacking dimer with a π–π distance of 4.375 Å, which was estimated by using the average distance between mean planes of five- and six-membered rings (pyrrole and core 1,3-diketone boron complex, respectively), and (c) packing diagram through the *c* axis. Atom color code: brown, pink, yellow, blue, red, green, and purple refer to carbon, hydrogen, boron, nitrogen, oxygen, fluorine, and iodine, respectively. Solvent molecules are omitted for clarity for (b) and (c).



Supporting Figure 25 Packing diagrams of **3a**: (a) a hydrogen-bonding dimer with N(–H)···F distances of 2.991 and 3.042 Å, (b) a stacking dimer with a π–π distance of 5.343 Å, which was estimated by using the average distance between mean planes of five- and six-membered rings (pyrrole and core 1,3-diketone boron complex, respectively), suggesting the absence of π–π interaction in the solid state, and (c) packing diagram through the *a* axis. Atom color code: brown, pink, yellow, blue, red, and green refer to carbon, hydrogen, boron, nitrogen, oxygen, and fluorine, respectively.



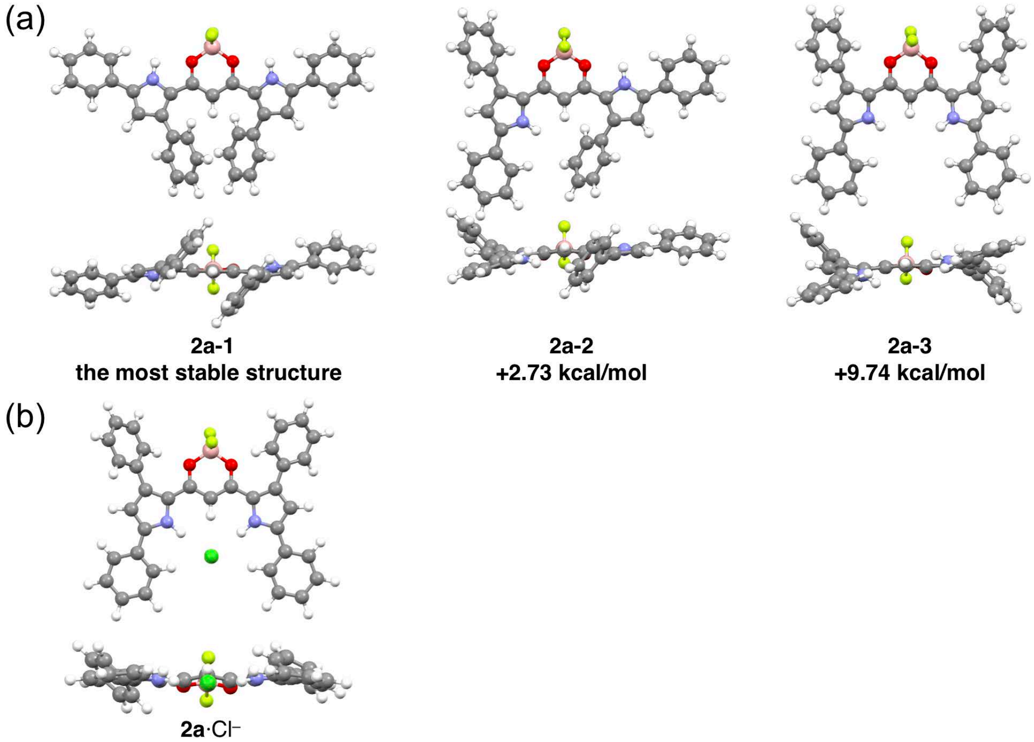
Supporting Figure 26 Packing diagrams of $\mathbf{2a}_2\cdot Cl^-$-TBA^+: (a) a [2+1]-type complex with pyrrole N(–H)···Cl distances of 3.379, 3.412, 3.384, and 3.421 Å, bridging C(–H)···Cl distances of 3.580 and 3.560 Å, and phenyl C(–H)···Cl distances of 3.601, 3.669, 3.627, and 3.667 Å, (b) an ion pair with a TBA-N···Cl distance of 5.427 Å, (c) two interlocked receptors with the dihedral angle θ based on the core planes, consisting of five- and six-membered rings (pyrrole and core 1,3-diketone boron complex, respectively), as 54.85°, and (d) packing diagram. Atom color code: brown, pink, yellow, blue, red, green, and green (sphere) refer to carbon, hydrogen, boron, nitrogen, oxygen, fluorine, and chlorine, respectively. Solvent molecules are omitted for clarity.

[S5] (a) N. Yasuda, H. Murayama, Y. Fukuyama, J. E. Kim, S. Kimura, K. Toriumi, Y. Tanaka, Y. Moritomo, Y. Kuroiwa, K. Kato, H. Tanaka and M. Takata, *J. Synchrotron Rad.*, 2009, **16**, 352–357; (b) N. Yasuda, Y. Fukuyama, K. Toriumi, S. Kimura and M. Takata, *AIP Conf. Proc.*, 2010, **1234**, 147–150.

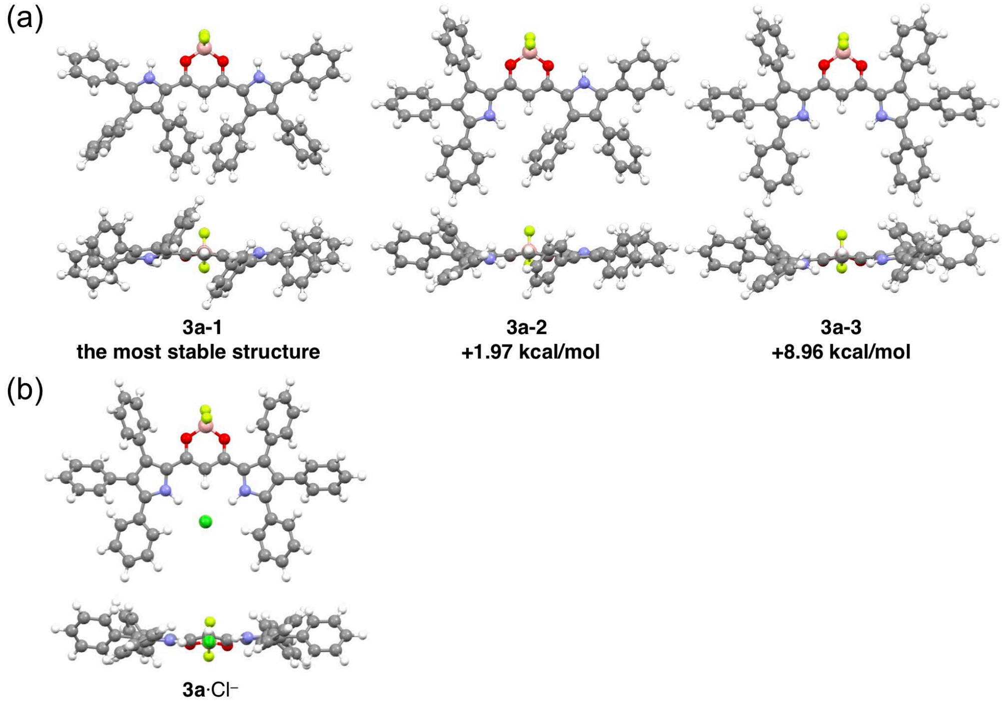
[S6] (a) *Yadokari-XG*, Software for Crystal Structure Analyses, K. Wakita, 2001; (b) C. Kabuto, S. Akine, T. Nemoto and E. Kwon, *J. Cryst. Soc. Jpn.*, 2009, **51**, 218–224.

3. Theoretical study

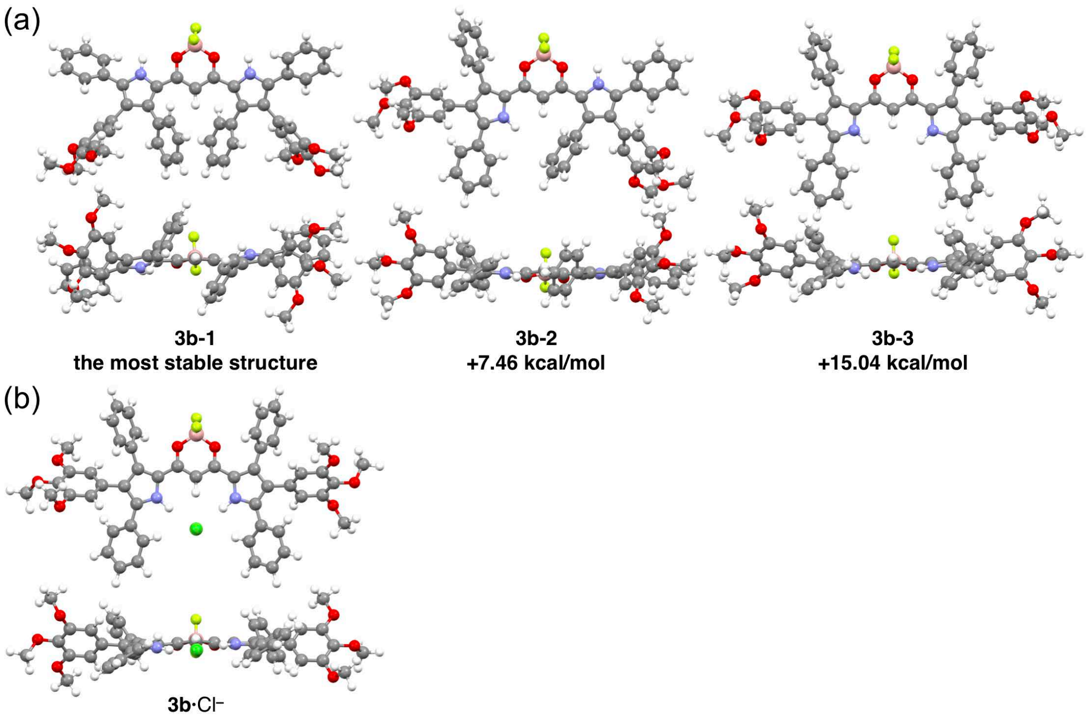
DFT calculations. DFT calculations of the geometrical optimizations of receptors and receptor–anion complexes were carried out using the Gaussian 09 program.[S7]



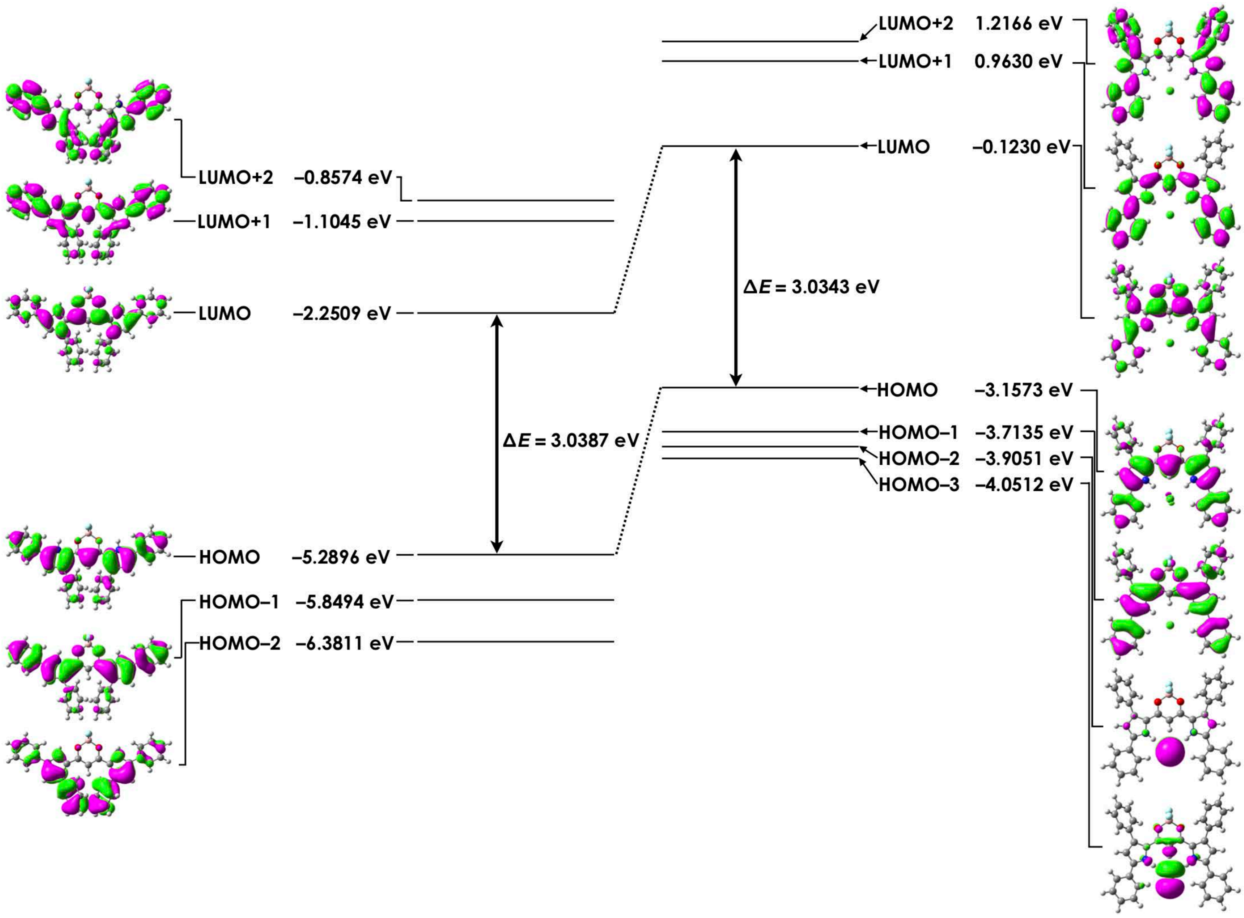
Supporting Figure 27 Optimized structures (top and side views) of (a) **2a** (**2a-1**: pyrrole-non-inverted conformation; **2a-2**: one-pyrrole-inverted conformation; **2a-3**: two-pyrrole-inverted conformation) and (b) **2a**$\cdot Cl^-$ at B3LYP/6-31+G(d,p). The difference in energy changes by the pyrrole inversion from **2a-1** to **2a-2** and that from **2a-2** to **2a-3** is probably due to the release of sterical hindrance of 3-phenyl moieties in **2a-1** by the first pyrrole inversion.



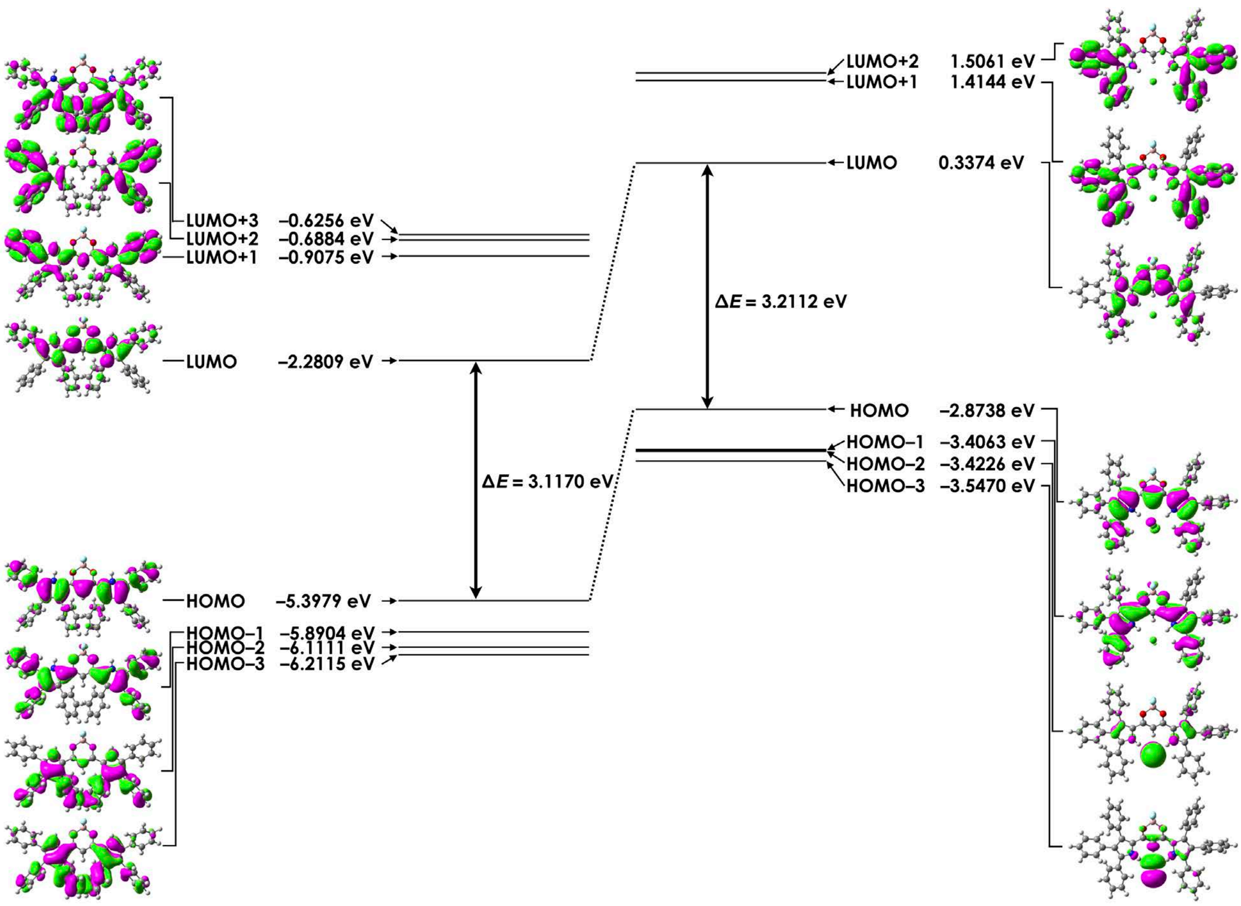
Supporting Figure 28 Optimized structures (top and side views) of (a) **3a** (**3a-1**: pyrrole-non-inverted conformation; **3a-2**: one-pyrrole-inverted conformation; **3a-3**: two-pyrrole-inverted conformation) and (b) **3a**·Cl^{-} at B3LYP/6-31+G(d,p). The difference in energy changes by the pyrrole inversion from **3a-1** to **3a-2** and that from **3a-2** to **3a-3** is probably due to the release of sterical hindrance of 3-phenyl moieties in **3a-1** by the first pyrrole inversion.



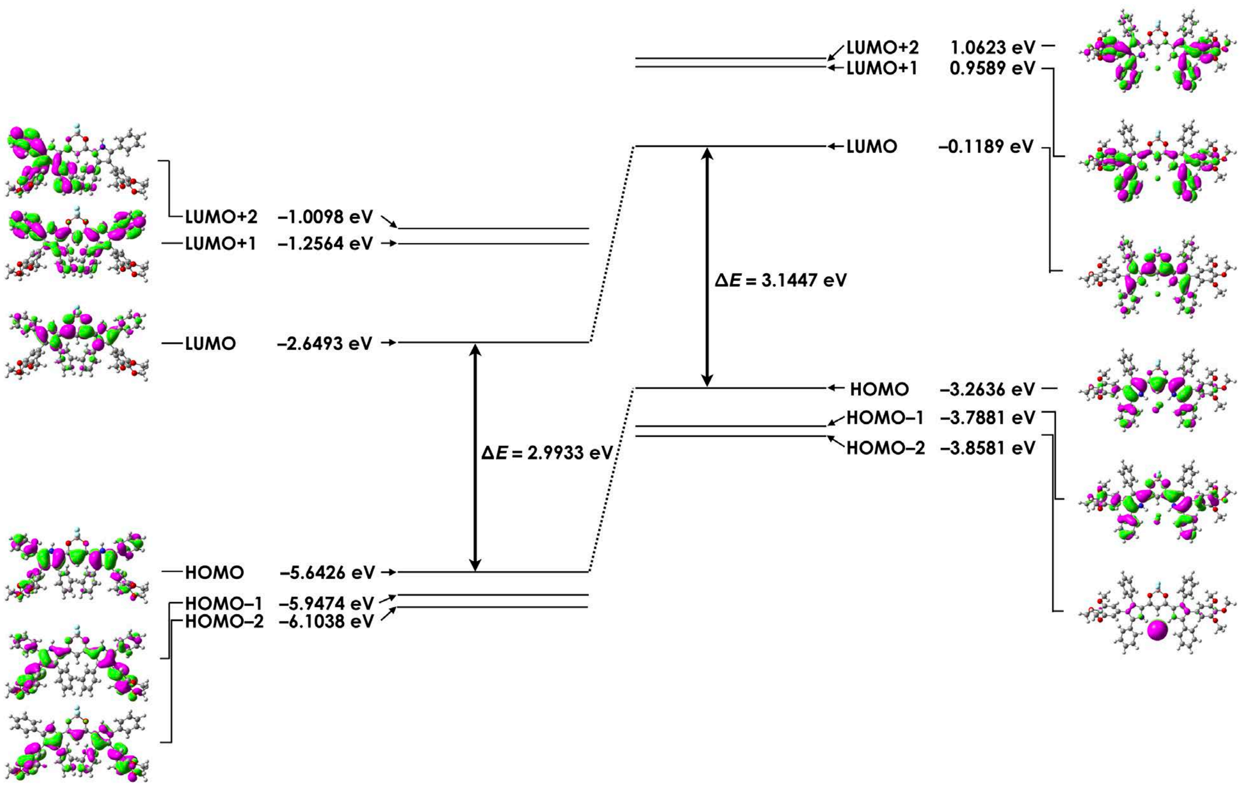
Supporting Figure 29 Optimized structures (top and side views) of (a) **3b** (**3b-1**: pyrrole-non-inverted conformation; **3b-2**: one-pyrrole-inverted conformation; **3b-3**: two-pyrrole-inverted conformation) and (b) **3b**·Cl^{-} at B3LYP/6-31+G(d,p). The differences in energy changes by the pyrrole inversion are currently under investigations.



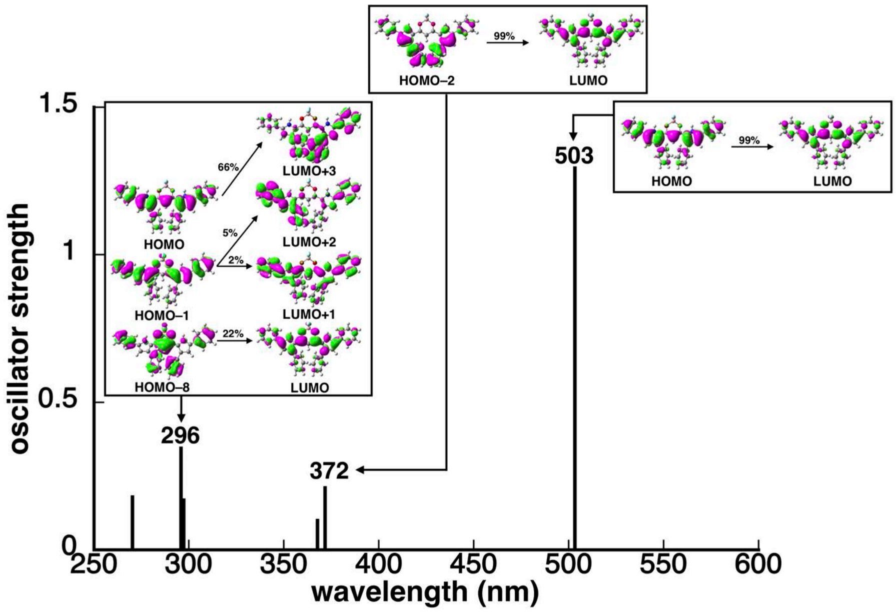
Supporting Figure 30 Molecular orbitals (HOMO/LUMO) of **2a** (left) and **2a**·Cl^- (right) estimated at B3LYP/6-31+G(d,p).



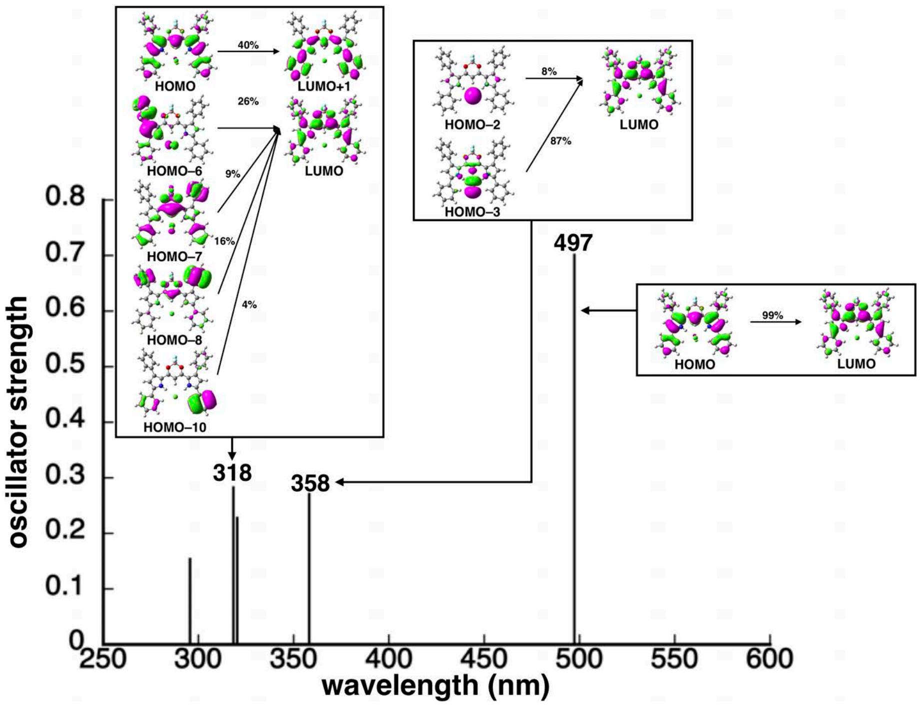
Supporting Figure 31 Molecular orbitals (HOMO/LUMO) of **3a** (left) and **3a**·Cl^- (right) estimated at B3LYP/6-31+G(d,p).



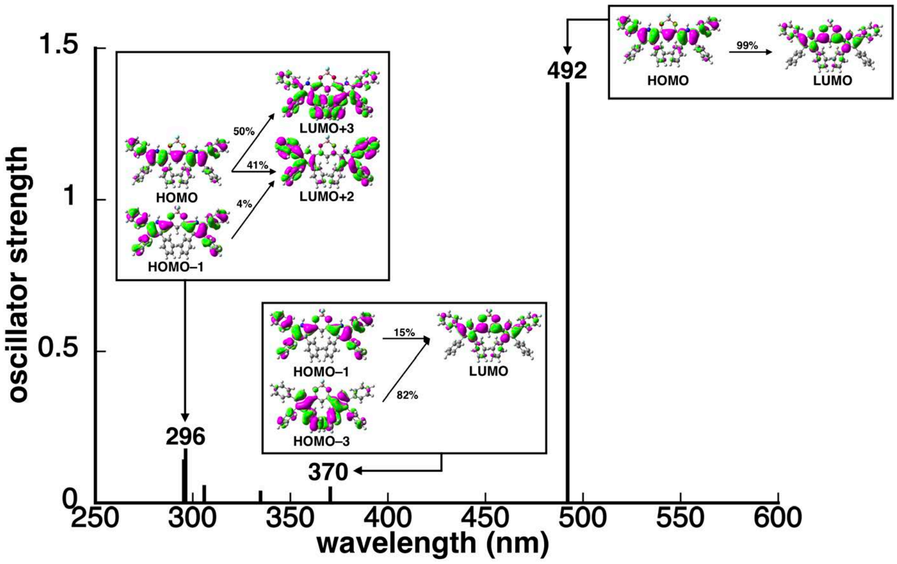
Supporting Figure 32 Molecular orbitals (HOMO/LUMO) of **3b** (left) and **3b**·Cl^- (right) estimated at B3LYP/6-31+G(d,p).



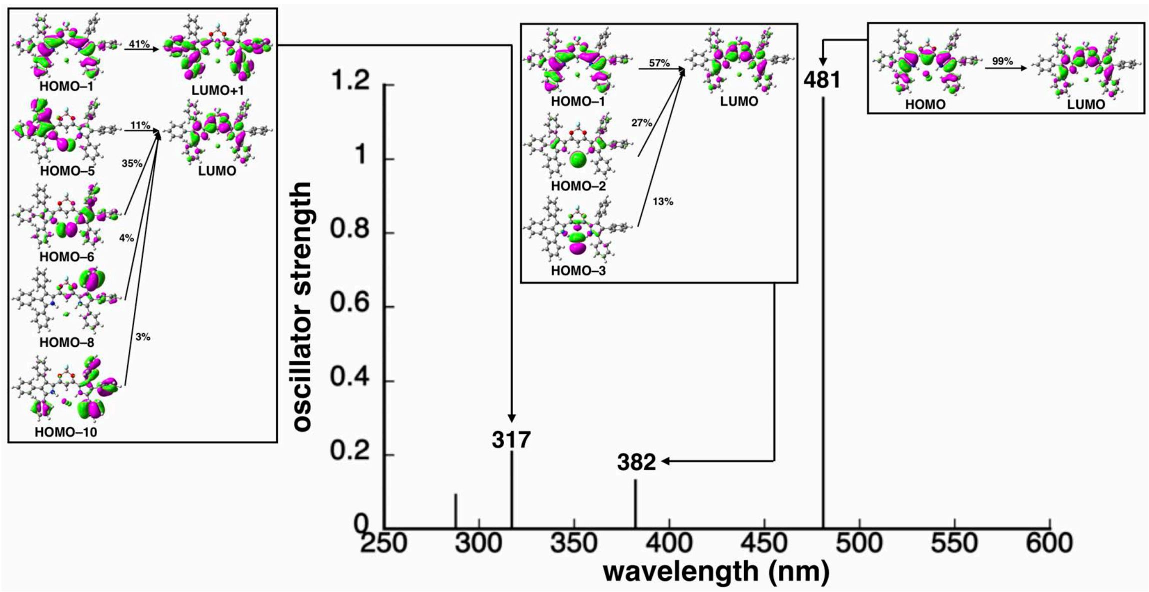
Supporting Figure 33 TD-DFT-based UV/vis absorption stick spectrum of **2a** with the transitions correlated with molecular orbitals estimated at PCM-B3LYP/6-31+G(d,p) in CH_2Cl_2//B3LYP/6-31+G(d,p).



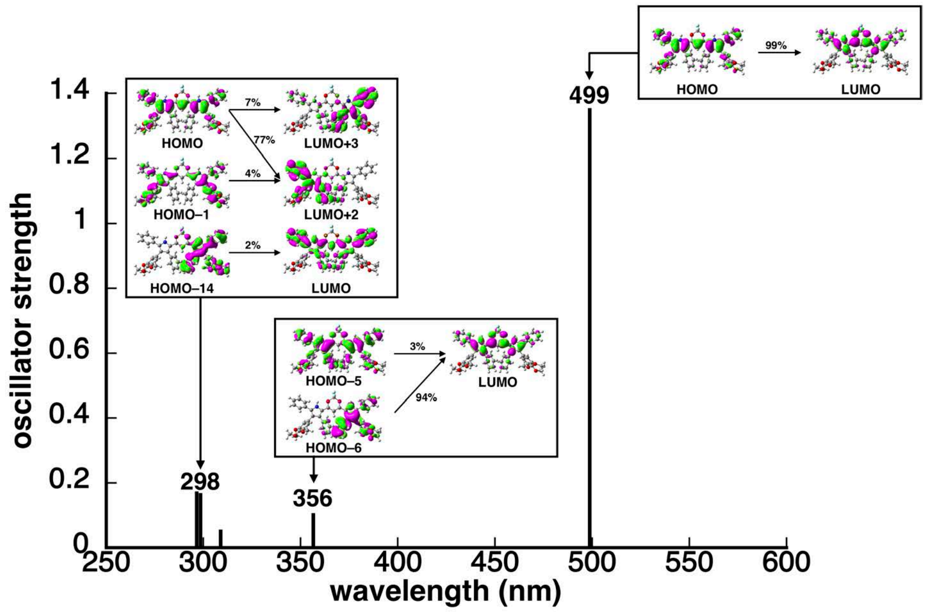
Supporting Figure 34 TD-DFT-based UV/vis absorption stick spectrum of **2a**·Cl^- with the transitions correlated with molecular orbitals estimated at PCM-B3LYP/6-31+G(d,p) in CH_2Cl_2//B3LYP/6-31+G(d,p).



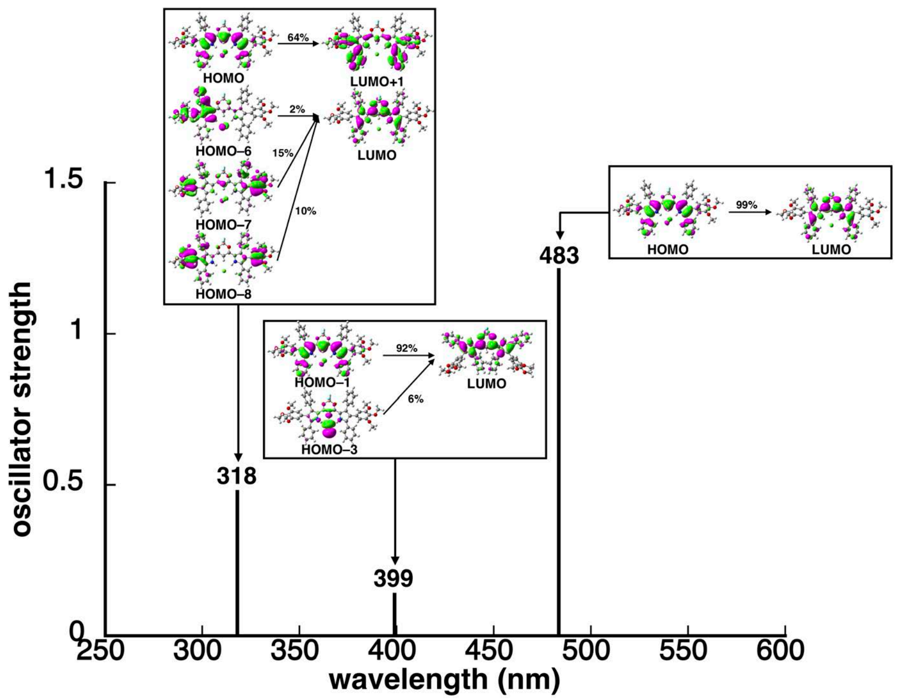
Supporting Figure 35 TD-DFT-based UV/vis absorption stick spectrum of **3a** with the transitions correlated with molecular orbitals estimated at PCM-B3LYP/6-31+G(d,p) in CH_2Cl_2//B3LYP/6-31+G(d,p).



Supporting Figure 36 TD-DFT-based UV/vis absorption stick spectra of **3a**·Cl^- with the transitions correlated with molecular orbitals estimated at PCM-B3LYP/6-31+G(d,p) in CH_2Cl_2//B3LYP/6-31+G(d,p).



Supporting Figure 37 TD-DFT-based UV/vis absorption stick spectra of **3b** with the transitions correlated with molecular orbitals estimated at PCM-B3LYP/6-31+G(d,p) in CH_2Cl_2//B3LYP/6-31+G(d,p).



Supporting Figure 38 TD-DFT-based UV/vis absorption stick spectra of **3b**·Cl^- with the transitions correlated with molecular orbitals estimated at PCM-B3LYP/6-31+G(d,p) in CH_2Cl_2//B3LYP/6-31+G(d,p).

Cartesian Coordination of 2a-1

-1833.5438533 hartree

H,-3.4559864894,2.8766479071,-0.2996814457
H,3.4563163177,2.8766986882,0.2998874133
O,-1.2280943595,2.950933062,0.0058637448
O,1.2282128065,2.9509962161,-0.0048034137
F,-0.0078395447,4.5767722965,-1.1439482079
F,0.0078966457,4.5728505496,1.1506632564
C,-1.2021996788,1.6390144028,0.0507088119
C,-2.5205307887,1.0489341278,0.1012269507
C,0.0000938507,0.9277712163,0.0008655847
C,1.2023315485,1.6390778428,-0.049478742
C,2.5206446724,1.0490216493,-0.1006957237
B,0.0000376846,3.8262827816,0.0020548717
N,-3.5864644386,1.883856453,-0.1690117622
N,3.5867227625,1.8839206883,0.1690464723
C,-3.0525326568,-0.2410915054,0.3154310241
C,3.0525204922,-0.2409945963,-0.3152299111
H,0.0001326271,-0.1502473498,0.0008957452
C,2.3776794187,-1.4906446651,-0.7187216033
C,1.4550426622,-1.5191517534,-1.7782816769
C,2.7247767085,-2.7042791324,-0.1014580409
C,0.8899356164,-2.7222434878,-2.1974454059
H,1.197651237,-0.5946853253,-2.2852300009
C,2.1623044392,-3.9069135626,-0.5250829952
H,3.4332325282,-2.6958902204,0.7216213495

C,1.2417533059,-3.9204273852,-1.5739018991
H,0.1815464257,-2.7238368612,-3.0206145458
H,2.441236984,-4.8340589679,-0.032625792
H,0.8028700969,-4.8572039842,-1.9039319317
C,-2.3779511687,-1.4907599945,0.7192966486
C,-1.4559587738,-1.5193193437,1.7794180536
C,-2.7247309606,-2.7043783947,0.1018212199
C,-0.8911359302,-2.7224354188,2.1988957792
H,-1.1988641116,-0.5948781646,2.2865611879
C,-2.1625515476,-3.9070372873,0.525763081
H,-3.4327009753,-2.6959573753,-0.7216757442
C,-1.2426168711,-3.9205977636,1.5751221712
H,-0.1832465487,-2.7240645612,3.022494854
H,-2.4412294482,-4.834167209,0.0331325145
H,-0.8039632901,-4.8573942014,1.9054012316
C,4.7646307921,1.2004696583,0.1514542309
C,-4.7643831203,1.2004048306,-0.1521187369
C,6.0570098891,1.8348083481,0.4146267806
C,6.1480291156,3.0436449359,1.127688858
C,7.2442203986,1.2371920666,-0.0447819501
C,7.385167491,3.6374975843,1.3657225826
H,5.2513713333,3.5115352605,1.5240172705
C,8.4794120316,1.8295671581,0.201683032
H,7.1921834518,0.3152632203,-0.6151248128
C,8.5563263055,3.0336679927,0.905133047
H,7.4339060368,4.5696715835,1.920482292
H,9.3845516051,1.3545838421,-0.1650011189
H,9.5202000013,3.4966448919,1.093060477
C,-6.0566165046,1.8347629566,-0.4159554511
C,-6.1472382433,3.0436674281,-1.1289535444
C,-7.2440842641,1.2370986261,0.0427262474
C,-7.3842441768,3.6375374194,-1.3676297768
H,-5.2503579755,3.5116002544,-1.5247277253
C,-8.4791388938,1.829492053,-0.2043801631
H,-7.192365841,0.3151175703,0.6130135451
C,-8.5556604285,3.0336592535,-0.907759854
H,-7.4326738653,4.5697642972,-1.9223276447
H,-9.3844834464,1.3544708908,0.1617483386
H,-9.5194295693,3.4966500521,-1.0961885537
C,-4.450222508,-0.1279315223,0.1450279923
C,4.4503078894,-0.1278432261,-0.145635943
H,-5.1590411165,-0.9368572914,0.2456213655
H,5.1590669641,-0.9367667149,-0.2466674088

Cartesian Coordination of 2a-2

-1833.5406601 hartree
H,-1.6887311533,-0.8014869475,-0.7479437492
H,3.5619150656,2.9056536006,0.2516194639
O,-1.1889185923,3.0315592717,0.1120021269
O,1.2638996647,3.0392052382,0.0377515116
F,0.0164665371,4.9893717083,-0.2657493704
F,0.093956119,4.0172533532,1.8182020826
C,-1.1744081253,1.7287270447,0.0841138171
C,-2.4404367844,1.0505897142,-0.0317940629
C,0.0397816167,1.0219483718,0.1204984696
C,1.238051599,1.7274085462,0.0265661687
C,2.5400755747,1.1116487774,-0.0824342886
B,0.0433138202,3.8356763342,0.4602232025
N,-2.4725775743,-0.2998045289,-0.3575418514
N,3.6465362934,1.9077383227,0.1202408462
C,-3.7732731783,1.4443730419,0.2263571369
C,3.0078449174,-0.1998912556,-0.2980306067
H,0.060635158,-0.0528593801,0.1973246018
C,2.2350836071,-1.4222703085,-0.6064125881
C,1.3262747704,-1.4620099901,-1.6792910797
C,2.438417054,-2.5933767578,0.1406309302
C,0.6310663802,-2.6329620306,-1.9817248741
H,1.1820371542,-0.5721605125,-2.2842349081
C,1.7450091057,-3.7654172831,-0.1637352602
H,3.1357575699,-2.5752627207,0.9727553938
C,0.8372888816,-3.7894187851,-1.2230299411
H,-0.0551552972,-2.6503758044,-2.8238779262
H,1.9136971536,-4.6592700041,0.4296298096
H,0.3026734484,-4.7030735786,-1.4655338321
C,-4.3278206023,2.7371894963,0.6797519447
C,-3.9735449504,3.9652343894,0.0970743689
C,-5.3083514658,2.7338606729,1.688768073
C,-4.5761604982,5.1487938529,0.5192552532
H,-3.2231563248,3.9924198321,-0.6818199193
C,-5.9066655314,3.9188464693,2.1107154299
H,-5.5830219026,1.7942762466,2.1590060533
C,-5.5423653857,5.13264416,1.5259315479
H,-4.2856128832,6.0877899995,0.0577237386
H,-6.6522790002,3.8941193408,2.9002638148
H,-6.0053247048,6.0585739701,1.8545815549
C,4.7954777584,1.1769628063,0.0550116939
C,-3.7551219731,-0.7702526442,-0.3480696672
C,6.1232785525,1.7628035708,0.245413012
C,6.2977371467,2.9669878644,0.9505974841
C,7.2604958362,1.1204829987,-0.2756910132
C,7.567480072,3.513360234,1.1212540719
H,5.4419242354,3.4677523981,1.3944228806
C,8.5287368304,1.6652552596,-0.0960338078
H,7.1431125682,0.2013552466,-0.8409864024
C,8.688631889,2.8653551182,0.6001955019
H,7.6810270565,4.4425453715,1.6714662287
H,9.3944231573,1.1562306985,-0.5093310419
H,9.6780794418,3.2910356648,0.7360309188
C,-4.0948939587,-2.1499915911,-0.6977866356
C,-3.1488948611,-3.1864085313,-0.5997537007
C,-5.3922096814,-2.4658511941,-1.1398777649
C,-3.4898796437,-4.4932027565,-0.9415253455
H,-2.148683339,-2.9798590181,-0.2301408724
C,-5.7308891552,-3.7744498659,-1.4716177566
H,-6.1285146498,-1.6749841453,-1.2410620118
C,-4.7811280894,-4.7942581243,-1.3776878214
H,-2.747293467,-5.2809022595,-0.8537257132
H,-6.7370392808,-3.9976350689,-1.8138175999
H,-5.0459561528,-5.8139362701,-1.6401297969
C,-4.570907957,0.2919315502,0.0328486316
C,4.4155134337,-0.1436567527,-0.2008446712
H,-5.6416699545,0.2457851616,0.166995576
H,5.086614929,-0.9830753983,-0.3115503892

Cartesian Coordination of 2a-3

-1833.5290259 hartree
H,-1.845823174,-0.6832910222,-1.0048890286
H,1.8026114074,-1.0008278616,0.5181294105
O,-1.2129310304,2.9878228094,0.2381265282
O,1.2380137117,2.942398916,0.0896147114

F,0.0105147133,4.8953790202,-0.2912162365
F,0.1531058376,4.0390209528,1.8394200284
C,-1.2169408705,1.6901175798,0.1517276153
C,-2.504068235,1.0461731621,0.0192530786
C,-0.0194967842,0.9574604261,0.1583079086
C,1.2070172667,1.6412475221,0.1160584734
C,2.479500995,0.9624533338,0.0740473951
B,0.0503837941,3.7833337584,0.4950767594
N,-2.5763951771,-0.2580045448,-0.4552570087
N,2.5462732042,-0.4232928181,0.1601509835
C,-3.8114390554,1.4244157924,0.3908048002
C,3.7963651938,1.4237064729,-0.1457357967
H,-0.0560805384,-0.1221320591,0.1647707652
C,4.3226043155,2.7902968351,-0.3499563924
C,3.9719173677,3.8682598183,0.4797782809
C,5.2773740203,3.0041567546,-1.3596257615
C,4.5557026886,5.1195973795,0.2959859607
H,3.2386188419,3.7280482841,1.2640247781
C,5.8555112475,4.2585435634,-1.5445932742
H,5.5498266551,2.1827528141,-2.0159390369
C,5.4968178316,5.3216018967,-0.7152673023
H,4.269594772,5.9409094318,0.9460220609
H,6.5817973975,4.4050253175,-2.3389191744
H,5.9443892555,6.3009526075,-0.8573680827
C,-4.3155710233,2.6552273508,1.0360112023
C,-3.9713749133,3.9440687151,0.5955227203
C,-5.2383983451,2.5328171159,2.0912801662
C,-4.5274492461,5.0698477298,1.2006936843
H,-3.266326207,4.0626806201,-0.216330003
C,-5.7898421173,3.660012409,2.6956561739
H,-5.5048556287,1.5436304822,2.4518250515
C,-5.4359080046,4.9348940486,2.2511430734
H,-4.2460923675,6.0571656163,0.8469778323
H,-6.4909356226,3.5421335629,3.5169358707
H,-5.8626587484,5.8158707728,2.7217122669
C,3.8387094281,-0.8548849587,0.0416363074
C,-3.8713335646,-0.7046605455,-0.446374758
C,4.207156439,-2.2671929634,0.142295747
C,3.2793346344,-3.2866027818,-0.1372565251
C,5.5106148809,-2.6335497089,0.5222131507
C,3.6404249823,-4.6275905179,-0.0297587532
H,2.278765454,-3.0298145324,-0.4745930063
C,5.8711272953,-3.9744861963,0.6185925597
H,6.2329796449,-1.8598526722,0.7617446458
C,4.9377604435,-4.9777901882,0.347747205
H,2.9109180896,-5.4002530659,-0.2536679626
H,6.8815487345,-4.2377863964,0.916651263
H,5.2199085688,-6.0230180364,0.428106654
C,-4.2499698179,-2.0231825145,-0.9545417602
C,-3.3225012404,-3.0790988162,-1.0095051986
C,-5.5624997266,-2.2612283993,-1.3998530074
C,-3.6927520787,-4.3278825514,-1.5031417912
H,-2.3138219115,-2.9323118863,-0.6329082672
C,-5.9321340599,-3.5133723837,-1.8824317104
H,-6.2851875104,-1.4517010641,-1.3844451616
C,-4.9991351449,-4.5513018509,-1.9409193301
H,-2.9629463745,-5.1315076421,-1.5342055378
H,-6.9496547236,-3.6769164628,-2.2245998762
H,-5.288408923,-5.5256313977,-2.3224816272
C,-4.6427693831,0.3123494732,0.1026516254
C,4.6222525599,0.2740581842,-0.1729197493
H,-5.7053061722,0.2642884473,0.2912927238
H,5.6897253084,0.2775039917,-0.3378214312

Cartesian Coordination of 2a·Cl⁻

-2293.9528391 hartree
H,1.7662997415,1.7470899362,-0.0073469616
H,-1.8201659898,1.7100251799,-0.056950084
O,1.2332904369,-2.2461319037,-0.2714167917
O,-1.2097929737,-2.263470761,-0.2557824266
F,0.0262293132,-4.1318766949,-0.9370476699
F,0.0226258915,-3.5307801489,1.2913225306
C,1.2131113277,-0.9540695163,-0.0360597899
C,2.4874860888,-0.2743388551,-0.0704095603
C,0.0034553774,-0.289942574,0.1999832535
C,-1.2000906736,-0.9773105807,0.0154572436
C,-2.4895007027,-0.3253485624,0.0629735294
B,0.0173807315,-3.0868246599,-0.033586728
N,2.5750742905,1.1083948056,0.0051769726
N,-2.6122556017,1.0550991888,0.0191336374
C,3.8101662593,-0.7805765093,-0.0803330086
C,-3.7957631446,-0.8658194033,0.10105578
C,-4.2535481559,-2.2676554049,0.2111433724
C,-3.6855504542,-3.1783553589,1.1190617875
C,-5.3451745381,-2.6976775824,-0.5648766886
C,-4.1889707462,-4.4731802525,1.2393865234
H,-2.8386968197,-2.8764362215,1.7243901142
C,-5.8512370318,-3.9936342696,-0.4426730685
H,-5.7839346396,-2.0132358449,-1.285571077
C,-5.2748449408,-4.8885069335,0.4619110459
H,-3.7237559889,-5.1612973502,1.9395787227
H,-6.688621691,-4.3049949408,-1.0621064485
H,-5.6607493374,-5.9002058035,0.5550023866
C,4.3248226742,-2.167542133,-0.1334064401
C,3.8973057946,-3.1035161527,-1.0909229082
C,5.3455520836,-2.5492010982,0.7575160967
C,4.4667591852,-4.3757385812,-1.1488004882
H,3.1072980272,-2.8361805199,-1.7815119135
C,5.9153143945,-3.822647316,0.7000016966
H,5.6764083132,-1.8437116257,1.5144958145
C,5.4778546148,-4.7430349973,-0.2558680079
H,4.110306831,-5.0848328534,-1.890733562
H,6.6927367016,-4.0970903068,1.4085305186
H,5.9133527405,-5.737821097,-0.2996571251
C,-3.9299229681,1.4146922484,0.0137508858
C,3.8817572027,1.5018148941,0.044518126
C,-4.4102247485,2.8010799378,-0.0306515335
C,-3.5367713506,3.902751535,0.0523865065
C,-5.791778229,3.0551521501,-0.1583142387
C,-4.0353608377,5.2057842226,0.0100976842
H,-2.4637370834,3.7564765672,0.1426759951
C,-6.2833531299,4.3582836399,-0.1957070623
H,-6.4872856872,2.2257449964,-0.236095779
C,-5.4065716161,5.4452692931,-0.1110955134
H,-3.3376207166,6.0362065859,0.0729105732
H,-7.3529564481,4.5246105021,-0.2952068065
H,-5.7879257207,6.4624154778,-0.1423155196
C,4.3278070873,2.8996373671,0.0984362414
C,3.4279768216,3.9805071283,0.0258128979
C,5.7031999672,3.1860025331,0.2248058664

C,3.8952643188,5.2948422711,0.0769322104
H,2.358710867,3.8097110306,-0.0666449778
C,6.1632519938,4.5001834736,0.2728029783
H,6.4194412839,2.3734832574,0.2909919712
C,5.2603782012,5.566353129,0.198426177
H,3.1776724637,6.1086027066,0.0201843658
H,7.2288215894,4.6913390104,0.3708399377
H,5.6172800429,6.5921057891,0.2365393843
C,4.6607147538,0.3399266405,0.0028428789
C,-4.6780718322,0.2329339948,0.0662252637
H,5.7399402461,0.2975756771,-0.0104794656
H,-5.7542741007,0.1651804892,0.1298146886
H,-0.0054661266,0.7662192035,0.4282676352
Cl,-0.040853633,3.1356418638,-0.0435596491

Cartesian Coordination of 3a-1

-2295.6609384 hartree
H,-3.4425659445,2.7713921762,0.0397211226
H,3.5008850902,2.6607618972,0.7129235493
O,-1.2052380187,2.8101918774,0.4092310753
O,1.2443188052,2.8122606876,0.3976971266
F,0.0129944588,4.7478151645,-0.0381829883
F,0.0295540596,3.8807424085,2.0887976496
C,-1.1852338938,1.4994637154,0.3191008718
C,-2.506766647,0.9137249041,0.2841550158
C,0.0170721125,0.7959589434,0.2030170083
C,1.2155504504,1.5161159769,0.1936453085
C,2.5306848195,0.9451087549,0.0025773138
B,0.0194034455,3.6253715924,0.7401461726
N,-3.5640560591,1.7689427093,0.066188873
N,3.6073866359,1.7060883038,0.4005552123
C,-3.0400537105,-0.3835158646,0.3950068871
C,3.0412874497,-0.2705258977,-0.4865269458
H,0.0192195942,-0.2752692298,0.0801559162
C,2.2840312345,-1.3827073911,-1.1034375939
C,1.4443662315,-1.1463978403,-2.20546123
C,2.436904629,-2.7017578195,-0.6474724974
C,0.7792199309,-2.1986581288,-2.832897472
H,1.3279108945,-0.1326236707,-2.5760679132
C,1.771682398,-3.7525772586,-1.2766156166
H,3.0842229428,-2.8991942919,0.2006773237
C,0.9435027089,-3.5058786455,-2.3724833842
H,0.1391635234,-1.9969452373,-3.6869464686
H,1.9020024565,-4.7663645397,-0.9096553674
H,0.4298265448,-4.3264818261,-2.864634395
C,-2.3135726398,-1.6339308857,0.7105606288
C,-1.5158440436,-1.7225546346,1.8644167413
C,-2.4561725167,-2.7748807455,-0.0951666403
C,-0.8783705098,-2.9161591043,2.1997495172
H,-1.4085323681,-0.8519155216,2.504050701
C,-1.8209958992,-3.9681707487,0.2438206238
H,-3.0718168553,-2.7220253222,-0.9870418459
C,-1.0315817965,-4.04401213,1.3921724882
H,-0.2693819885,-2.9661036309,3.0977172829
H,-1.9433406548,-4.8403182963,-0.3916476243
H,-0.5400715361,-4.9756249672,1.65673836
C,4.7792852996,1.0432013006,0.2042253397
C,-4.7442180753,1.0932520897,0.0217319999
C,6.0618657933,1.6768723518,0.5412908389
C,6.1563489017,2.5311539929,1.6551263528
C,7.2050531512,1.4779766616,-0.2525420496
C,7.3555519676,3.1703965763,1.9625919917
H,5.2927899262,2.6753794927,2.2984400687
C,8.4029341534,2.1147747293,0.0622908482
H,7.145901898,0.8350006253,-1.1231295616
C,8.4841549499,2.963841595,1.1681337043
H,7.4090362389,3.8233708526,2.8286176846
H,9.2746425896,1.9539464477,-0.5651189825
H,9.4195546064,3.4600148099,1.4086945733
C,-6.0100039725,1.8126322934,-0.1780951695
C,-6.0533627744,2.9488133132,-1.0067833091
C,-7.1886053978,1.4118896232,0.4754724638
C,-7.2371264004,3.6645340666,-1.172823622
H,-5.1611484158,3.2585222396,-1.5438204846
C,-8.3706832235,2.1274421292,0.3018417973
H,-7.1696144274,0.548095632,1.1298375956
C,-8.4010772655,3.2560509368,-0.5201538451
H,-7.2507753903,4.536933075,-1.8193319015
H,-9.2702219884,1.8068315153,0.818952653
H,-9.3244162863,3.8122494107,-0.65094759
C,-4.4516345578,-0.2689122918,0.220757567
C,4.4604675911,-0.2104977027,-0.3501423683
C,5.4281376503,-1.2735967136,-0.7121816236
C,6.3199463786,-1.7861733154,0.2446889774
C,5.4760787836,-1.7929945418,-2.0163257957
C,7.2350801269,-2.7824283463,-0.0933769897
H,6.2899385381,-1.3987358012,1.2584970362
C,6.3896482319,-2.7913794918,-2.3528638421
H,4.793090158,-1.4079742068,-2.7667980897
C,7.2731330737,-3.2890544332,-1.3935749227
H,7.9160008705,-3.1656853319,0.6612417109
H,6.4123078592,-3.1788091849,-3.3674078842
H,7.9846977997,-4.0662154579,-1.6568663702
C,-5.4358940234,-1.3774916822,0.2349375741
C,-6.2821394155,-1.5977529933,-0.8645637154
C,-5.5444761773,-2.2324428949,1.3439743664
C,-7.212528697,-2.6362988615,-0.8528051647
H,-6.2045296606,-0.9487151,-1.7315130194
C,-6.4734087794,-3.2724750328,1.3538976958
H,-4.8965186497,-2.0758057527,2.2004494619
C,-7.3114939887,-3.4777403707,0.2566066226
H,-7.8577080331,-2.790170072,-1.7130756523
H,-6.5435962196,-3.9216709096,2.2219484887
H,-8.0350474618,-4.2876860245,0.2655443744

Cartesian Coordination of 3a-2

-2295.6584808 hartree
H,-1.7152853359,-0.8716411394,-0.6342409311
H,3.5691302797,2.8872428857,0.16540974
O,-1.1968925988,3.0039143513,0.0581924705
O,1.2573910843,3.0101417262,-0.0162397187
F,0.0101447923,4.9409340912,-0.4193542086
F,0.0851402944,4.076101205,1.7114419504
C,-1.1780967305,1.7021415604,0.0894466694
C,-2.4452506003,1.0166371732,0.0112794451
C,0.0357750882,0.9972866537,0.1492650789
C,1.232721759,1.6996938315,0.0211049844
C,2.5363722559,1.0824281789,-0.0794704189
B,0.0343283723,3.826143627,0.3644769406
N,-2.4866097158,-0.3432044955,-0.2520691945

N,3.6426933333,1.8830092097,0.0818731764
C,-3.7686957529,1.4322794013,0.2514104216
C,2.9991439351,-0.2304061704,-0.2696328216
H,0.0562559918,-0.0742049972,0.2617497516
C,2.1705779731,-1.4362349545,-0.5069819363
C,1.3272746253,-1.5135967976,-1.6296673577
C,2.2165930817,-2.5288633585,0.3724133146
C,0.5415840462,-2.6440794715,-1.8562265479
H,1.2960642653,-0.6806289207,-2.3256006202
C,1.4324159161,-3.6605799464,0.1446890345
H,2.8685357972,-2.4854424772,1.2388698414
C,0.5911751718,-3.7218834502,-0.9671635857
H,-0.0962253835,-2.6916206853,-2.7344370793
H,1.4807233745,-4.4951878052,0.8379594156
H,-0.0169145564,-4.6032899904,-1.1470434476
C,-4.2418652611,2.77267319,0.6714060513
C,-3.9940643526,3.9168296297,-0.1026691015
C,-4.9918843913,2.9086099307,1.8513706587
C,-4.4801852823,5.1610119013,0.2951632753
H,-3.409341856,3.830766997,-1.0107744919
C,-5.4710381836,4.1544459738,2.2511142986
H,-5.1919714671,2.0323482531,2.4595260122
C,-5.2184292018,5.2849979588,1.4728576703
H,-4.2731929594,6.0357591369,-0.314021927
H,-6.0402033881,4.2411452588,3.1721517929
H,-5.5908701238,6.256707302,1.7840692912
C,4.7916743177,1.155728484,0.0095963288
C,-3.7718111785,-0.8023850699,-0.2279450163
C,6.1015447064,1.8117911129,0.1274785371
C,6.2689393182,2.9053396537,0.9964385288
C,7.1990902621,1.3906248701,-0.6436668722
C,7.4954758317,3.5600203208,1.0884098283
H,5.4417372016,3.2280868878,1.6225661334
C,8.4246172072,2.0443930231,-0.5435225079
H,7.0825271288,0.559487662,-1.3297459745
C,8.5786406752,3.1311943936,0.319986461
H,7.6058940205,4.3999160233,1.7677683258
H,9.2605607915,1.7090599556,-1.1502412513
H,9.5353579049,3.639424397,0.3933103381
C,-4.068107086,-2.2019077802,-0.564303746
C,-3.1843979849,-3.2257045875,-0.1766695065
C,-5.2145453953,-2.5460578651,-1.3022761671
C,-3.4397228979,-4.5524725203,-0.5186931698
H,-2.3057861442,-2.9843569035,0.414463205
C,-5.4664486589,-3.8737373591,-1.638395415
H,-5.898872803,-1.7671961636,-1.6185733959
C,-4.5817376847,-4.8823520526,-1.2497819407
H,-2.7516825476,-5.3306665172,-0.2011342979
H,-6.3546913966,-4.1206613875,-2.212262962
H,-4.7825791889,-5.9165760011,-1.5127146275
C,-4.6000467853,0.2792066396,0.1099797752
C,4.4225954877,-0.1865148772,-0.2031224594
C,5.34075296,-1.3445876957,-0.3065119081
C,6.2873701146,-1.6009542216,0.6999459254
C,5.2813689381,-2.2175287557,-1.4053412215
C,7.1515148769,-2.6907763117,0.6062474922
H,6.3398093628,-0.9401047163,1.5596385983
C,6.1437834097,-3.3096943972,-1.4963548088
H,4.5569813392,-2.0326704208,-2.1921273989
C,7.0830411296,-3.5497005571,-0.4922213731
H,7.8758243641,-2.8717482399,1.3952522944
H,6.0835332695,-3.9714644973,-2.3556154988
H,7.755253999,-4.3996684443,-0.5643741118
C,-6.0671020615,0.2181477621,0.3077713674
C,-6.6355711494,-0.715255783,1.1904666469
C,-6.9225094908,1.0923597583,-0.3830118595
C,-8.0166865872,-0.777842818,1.3710530298
H,-5.9863940883,-1.3899510762,1.7401765699
C,-8.3032467625,1.030023409,-0.2004154919
H,-6.4979298799,1.8237784675,-1.063093472
C,-8.8559500825,0.0941859564,0.6757488086
H,-8.436353041,-1.5052885332,2.0600421759
H,-8.9480116253,1.7143839348,-0.7442161022
H,-9.9316643533,0.047344004,0.817981218

Cartesian Coordination of 3a-3

-2295.646495 hartree
H,-1.8605560867,-0.8790136822,-0.7646410371
H,1.7631152348,-1.0030130902,-0.6071466439
O,-1.2222247185,2.9646801362,-0.1710470534
O,1.2173961716,2.9279089132,-0.3667740903
F,-0.0150561323,4.8813735735,-0.7219150319
F,0.1651602052,4.0212634973,1.4099551496
C,-1.2177533013,1.669340765,-0.0575877165
C,-2.4999312272,1.0040321011,-0.0401298413
C,-0.0084935493,0.9552080918,0.0149870242
C,1.2011576174,1.6391037828,-0.1866108006
C,2.4775879591,0.9620100714,-0.2228683958
B,0.0416293892,3.773516636,0.0633998436
N,-2.5791561943,-0.3567460665,-0.2878668683
N,2.5526394133,-0.4006283785,-0.4412014129
C,-3.7943591549,1.4393772579,0.2955411805
C,3.7946227047,1.4260122712,-0.0503482485
H,-0.0144296466,-0.0944270857,0.2750371499
C,4.2346339221,2.8143109538,0.2204669603
C,3.6495511115,3.5832118573,1.2397015249
C,5.2747133257,3.3803280755,-0.5343269643
C,4.0932480846,4.8789721806,1.4934544695
H,2.8298501513,3.178158939,1.8223804644
C,5.7162221133,4.6775785777,-0.2792613822
H,5.7324442959,2.8022545372,-1.3302302654
C,5.1290109967,5.4308107949,0.7374738032
H,3.620558732,5.4598484692,2.2795708537
H,6.5171874848,5.0996180978,-0.8794109618
H,5.4709277198,6.4425043722,0.9357179284
C,-4.2130029329,2.7852048665,0.7538532411
C,-4.0017528341,3.9294324375,-0.0310407818
C,-4.8718411055,2.9271132133,1.9867238478
C,-4.4336267084,5.1797820045,0.408406088
H,-3.4876586629,3.8386571473,-0.9801757259
C,-5.2966603895,4.1787803908,2.4269589464
H,-5.0430177438,2.050906597,2.6037463133
C,-5.0805723183,5.3095658386,1.6378285892
H,-4.2556202505,6.0543943791,-0.2099681792
H,-5.7948782387,4.2700702188,3.3877745213
H,-5.4107248486,6.2858792931,1.9806756844
C,3.8479472513,-0.8301617673,-0.4178625979
C,-3.8690217309,-0.796905657,-0.1760780963
C,4.1608348469,-2.2534135135,-0.6112811344
C,3.4236684564,-3.024295809,-1.5286732858

C,5.1704890107,-2.8841549819,0.13683006
C,3.6815780729,-4.384773986,-1.6871851194
H,2.6675807446,-2.5482644128,-2.1478449216
C,5.4288261588,-4.2424590415,-0.0292870404
H,5.7412752464,-2.3068788019,0.8550780895
C,4.6856978966,-4.9993107438,-0.9379852066
H,3.1062958316,-4.9610340317,-2.4058688473
H,6.2095316428,-4.7137889365,0.5602768326
H,4.8902464488,-6.0582334635,-1.0635252938
C,-4.2038273127,-2.1887198875,-0.5051570813
C,-3.2967086924,-3.2231490433,-0.2102902956
C,-5.4085752453,-2.5154525547,-1.1527528434
C,-3.5816834492,-4.5421187078,-0.5581987445
H,-2.3780495162,-2.9948226117,0.3235282923
C,-5.6916075196,-3.8356619565,-1.4929309296
H,-6.1130618181,-1.7284623767,-1.396067918
C,-4.780759109,-4.8535826464,-1.2005942929
H,-2.8721000335,-5.327834359,-0.3160085711
H,-6.624828751,-4.0695228829,-1.9965128678
H,-5.0055752154,-5.8814458664,-1.4686977726
C,-4.651869914,0.2963276809,0.2199963748
C,4.6547401836,0.2906863418,-0.1686022559
C,6.1323362209,0.2794692418,-0.0467580088
C,6.9366085913,-0.2278639752,-1.0802889771
C,6.759483776,0.772752976,1.1090975717
C,8.3257815017,-0.2475008328,-0.9590513142
H,6.4663377943,-0.6028081194,-1.9842922672
C,8.1484184073,0.7544496814,1.2285403413
H,6.1507253369,1.1740682576,1.9130042213
C,8.9367179849,0.2432757494,0.1959475365
H,8.930823522,-0.6418210557,-1.7704721694
H,8.6148483192,1.1404915571,2.1302882622
H,10.0186784902,0.2304038648,0.2894890931
C,-6.1006996843,0.258143273,0.5269694772
C,-6.6161793876,-0.6674602758,1.4493899145
C,-6.9909421604,1.1463716132,-0.0987585511
C,-7.9808967703,-0.7086418492,1.7320717653
H,-5.9383394894,-1.3526052388,1.9494011647
C,-8.3551000291,1.1051834105,0.1857669832
H,-6.6065715246,1.8715875093,-0.8087044507
C,-8.8556017975,0.1771413305,1.1007674064
H,-8.3597209904,-1.4300665634,2.4503910913
H,-9.0277349537,1.7998786003,-0.3088597459
H,-9.9183644505,0.1468688454,1.3224481202

Cartesian Coordination of 3a·Cl⁻

-2756.0804838 hartree
H,-1.7718268944,1.6861160814,0.1399741897
O,1.2173817248,-2.3265617256,-0.269222549
O,-1.2292468852,-2.3078703644,-0.2676885737
F,-0.0159201717,-4.1905673904,-0.9513898972
F,-0.0218133442,-3.600011766,1.279882471
C,1.2077059225,-1.0368140868,-0.0301251945
C,2.4844614011,-0.3567215807,-0.0784612857
C,0.0091508287,-0.3583060417,0.2111638735
C,-1.2034588209,-1.0256275968,0.0116712875
C,-2.4804197281,-0.3466222533,0.0547865375
B,-0.0138055956,-3.1522283631,-0.0416757144
N,2.5661838372,1.0237104293,-0.1161631501
N,-2.5726329958,1.0315422609,0.1257397254
C,3.8005921068,-0.8587091509,-0.0345769123
C,-3.7924408587,-0.8581017085,0.0094928599
C,-4.2149873919,-2.2776775886,-0.0790210187
C,-3.8664230275,-3.2064187161,0.9151904134
C,-5.0103305665,-2.7133362049,-1.1510511316
C,-4.2982126541,-4.5306329521,0.8378300921
H,-3.2371067789,-2.8922245597,1.7415736037
C,-5.4422532498,-4.0389676763,-1.2304013151
H,-5.2832264416,-2.0082262254,-1.9303580286
C,-5.0898621198,-4.9529658455,-0.2345015272
H,-4.00307026,-5.2354282356,1.61012636
H,-6.0502991213,-4.3566789784,-2.0734530405
H,-5.4198216165,-5.9865382063,-0.2974764422
C,4.2416551315,-2.2702140965,0.0991644892
C,3.9633188319,-3.2284086464,-0.8888172229
C,4.9948174065,-2.66462519,1.2178552389
C,4.4239891714,-4.5395096899,-0.7618813945
H,3.36603298,-2.9466009138,-1.7486918294
C,5.4529692119,-3.9770299177,1.3482061939
H,5.2148811518,-1.9363002447,1.9925796288
C,5.1717331356,-4.9198578427,0.3562699618
H,4.183872962,-5.2674369655,-1.5318248991
H,6.0260915562,-4.2619087629,2.2266594467
H,5.5227916993,-5.9433964186,0.4577339532
C,-3.8773899868,1.4208372341,0.131497935
C,3.867991255,1.4237811881,-0.1156469356
C,-4.2612543953,2.8386678427,0.2542119848
C,-3.4775099011,3.8534116679,-0.3267190285
C,-5.4081682276,3.2106291388,0.9825506035
C,-3.840003653,5.1942481452,-0.1908204282
H,-2.5666697571,3.6026856873,-0.8605641735
C,-5.7690713101,4.551565451,1.1096368322
H,-6.0107639933,2.4462976163,1.460041346
C,-4.9887054076,5.5512080725,0.5200286143
H,-3.2117656478,5.9591906137,-0.6380677585
H,-6.6559439427,4.8152140401,1.6799681056
H,-5.26745569,6.5965770169,0.6236996952
C,4.2401817864,2.8443489919,-0.2390547722
C,3.4418085722,3.8528141472,0.3325974897
C,5.3891613653,3.2255658131,-0.9593461032
C,3.7916683634,5.1967835259,0.1955834415
H,2.5289420686,3.594043613,0.8588798047
C,5.737846585,4.5696249059,-1.0871015109
H,6.0028400411,2.4657437208,-1.4298869714
C,4.9426553174,5.5630545582,-0.5068042077
H,3.1517991117,5.9567600614,0.6346893607
H,6.6266210704,4.8406490128,-1.6509664284
H,5.2116615672,6.6108664438,-0.6115058971
C,4.6730469289,0.2677106407,-0.0428890034
C,-4.6742819563,0.2589124654,0.0501602835
C,-6.1535571003,0.2039021638,-0.0187328643
C,-6.8588769658,0.939437346,-0.9885777681
C,-6.8925576026,-0.5970498933,0.8699916808
C,-8.2518338664,0.8847287872,-1.0611133056
H,-6.3050865597,1.558096339,-1.6883834876
C,-8.2857094272,-0.6568218905,0.7954811498
H,-6.3666871547,-1.1774304318,1.6215054187
C,-8.9732793103,0.0855050721,-0.1689286924
H,-8.7731146447,1.4639747804,-1.8188610547
H,-8.833369208,-1.2853294893,1.4928273508

H,-10.0574970444,0.0394599208,-0.2269098305
C,6.1507115062,0.2244940034,0.0528800982
C,6.834374503,0.9685498372,1.0318038467
C,6.9107691834,-0.574339361,-0.820122402
C,8.2262172388,0.9241691677,1.1279858455
H,6.2645436414,1.5852423662,1.7203618002
C,8.3027496081,-0.6236117339,-0.7220398675
H,6.4018768623,-1.1611758809,-1.5782783001
C,8.9685804305,0.1271518104,0.2510986053
H,8.7303806255,1.5097762623,1.892401978
H,8.8666423596,-1.2504929241,-1.4078262037
H,10.0519549954,0.0892855465,0.3276006992
H,0.0202364938,0.697877731,0.4393951347
Cl,-0.0123403716,3.0559035256,-0.0449286648

Cartesian Coordination of 3b-1
-2982.8901142 hartree
H,-3.4471847728,3.5315313319,-0.6987837249
H,3.4482957976,3.5714258931,0.4900582573
O,-1.2236696663,3.6442992103,-0.1956893533
O,1.2084806478,3.6580496552,-0.0322731422
F,0.0153583542,5.5722564303,-0.6596561597
F,-0.1200057276,4.8152689333,1.5161788829
C,-1.2170866958,2.3351370344,-0.0356582574
C,-2.5373353732,1.7517026855,-0.0589397919
C,-0.0126957344,1.6307619462,0.068476479
C,1.1909060923,2.3424010684,0.0039486809
C,2.5119701799,1.7578357132,-0.0003707241
B,-0.0331234457,4.4787897514,0.1718405246
N,-3.5742216858,2.5497448354,-0.4932371803
N,3.5662504762,2.5787573716,0.3391274826
C,-3.0882571838,0.4952883997,0.2599019506
C,3.0466463003,0.480273131,-0.2531013077
H,-0.0087509327,0.554993219,0.1491142866
C,2.3328110914,-0.7192280946,-0.7483954932
C,1.5820765731,-0.6613943472,-1.9363283236
C,2.4542080492,-1.9553310656,-0.0916113601
C,0.9740194158,-1.8065794683,-2.4536711507
H,1.4895610336,0.2842690749,-2.4624559609
C,1.8486812409,-3.1004260948,-0.6112165326
H,3.031035873,-2.0172960551,0.8255918743
C,1.1094689659,-3.0318624491,-1.7949742211
H,0.4009801114,-1.7414954043,-3.3743898963
H,1.9560657102,-4.0469890543,-0.0894726625
H,0.641197579,-3.924511,-2.1997175823
C,-2.3969149253,-0.6716113896,0.8559797794
C,-1.7092035768,-0.5452843203,2.076264793
C,-2.4765481201,-1.9407170043,0.2589804633
C,-1.1178125912,-1.6562547244,2.6806298229
H,-1.6502692313,0.426996094,2.5568298083
C,-1.887978748,-3.0512949124,0.8654241477
H,-3.0059557217,-2.0538753563,-0.6816795811
C,-1.2086784742,-2.9144185228,2.0787725596
H,-0.5911949683,-1.5384651628,3.6234914681
H,-1.9601678232,-4.0243980099,0.3883965328
H,-0.7513437596,-3.779637809,2.5500336022
C,4.7438666946,1.8953183539,0.333150636
C,-4.7550963417,1.8725112124,-0.4825098847
C,6.0078430428,2.5743605285,0.6553706849
C,6.038239497,3.5944811882,1.6251807013
C,7.2005455784,2.2492026681,-0.0163499237
C,7.223734507,4.2729458553,1.9101716653
H,5.1365045137,3.8417476787,2.1787183576
C,8.3838184851,2.927338761,0.2739722634
H,7.1937496055,1.4727614034,-0.7731903201
C,8.401858514,3.9420016234,1.2359987123
H,7.2268418103,5.053985726,2.6647708316
H,9.2938552874,2.6675851239,-0.2591815669
H,9.3251898891,4.468680951,1.4581956002
C,-6.0027221082,2.5357157521,-0.8902612283
C,-5.9943157285,3.4823261351,-1.9324738221
C,-7.2175132155,2.2708075102,-0.2318341798
C,-7.1642737375,4.1467538469,-2.3019848839
H,-5.0740699884,3.6814842581,-2.4749195927
C,-8.3851755999,2.9338941919,-0.6069927674
H,-7.2409507661,1.5528187199,0.5802353119
C,-8.3648502908,3.874601028,-1.6412778938
H,-7.1380484396,4.8697601976,-3.1119537882
H,-9.3132786084,2.7191287538,-0.0853924663
H,-9.2765258069,4.3889094437,-1.9303556604
C,-4.4859929866,0.5708957741,-0.0170986649
C,4.4536779937,0.5671732398,-0.0314356998
C,5.4337843834,-0.5409780855,-0.1489639595
C,6.1914292847,-0.9365436819,0.9527245945
C,5.6063903939,-1.2063777227,-1.3755758954
C,7.1251917574,-1.9788077144,0.8503613028
H,6.0786943656,-0.4492012481,1.9148444775
C,6.5156901258,-2.2598516335,-1.4817255604
H,5.0105117154,-0.9051338306,-2.2273352904
C,7.3004086659,-2.6534108784,-0.3704757458
C,-5.4790507658,-0.5191136346,0.1464662101
C,-6.2495673778,-0.9487948854,-0.9388978761
C,-5.6494031201,-1.137553846,1.3976417376
C,-7.1936513506,-1.9690075586,-0.7788949372
H,-6.1393365654,-0.4964374162,-1.9184505575
C,-6.5823413668,-2.1658183414,1.5600999471
H,-5.0438475243,-0.8095195617,2.2327612229
C,-7.3794403319,-2.5799227261,0.4698482804
O,-7.9738773685,-2.3121388771,-1.8581724453
O,-8.283027721,-3.6062570557,0.6020441577
O,-6.8077487041,-2.8222186367,2.7361074491
O,7.7557432247,-2.3175610039,2.0165185956
O,8.1183013719,-3.7569278456,-0.4285967473
O,6.6991403617,-2.9957916748,-2.6198650954
C,-7.7590280283,-3.6247722324,-2.3963395738
H,-6.7294939485,-3.721547748,-2.7646666485
H,-7.9633126015,-4.3971223815,-1.6496762421
H,-8.4532614971,-3.7226175877,-3.2331865911
C,-9.4976839564,-3.2660769419,1.2862836028
H,-10.1083674691,-4.1710057923,1.2857399174
H,-9.2927348874,-2.961579368,2.3174780614
H,-10.0255595515,-2.4659519234,0.7537383281
C,-5.9984946675,-2.4939765684,3.8614136671
H,-4.9363155983,-2.6650461696,3.6509512701
H,-6.1479419065,-1.4521984188,4.17150306
H,-6.3235769053,-3.1600828423,4.6615594415
C,9.1388224124,-2.6841963489,2.0124056618
H,9.2779655267,-3.721541259,1.7022544386
H,9.7162871527,-2.0208476321,1.3571018624
H,9.4769794587,-2.5526644504,3.0424505753

C,9.2484145854,-3.6887295858,-1.3096273924
H,9.7894365531,-4.6272928357,-1.1734639517
H,8.9339335237,-3.5899110529,-2.350894828
H,9.9002454518,-2.8484274828,-1.0369237517
C,5.8645434696,-2.7298695195,-3.743203569
H,4.8057756297,-2.8594899264,-3.4909658418
H,6.0280340034,-1.7174729881,-4.1327978564
H,6.1513516617,-3.4597815436,-4.5013469175

Cartesian Coordination of 3b-2

-2982.8782282 hartree
H,-1.2904590731,-1.0764214902,-0.5443036995
H,3.4071188986,3.5217820877,-0.1934194528
O,-1.3048239645,2.9125900008,-0.3632364977
O,1.1153226126,3.2640773236,-0.384083205
F,-0.373735201,4.9785113272,-0.9444281077
F,-0.2446012201,4.2622913123,1.2477653947
C,-1.108330126,1.6335581613,-0.1879657547
C,-2.2723114142,0.7833768778,-0.2142360841
C,0.1919448982,1.1207679953,-0.0282354254
C,1.2838304652,1.9733969819,-0.1955014944
C,2.6675959874,1.5591208996,-0.1842838835
B,-0.216504943,3.9127356451,-0.0932706707
N,-2.1404029895,-0.5955610146,-0.2859350194
N,3.6339761537,2.5384187001,-0.1285238052
C,-3.6479063666,1.0612417467,-0.091072222
C,3.3325729888,0.3203242945,-0.1717497039
H,0.3624296481,0.0793758442,0.1931392213
C,2.7166275533,-1.028410003,-0.2285493737
C,2.0201948624,-1.4513121748,-1.3745375566
C,2.8431170575,-1.9211531853,0.8477129589
C,1.4596370636,-2.7290849045,-1.4387393723
H,1.9287980343,-0.7756092201,-2.2203126225
C,2.2836916826,-3.1998046033,0.7839225801
H,3.3835643437,-1.6087510539,1.7359661061
C,1.5903458723,-3.6081368255,-0.3584064635
H,0.935391658,-3.0437815002,-2.3368555299
H,2.3949479693,-3.8775764769,1.6254824397
H,1.1632612288,-4.6051173791,-0.4127532174
C,-4.2986428793,2.3783569219,0.1160123544
C,-4.2082544399,3.4015973363,-0.840377429
C,-5.0589322259,2.6041739741,1.2755337192
C,-4.8600430247,4.6190635696,-0.6412990102
H,-3.6159435907,3.2467908682,-1.7354394066
C,-5.7036887457,3.8250719137,1.4783267816
H,-5.137080303,1.8204001134,2.0229181284
C,-5.6084138794,4.8359291456,0.5185187598
H,-4.772661474,5.4017311963,-1.3890365008
H,-6.2789093692,3.9860325584,2.3856750715
H,-6.1093923835,5.7869074224,0.6752000522
C,4.8820804288,1.9956976732,-0.0774120596
C,-3.3637601097,-1.2007509248,-0.2507104183
C,6.0743798178,2.8552283769,-0.0342944328
C,6.0463119641,4.0726364737,0.6724880327
C,7.2515286188,2.501239365,-0.7186307436
C,7.1603198486,4.9125308503,0.6897034147
H,5.1588828707,4.3529246034,1.2334341268
C,8.3643144806,3.3410343316,-0.6944664522
H,7.2864787834,1.5728475791,-1.2778975881
C,8.3243338774,4.5497880582,0.0073036814
H,7.1203347431,5.8453646648,1.2443665229
H,9.2633565374,3.0536844037,-1.2319208458
H,9.1925726026,5.2018392453,0.0230492244
C,-3.4827062102,-2.6594523035,-0.3941767844
C,-2.5387051974,-3.5139766073,0.2057902826
C,-4.5203388633,-3.2299593993,-1.1542508882
C,-2.6294067383,-4.8977960664,0.0484501781
H,-1.745835784,-3.0963783005,0.8201520398
C,-4.6082771857,-4.6129872364,-1.3070335368
H,-5.2500151321,-2.584879683,-1.631275833
C,-3.6645826152,-5.4532383602,-0.7078707795
H,-1.8978905225,-5.5417630341,0.5280527502
H,-5.4139479205,-5.035700111,-1.9002205019
H,-3.737808091,-6.5301978621,-0.8267468995
C,-4.3304381609,-0.1926642186,-0.1052261487
C,4.72900405,0.5950946325,-0.0942953358
C,5.8154845002,-0.4093010227,-0.0041168731
C,6.7217562823,-0.3855563461,1.0684331871
C,5.9543912769,-1.4061248889,-0.9758849451
C,7.7333117876,-1.3379274237,1.15662688
H,6.6446258885,0.361063316,1.8516770249
C,6.9789991631,-2.3593526399,-0.9071035026
H,5.2752391048,-1.4604361285,-1.8194362163
C,7.894051283,-2.3274817208,0.1645998437
C,-5.790279238,-0.4058395503,0.0375277919
C,-6.2959844684,-1.2525938522,1.0371245743
C,-6.6921095394,0.2312868022,-0.8207219568
C,-7.6681683653,-1.4475507234,1.1647772697
H,-5.6349091242,-1.7550012383,1.7352987405
C,-8.0744822807,0.0287136849,-0.7134689647
H,-6.3422880993,0.9003114944,-1.5989530811
C,-8.5799719996,-0.8308812703,0.2832778218
O,8.6005733672,-1.2957189407,2.2311781411
O,8.8533236542,-3.308054466,0.2867598142
O,6.9675551448,-3.3144288761,-1.8874732045
O,-8.8440874305,0.7591033588,-1.5765333603
O,-9.9393669342,-0.975144141,0.4557736702
O,-8.136261094,-2.2757117687,2.1673033161
C,8.323178021,-2.2574640718,3.2601193008
H,7.3334428909,-2.0766822595,3.6972335166
H,8.3732669125,-3.2793047441,2.8687592754
H,9.0894021151,-2.1149715578,4.0245978778
C,10.2209394007,-2.8699694813,0.212666385
H,10.83027863,-3.7637594288,0.3600113383
H,10.43252318,-2.4421279859,-0.775307079
H,10.4416017871,-2.1328626717,0.9885499029
C,8.1948881467,-3.747160492,-2.4830963835
H,8.8408635239,-2.8898256698,-2.709655469
H,8.726538228,-4.4517186575,-1.8406524095
H,7.9087002084,-4.2355641448,-3.416775043
C,-8.6567004294,-1.5864588541,3.3142796157
H,-9.4970763828,-0.9405160371,3.038298124
H,-8.9948248872,-2.3599111068,4.0067039508
H,-7.8711339544,-0.9873157734,3.7908486442
C,-10.4695689305,-2.2915502929,0.2287462949
H,-9.9901016953,-3.0272928643,0.879181419
H,-11.5357436897,-2.2291297639,0.4555062878
H,-10.3361445775,-2.5824426993,-0.8209514921
C,-10.0198061629,0.1915903069,-2.1610454768
H,-9.8251149767,-0.8277057098,-2.5172657734

H,-10.8552172279,0.1841796497,-1.458410256
H,-10.2550635143,0.8297931171,-3.0151881253

Cartesian Coordination of 3b-3

-2982.8661436 hartree
H,1.8264040388,1.6329450177,-0.6880466796
H,-1.7924875075,1.6774108316,-0.2695298262
O,1.2124503221,-2.28142714,-0.7035557614
O,-1.2331463873,-2.2605231477,-0.6612780497
F,-0.0345852426,-4.1249748887,-1.4158040791
F,-0.0014600061,-3.5862353086,0.8324863526
C,1.2180786462,-1.0171184698,-0.3880751441
C,2.5003135487,-0.3530530793,-0.3687567157
C,0.015331859,-0.3398341412,-0.1159838793
C,-1.2077166202,-1.0021233227,-0.3209098307
C,-2.4851493593,-0.3360056387,-0.2064147696
B,-0.0163751313,-3.1287649157,-0.4762985825
N,2.5744206419,1.0320472487,-0.3761664955
N,-2.5746310011,1.045356023,-0.208979708
C,3.8138305788,-0.8369671551,-0.2275557003
C,-3.7969471393,-0.8324139377,-0.0958110715
H,0.0385558442,0.6662172342,0.2798815039
C,-4.2221223254,-2.2513932258,-0.0450643068
C,-3.7158145307,-3.1263472379,0.9289090044
C,-5.1667644683,-2.7375314331,-0.963061787
C,-4.1391821395,-4.454340076,0.9795264212
H,-2.9787329799,-2.7704197666,1.6416235562
C,-5.5879176957,-4.0672421241,-0.9138602024
H,-5.5640974095,-2.0726142192,-1.7237894673
C,-5.0768169838,-4.929906753,0.0588364517
H,-3.7278444283,-5.1184522363,1.7337919747
H,-6.3133138428,-4.4285615481,-1.6373127079
H,-5.4023812503,-5.9654494782,0.0964969114
C,4.2536468964,-2.2430173742,-0.0563715066
C,4.0214532685,-3.2110285911,-1.0459600701
C,4.9525110908,-2.6183244764,1.1036049472
C,4.4756061065,-4.5198739931,-0.8788359342
H,3.4746040676,-2.9402050267,-1.9420276739
C,5.3993778831,-3.9290291154,1.2735007728
H,5.1373996992,-1.879963972,1.8779302266
C,5.1648883065,-4.8838121655,0.2805376255
H,4.2799811522,-5.2568235784,-1.6520407833
H,5.9293836438,-4.2037530156,2.1810649425
H,5.5122829206,-5.904592553,0.4115210497
C,-3.8741531136,1.4516765439,-0.1044613403
C,3.8752449722,1.4477310283,-0.2950554063
C,-4.2059404068,2.8842153844,-0.0685360084
C,-3.502108297,3.7998470782,-0.8739401186
C,-5.2056308579,3.3757349654,0.7907666331
C,-3.7836232945,5.1657790297,-0.8165929883
H,-2.7561769995,3.4387855198,-1.5775708275
C,-5.4874972862,4.7403029558,0.8415723438
H,-5.7526858879,2.6852828914,1.4232401356
C,-4.7779849404,5.6415668411,0.0417278587
H,-3.2359089695,5.8548246414,-1.4529849929
H,-6.2607144653,5.1020007597,1.5130659787
H,-5.0015128365,6.7033744878,0.0838039116
C,4.2028600371,2.8776942087,-0.3885455235
C,3.3622775334,3.8394285729,0.204161424
C,5.3354470378,3.3193006909,-1.0969891469
C,3.641639074,5.2017366795,0.0862515397
H,2.5055800828,3.5170534737,0.7902861395
C,5.6135223977,4.6809356863,-1.2087686956
H,5.9885239793,2.5914275933,-1.5656619743
C,4.7686646184,5.6278865959,-0.6210544163
H,2.9864647681,5.9281881178,0.5582595852
H,6.4903079968,5.0042359051,-1.76221198
H,4.9896189614,6.6873516585,-0.7099819907
C,4.6757497586,0.3034488885,-0.1697059275
C,-4.6689826502,0.296772497,-0.0290945987
C,-6.1468989579,0.2665477266,0.088918893
C,-6.9556992491,0.9109924258,-0.8605770287
C,-6.7622654157,-0.4058213656,1.1494694084
C,-8.3421979066,0.8760194419,-0.7415092036
H,-6.5225025469,1.4295659541,-1.7093125303
C,-8.1562045235,-0.4318451007,1.2904068987
H,-6.1721466814,-0.9259894941,1.8957340915
C,-8.9670988858,0.2257796924,0.3426804509
C,6.1446293679,0.2909629693,0.0278278707
C,6.7295784413,1.0170283738,1.0779268702
C,6.9743827462,-0.4456670056,-0.82311387
C,8.1086413143,0.9946526456,1.2637096334
H,6.1225495924,1.5887094541,1.7718714265
C,8.3661232274,-0.459190844,-0.658638106
H,6.5599315219,-1.0279789113,-1.6385198458
C,8.9529241717,0.2770441724,0.3913116387
O,-10.3396504437,0.1364904175,0.4206813405
O,-8.6271595262,-1.1731593887,2.338383323
O,-9.1116134789,1.5065458649,-1.7006937035
O,8.6540020884,1.7032812806,2.317508243
O,10.3092385462,0.2024241085,0.621081433
O,9.050243215,-1.2652561647,-1.5253861488
C,10.3374585346,-0.8836104868,-2.0189140208
H,11.1219747701,-1.0683279078,-1.2826972853
H,10.5018728099,-1.5016945759,-2.9038702392
H,10.3460044593,0.1733260638,-2.3122536123
C,11.0454411852,1.4281771468,0.4763500974
H,11.0022272262,1.7804293397,-0.5620963819
H,10.6588279369,2.201545454,1.1447074742
H,12.0787415364,1.1901746157,0.7363628618
C,9.0130167415,0.8991004836,3.4517419553
H,8.1252521503,0.4103753461,3.8714368829
H,9.7564233876,0.1424165695,3.1789186166
H,9.4344026519,1.5844391314,4.1897657489
C,-9.7647765693,-0.7353591068,3.0871074431
H,-10.6981629228,-0.9466438368,2.5618872905
H,-9.7277048252,-1.2956150468,4.0235688105
H,-9.6976977412,0.3372712021,3.3074443836
C,-11.0448077642,1.3707949302,0.632384335
H,-10.832265634,2.0883207575,-0.1640749295
H,-12.1059590189,1.113966488,0.6323664412
H,-10.7744062067,1.8046760888,1.6034103588
C,-9.7045303087,0.6222461587,-2.6644505687
H,-10.3654822271,-0.1037434733,-2.1790190258
H,-10.2811863678,1.2540671584,-3.3428483977
H,-8.9268596993,0.0938803019,-3.229419945

Cartesian Coordination of 3b·Cl⁻

-3443.2272882 hartree
H,1.7688401668,1.7016859428,-0.2083565548

H,-1.7701363542,1.7213935847,0.1128767078
O,1.2181249085,-2.293008267,-0.2885285582
O,-1.2285910617,-2.2737779742,-0.2841965877
F,-0.0162973457,-4.1561545381,-0.9708533359
F,-0.0199307431,-3.567530667,1.2608510155
C,1.209241099,-1.0029395957,-0.0485124306
C,2.4861919562,-0.3242297665,-0.0948378913
C,0.0110793577,-0.3241811179,0.1928544738
C,-1.201617867,-0.9911159976,-0.0050636147
C,-2.4780258793,-0.3121488758,0.0423834118
B,-0.0130237834,-3.1179689315,-0.0606135463
N,2.571777988,1.0561359136,-0.1231010771
N,-2.5710154834,1.0660354946,0.1072388357
C,3.8010457649,-0.829654194,-0.0570775561
C,-3.7898910663,-0.8250618076,0.0126225572
C,-4.2137716766,-2.2450918158,-0.0594561796
C,-3.8499318701,-3.1672416344,0.9356387476
C,-5.0295517905,-2.6871115193,-1.1136287682
C,-4.288071545,-4.4906812228,0.8775482176
H,-3.2028414941,-2.8491529745,1.7467020656
C,-5.4675366809,-4.0118399891,-1.1739850172
H,-5.3137367141,-1.987456922,-1.8937397211
C,-5.1011806933,-4.9189836555,-0.176432733
H,-3.9792206569,-5.1907328955,1.6489093335
H,-6.0905245199,-4.3346497013,-2.0041053427
H,-5.4347317532,-5.9521784537,-0.2255514651
C,4.2388045946,-2.2437228944,0.0602944551
C,3.9586524356,-3.1891649358,-0.9395794211
C,4.9925001099,-2.6534098515,1.1731240086
C,4.4200854209,-4.5019656629,-0.8310457581
H,3.3579620718,-2.8965663522,-1.7935918478
C,5.4518215839,-3.9671728119,1.2850933247
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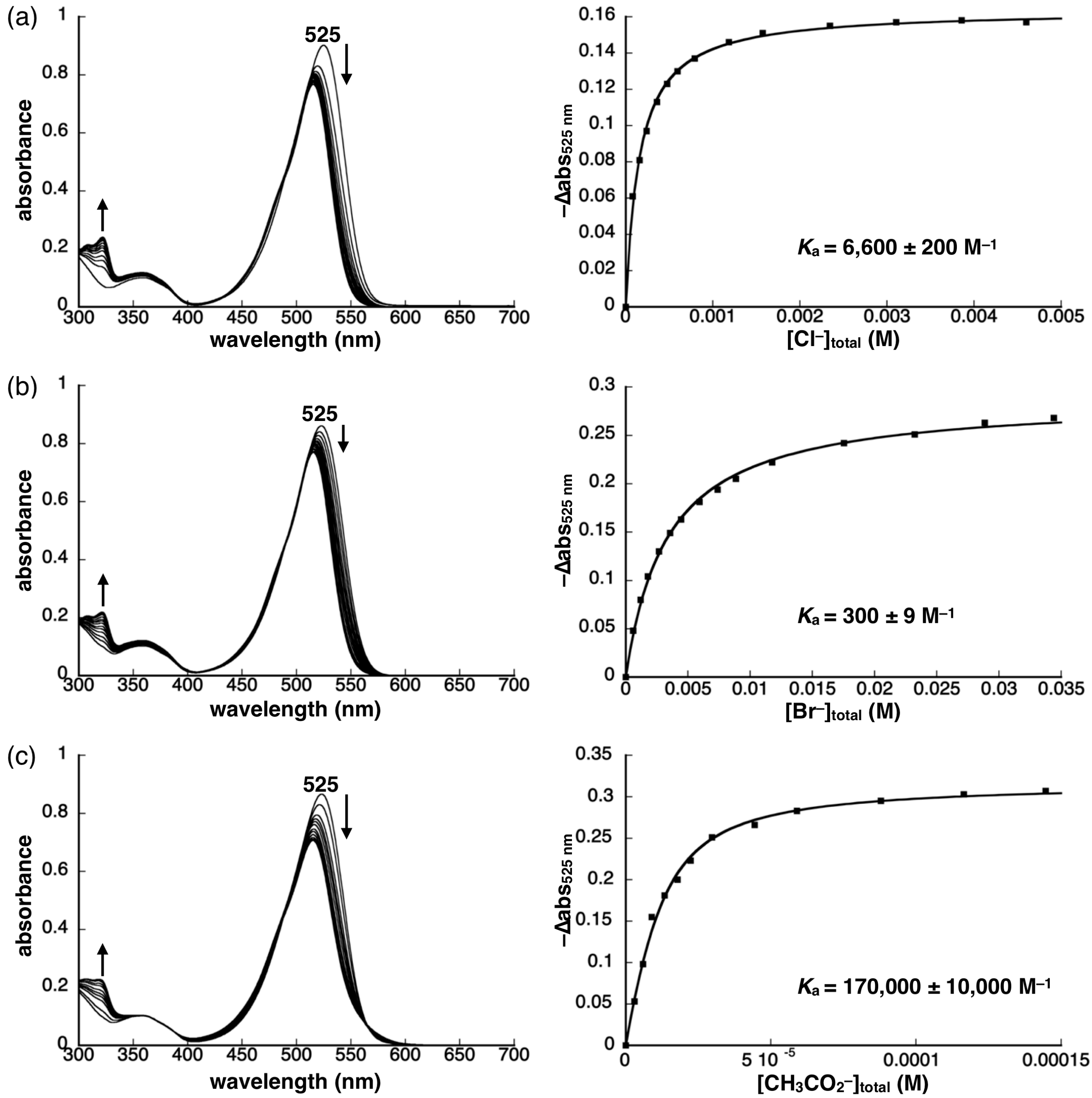
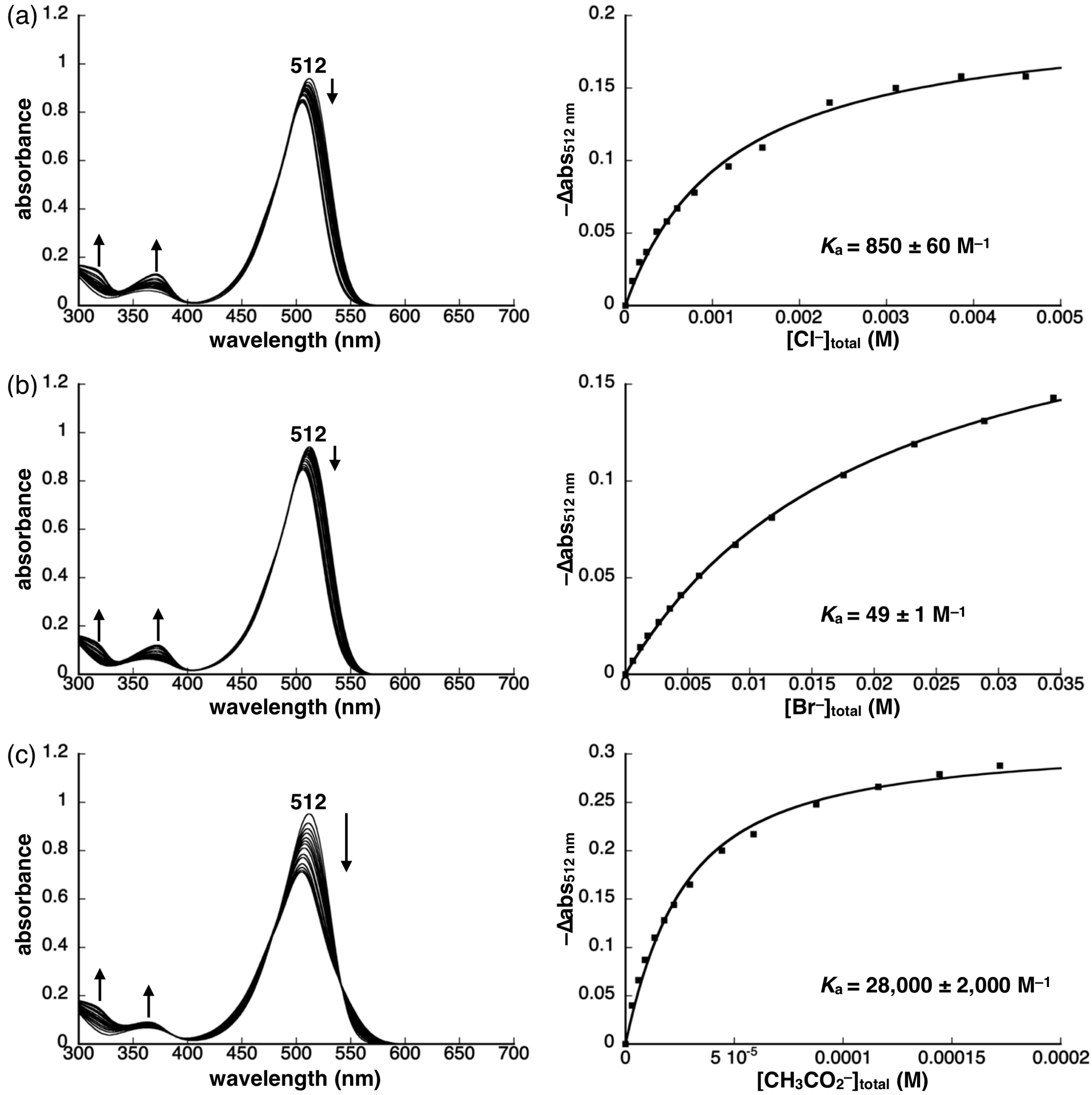
[S7 (the complete form of ref. 7)] *Gaussian 09* (Revision D.01), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R.

Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

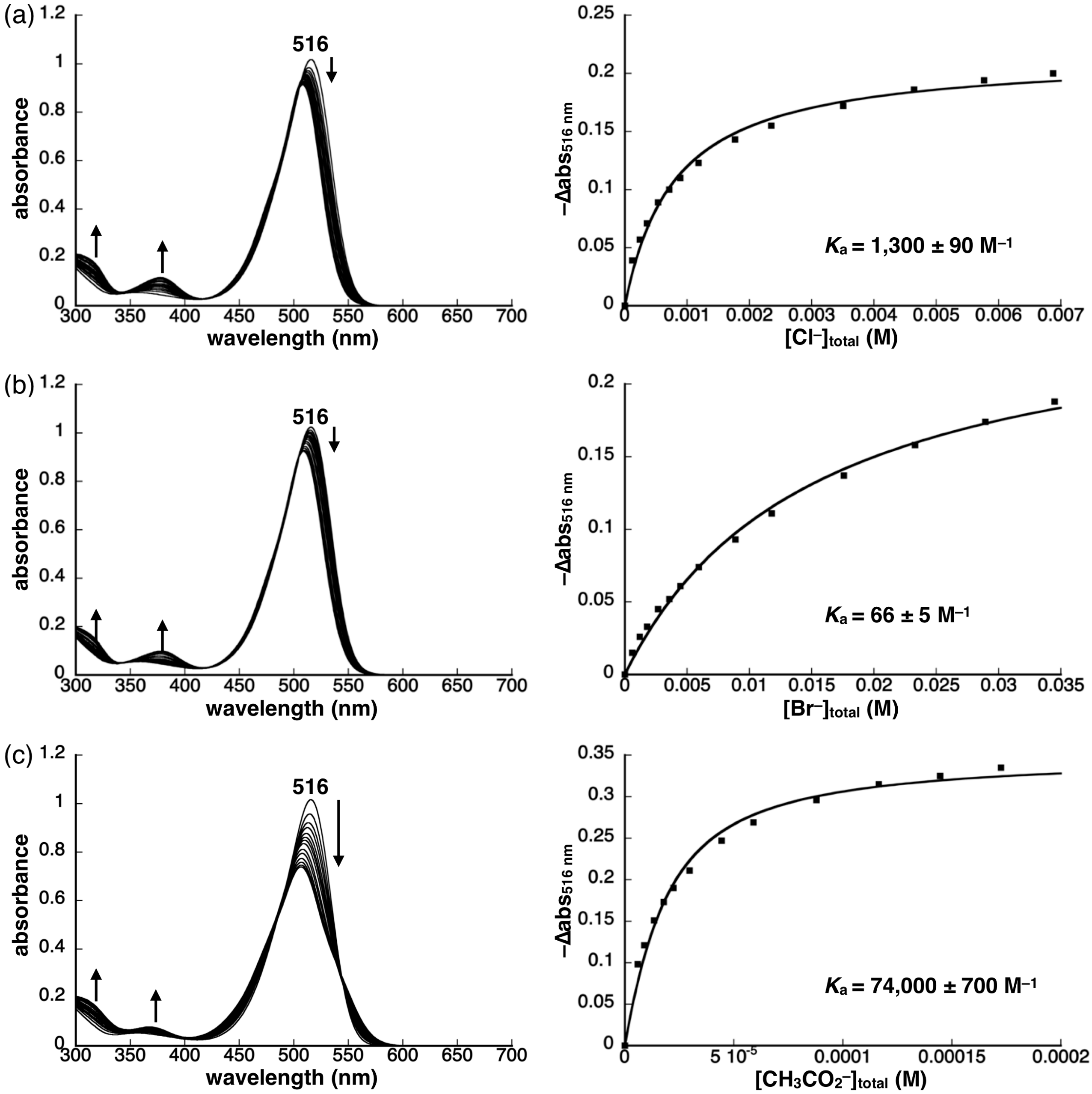
4. Anion-binding behaviors



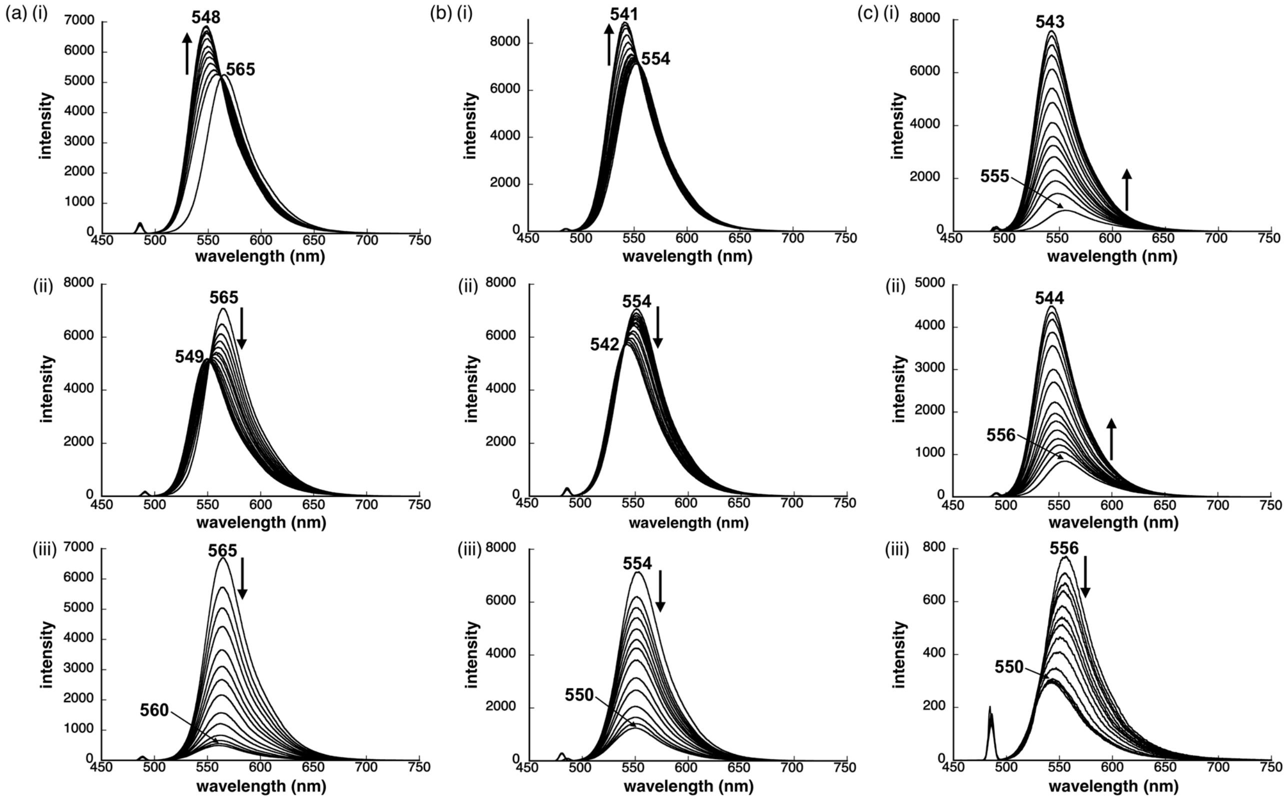
Supporting Figure 39 UV/vis absorption spectral changes (left) and titration plots and 1:1 fitting curves (right) of **2a** (1.0×10^{-5} M) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as tetrabutylammonium (TBA) salts in CH_2Cl_2.



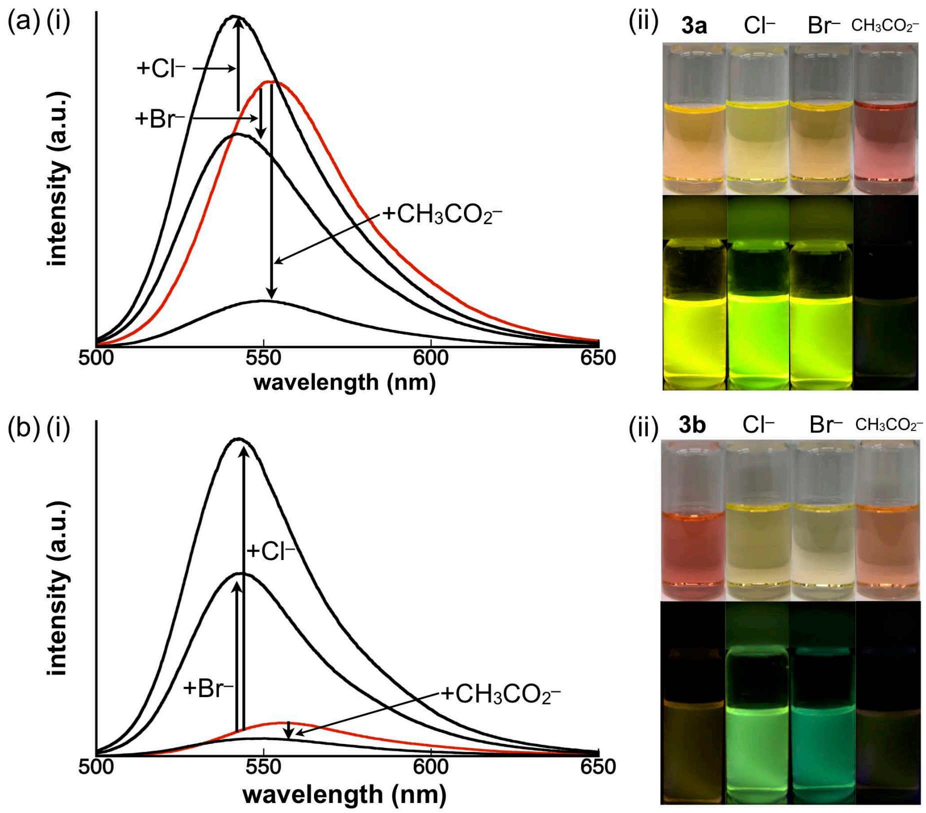
Supporting Figure 40 UV/vis absorption spectral changes (left) and titration plots and 1:1 fitting curves (right) of **3a** (1.0×10^{-5} M) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2.



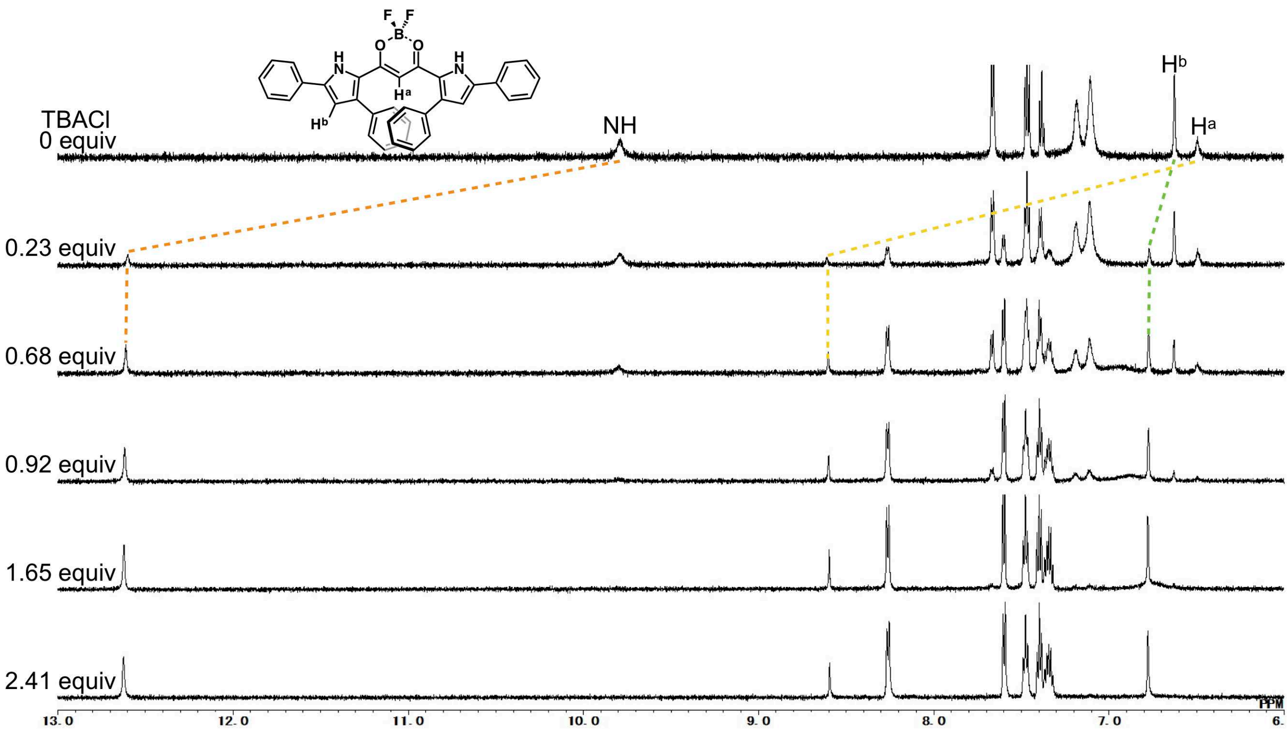
Supporting Figure 41 UV/vis absorption spectral changes (left) and titration plots and 1:1 fitting curves (right) of **3b** (1.0×10^{-5} M) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2.



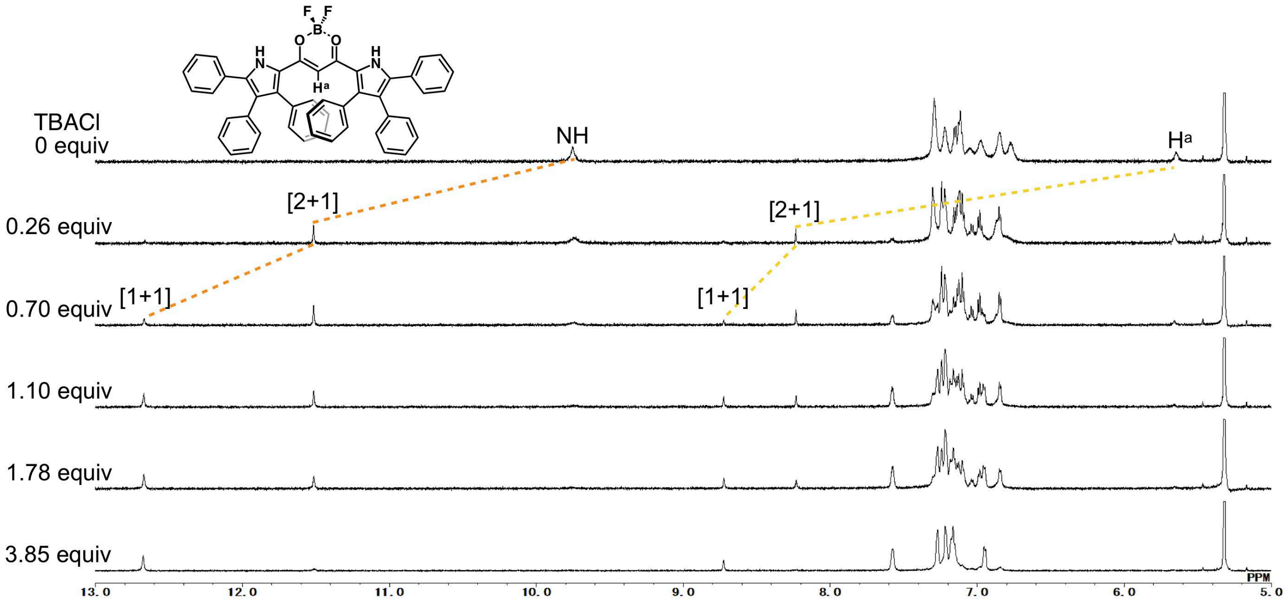
Supporting Figure 42 Fluorescence spectral changes of (a) **2a**, (b) **3a**, and (c) **3b** (1.0×10^{-5} M) upon the addition of (i) Cl^-, (ii) Br^-, and (iii) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2 excited at respective isosbestic points of UV/vis absorption spectral changes at 485 (**2a**), 480 (**3a**), and 490 (**3b**) nm for Cl^- and Br^- and 488 (**2a**), 478 (**3a**), and 485 (**3b**) nm for $CH_3CO_2^-$.



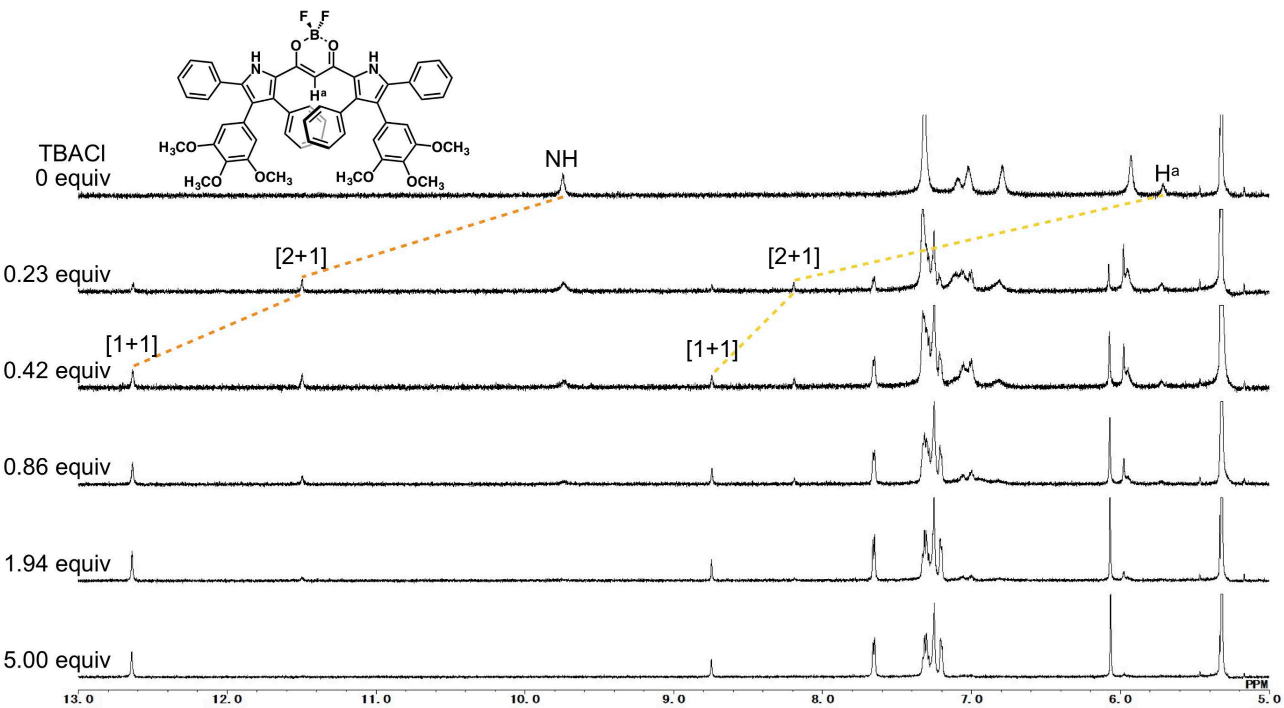
Supporting Figure 43 Fluorescence spectra of (a) **3a** and (b) **3b**: (i) fluorescence spectra in CH_2Cl_2 (1.0×10^{-5} M) in the states in the absence of anions (red line) and upon the addition of Cl^-, Br^-, and $CH_3CO_2^-$ as TBA salts, wherein the spectra, derived from those in Supporting Figure 41, were normalized by the intensity of anion-free spectrum, and (ii) photographs in CH_2Cl_2 (1.0×10^{-5} M) in the absence and presence of anions as TBA salts (Cl^-, Br^-, and $CH_3CO_2^-$) under the visible light (top) and 365 nm UV light (bottom) from left to right. Fluorescence quantum yields of **3a** upon the addition of Cl^-, Br^-, and $CH_3CO_2^-$ as TBA salts are 0.72 (Cl^-), 0.63 (Br^-), and 0.38 ($CH_3CO_2^-$), and those of **3b** are 0.71, 0.52, and 0.010, respectively.



Supporting Figure 44 ^1H NMR spectral changes of **2a** (1×10^{-3} M) upon the addition of Cl^- (0–2.41 equiv) added as a TBA salt in CD_2Cl_2 at –50 °C.



Supporting Figure 45 ^{1}H NMR spectral changes of **3a** (1×10^{-3} M) upon the addition of Cl^- (0–3.85 equiv) added as a TBA salt in CD_2Cl_2 at –50 °C.



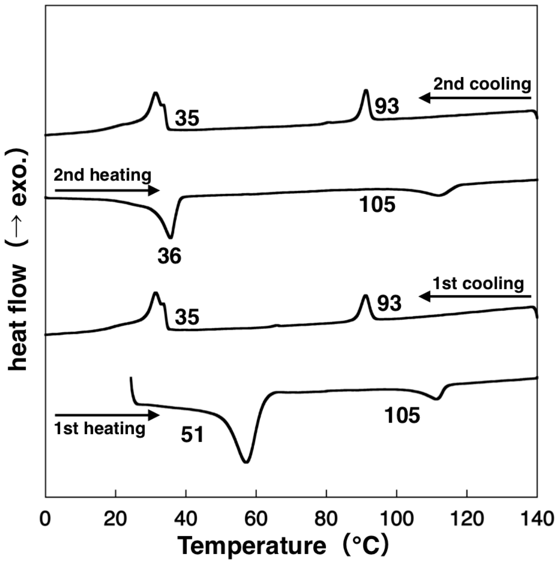
Supporting Figure 46 ^{1}H NMR spectral changes of **3b** (1×10^{-3} M) upon the addition of Cl^- (0–5.00 equiv) added as a TBA salt in CD_2Cl_2 at –50 °C.

5. Assembled behaviors

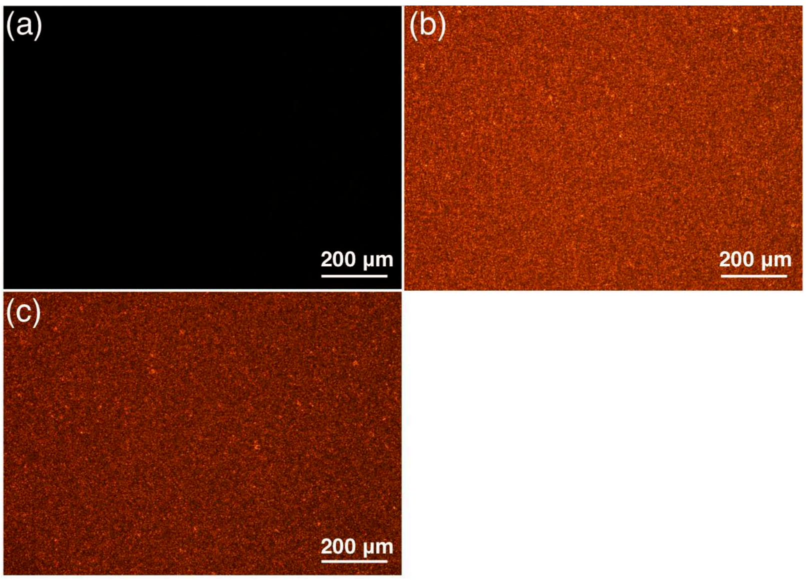
Differential scanning calorimetry (DSC). The phase transitions were measured on a differential scanning calorimetry (Shimadzu DSC-60).

Polarizing optical microscopy (POM). POM observations were carried out with a Nikon ECLIPSE LV100N-POL polarizing optical microscope equipped with a Mettler-Toledo HS82 hot stage system.

Synchrotron X-ray diffraction analysis (XRD). High-resolution XRD analysis was carried out using a synchrotron radiation X-ray beam with a wavelength of 1.00 Å on BL40B2 at SPring-8 (Hyogo, Japan). A large Debye-Scherrer camera with camera lengths of 428.7 mm for VT-XRD of **3c** (Supporting Figure 49), using a quartz capillary, was used with an imaging plate as a detector, where the diffraction patterns were obtained with a 0.01° step in 2θ. The exposure time of the X-ray beam was 10 sec.



Supporting Figure 47 DSC trace of **3c** (a scan rate of 5 °C/min).

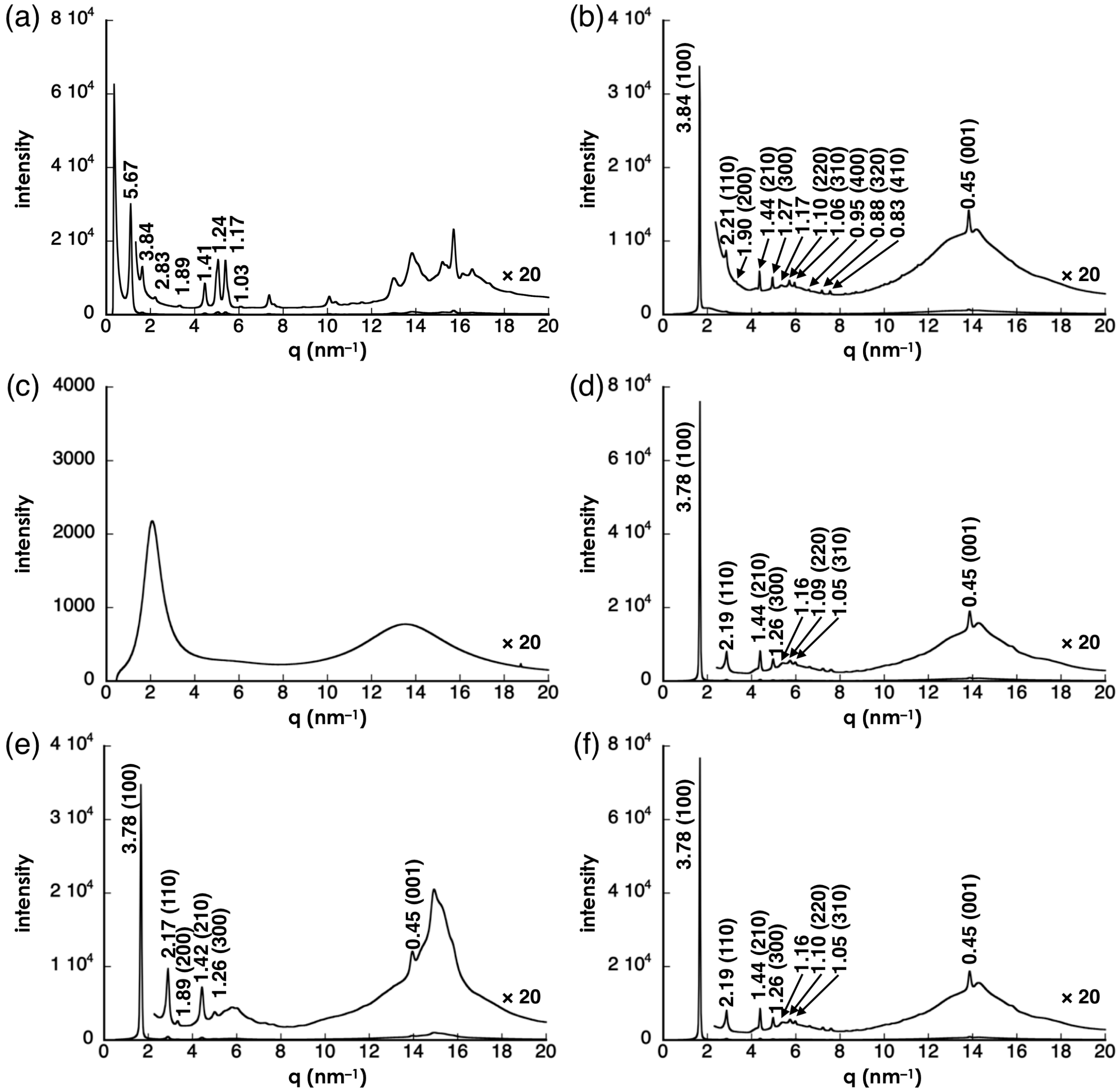


Supporting Figure 48 POM images of **3c** at (a) 130 °C, (b) 90 °C, and (c) 30 °C upon 1st cooling.

Supporting Table 2 Summarized phase transition behaviors of **3c**. The details of the packing structures such as XRD patterns are shown in Supporting Figure 49 and Supporting Table 3. Crystalline states are described in italic.

derivative	cooling[a]	heating[a]
3c	*Col_h* 35 Col_h 93 Iso	*Col_h* 36 Col_h 105 Iso

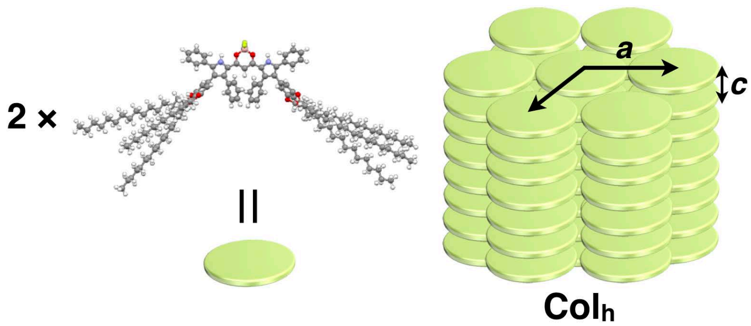
[a] Transition temperatures (°C, the onset of the peak) from DSC 1st cooling and 2nd heating scans (5 °C min^{-1}).



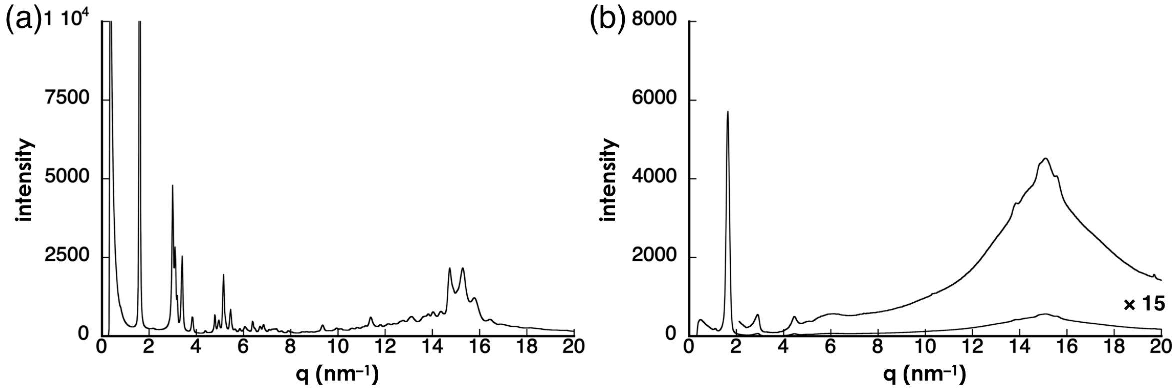
Supporting Figure 49 Synchrotron XRD patterns of **3c** at (a) 25 °C upon 1st heating, (b) 50 °C upon 1st heating, (c) 120 °C upon 1st heating, (d) 40 °C upon 1st cooling, (e) 0 °C upon 1st cooling, and (f) 40 °C upon 2nd heating.

Supporting Table 3 XRD peaks of **3c**. The peaks which can be indexed are represented.

	q (nm^{-1})	*d*-spacing (nm)	ratio	ratio (calc.)	*hkl*
	1.64	3.84	1	1	100
	2.85	2.21	0.57	0.577	110
	3.30	1.90	0.49	0.500	200
(b) **3c**	4.35	1.44	0.38	0.378	210
50 °C (1st heating)	4.95	1.27	0.33	0.333	300
Col$_h$	5.70	1.10	0.29	0.289	220
a = 4.43 nm, c = 0.45 nm	5.93	1.06	0.28	0.277	310
M = 2149.19, Z = 2 for ρ = 0.81	6.60	0.95	0.25	0.250	400
	7.17	0.88	0.23	0.229	320
	7.55	0.83	0.22	0.218	410
	13.83	0.45	—	—	001
	1.66	3.78	1	1	100
(d) **3f**	2.87	2.19	0.58	0.577	110
60 °C (1st heating)	4.38	1.44	0.38	0.378	210
Col$_h$	4.98	1.26	0.33	0.333	300
a = 4.36 nm, c = 0.45 nm	5.75	1.09	0.29	0.289	220
M = 2149.19, Z = 2 for ρ = 0.84	5.98	1.05	0.28	0.277	310
	13.88	0.45	—	—	001
	1.66	3.78	1	1	100
(e) **3f**	2.90	2.17	0.57	0.577	110
60 °C (1st heating)	3.32	1.89	0.50	0.500	200
Col$_h$	4.43	1.42	0.38	0.378	210
a = 4.36 nm, c = 0.45 nm	5.00	1.26	0.33	0.333	300
M = 2149.19, Z = 2 for ρ = 0.84	13.95	0.45	—	—	001
	1.66	3.78	1	1	100
(f) **3f**	2.87	2.19	0.58	0.577	110
75 °C (2nd heating)	4.35	1.44	0.38	0.378	210
Col$_h$	4.98	1.26	0.33	0.333	300
a = 4.36 nm, c = 0.45 nm	5.73	1.10	0.29	0.289	220
M = 2149.19, Z = 2 for ρ = 0.84	5.98	1.05	0.28	0.277	310
	13.86	0.45	—	—	001



Supporting Figure 50 Possible packing model of **3c** in a Col$_h$ structure.



Supporting Figure 51 Synchrotron XRD patterns of **3c** at 25 °C for the sample prepared by the evaporation from (a) CH_2Cl_2 and (b) *n*-hexane.