Electronic Supplementary Information

Dimension-controlled assemblies of anion-responsive π-electronic systems bearing aryl substituents with fan-shaped geometries

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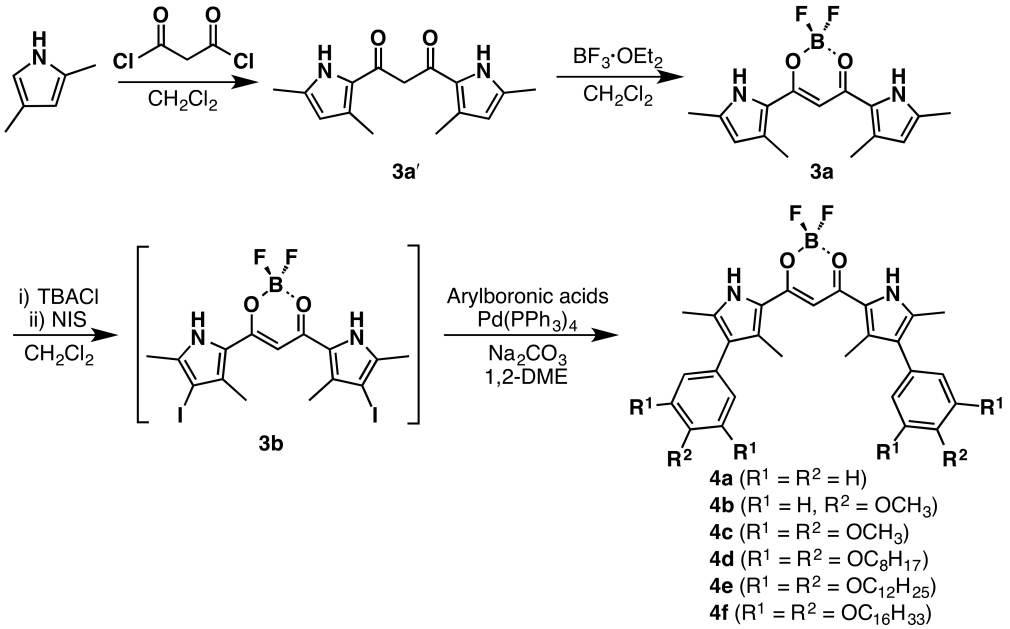
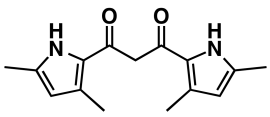
1. Synthetic procedures and spectroscopic data



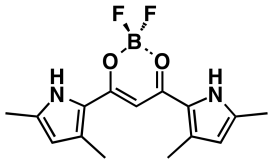
Supporting Figure 1 Synthesis of β-aryl-substituted anion receptors.

General Procedures. Starting materials were purchased from Wako Pure Chemical Industries Ltd., 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 spectrometers. All NMR spectra were referenced to solvent. UV-visible 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. Matrix-assisted laser desorption ionization time-of-flight mass spectrometries (MALDI-TOF-MS) were recorded on a Shimadzu Axima-CFRplus. TLC analyses were carried out on aluminum sheets coated with silica gel 60 (Merck 5554). Column chromatography was performed on Wakogel C-300.

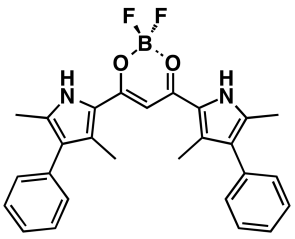
1,3-Bis(3,5-dimethylpyrrol-2-yl)-1,3-propanedione, 3a′. Following the literature procedure,[S1] a CH_2Cl_2 solution of 2,4-dimethylpyrrole[S2] (710 mg, 7.46 mmol) was treated with malonyl chloride (0.36 mL, 3.73 mmol) at r.t. and stirred for 2 h. After the consumption of starting pyrrole, the mixture was washed with saturated aq. Na_2CO_3 and water, dried over anhydrous Na_2SO_4, filtered and evaporated to dryness. The residue was purified by silica gel column chromatography (eluent: 4% MeOH/CH_2Cl_2) and recrystallized using CH_2Cl_2/*n*-hexane to afford **3a′** (241 mg, 0.93 mmol, 25%) as a light yellow solid. R_f = 0.33 (4% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; diketone **3a′** is obtained as keto and enol tautomers in the ratio of 1:0.4): δ (ppm) keto form 8.90 (br, 2H, NH), 5.85 (d, J = 2.4 Hz, 2H, pyrrole-H), 4.14 (s, 2H, CH), 2.38 (s, 6H, CH_3), 2.27 (s, 6H, CH_3); enol form 17.30 (s, 1H, OH), 9.56 (br, 2H, NH), 6.04 (s, 1H, bridged-CH), 5.86 (d, J = 2.4 Hz, 2H, pyrrole-H), 2.34 (s, 6H, CH_3), 2.28 (s, 6H, CH_3). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 174.93, 132.86, 126.42, 124.34, 113.26, 112.95, 92.34, 14.50, 14.09, 13.41, 13.22. MALDI-TOF-MS: *m/z* (% intensity): 257.3 (100), 258.3 (44). Calcd for $C_{15}H_{17}N_2O_2$ ([M – H]$^-$): 257.13.



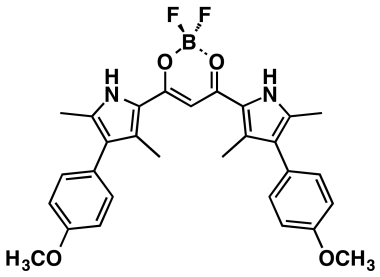
BF_2 complex of 1,3-bis(3,5-dimethylpyrrol-2-yl)-1,3-propanedione, 3a. To a CH_2Cl_2 solution (40 mL) of **3a′** (100 mg, 0.39 mmol) was added BF_3·OEt_2 (0.21 mL, 1.94 mmol) and stirred at r.t. for 15 min. The solvent was removed and subjected to silica gel column chromatography (eluent: 2% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/*n*-hexane to afford **3a** (101 mg, 0.33 mmol, 85%) as a red solid. R_f = 0.28 (2% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.16 (s, 2H, NH), 6.20 (s, 1H, CH), 5.98 (d, J = 3.0 Hz, 2H, pyrrole-H), 2.37 (s, 6H, CH_3), 2.33 (s, 6H, CH_3). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 166.60, 137.01, 131.99, 122.45, 114.75, 90.38, 14.65, 13.27. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 336 (0.09), 457 (1.5). MALDI-TOF-MS: *m/z* (% intensity): 304.1 (23), 305.1 (100), 306.1 (73), 307.1 (14). Calcd for $C_{15}H_{16}BF_2N_2O_2$ ([M – H]$^-$): 305.13. This compound was further characterized by single-crystal X-ray analysis.



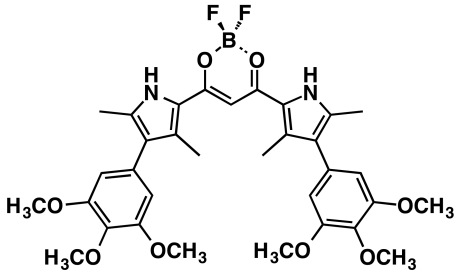
BF_2 complex of 1,3-bis(3,5-dimethyl-4-phenylpyrrol-2-yl)-1,3-propanedione, 4a. To a CH_2Cl_2 solution (8 mL) of **3a** (15.0 mg, 0.049 mmol) was added tetrabutylammonium chloride (TBACl) (27.2 mg, 0.098 mmol) and stirred for 5 min at r.t. *N*-Iodosuccinimide (23.2 mg, 0.10 mmol) was added to the reaction and stirring continued for another 6 h at r.t. After the consumption of **3a** elucidated by MALDI-TOF-MS, solvent was removed under vacuum and mixture was washed with saturated aq. $NaHCO_3$ solution, water (3 × 20 mL), and CH_2Cl_2. Organic phase was filtered over Na_2SO_4, evaporated and dried under vacuum. The resultant crude iodinated species **3b** was used without further purification. To the crude iodinated species were added phenylboronic acid (17.9 mg, 0.15 mmol), $Pd(PPh_3)_4$ (2.83 mg, 2.45 μmol), and Na_2CO_3 (31.2 mg, 0.29 mmol) and flushed with N_2. The mixture was charged with a mixture of degassed DME/water (4/0.4 mL) and heated at 85 °C for 13 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (eluent: 2% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/*n*-hexane to give **4a** (11.6 mg, 0.025 mmol, 51%) as a yellow solid. R_f = 0.36 (2% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.34 (s, 2H, NH), 7.43 (t, J = 7.8 Hz, 4H, phenyl), 7.34 (t, J = 7.2 Hz, 2H, phenyl), 7.23 (d, J = 7.2 Hz, 4H, phenyl), 6.40 (s, 1H, CH), 2.33 (s, 6H, CH_3), 2.32 (s, 6H, CH_3). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 166.78, 135.36, 133.84, 130.34, 129.26, 128.60, 128.17, 127.10, 122.50, 91.33, 13.11, 12.68. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 341 (0.07), 472 (1.5). MALDI-TOF-MS: *m/z* (% intensity): 456.3 (23), 457.3 (100), 458.3 (70), 459.3 (18). Calcd for $C_{27}H_{24}BF_2N_2O_2$ ($[M - H]^-$): 457.19. This compound was further characterized by single-crystal X-ray analysis.



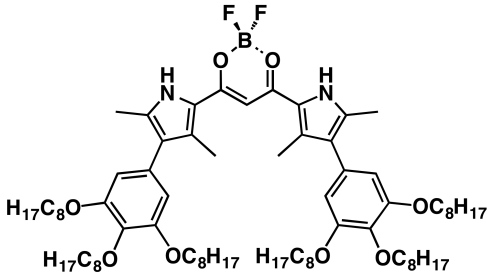
BF_2 complex of 1,3-bis(4-(4-methoxyphenyl)-3,5-dimethylpyrrol-2-yl)-1,3-propanedione, 4b. To the crude iodinated species **3b** from **3a** (21.5 mg, 0.070 mmol) were added 4-methoxyphenylboronic acid (32.0 mg, 0.21 mmol), $Pd(PPh_3)_4$ (4.06 mg, 3.51 μmol), and Na_2CO_3 (44.7 mg, 0.42 mmol) and flushed with N_2. The mixture was charged with a mixture of degassed DME/H_2O (5/0.5 mL) and heated at 85 °C for 15 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (eluent: 1.5% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/*n*-hexane to give **4b** (23.5 mg, 0.045 mmol, 65%) as a yellow solid. R_f = 0.28 (1.5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.28 (s, 2H, NH), 7.14 (d, J = 7.8 Hz, 4H, Ar-H), 6.97 (d, J = 8.4 Hz, 4H, Ar-H), 6.38 (s, 1H, CH), 3.86 (s, 6H, OCH_3), 2.31 (s, 6H, CH_3), 2.30 (s, 6H, CH_3). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 166.63, 158.76, 135.37, 131.42, 129.30, 127.82, 126.08, 122.37, 114.06, 91.21, 55.46, 13.11, 12.65. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 323 (0.06), 476 (1.3). MALDI-TOF-MS: *m/z* (% intensity): 516.4 (28), 517.4 (100), 518.4 (62), 519.4 (16). Calcd for $C_{29}H_{28}BF_2N_2O_4$ ($[M - H]^-$): 517.21.



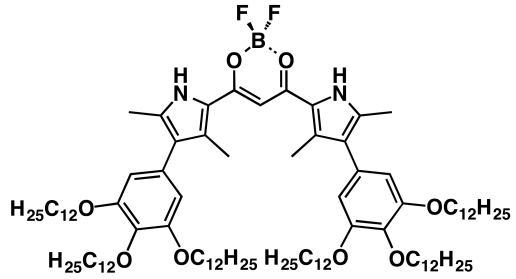
BF_2 complex of 1,3-bis(4-(3,4,5-trimethoxyphenyl)-3,5-dimethylpyrrol-2-yl)-1,3-propanedione, 4c. To the crude iodinated species **3b** from **3a** (30.4 mg, 0.099 mmol) were added 3,4,5-trimethoxyphenylboronic acid[S3] (63.2 mg, 0.30 mmol), $Pd(PPh_3)_4$ (5.73 mg, 4.96 μmol), and Na_2CO_3 (63.1 mg, 0.59 mmol) and flushed with N_2. The mixture was charged with a mixture of degassed DME/water (5/0.5 mL) and heated at 85 °C for 16 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (eluent: 2% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/*n*-hexane to give **4c** (37.7 mg, 0.059 mmol, 60%) as a yellow solid. R_f = 0.25 (2% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.31 (s, 2H, NH), 6.41 (s, 4H, Ar-H), 6.38 (s, 1H, CH), 3.91 (s, 6H, OCH_3), 3.87 (s, 12H, OCH_3), 2.35 (s, 6H, CH_3), 2.34 (s, 6H, CH_3). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 166.81, 153.33, 137.30, 135.28, 129.37, 129.14, 128.36, 122.43, 107.50, 91.28, 61.10, 56.35, 30.47, 13.19, 12.73. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 324 (0.06), 474 (1.3). MALDI-TOF-MS: *m/z* (% intensity): 636.4 (13), 637.4 (71), 638.4 (100), 639.4 (30), 640.4 (3). Calcd for $C_{33}H_{37}BF_2N_2O_8$ ($[M]^-$): 638.26.



BF_2 complex of 1,3-bis(3,5-dimethyl-4-(3,4,5-trioctyloxyphenyl)pyrrol-2-yl)-1,3-propanedione, 4d. To the crude iodinated species **3b** from **3a** (52.4 mg, 0.17 mmol) were added 3,4,5-trioctyloxyphenylboronic acid[S4] (302 mg, 0.51 mmol), $Pd(PPh_3)_4$ (9.89 mg, 8.56 μmol), and Na_2CO_3 (109 mg, 1.03 mmol) and flushed with N_2. The mixture was charged with a mixture of degassed DME/water (8/0.8 mL) and heated at 85 °C for 18 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (eluent: 1% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/*n*-hexane to give **4d** (122 mg, 0.099 mmol, 58%) as a red solid. R_f = 0.39 (1% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.27 (s, 2H, NH), 6.37–6.36 (m, 5H, Ar-H and CH), 4.00 (t, J = 6.6 Hz, 4H, OCH_2), 3.96 (t, J = 6.6 Hz, 8H, OCH_2), 2.33 (s, 6H, CH_3), 2.32 (s, 6H, CH_3), 1.83–1.75 (m, 12H, OCH_2CH_2), 1.51–1.44 (m, 12H, $OC_2H_4CH_2$), 1.36–1.25 (m, 48H, $OC_3H_6C_4H_8$), 0.90–0.86 (m, 18H, $OC_7H_{14}CH_3$). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 166.67, 153.16, 137.58, 135.27, 129.15, 128.71, 128.54, 122.37, 109.06, 73.63, 69.41, 32.07, 31.98, 30.54, 29.72, 29.61, 29.55, 29.45, 26.30, 26.27, 22.862, 22.82, 14.27, 14.25, 13.20, 12.76. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^4 $M^{-1}cm^{-1}$)): 324 (0.066), 476 (1.2). MALDI-TOF-MS: *m/z* (% intensity): 1225.5 (20), 1226.5 (100), 1227.5 (92), 1228.6 (43), 1229.6 (18). Calcd for $C_{75}H_{121}BF_2N_2O_8$ ($[M]^-$): 1226.92.

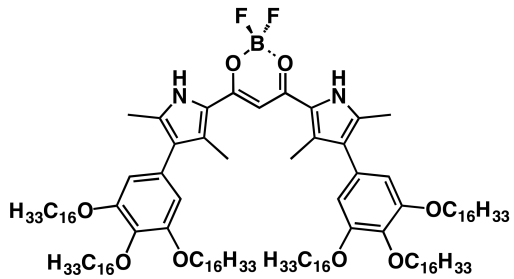


BF_2 complex of 1,3-bis(4-(3,4,5-tridodecyloxyphenyl)-3,5-dimethylpyrrol-2-yl)-1,3-propanedione, 4e. To the crude iodinated species **3b** from **3a** (62.8 mg, 0.21 mmol) were added 3,4,5-tridodecyloxyphenylboronic acid[S4] (466 mg, 0.62 mmol), $Pd(PPh_3)_4$ (11.9 mg, 10.3 μmol), and Na_2CO_3 (130 mg, 1.23 mmol) and flushed with N_2. The mixture was charged with a mixture of degassed DME/water (9/1 mL) and heated at 85 °C for 28 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/*n*-hexane to give **4e** (184 mg, 0.12 mmol, 56%) as an orange solid. R_f = 0.40 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.27 (s, 2H, NH), 6.37–6.36 (m, 5H, Ar-H and CH), 3.99 (t, J = 6.6 Hz, 4H, OCH_2), 3.96 (t, J = 6.6 Hz, 8H, OCH_2), 2.33 (s, 6H, CH_3), 2.32 (s, 6H, CH_3), 1.83–1.76 (m, 12H, OCH_2CH_2), 1.52–1.45 (m, 12H, $OC_2H_4CH_2$), 1.37–1.23 (m, 96H, $OC_3H_6C_8H_{16}$), 0.89–0.85 (m, 18H, $OC_{11}H_{22}CH_3$). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 166.66, 153.18, 137.59, 135.27, 129.14, 128.71, 128.54, 122.37, 109.05, 73.63, 69.41, 32.10, 32.07, 30.55, 29.93, 29.91, 29.86, 29.79, 29.74, 29.63, 29.61, 29.55, 29.52, 26.32, 26.30, 22.86, 14.27, 13.20, 12.76. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 326 (0.06), 475 (1.2). MALDI-TOF-MS: *m/z* (% intensity): 1562.2 (20), 1563.2 (87), 1564.2 (100), 1565.2 (52), 1566.2 (21). Calcd for $C_{99}H_{169}BF_2N_2O_8$ ($[M]^-$): 1564.30.



BF_2 complex of 1,3-bis(4-(3,4,5-trihexadecyloxyphenyl)-3,5-dimethylpyrrol-2-yl)-1,3-propanedione, 4f. To the crude iodinated species **3b** from **3a** (83.8 mg, 0.27 mmol) were added 3,4,5-trihexadecyloxyphenylboronic acid[S4] (760 mg, 0.82 mmol), $Pd(PPh_3)_4$ (15.8 mg, 13.7 μmol), and Na_2CO_3 (175 mg, 1.64 mmol) and flushed with N_2. The mixture was charged with a mixture of degassed DME/water (9/1 mL) and heated at 85 °C for 24 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (eluent: CH_2Cl_2/*n*-hexane = 8/2) and recrystallized from CH_2Cl_2/*n*-hexane to give **4f** (261 mg, 0.14 mmol, 51%) as a yellow solid. R_f = 0.30 (eluent: CH_2Cl_2/*n*-hexane = 8/2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.28 (s, 2H, NH), 6.37–6.36 (m, 5H, Ar-H and CH), 3.99 (t, J = 6.6 Hz, 4H, OCH_2), 3.96 (t, J = 6.6 Hz, 6H, OCH_2), 2.33 (s, 6H, CH_3), 2.32 (s, 6H, CH_3), 1.81–1.76 (m, 12H, OCH_2CH_2), 1.50–1.45 (m, 12H, $OC_2H_4CH_2$), 1.35–1.22 (m, 144H, $OC_3H_6C_{12}H_{24}$), 0.89–0.85 (m, 18H, $OC_{15}H_{30}CH_3$). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 166.67, 153.18, 137.59, 135.26, 129.14, 128.71, 128.54, 122.37, 109.05, 73.63, 69.42, 32.08, 30.56, 29.94, 29.92, 29.89, 29.87, 29.84, 29.80, 29.62, 29.57, 29.53, 29.48, 26.31, 26.24, 22.84, 14.27, 13.20, 12.76. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 328 (0.06), 475

(1.2). MALDI-TOF-MS: *m/z* (% intensity): 1898.2 (13) 1899.3 (60), 1900.3 (100), 1901.3 (70), 1902.3 (24). Calcd for $C_{123}H_{217}BF_2N_2O_8$ ([M]$^-$): 1900.68.



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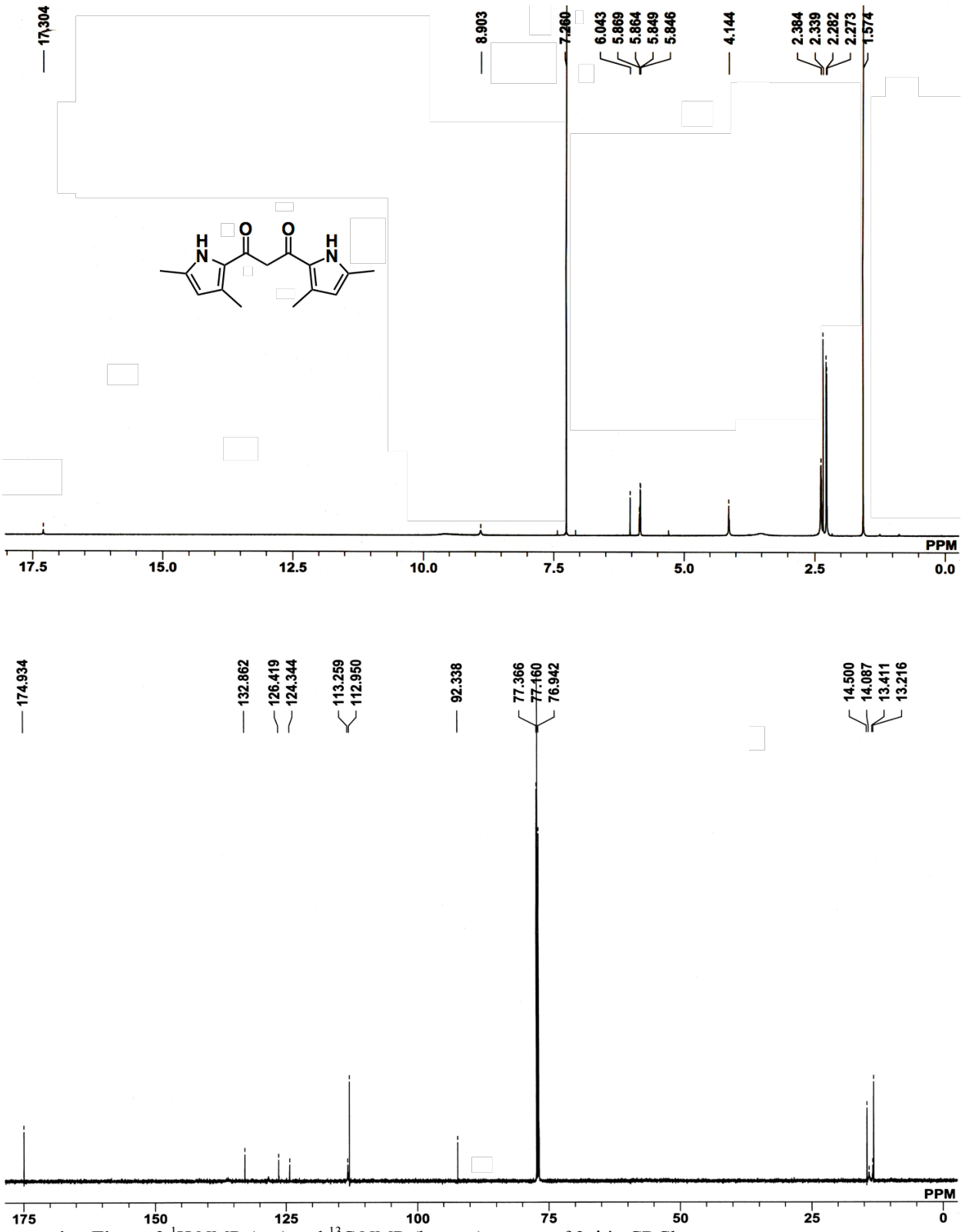
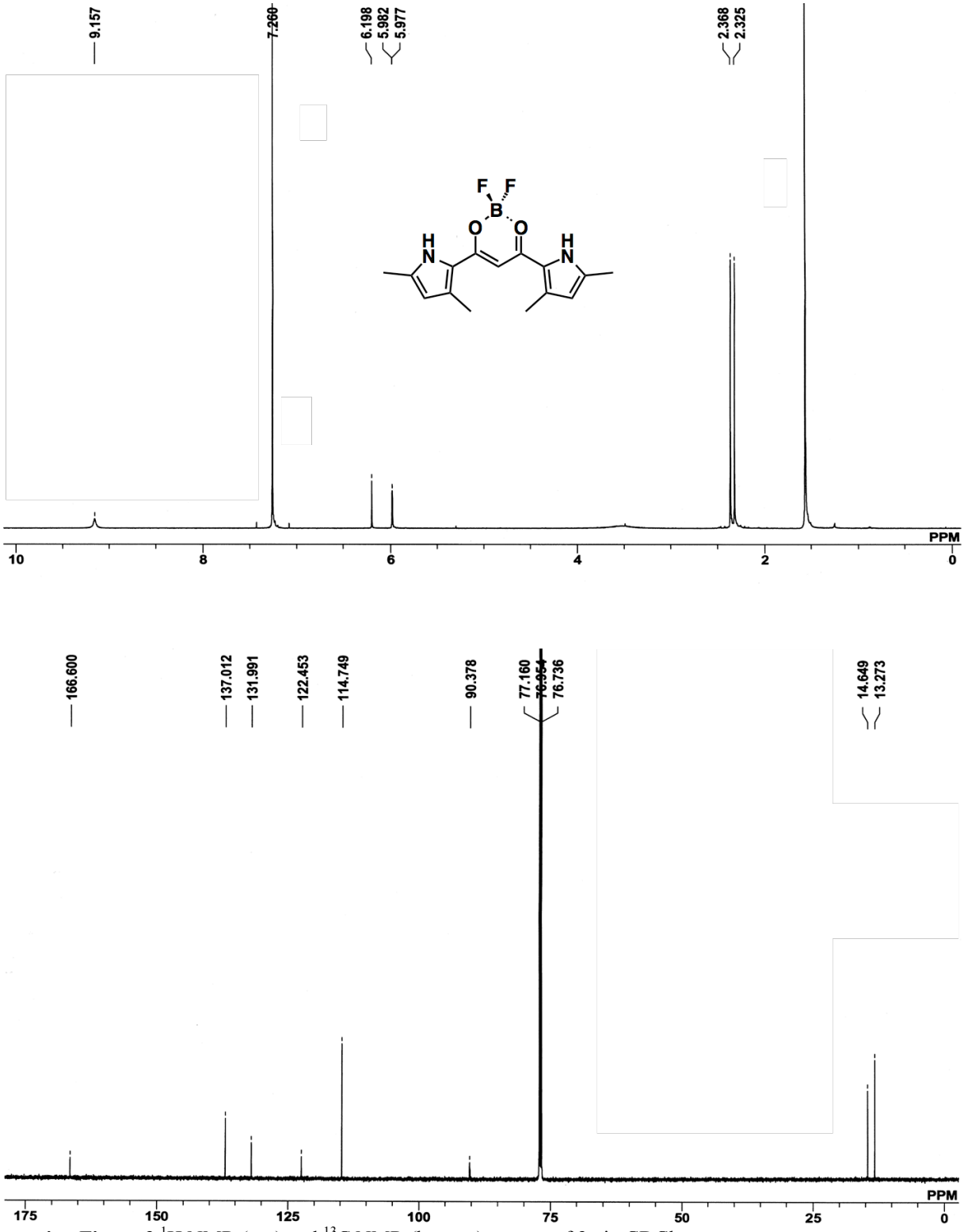
[S2] (a) E. V. Antina, G. B. Guseva, A. E. Loginova, A. S. Semeikin and A. I. V'yugin, *Russ. J. Gen. Chem*., 2010, **80**, 2374–2381; (b) Y. He, M. Lin, Z. Li, X. Liang, G. Li and J. C. Antilla, *Org. Lett.,* 2011, **13**, 4490–4493; (c) J. L. Hickey, J. L. James, C. A. Henderson, K. A. Price, A. I. Mot, G. Buncic, P. J. Crouch, J. M. White, A. R. White, T. A. Smith and P. S. Donnelly, *Inorg. Chem.,* 2015, **54**, 9556–9567.

[S3] (a) S. S. Moleele, J. P. Michael and C. B. de Koning, *Tetrahedron,* 2006, **62**, 2831–2844; (b) B. M. Rosen, D. A. Wilson, C. J. Wilson, M. Peterca, B. C. Won, C. Huang, L. R. Lipski, X. Zeng, G. Ungar, P. A. Heiney and V. Percec, *J. Am. Chem. Soc.,* 2009, **131**, 17500–17521.

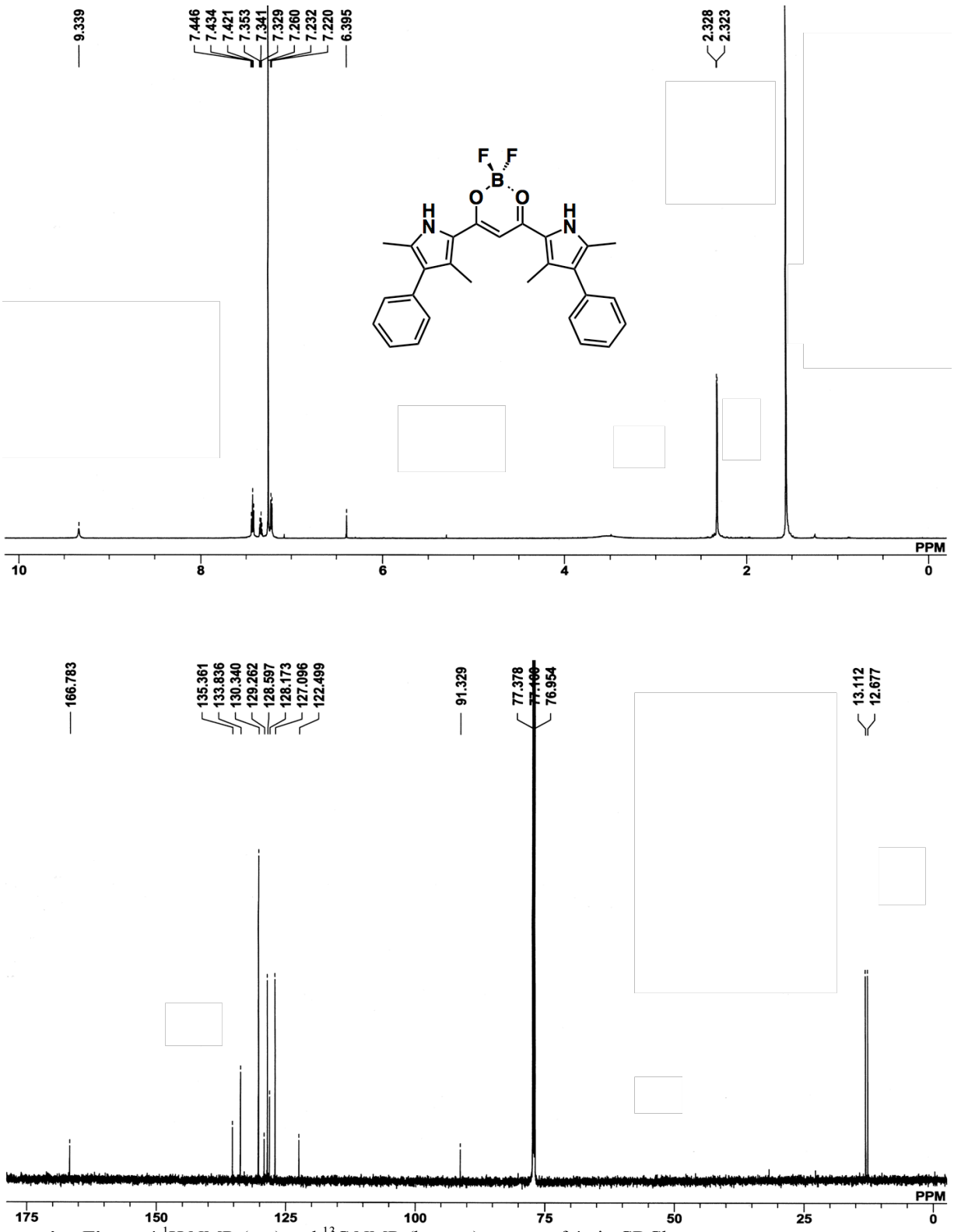
[S4] (a) Y. Haketa, S. Sakamoto, K. Chigusa, T. Nakanishi and H. Maeda, *J. Org. Chem*., 2011, **76**, 5177–5184; (b) H. Maeda, K. Chigusa, T. Sakurai, K. Ohta, S. Uemura and S. Seki, *Chem. Eur. J*., 2013, **19**, 9224–9233.



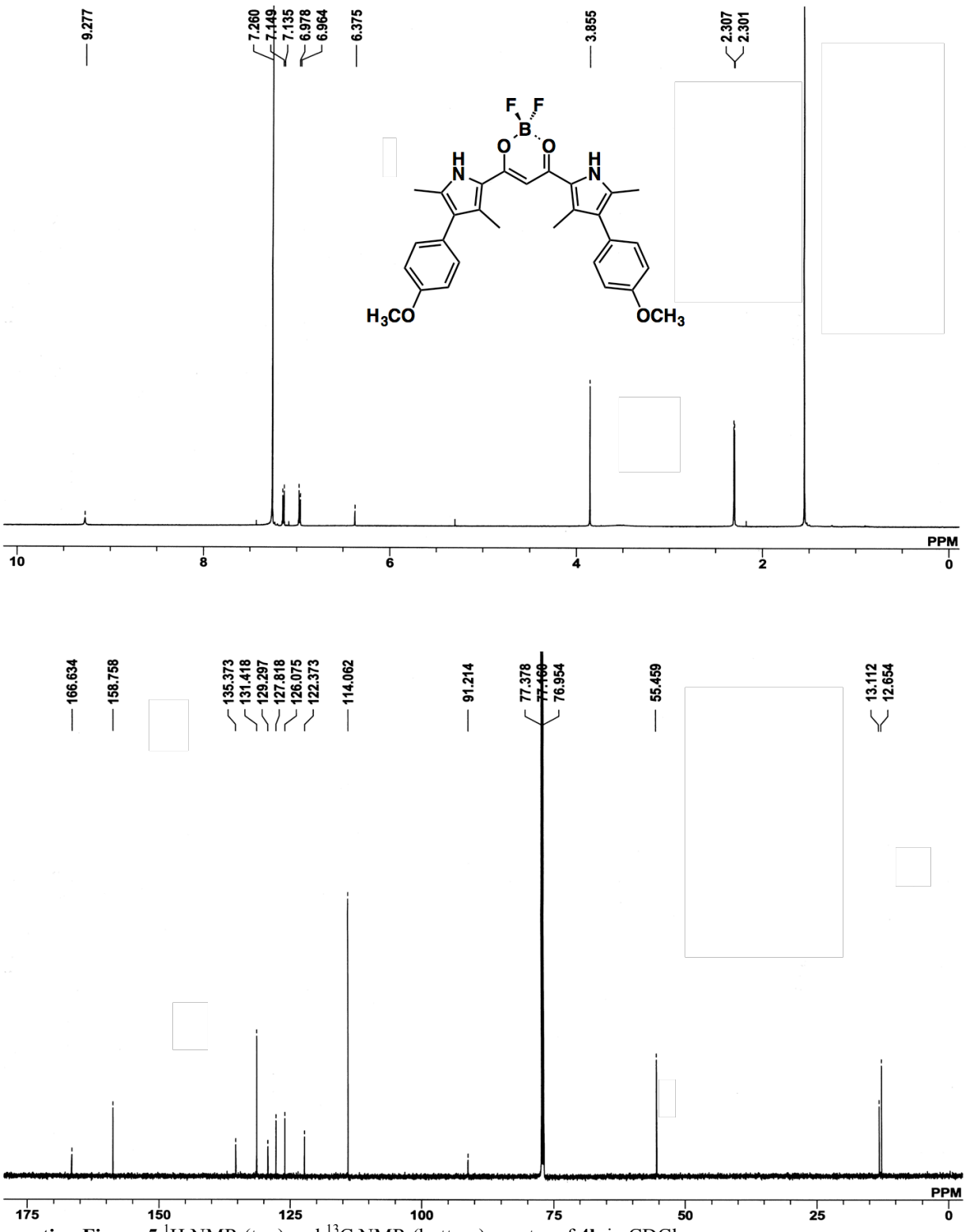
Supporting Figure 2 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **3a′** in $CDCl_3$.



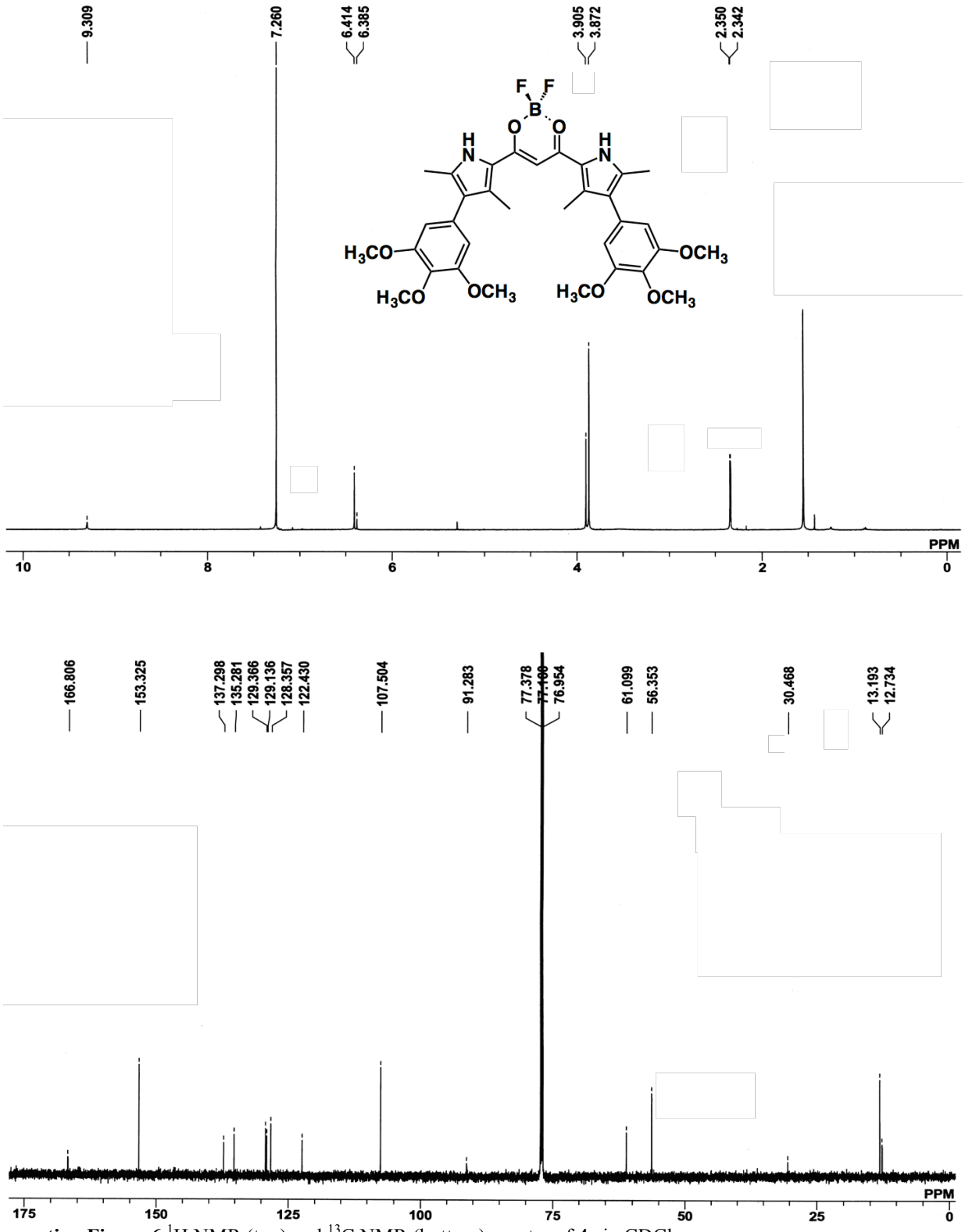
Supporting Figure 3 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **3a** in $CDCl_3$.



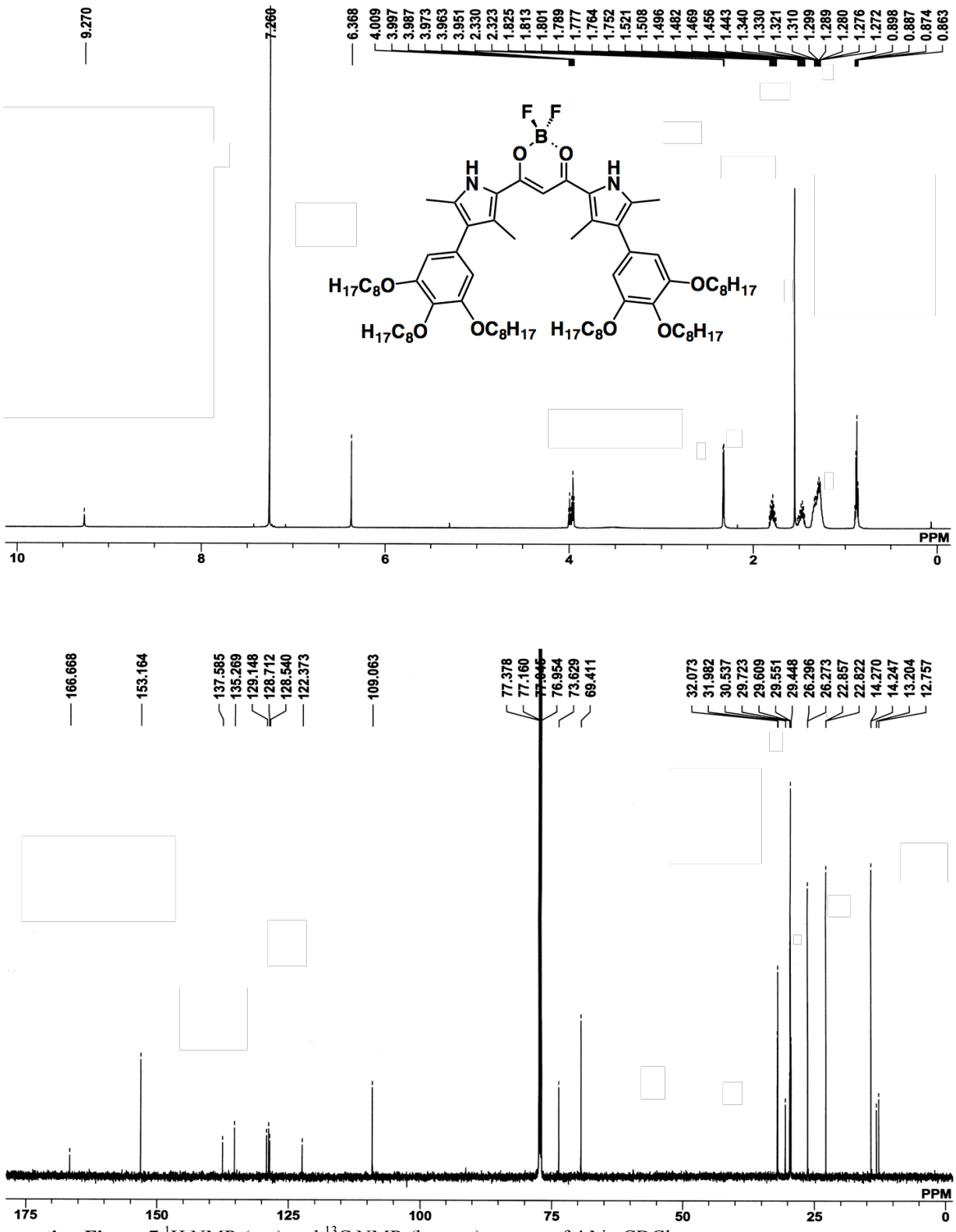
Supporting Figure 4 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **4a** in $CDCl_3$.



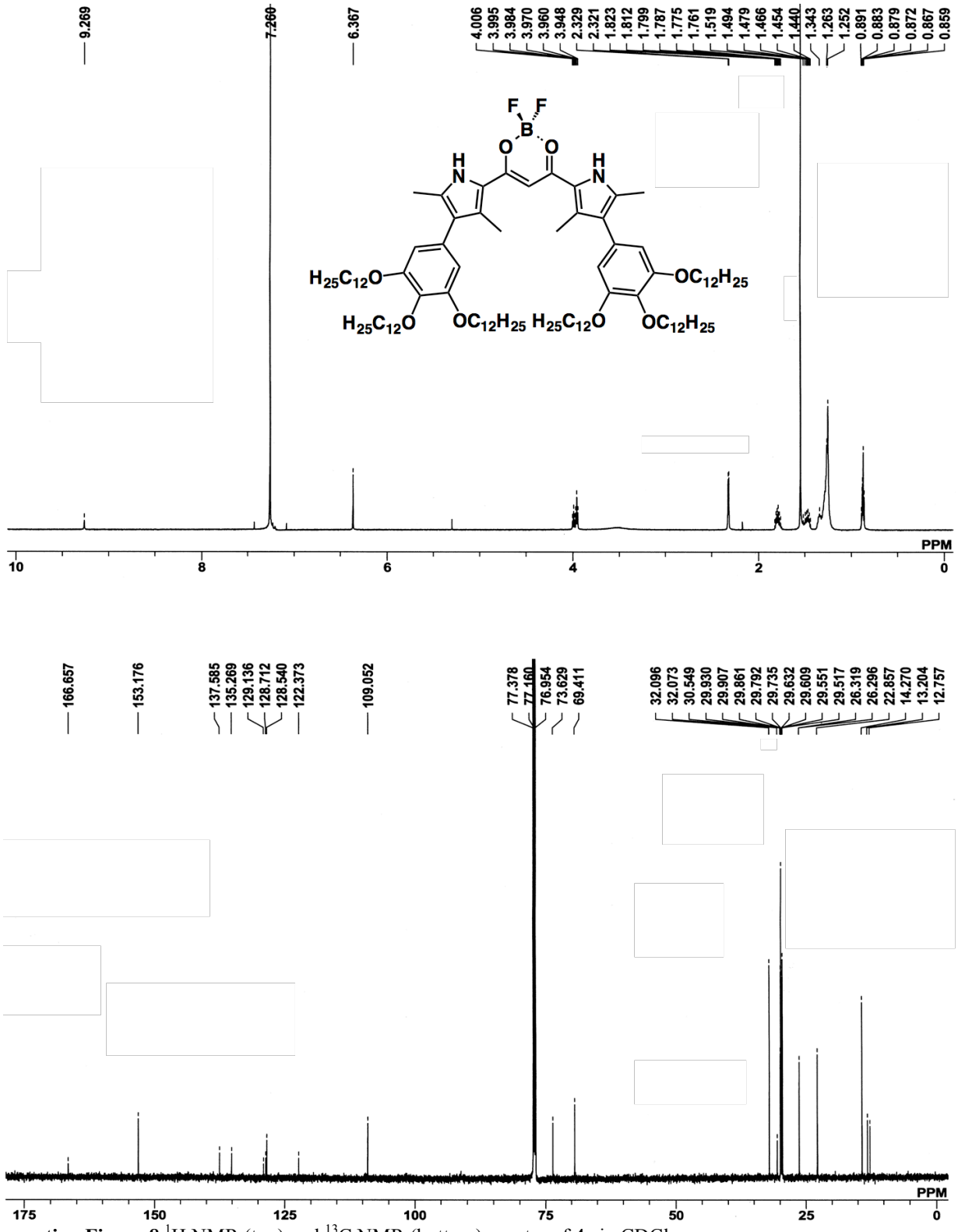
Supporting Figure 5 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **4b** in $CDCl_3$.



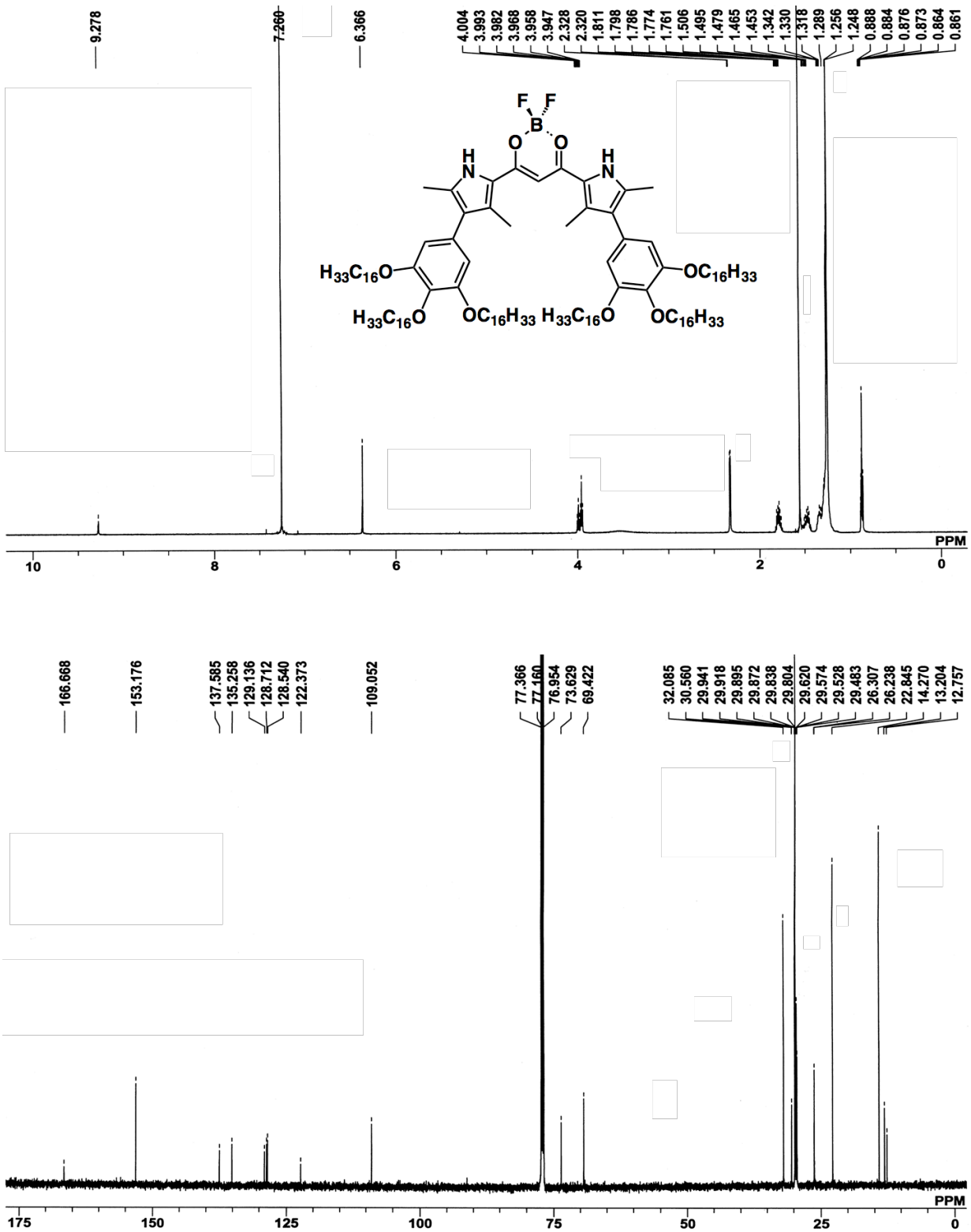
Supporting Figure 6 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **4c** in $CDCl_3$.



Supporting Figure 7 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **4d** in $CDCl_3$.



Supporting Figure 8 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **4e** in $CDCl_3$.



Supporting Figure 9 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **4f** in $CDCl_3$.

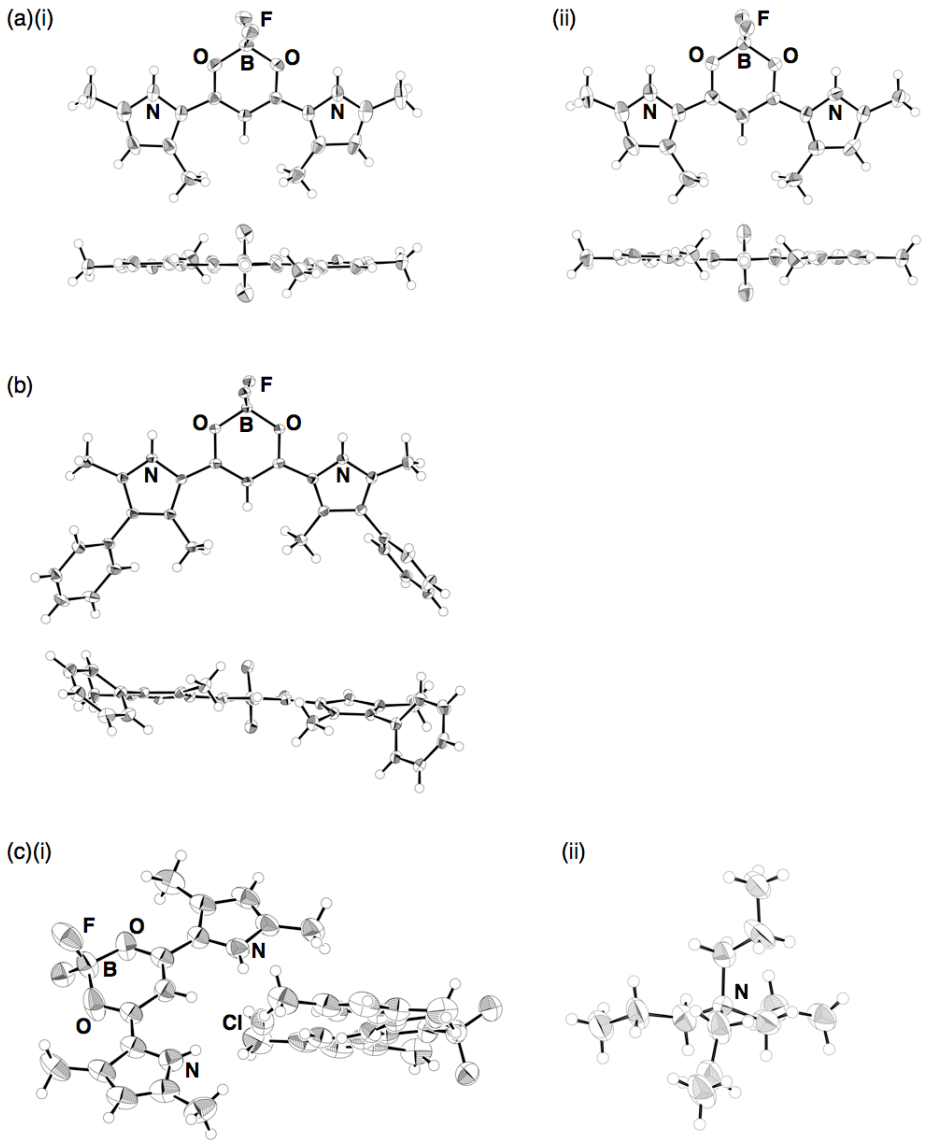
2. X-ray crystallographic data

Method for single-crystal X-ray analysis: Crystallographic data for receptors and anion complexes are summarized in Supporting Table 1. A single crystal of **3a** was obtained by vapor diffusion of *n*-hexane into an EtOAc solution. The data crystal was a yellow block of approximate dimensions 0.10 mm × 0.05 mm × 0.05 mm. A single crystal of **4a** was obtained by vapor diffusion of *n*-hexane into an EtOAc solution. The data crystal was a red prism of approximate dimensions 0.14 mm × 0.10 mm × 0.06 mm. A single crystal of **3a**·Cl^--TPA^+ was obtained by vapor diffusion of *n*-hexane into a CH_2Cl_2 solution of the 1:1 mixture of **3a** and TPACl. The data crystal was a yellow prism of approximate dimensions 0.06 mm × 0.05 mm × 0.01 mm. Single crystal of **4a**·Cl^--$TATA^+$ was obtained by vapor diffusion of *n*-hexane into a CH_2Cl_2 solution of the 1:1 mixture of **4a** and TATACl.[S5,6] The data crystal was an orange prism of approximate dimensions 0.22 mm × 0.09 mm × 0.01 mm. Data were collected at 100 K on a Rigaku Mercury CCD2 diffractometer for **3a** with Si(311) monochromated synchrotron radiation (λ = 0.6999 Å) at BL02B1 (SPring-8) and at 93 K on a Rigaku XtaLAB P200 diffractometer for **4a**, **3a**$_2$·Cl^--TPA^+, and **4a**·Cl^--$TATA^+$ with graphite monochromated Cu-Kα radiation (λ = 1.54187 Å), and structures were solved by direct method. The non-hydrogen atoms were refined anisotropically. The calculations were performed using the Crystal Structure crystallographic software package of Molecular Structure Corporation.[S7] CIF files (CCDC-1533939–1533942) can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

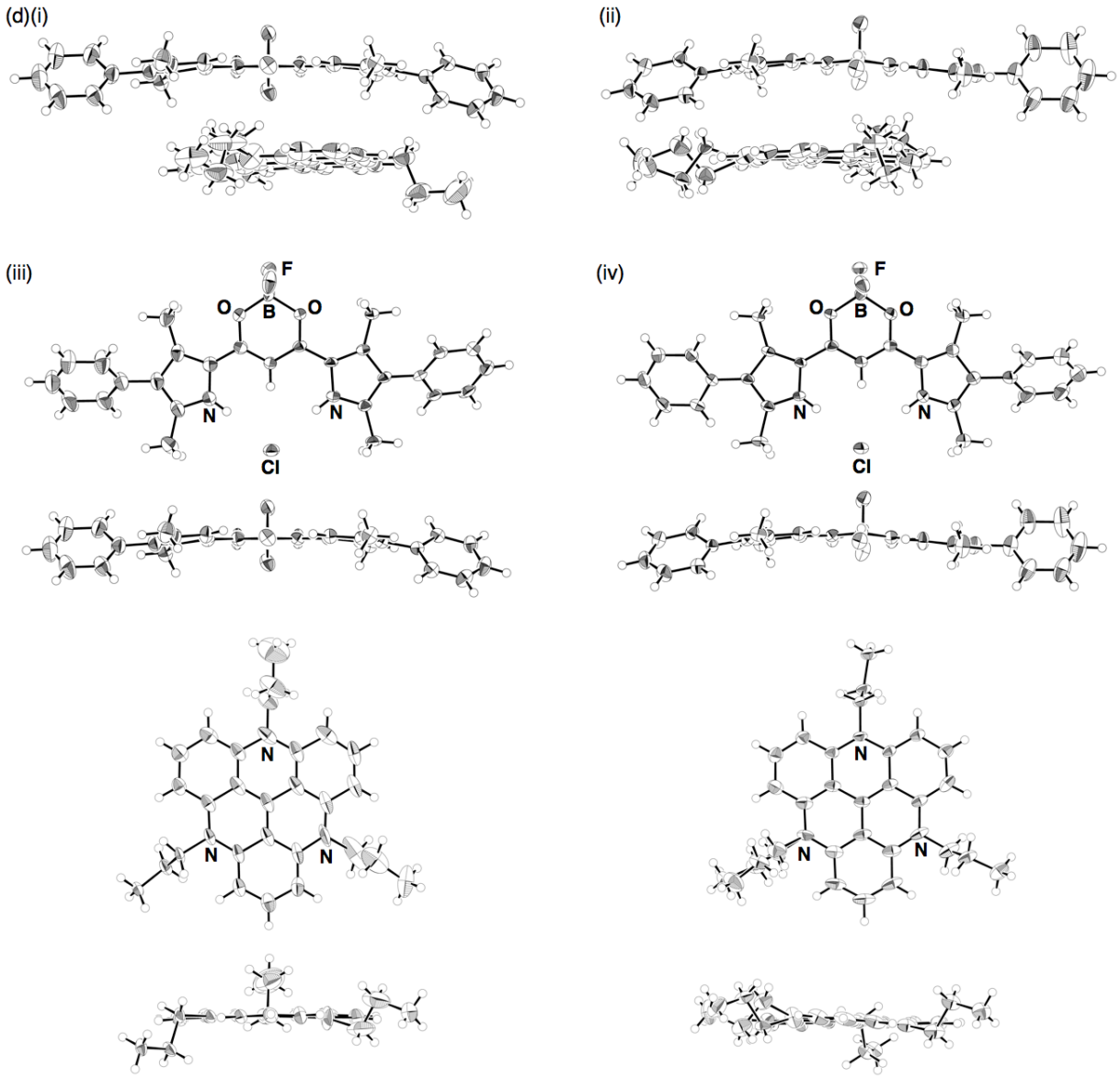
Supporting Table 1 Crystallographic details.

	3a	**4a**	**3a**$_2$·Cl^--TPA^+	**4a**·Cl^--$TATA^+$
formula	$C_{15}H_{17}BF_2N_2O_2$	$C_{27}H_{24}BF_2N_2O_2$	$(C_{15}H_{17}BF_2N_2O_2)_2Cl·C_{12}H_{28}N·C_6H_{14}$	$C_{27}H_{25}BF_2N_2O_2Cl·C_{28}H_{30}N_3·0.191C_6·1.309CCl_2$
fw	306.11	458.30	920.20	1024.59
crystal size, mm	0.10 × 0.05 × 0.05	0.14 × 0.10 × 0.06	0.06 × 0.05 × 0.01	0.22 × 0.09 × 0.01
crystal system	monoclinic	monoclicnic	monoclinic	triclinic
space group	*C*2/*c* (no. 15)	*P*2$_1$/*a* (no. 14)	*P*2$_1$/*c* (no. 14)	*P*-1 (no. 2)
a, Å	11.382(4)	8.1530(19)	11.592(4)	8.5862(12)
b, Å	13.964(5)	17.336(3)	29.363(9)	19.717(2)
c, Å	27.457(9)	17.063(5)	15.588(5)	31.483(3)
α, °	90	90	90	72.702(9)
β, °	91.853(7)	103.3167(10)	104.696(5)	85.311(12)
γ, °	90	90	90	88.492(10)
V, Å^3	4362(2)	2346.8(10)	5132(3)	5071.8(10)
ρ_{calcd}, gcm^{-3}	1.398	1.297	1.191	1.342
Z	12	4	4	4
T, K	100(2)	93(2)	93(2)	93(2)
μ, mm^{-1} (Cu-Kα)	0.104 [a]	0.756	1.150	2.389
no. of reflns	20846	30070	63179	62082
no. of unique reflns	4937	4301	8887	16843
variables	305	311	591	1306
λ, Å (Cu-Kα)	0.6999 [a]	1.54187	1.54187	1.54187
R_1 ($I > 2\sigma(I)$)	0.0970	0.0307	0.1070	0.0934
wR_2 ($I > 2\sigma(I)$)	0.2446	0.0815	0.2918	0.2549
GOF	0.993	1.038	1.047	1.012

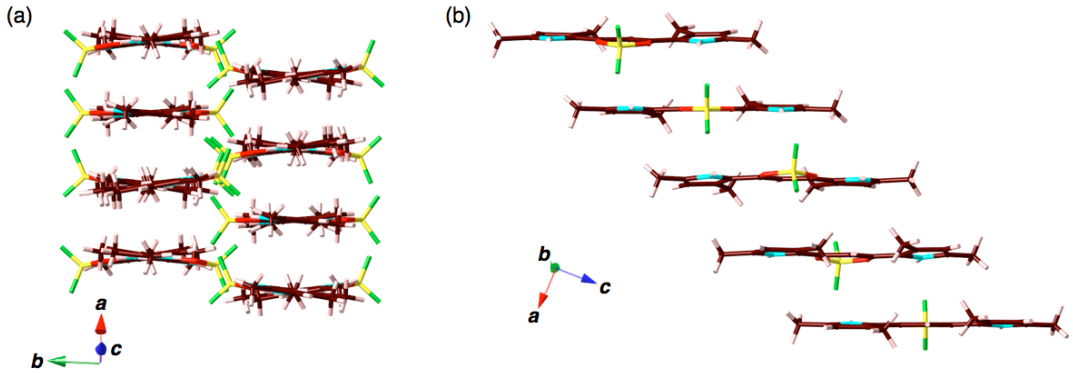
[a] The values under the synchrotron radiation.



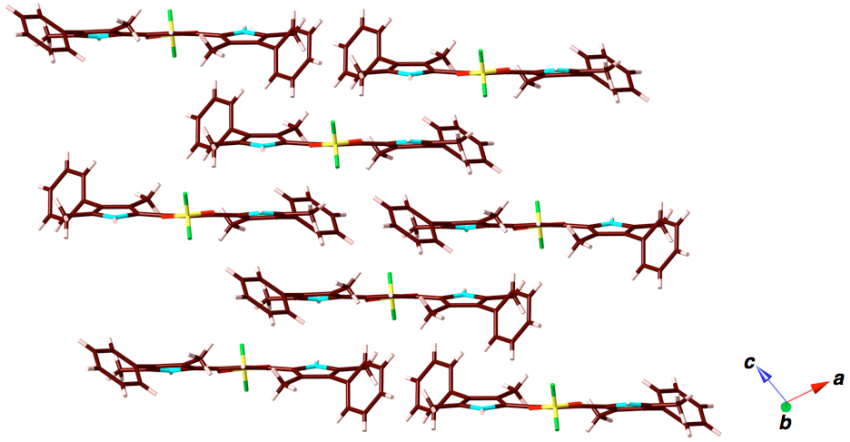
Supporting Figure 10 Ortep drawing of single-crystal X-ray structures (top and side views) of (a) **3a** with two independent structures in (i) and (ii), (b) **4a**, (c) $\mathbf{3a}_2 \cdot Cl^-$-TPA^+, wherein the [2+1]-type complex $\mathbf{3a}_2 \cdot Cl^-$ and TPA^+ were independently shown in (i) and (ii), respectively, and (d) $\mathbf{4a} \cdot Cl^-$-$TATA^+$ with two independent structures of Cl^- complexes in (i) and (ii), wherein $\mathbf{4a} \cdot Cl^-$ and $TATA^+$ for both independent Cl^- complexes were separately shown ((iii) and (iv)). In (d), a propyl-C–N bond in an independent $TATA^+$ structure (left) has a longer length (1.62 Å) than the other two C–N bonds (1.46 and 1.48 Å) and the C–N bonds in the other independent structure (right), which has a disordered N-propyl moiety in the ratio of 51:49. Thermal ellipsoids are scaled to the 50% probability level. Solvent molecules are omitted for clarity in the Cl^- complexes.



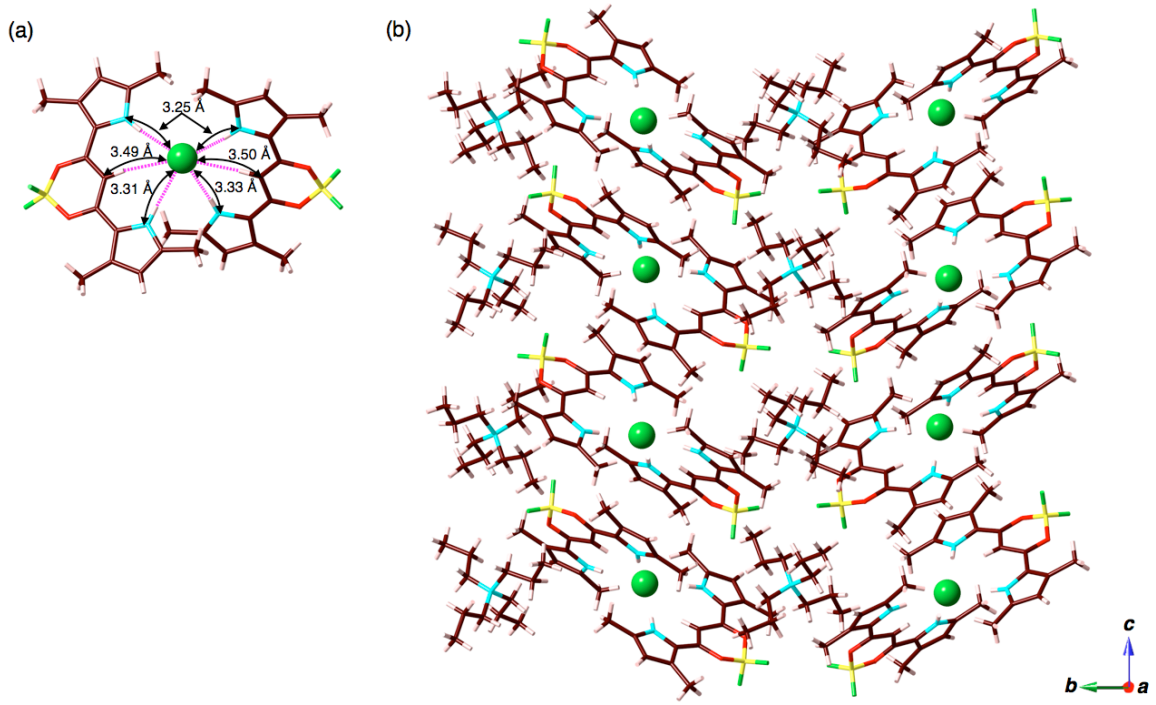
Supporting Figure 10 (Continued)



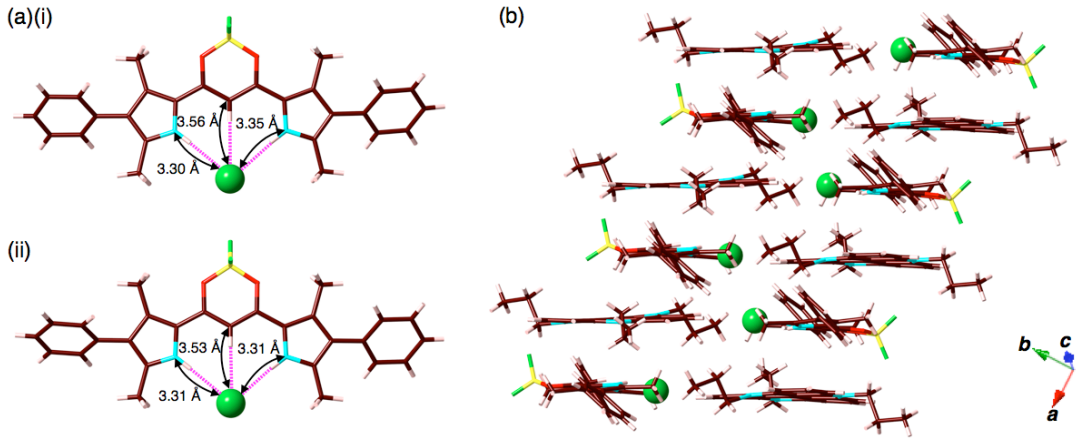
Supporting Figure 11 Packing diagrams of **3a** with a π–π stacking distance of 3.24 Å through the stacking of five- and six-membered rings (pyrrole and core 1,3-diketone boron complex, respectively). Atom color code: brown, pink, yellow, green, blue, and red refer to carbon, hydrogen, boron, fluorine, nitrogen, and oxygen, respectively.



Supporting Figure 12 Packing diagram of **4a** with a π–π stacking distance of 3.51 Å through the stacking of pyrrole moieties. Atom color code: brown, pink, yellow, green, blue, and red refer to carbon, hydrogen, boron, fluorine, nitrogen, and oxygen, respectively.



Supporting Figure 13 (a) [2+1]-Type anion complex and (b) packing diagram of **3a**$_2$·Cl$^-$-TPA$^+$, which formed a charge-segregated assembly, wherein the hydrogen-bonding distances of N(–H)···Cl$^-$ and C(–H)···Cl$^-$ are 3.25/3.25/3.31/3.33 and 3.49/3.50 Å, respectively. Solvent molecules are omitted for clarity. Atom color code: brown, pink, yellow, yellow green (spherical), green, blue, and red refer to carbon, hydrogen, boron, chlorine, fluorine, nitrogen, and oxygen, respectively.



Supporting Figure 14 (a) Two independent structures of anion-binding [1+1]-type complex and (b) packing diagram of **4a**·Cl$^-$-TATA$^+$, wherein the hydrogen-bonding distances of N(–H)···Cl$^-$ are 3.30/3.35 and 3.31 Å, and C(–H)···Cl$^-$ are 3.56 and 3.53 Å for each of independent structures, respectively. The [1+1]-type Cl$^-$ complex formed the charge-by-charge assembly by ion-pairing with the planar TATA$^+$ cation. Solvent molecules are omitted for clarity. Atom color code: brown, yellow, yellow green (spherical), green, blue, and red refer to carbon, hydrogen, boron, chlorine, fluorine, nitrogen, and oxygen, respectively.

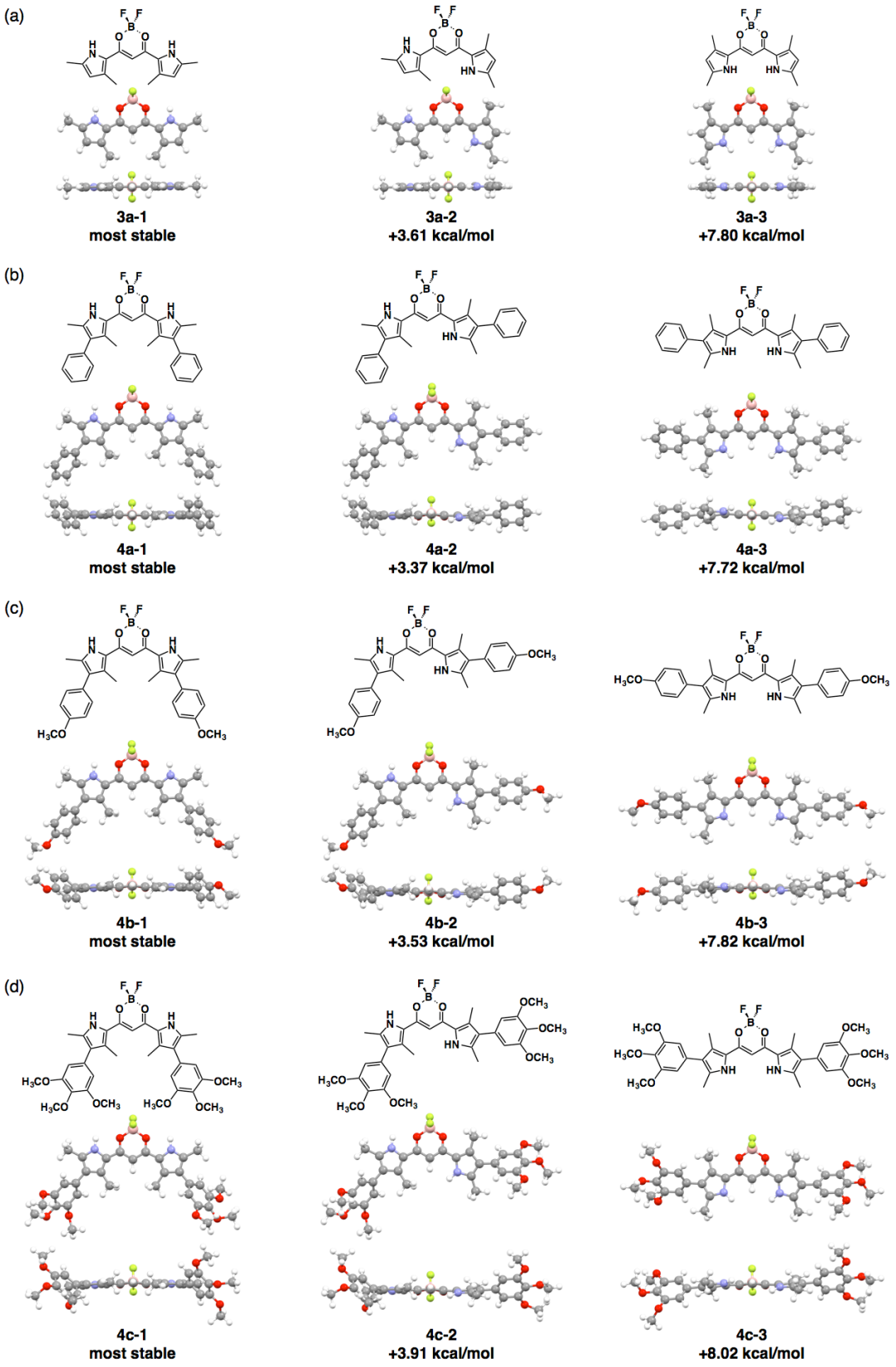
[S5] (a) B. W. Laursen and F. C. Krebs, *Angew. Chem. Int. Ed.*, 2000, **39**, 3432–3434; (b) B. W. Laursen and F. C. Krebs, *Chem. Eur. J.*, 2001, **7**, 1773–1783.

[S6] Y. Haketa, S. Sasaki, N. Ohta, H. Masunaga, H. Ogawa, N. Mizuno, F. Araoka, H. Takezoe and H. Maeda, *Angew. Chem. Int. Ed.,* 2010, **49**, 10079–10083.

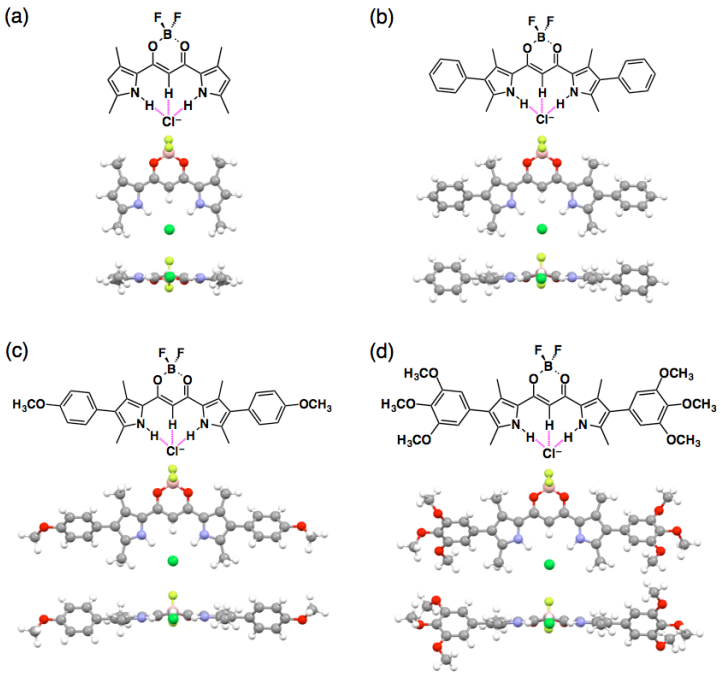
[S7] *CrystalStructure (Ver. 3.8), Single Crystal Structure Analysis Software*, Rigaku/MSC and Rigaku Corporation, 2006.

3. Theoretical studies

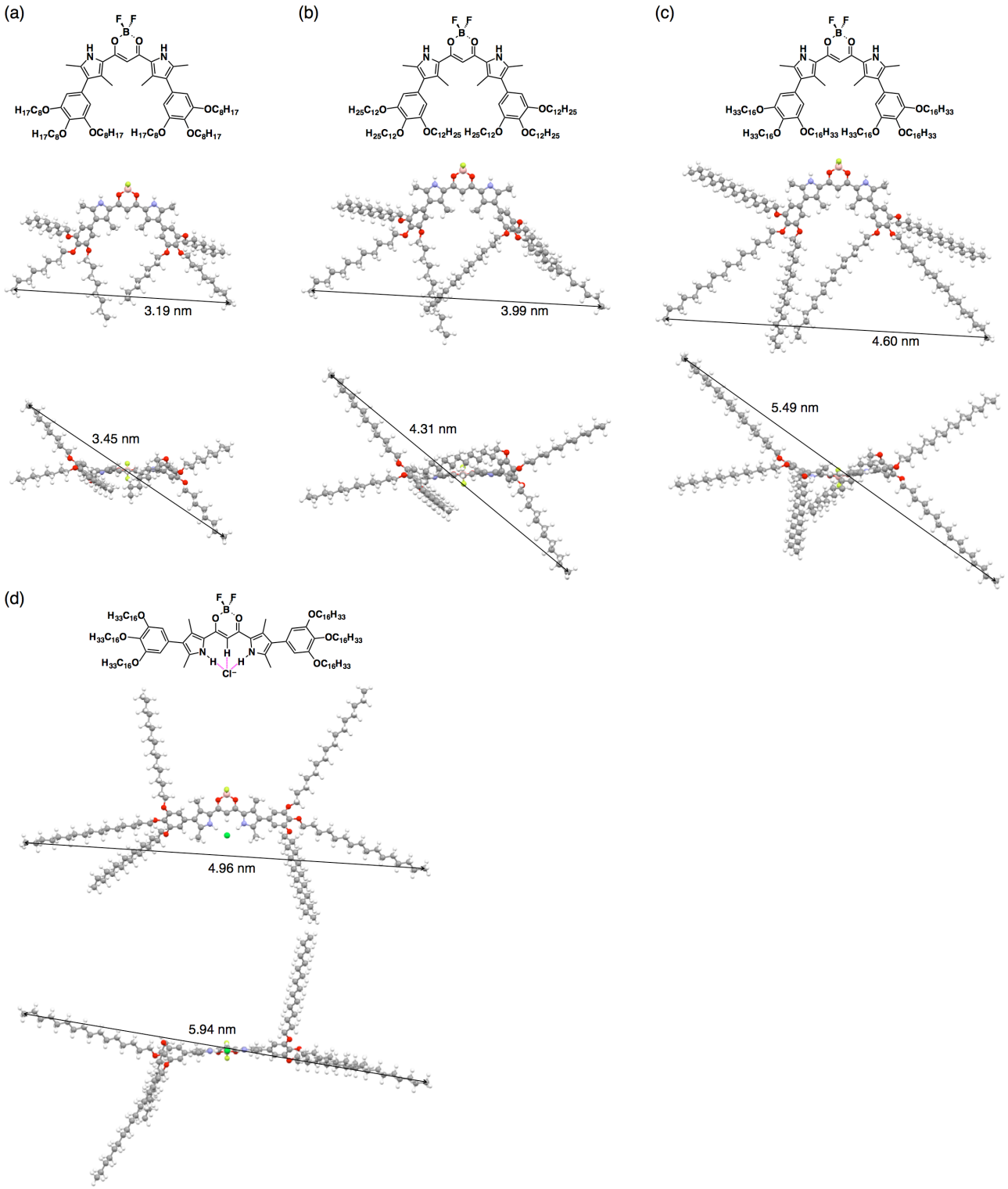
DFT and semi-empirical calculations. Ab initio and semi-empirical calculations for the geometrical optimizations were carried out by using the Gaussian 09 program.[S8]



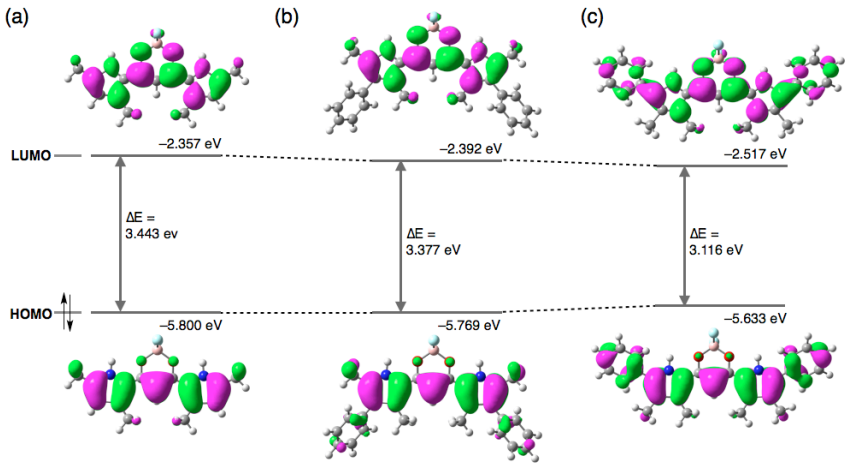
Supporting Figure 15 Optimized structures (top and side views) of (a) **3a**, (b) **4a**, (c) **4b**, and (d) **4c** at B3LYP/6-31G(d,p) level.



Supporting Figure 16 Optimized structures (top and side views) of (a) **3a**·Cl^-, (b) **4a**·Cl^-, (c) **4b**·Cl^-, and (d) **4c**·Cl^- at B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) level.



Supporting Figure 17 Optimized structures (top and side view) of (a) **4d**, (b) **4e**, (c) **4f**, and (d) **4f**·Cl^- at AM1 level. Estimated molecular sizes were consistent with the packing modes of receptors and receptor–anion complexes as discussed in the Section 5 in the ESI.



Supporting Figure 18 Molecular orbitals (HOMO/LUMO) of (a) **3a** and (b) **4a** along with (c) reference **2b**[S4] at B3LYP/6-31+G(d,p) basis set for the optimized geometries obtained by DFT with B3LYP/6-31G(d,p) level. Smaller HOMO–LUMO gaps were observed for phenyl-substituted **2b** and **4a** than the unsubstituted derivative **3a**.

Cartesian Coordination of 3a-1 at DFT

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H,5.0692119432,2.4954163026,-0.0003645204
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Cartesian Coordination of 3a-2 at DFT

–1066.5697044 hartree

F,1.1662892948,-0.6270692932,-1.5174019976
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Cartesian Coordination of 3a-3 at DFT
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Cartesian Coordination of 4a-1 at DFT
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C,-4.7610047938,0.9871817636,-0.10794178
C,-4.408434428,-0.3715118284,-0.0846179239
C,-2.9869056489,-0.4480566504,-0.0411981971
C,2.9868928233,-0.4481553009,0.041269651
C,4.4084176642,-0.3716126629,0.0848381163
C,-1.2057470751,1.4794332816,-0.0176715635
C,4.7610026158,0.9870823499,0.1078380788
C,0.0000056802,0.7711965912,-0.0007331926
C,5.3614252346,-1.5028102435,0.113442828
C,6.4005950243,-1.5989255676,-0.8280631357
C,5.2585755407,-2.5083648524,1.0906959587
C,7.3077072922,-2.6578392485,-0.7903821953
H,6.4829858541,-0.844470887,-1.6050124562
C,6.1591177366,-3.5724202667,1.1227998414
H,4.4765992261,-2.4399139685,1.8411718744
C,7.1889540516,-3.6501891149,0.1836740245
H,8.1021711935,-2.7120798927,-1.5292420899
H,6.0621227966,-4.3364318799,1.8889068077
H,7.8926657581,-4.4768714459,0.2108037091
C,-5.3614531635,-1.5027058153,-0.1127983663
C,-5.2586234314,-2.5086151162,-1.08969142
C,-6.4006106211,-1.5984787989,0.8287548769
C,-6.1591758821,-3.572672928,-1.1214064451
H,-4.4766511076,-2.440446868,-1.840197005
C,-7.3077357104,-2.6573947293,0.7914589651
H,-6.482986717,-0.8437519517,1.6054415079
C,-7.189006507,-3.650092897,-0.1822456888
H,-6.0621940704,-4.3369590899,-1.8872412283
H,-8.1021919556,-2.7113629227,1.5303470537
H,-7.8927291462,-4.4767757122,-0.2090727859
C,-2.1757418722,-1.7071598901,0.0476162788
H,-1.5612114219,-1.8663147148,-0.8470996258
H,-1.4984267025,-1.6880739671,0.9088105593
H,-2.826854596,-2.576267815,0.1580707296
C,-6.1003945746,1.6465138955,-0.1799873699
H,-6.867175285,0.9170530071,-0.4459759582
H,-6.386275717,2.0972192582,0.778504859
H,-6.1094257356,2.4430057594,-0.9323317435
C,6.100388141,1.6464167923,0.1799451378
H,6.8671516218,0.916955562,0.4459761025
H,6.3863109383,2.0971256566,-0.7785318607
H,6.1093837202,2.4429100998,0.9322912398
C,2.1757378348,-1.7072871418,-0.0472366216
H,1.5608158936,-1.8659454624,0.8472965846
H,1.4987983789,-1.6886530017, -0.9087386648
H,2.8268756676,-2.5764689248,-0.1569535443

Cartesian Coordination of 4a-2 at DFT
–1528.6942057 hartree
F,-0.1374586433,4.8634509406,-0.8638375696
H,-3.5208703565,2.6777576208,-0.2619042566
H,2.1028361955,-0.831891881,-0.4487179343
H,0.1771979108,-0.0652778941,0.2347579179
N,-3.5513673264,1.6716265744,-0.1759904923
N,2.8138220837,-0.1585973416,-0.2109084161
O,-1.2390366471,2.9085954644,-0.2310460714
O,1.2087814342,3.0728214672,-0.208300579
F,-0.1105669566,4.2288380686,1.3462529515
B,-0.0727271162,3.8352385235,0.0305481269

C,1.2744780956,1.7757214123,-0.0733595535
C,-2.3979916367,0.9161152,-0.0732779913
C,2.5950971134,1.2087776044,-0.0963596158
C,-4.650953566,0.8799606262,-0.1648509786
C,-4.2118299434,-0.4487963475,-0.0546885669
C,-2.7887961522,-0.4293644335,0.0037896258
C,3.8487487157,1.8210617529,0.0320380367
C,4.8257437003,0.7823982768,-0.0169148598
C,-1.1363100506,1.6085088782,-0.0720079032
C,4.1469973041,-0.4308814889,-0.183790166
C,0.1128312682,0.9962537472,0.057913108
C,6.2924478939,0.9346447715,0.0857598971
C,7.0422749674,0.1468960749,0.9764785126
C,6.9781671477,1.8686317181,-0.7105959433
C,8.4278173465,0.2809536375,1.0619862675
H,6.5285207007,-0.559564328,1.6218670086
C,8.3620495497,2.0091621307,-0.6187187425
H,6.4195542601,2.4750371453,-1.416743485
C,9.0931120084,1.2140187489,0.2656973157
H,8.9861870967,-0.3365439902,1.7598411562
H,8.8710817718,2.7361773217,-1.2450101875
H,10.1714213396,1.322582613,0.3352451635
C,-5.0903571231,-1.6387764669,-0.011177343
C,-4.9308785248,-2.6919181136,-0.9287803405
C,-6.1142374148,-1.7441905366,0.9458957786
C,-5.7610757792,-3.8116538172,-0.886790767
H,-4.1608763313,-2.6180122996,-1.6911543579
C,-6.9512919498,-2.859242036,0.9820484524
H,-6.2395074258,-0.950890103,1.6770705594
C,-6.7759907474,-3.898821985,0.0676131867
H,-5.6212835095,-4.6123480284,-1.6074875663
H,-7.7351012714,-2.91971125,1.7317116398
H,-7.4248240402,-4.7691307892,0.0978254971
C,-1.8988049411,-1.6256659221,0.1734489187
H,-1.2167165413,-1.7538073651,-0.6763110085
H,-1.2858899535,-1.5458854799,1.0788352009
H,-2.492612605,-2.5373410817,0.2595804614
C,-6.0296450863,1.4447541924,-0.2845439559
H,-6.7484227207,0.6483047999,-0.4838138294
H,-6.3426223738,1.9556353155,0.6344098969
H,-6.0903862391,2.172914487,-1.1011232639
C,4.6599404463,-1.8244045676,-0.3555576115
H,5.7245827995,-1.8077939818,-0.5941878333
H,4.5320235133,-2.4252505908,0.553621646
H,4.1373854602,-2.3430243092,-1.1678233204
C,4.1081745354,3.2819351581,0.2513535874
H,4.0232461786,3.8479583998,-0.6831273997
H,3.3760414904,3.7136494803,0.9367389451
H,5.1122778955,3.4383836862,0.6519500317

Cartesian Coordination of 4a-3 at DFT

–1528.6872704 hartree

F,-0.0276805395,4.8440574244,-1.1483255801
H,-1.8885337354,-0.6847861255,0.6801587024
H,1.888478806,-0.6847970652,-0.6798180399
H,-0.0000173291,0.1377351553,0.0000767259
N,-2.63128468,-0.084491508,0.3591117098
N,2.6312453303,-0.0845139073,-0.3587854031
O,-1.2353865962,3.2279854521,0.0290327725
O,1.2353821987,3.227975936,-0.0286258081
F,0.0276815533,4.8442915349,1.1483920858
B,-0.0000010899,4.0996451629,0.0001111574
C,1.2107260643,1.9248588187,-0.0490586931
C,-2.4956272482,1.2791485267,0.1256071051
C,2.4956116006,1.2791260631,-0.1252625267
C,-3.9475751342,-0.4366427749,0.365803605
C,-4.6961556572,0.7126311774,0.09239161
C,-3.7826815337,1.800330529,-0.0532371614
C,3.7826755888,1.8002703809,0.0536491169
C,4.6961433844,0.7126049665,-0.0922617543
C,-1.2107344797,1.9248679643,0.0494025981
C,3.9475303617,-0.4366822813,-0.3655245929
C,-0.0000089426,1.2188474031,0.0001275799
C,6.1694513147,0.7676697366,0.0191287868
C,6.8667271751,-0.1237463163,0.8527603189
C,6.913231445,1.7107781168,-0.7114341939
C,8.2575854185,-0.0801346101,0.9468124854
H,6.3083989736,-0.8411076819,1.4472369953
C,8.3028279474,1.7600575573,-0.6111525931
H,6.3951208829,2.3978524774,-1.3733623166
C,8.9811413692,0.8632170636,0.2161777323
H,8.7749174357,-0.7769521993,1.6001911452
H,8.8571332012,2.4962306989,-1.1861843197
H,10.0637733864,0.901065082,0.2924105315
C,-6.1694432392,0.7676790113,-0.0192771237
C,-6.9133699828,1.7107444473,0.711191043
C,-6.866557473,-0.1237088913,-0.8530763799
C,-8.3029490111,1.7600067804,0.6106609676
H,-6.3953906591,2.3977956808,1.373245641
C,-8.2573992552,-0.0801132885,-0.9473790209
H,-6.3081126875,-0.8410324906,-1.4474885117
C,-8.9811008126,0.8631949829,-0.2168327559
H,-8.8573684254,2.4961457155,1.1856262731
H,-8.7746030945,-0.7769078176,-1.6008839291
H,-10.0637195131,0.9010315539,-0.2932599186
C,-4.1337192774,3.2166357097,-0.4006517959
H,-4.065676273,3.8710215275,0.4755681768
H,-3.4424550566,3.6259719872,-1.140011865
H,-5.1524175467,3.2748787512,-0.7902206823
C,-4.377167086,-1.8352318457,0.6721588666
H,-5.4495239239,-1.8640883423,0.8716407129
H,-4.174599503,-2.5205976004,-0.160500873
H,-3.857439101,-2.2275746108,1.5544069872
C,4.377095962,-1.8352661945,-0.6719363523
H,5.4494350016,-1.8641172432,-0.8715162747
H,4.1746057614,-2.5206443007,0.1607321394
H,3.8572880166,-2.2275960107,-1.5541427491
C,4.1337583694,3.2165550303,0.4011071428
H,4.0655274984,3.8710072648,-0.4750486019
H,3.4426375025,3.6258232625,1.1406377959
H,5.1525354971,3.2747847234,0.790472206

Cartesian Coordination of 4b-1 at DFT

–1757.7500494 hartree

F,-0.0701162285,3.4331878563,0.8521516941
H,3.4926280321,1.5011264649,0.4757219162
H,-3.5092343642,1.5072338132,-0.2406612877
H,0.0199152199,-1.4947773196,-0.2012351486
N,3.5916161871,0.4974191471,0.4211438291
N,-3.6007312679,0.5015164094,-0.2599215097

O,1.213719471,1.5849972692,0.2361287317
O,-1.2297823166,1.5857485993,0.0237297951
F,0.1227163718,2.8954472313,-1.3725177417
B,0.0106267114,2.4382558585,-0.081373866
C,-1.1991578724,0.276984885,-0.0929423171
C,2.499970743,-0.332243222,0.2397331266
C,-2.4974801796,-0.3305936046,-0.2025026916
C,4.7334908838,-0.2242521387,0.5292017604
C,4.3889130687,-1.5804383584,0.4163342092
C,2.9788340163,-1.6524507177,0.2322937195
C,-2.9698483531,-1.6511599162,-0.2712611276
C,-4.3880214802,-1.577047842,-0.3767492548
C,1.2035371586,0.2763556386,0.114529081
C,-4.7436008994,-0.2187877063,-0.3661684724
C,0.0108497012,-0.4251953549,-0.0920802209
C,-5.3328974414,-2.709295485,-0.4875188729
C,-6.4103463118,-2.8518141926,0.3970979184
C,-5.1890776324,-3.6837431969,-1.4949691116
C,-7.3176554346,-3.9090121251,0.2915901913
H,-6.5368722838,-2.130882,1.1996262328
C,-6.07540933,-4.7455550914,-1.6081292946
H,-4.3768002868,-3.5924748815,-2.2099727691
C,-7.150502063,-4.8658014955,-0.7152635488
H,-8.1340847971,-3.9794530696,1.0004796389
H,-5.9640585384,-5.4917075712,-2.3880124533
C,5.3372477854,-2.7138661976,0.4898115756
C,5.1743694599,-3.7401543173,1.4410439388
C,6.4355556683,-2.8051108243,-0.3753761293
C,6.0623558696,-4.8038452402,1.5184674082
H,4.3450954434,-3.6887493093,2.1403750981
C,7.3445422627,-3.8639822491,-0.3052062207
H,6.5779299759,-2.0405101505,-1.1336601261
C,7.1577852794,-4.8735052838,0.6451157974
H,5.9364034759,-5.5908280348,2.2547744838
H,8.1778247793,-3.8942022689,-0.9971489726
C,-6.0812826127,0.4384273987,-0.4761409676
H,-6.8277115037,-0.2816206673,-0.8159657291
H,-6.4203291045,0.8420382583,0.4861489913
H,-6.0568164661,1.2697382478,-1.1895059942
C,-2.1599045396,-2.9113416699,-0.1911261742
H,-1.5357171696,-3.0600112901,-1.0811849613
H,-1.4916059959,-2.9036368455,0.6770306756
H,-2.8136171518,-3.7810624839,-0.1003049753
C,2.1838027107,-2.9074648306,0.0239597092
H,1.4525955502,-3.070046727,0.8251800087
H,1.6298915287,-2.8811596622,-0.9215629389
H,2.8423027359,-3.777633194,-0.0042437797
C,6.0598205747,0.4266921137,0.7535251039
H,6.8008071605,-0.3201322125,1.0436810068
H,6.4271716801,0.9293251115,-0.149860493
H,6.0030801982,1.1801730374,1.5471693045
O,-7.9680206151,-5.941156407,-0.9120212318
O,7.9744049562,-5.9558691181,0.8033391047
C,-9.0752649346,-6.1104240745,-0.041033148
H,-9.5872070606,-7.0133346331,-0.3766932864
H,-8.7555656384,-6.243768522,1.0004136757
H,-9.7685707669,-5.2613717136,-0.0965438433
C,9.0988976729,-6.0791099346,-0.0531484882
H,9.604652856,-6.998764408,0.2442469307
H,8.7999879131,-6.1568240311,-1.1063249106
H,9.7905635888,-5.2345706504,0.0610198311

Cartesian Coordination of 4b-2 at DFT

–1757.7444172 hartree

F,0.1067814259,3.7683897609,0.4847038418
H,3.4695443596,1.5122905429,0.066742731
H,-2.131883048,-1.9159867385,0.936721292
H,-0.239904269,-1.2609110362,0.0593840296
N,3.4985178409,0.5032174862,0.1033286842
N,-2.8531015068,-1.2856244451,0.6238983353
O,1.1873047554,1.7442060707,0.0741460109
O,-1.2601496665,1.9115441122,0.1190506554
F,-0.0004532573,2.8498364308,-1.6205785445
B,0.0105845316,2.6314022056,-0.2638467778
C,-1.3278950107,0.6078996606,0.1615919346
C,2.3433549878,-0.2558493589,0.1329941597
C,-2.6448032376,0.0518521236,0.3098241698
C,4.5978404301,-0.2880370288,0.1509001827
C,4.1575817417,-1.6194565788,0.214364823
C,2.7334875413,-1.60218461,0.2033740311
C,-3.9050159015,0.6390116928,0.1358441214
C,-4.8758453855,-0.3813218704,0.364884156
C,1.0816269035,0.4343881155,0.0907477846
C,-4.1859255754,-1.5573653263,0.6828402377
C,-0.1704108945,-0.1855624939,0.0913195194
C,-6.3451125034,-0.2446709219,0.2854157965
C,-7.1236459959,-1.1395360192,-0.4611051912
C,-7.0189574791,0.7906302104,0.9632270546
C,-8.5143913811,-1.0274328553,-0.5319690424
H,-6.6341807764,-1.9318129803,-1.0200830508
C,-8.3985163936,0.9213409533,0.8965442582
H,-6.4480832614,1.4932100351,1.5623034421
C,-9.159411665,0.0103388657,0.1489962359
H,-9.074649717,-1.7397099554,-1.1257626759
H,-8.9142951701,1.7181377635,1.4222323093
C,5.0359353372,-2.8081855838,0.2785800347
C,4.9244927508,-3.7484394414,1.3217362126
C,6.0190258022,-3.0379030086,-0.6933344303
C,5.7500765378,-4.8625011588,1.3844517761
H,4.1882756245,-3.5886400558,2.1040368353
C,6.8650843745,-4.1482185023,-0.6400651102
H,6.1177777692,-2.3429610318,-1.5222517333
C,6.7302845519,-5.0708740036,0.4029775504
H,5.6643931081,-5.5823535228,2.1918387623
H,7.6094323028,-4.2857004282,-1.4151919764
C,-4.6883940596,-2.9103188939,1.0710652202
H,-5.7437048269,-2.8544655937,1.3433184043
H,-4.5932107286,-3.6366904261,0.2540295944
H,-4.1359043985,-3.3089751987,1.9300323409
C,-4.1802657722,2.0529068503,-0.2814748629
H,-4.0860125954,2.7455880015,0.5626053951
H,-3.4638909852,2.3892677202,-1.0336068117
H,-5.1926196963,2.1441507203,-0.6818967197
C,1.8408462617,-2.8084429574,0.2106602504
H,1.1968169359,-2.8386433127,1.0985355455
H,1.1883528336,-2.8320983426,-0.6699293926
H,2.4343899195,-3.7244976224,0.2032607562
C,5.9797150035,0.2811747096,0.1541568396
H,6.7017447628,-0.4857735411,0.4395864275
H,6.2684741775,0.6613347981,-0.8336665524

H,6.0646525805,1.112886969,0.8625281889
O,-10.507991632,0.2224535025,0.1493253135
O,7.4945274542,-6.1916049723,0.5551124257
C,-11.3266565322,-0.6627144753,-0.5983760787
H,-12.3511257338,-0.3137837254,-0.4614875872
H,-11.0780789517,-0.6398429753,-1.6671676859
H,-11.2461914264,-1.6951970693,-0.2344658177
C,8.5077358922,-6.4480101642,-0.4049423731
H,8.9906617772,-7.3750155242,-0.0928974252
H,8.0892332268,-6.580560271,-1.4108735087
H,9.2540473525,-5.64370388,-0.4310347119

Cartesian Coordination of 4b-3 at DFT

–1757.7375881 hartree

F,0.0654060591,3.9646498098,0.8827803221
H,1.8681911045,-1.9144603236,-0.2253786804
H,-1.8573271531,-1.8344523736,0.8583505919
H,-0.0477462288,-0.9939500493,-0.1095201952
N,2.6270754349,-1.2629962216,-0.1113157921
N,-2.6157945545,-1.2311047939,0.5827966255
O,1.2370738734,2.0621708639,0.2167740143
O,-1.2144487415,2.0833896989,0.3653957304
F,-0.0778212756,3.2689140916,-1.3055268721
B,0.0018579499,2.9118073035,0.018700389
C,-1.2098387827,0.7826703041,0.2550972321
C,2.4884576409,0.1140544412,0.0140793759
C,-2.4908058654,0.1387983501,0.3832419609
C,3.9427942432,-1.6074239524,-0.164069948
C,4.6953749635,-0.4325268365,-0.0543985378
C,3.781330053,0.6561904725,0.0575889277
C,-3.7837253475,0.6646990644,0.2833071235
C,-4.6916270179,-0.4263499018,0.4426956385
C,1.2074816912,0.7629861167,0.0876110995
C,-3.9316651554,-1.5822918982,0.6479236988
C,-0.0161597398,0.075052955,0.0513021895
C,-6.1676203166,-0.3668369241,0.3995538722
C,-6.911114233,-1.2340730906,-0.4122774591
C,-6.883164304,0.563246318,1.1793440442
C,-8.3072288132,-1.1968164639,-0.4489806626
H,-6.3901346975,-1.9437598445,-1.0485070599
C,-8.2690475346,0.6188628555,1.1488788795
H,-6.3399311954,1.2421764862,1.8293271744
C,-8.9942573685,-0.2642722898,0.3353268736
H,-8.8395243506,-1.8842600861,-1.0956729126
H,-8.8166758167,1.3341010718,1.7537021763
C,6.1726781066,-0.3609347081,-0.0636202823
C,6.8573702574,0.4734933859,-0.9688942984
C,6.9457754724,-1.1250426502,0.8204735718
C,8.2432024075,0.5387576193,-0.9862904232
H,6.2890491923,1.0684569977,-1.6772820524
C,8.3421785836,-1.0777694462,0.8108276526
H,6.4486003552,-1.7592018196,1.5489191863
C,8.9985046685,-0.2396208984,-0.0966549009
H,8.7674443192,1.1804912127,-1.6867190287
H,8.8987422584,-1.6832236985,1.5162873485
C,-4.3485732722,-2.9881960489,0.9370102171
H,-5.4060524242,-3.0178994176,1.2049165656
H,-4.2053248022,-3.648536784,0.0722872272
H,-3.7752479982,-3.4109002081,1.7708359839
C,-4.1481826893,2.0895392243,-0.0110613317
H,-4.1077788901,2.7081201331,0.8927637357
H,-3.4497118976,2.5381502297,-0.7199510981
H,-5.1613132198,2.150077347,-0.4156689558
C,4.1394130967,2.1019157671,0.2340964232
H,3.8503449471,2.6955314578,-0.6396825708
H,3.6104341959,2.5383976662,1.0844450609
H,5.2145381258,2.2142076205,0.388207841
C,4.3712387153,-3.0280693684,-0.3422785896
H,5.4280769501,-3.0687792017,-0.611174617
H,4.2383839075,-3.6178746541,0.5736628346
H,3.7987501978,-3.5210206922,-1.1369236497
O,-10.3523835923,-0.1336427915,0.3802076024
O,10.3535706695,-0.1083553269,-0.1963590949
C,-11.1363074701,-1.0000481974,-0.4244630725
H,-12.1759364203,-0.7305723977,-0.2332672414
H,-10.9204141976,-0.8678687092,-1.4924238305
H,-10.9817574289,-2.0531209795,-0.156055654
C,11.1676005445,-0.8684195106,0.6825712163
H,12.1988956469,-0.6159405467,0.4322396115
H,10.9789227358,-0.6128532933,1.73312996
H,11.0168402977,-1.9468333756,0.5441234732

Cartesian Coordination of 4c-1 at DFT

–2215.8193915 hartree

F,0.0257772406,2.7008333646,1.7880296176
H,3.579533634,1.2820997688,0.4587407709
H,-3.4359032262,1.4720623786,-0.0268492885
H,-0.0201381146,-1.6337681643,0.4037507694
N,3.6475678288,0.2750519232,0.4208434689
N,-3.559749949,0.4697446302,-0.0070887053
O,1.2956967948,1.4248977439,0.2871547311
O,-1.153034512,1.4903348374,0.1630844176
F,0.1540341779,3.3343311741,-0.4159761068
B,0.0811933535,2.3004015318,0.4748490037
C,-1.1707934676,0.1775859856,0.221701045
C,2.5231806003,-0.5285889319,0.3670721111
C,-2.4858781834,-0.3936746103,0.1118627749
C,4.7761155932,-0.4746943355,0.4419120313
C,4.3879053703,-1.8231514719,0.3991706376
C,2.9650101689,-1.8611882724,0.3501424423
C,-2.9983404585,-1.7006057911,0.0800354606
C,-4.4104771604,-1.5846985449,-0.0634006007
C,1.2367884053,0.1131291872,0.3392842808
C,-4.7228185059,-0.2163708473,-0.1122414249
C,0.0106729711,-0.5604639039,0.3498944115
C,-5.3929794609,-2.6861751405,-0.1614962398
C,-6.5071587716,-2.73339241,0.6907882972
C,-5.2342761145,-3.7069741275,-1.1125360875
C,-7.4537597836,-3.753235706,0.5808651356
H,-6.6546188657,-1.9798566854,1.4568159561
C,-6.1691742516,-4.7365971474,-1.2215343137
H,-4.402822996,-3.695824984,-1.8087254051
C,-7.2942942254,-4.7646103356,-0.3805611795
C,5.3074636125,-2.9822309087,0.4110270911
C,5.1677462098,-3.9930971077,1.3614342588
C,6.3450086239,-3.0785844753,-0.5353743676
C,6.0360927141,-5.0948868079,1.3891077911
H,4.3999442109,-3.941043775,2.1247838921
C,7.2105578243,-4.1717447944,-0.5213524554
H,6.4333627894,-2.3162898997,-1.298719194

C,7.0735037603,-5.1947004941,0.4469243771
C,-6.0348671347,0.4806530813,-0.2748890842
H,-6.7985469234,-0.2227166303,-0.6105426367
H,-6.3815715175,0.9233701881,0.6671036457
H,-5.9642612208,1.2889801449,-1.0110826726
C,-2.2279392412,-2.9799144686,0.2247089008
H,-1.5384722,-3.1425936936,-0.6127680756
H,-1.6313625948,-2.9875807015,1.1439621988
H,-2.9060077175,-3.8342087511,0.2635300704
C,2.1207969565,-3.0964029836,0.2411415018
H,1.5254914331,-3.2701986349,1.1461510384
H,1.422735591,-3.0311467179,-0.6008483556
H,2.7481254938,-3.9766212835,0.0896108707
C,6.1313820256,0.1487973408,0.535750082
H,6.8803381865,-0.6106140816,0.7656823598
H,6.4240929607,0.63531982,-0.403200942
H,6.1627957946,0.9112593073,1.3222532869
O,-8.2284601422,-5.7725608672,-0.4980874978
O,-8.5697047198,-3.7038575569,1.382210616
O,-6.0155772878,-5.6644901788,-2.225041899
O,5.7434001807,-6.0294393449,2.3401997448
O,7.859959814,-6.3231851655,0.3969272907
O,8.2106437981,-4.3679083322,-1.4334601938
C,-8.695831516,-4.764452113,2.3369365304
H,-9.6152760839,-4.5647044212,2.890750586
H,-8.7645050176,-5.7382072399,1.8445725697
H,-7.8481024213,-4.7623021895,3.0337384426
C,-9.2759931676,-5.4750690132,-1.4316816241
H,-9.9399445425,-6.3419138604,-1.4363741553
H,-9.8353852448,-4.587174975,-1.1169689499
H,-8.867796843,-5.3206645028,-2.4363741882
C,-5.7515921685,-7.0034410418,-1.7908393676
H,-6.5705707229,-7.3935226025,-1.1802568852
H,-5.6502898651,-7.6018544235,-2.6983959277
H,-4.8137567016,-7.0500363375,-1.2226643084
C,6.7748903136,-6.8024138792,2.9522230726
H,7.1186422437,-7.6098602876,2.3034505885
H,7.6288646334,-6.1748551116,3.2345141177
H,6.3271389354,-7.2177184075,3.8580651852
C,9.2556612625,-6.1436677775,0.6596870613
H,9.722172523,-5.4961816874,-0.0858959968
H,9.4174312644,-5.7249974255,1.6616538316
H,9.701478899,-7.1393021401,0.6108760588
C,8.359097445,-3.4238202125,-2.4828036787
H,9.1857561465,-3.785558115,-3.0958097695
H,7.4532865868,-3.3598724731,-3.0979903708
H,8.6037960895,-2.4250846455,-2.099485426

Cartesian Coordination of 4c-2 at DFT

–2215.8131669 hartree

F,0.0463977591,2.7837580204,1.9219989377
H,2.0549331387,-1.9324637435,-0.8200136466
H,-3.4794330791,1.527999776,0.2940164841
H,0.1969394526,-1.2836932668,0.1278325676
N,2.7906844012,-1.3249200715,-0.495938908
N,-3.5212432183,0.5204477146,0.2328908963
O,1.2515268913,1.8776979786,0.1277525242
O,-1.1964950956,1.7350092923,0.231074736
F,-0.1043007155,3.7574874086,-0.1557792699
B,-0.0012680896,2.6014132427,0.5610612414
C,-1.1056839953,0.4254492313,0.1767813614
C,2.6091909012,0.0073761381,-0.144210311
C,-2.3764081236,-0.2501352879,0.1511205677
C,4.1178870111,-1.6164554522,-0.5812263008
C,4.8305428524,-0.460037692,-0.2439109618
C,3.88098825,0.5707888844,0.0241486196
C,-2.783651116,-1.5894995689,0.0555038795
C,-4.2077914438,-1.5896978864,0.0846639902
C,1.3031291672,0.5756026986,0.0485607393
C,-4.6310718065,-0.2557307887,0.1972233283
C,0.1384810137,-0.2073255554,0.1260328455
C,-5.1048947395,-2.763713062,0.0130204135
C,-6.0865663887,-2.9730135477,0.9946143216
C,-4.9958096539,-3.6949845101,-1.0315924054
C,-6.9502478624,-4.065489591,0.9223698658
H,-6.1873743916,-2.2957337016,1.83571727
C,-5.8531216201,-4.7942248934,-1.1097608517
H,-4.2692653842,-3.5588951486,-1.8252722615
C,-6.8482991259,-4.9838904298,-0.1360549639
C,6.303896264,-0.3511803494,-0.1735815806
C,6.9786107213,0.6636428552,-0.8503526962
C,7.0494747099,-1.2792465058,0.5780669532
C,8.3768235436,0.7726505294,-0.7978251893
H,6.4427781176,1.3847344765,-1.4565332163
C,8.4379625481,-1.175264098,0.6454123465
H,6.5286109473,-2.0426027209,1.1414302718
C,9.1250671978,-0.1523096955,-0.0496918331
C,-6.0043351151,0.3319967699,0.2503883136
H,-6.744973977,-0.4065246395,-0.0606121101
H,-6.2684739322,0.6620329826,1.2627314847
H,-6.0877578818,1.2018768542,-0.4104528826
C,-1.9024970518,-2.8029180464,-0.005286208
H,-1.2861716347,-2.8180934971,-0.9129580503
H,-1.223925661,-2.8502138058,0.8543432783
H,-2.502823414,-3.7143510733,-0.0010122097
C,4.1855703999,1.9696837491,0.4698219372
H,4.0758455794,2.6832634826,-0.3544781476
H,3.4944813934,2.2949691132,1.2501487165
H,5.2103768062,2.0393450644,0.8407272081
C,4.5912654005,-2.9649748937,-1.0191307987
H,5.6592798295,-2.9335025902,-1.2392014128
H,4.4301533823,-3.7288726348,-0.2479032359
H,4.0671379344,-3.2971245054,-1.9233030509
O,-7.7044030456,-6.0613214003,-0.2212251078
O,-7.9425585483,-4.1889114091,1.8685168812
O,-5.7560108585,-5.6207767485,-2.2029213659
O,8.8885926481,1.8444152677,-1.4692907577
O,10.4841332439,0.0094691941,0.0989153166
O,9.2311395636,-2.0013388667,1.3943720896
C,-7.8089032512,-5.308615831,2.7526889863
H,-8.6608598183,-5.2607910301,3.4336695502
H,-7.8266860313,-6.2544337001,2.2037678877
H,-6.8797484882,-5.2363051989,3.3316629796
C,-8.9931996046,-5.7337106032,-0.7609161119
H,-9.5657115449,-6.6632873073,-0.773574332
H,-9.5018882547,-4.9963440608,-0.1316172534
H,-8.8982934656,-5.3490365637,-1.7825608787
C,-5.3845831194,-6.9762189672,-1.9309268243
H,-6.1229753864,-7.4735075017,-1.2966802819
H,-5.3341060722,-7.4755988847,-2.900549154

H,-4.3978079543,-7.0205310353,-1.4519537861
C,10.1919209956,1.8012170869,-2.0474850168
H,10.9756148315,1.9162869446,-1.2969119928
H,10.3526611731,0.8673896984,-2.5998279875
H,10.2236461943,2.6371529826,-2.7500286027
C,11.3144529053,-1.0274069802,-0.4334512391
H,11.1406901664,-1.9786024765,0.0746275276
H,11.1475813381,-1.1518830922,-1.5115153969
H,12.3440939263,-0.7049842999,-0.2649202154
C,8.6038678612,-2.9845087898,2.2023946814
H,9.4089557499,-3.4914465506,2.7362436878
H,7.9175667182,-2.5310348418,2.9278846017
H,8.0541663619,-3.7179480341,1.5984060987

Cartesian Coordination of 4c-3 at DFT

–2215.8066042 hartree

F,-0.0903771017,2.7141290312,1.7593585467
H,2.0368828024,-1.9150164897,-1.0815661922
H,-1.7205730205,-2.3423929587,0.0085320949
H,0.1518294647,-1.3208852931,-0.1023212544
N,2.7521562788,-1.3221242442,-0.6914802957
N,-2.5010978455,-1.7233569256,-0.1380767092
O,1.1658832104,1.8455355367,-0.0166882552
O,-1.2851763103,1.6809520459,0.0264957965
F,-0.1986114717,3.7163659732,-0.3087924404
B,-0.1054112859,2.5526222909,0.3955628883
C,-1.1875390547,0.3808426908,-0.0435281199
C,2.5460862905,-0.0051196781,-0.2966691099
C,-2.4334518391,-0.3352968253,-0.1139531972
C,4.0866977608,-1.5924043962,-0.7607890998
C,4.7747607623,-0.4420762282,-0.3628924143
C,3.8047413916,0.5662195965,-0.0766488193
C,-3.7483755779,0.1436636851,-0.1944930563
C,-4.6039859026,-0.9961143777,-0.2559031762
C,1.228814963,0.5459060012,-0.1153096043
C,-3.7959154736,-2.1374178888,-0.2076429177
C,0.0693169697,-0.2430726694,-0.0714573389
C,-6.0800086011,-0.9995803629,-0.3475187754
C,-6.7369438304,-1.7404018811,-1.3417267649
C,-6.8565616852,-0.257126018,0.556526601
C,-8.1308114086,-1.7681746092,-1.4188511967
H,-6.1759819048,-2.303916263,-2.079457166
C,-8.2483497047,-0.2666067349,0.477162571
H,-6.3922828558,0.3164882038,1.3510005613
C,-8.9014952562,-1.0318150224,-0.5043102092
C,6.2445181071,-0.312844752,-0.2586410375
C,6.9134116588,0.7359551935,-0.8874816961
C,6.9922329411,-1.2533820066,0.4751527469
C,8.3081304683,0.8673068475,-0.804644718
H,6.3760062307,1.4688161483,-1.4779789854
C,8.3773779914,-1.1281913187,0.5717029677
H,6.4742261257,-2.0446218427,1.0015145612
C,9.0588893406,-0.0701749589,-0.074920729
C,-4.1518034983,-3.5889484927,-0.1907254846
H,-5.2182328285,-3.7126458329,0.003766764
H,-3.9309502384,-4.0783570749,-1.1477064542
H,-3.5988680169,-4.1256036809,0.5892935657
C,-4.1733696617,1.5806412076,-0.2606134122
H,-4.0404348314,2.0811233356,0.7047228482
H,-3.5677250023,2.1390561562,-0.9774088729
H,-5.2251197294,1.6566647625,-0.544039036
C,4.0819946724,1.9490329178,0.4331936105
H,4.0000830745,2.6927053624,-0.3673261711
H,3.3589495049,2.2409596541,1.1974504039
H,5.0911976604,2.0098559614,0.8461946747
C,4.5879995961,-2.9147009143,-1.2453822766
H,5.6653339391,-2.8682476338,-1.4110183409
H,4.3941375284,-3.7188965235,-0.5242268284
H,4.1110956272,-3.2006214274,-2.1908159313
O,-10.2778084703,-1.0542099512,-0.580071045
O,-8.7171483663,-2.5782603957,-2.3612728884
O,-8.9728891546,0.4163113773,1.4277268796
O,8.8120788969,1.9708714115,-1.4285777345
O,10.4119668183,0.1089473541,0.1052461963
O,9.1720231618,-1.9665409232,1.305213754
C,-9.4773597179,-1.9085758514,-3.3737372374
H,-9.8492417713,-2.6906993787,-4.0386781211
H,-10.3181621798,-1.3585071256,-2.9432829913
H,-8.8411659973,-1.2216167499,-3.9461918157
C,-10.8945839963,-1.9417472084,0.3632153827
H,-11.9713733062,-1.8620184158,0.2009204402
H,-10.5747581667,-2.9753653201,0.1886566886
H,-10.6541566652,-1.6462596289,1.3895337007
C,-9.6823220955,1.562745817,0.9424878714
H,-10.4152143328,1.2838152031,0.1797395941
H,-10.1937553351,1.9916648557,1.8063512098
H,-8.9861096054,2.3039060168,0.5306641617
C,10.1275247857,1.9738394515,-1.9801820618
H,10.8931388731,2.0776825098,-1.2096022424
H,10.318475741,1.063646987,-2.5615666791
H,10.1564669822,2.834703976,-2.6520646364
C,11.2697285706,-0.8920032818,-0.4518124719
H,11.1012148744,-1.8660934672,0.0128744857
H,11.1270827643,-0.9742427356,-1.5373962759
H,12.2903356949,-0.5610777148,-0.2484787612
C,8.5485684532,-2.9914858908,2.0628423179
H,9.3536990946,-3.5076354651,2.5877135583
H,7.8446685733,-2.5786560415,2.7957583848
H,8.019178783,-3.7075999606,1.4211611808

Cartesian Coordination of 3a·Cl⁻ at DFT

–1526.9544756 hartree

F,-0.000022435,3.9623207962,-0.789036829
H,-1.7281752872,-1.9692461972,0.04293283
H,1.7281526933,-1.9692390635,0.0430320159
H,-0.000001223,-0.9742562938,0.3952325464
N,-2.5296810495,-1.3177112089,0.0252976597
N,2.5296600547,-1.3177062941,0.0253248466
O,-1.2306743577,2.0713403227,-0.1633595095
O,1.2306489051,2.0713424319,-0.1633903272
F,0.0000054043,3.3073158938,1.4214660525
B,-0.0000111999,2.887315646,0.0867177319
C,1.2064262281,0.7667262366,0.0315696462
C,-2.4627662451,0.0716499164,-0.0150340505
C,2.4627455804,0.0716520822,-0.0150792548
C,-3.8214628347,-1.7207191327,-0.0370638616
C,-4.6220235859,-0.5767875475,-0.1155575336
C,-3.7799641031,0.5575131345,-0.1045501125
C,3.7799440139,0.5575105107,-0.1046270845
C,4.6219982981,-0.5767928458,-0.1156529514

C,-1.2064453271,0.7667242576,0.0316038781
C,3.8214359546,-1.720720708,-0.0371007371
C,-0.0000066215,0.0921159157,0.2225714074
H,5.7034930744,-0.5690295005,-0.1728518265
H,-5.7035205263,-0.5690205595,-0.1727145305
C,4.1953672274,-3.1692845698,0.0071522691
H,4.1837729467,-3.5550165095,1.0345926662
H,3.4906791511,-3.7762225245,-0.5700443699
H,5.2017430789,-3.3148399298,-0.3965637667
C,4.2225998365,1.9904942286,-0.175246228
H,3.8866894855,2.471064492,-1.1005355281
H,3.8060275627,2.5830520021,0.6451553508
H,5.315410507,2.0509996861,-0.1312943796
C,-4.2226177804,1.990499262,-0.1751352425
H,-3.806003685,2.5830472256,0.6452518847
H,-3.8867508152,2.4710773172,-1.1004365546
H,-5.3154261108,2.0510083573,-0.1311308673
C,-4.1954019686,-3.1692815062,0.0071539347
H,-3.4909007498,-3.7761757889,-0.5703185174
H,-4.1835013999,-3.555121233,1.03454971
H,-5.201901322,-3.3147729409,-0.3962752773
Cl,0.0000006251,-3.4200493611,0.0664719101

Cartesian Coordination of 4a·Cl⁻ at DFT

–1989.0955506 hartree

F,-0.0038019548,4.171919054,0.7895824062
H,1.6983440869,-1.7468790317,-0.0672771012
H,-1.6994091226,-1.7466400875,-0.0908203007
H,0.0032704002,-0.7451261234,-0.4690311231
N,2.5080519743,-1.1038677216,-0.0461291566
N,-2.5086046159,-1.1027807399,-0.0959551573
O,1.2288605509,2.2885627738,0.1486820413
O,-1.2312719777,2.2872548659,0.1393565546
F,0.0036433805,3.5396312111,-1.4278382289
B,-0.0004693437,3.1090509927,-0.098170953
C,-1.2064123937,0.9879830661,-0.0802161046
C,2.4624374538,0.2842799313,-0.0114639221
C,-2.4616571734,0.2849779997,-0.0535263192
C,3.7882368485,-1.5314573006,-0.0002204161
C,4.6267139811,-0.3995879047,0.0502930176
C,3.7857161003,0.751344151,0.0522197835
C,-3.784039048,0.7536863935,0.0065318944
C,-4.6272560352,-0.3962491738,-0.0034838609
C,1.2076355819,0.9877764191,-0.0595185756
C,-3.7900519464,-1.5285131014,-0.0683067676
C,0.0021769147,0.3167299301,-0.2725539033
C,-4.1073336682,-2.9922778618,-0.0701139826
H,-4.2945924898,-3.366418998,-1.0848415027
H,-3.2652109632,-3.5627156463,0.3322214927
H,-4.9997487476,-3.1981718599,0.5281935366
C,-4.2202371359,2.1913571634,0.009487864
H,-4.1884581851,2.6240593174,1.0176367305
H,-3.5579672967,2.802416761,-0.6068516397
H,-5.2444949161,2.2859850346,-0.3631425878
C,4.2236837699,2.1864161708,0.1393527776
H,4.1745475668,2.6858432013,-0.8369442723
H,3.5746491747,2.7540988106,0.8085492779
H,5.2543588079,2.2546118679,0.498647026
C,4.1073489271,-2.9944357572,-0.0288080466
H,4.2261039973,-3.4041613622,0.9824892198
H,3.2964591678,-3.5506433713,-0.50758715
H,5.0392584392,-3.1785809816,-0.5715539283
C,6.1022686889,-0.4276789599,0.07514303
C,6.8611785742,0.3939730956,-0.7819817129
C,6.8048759571,-1.2836819086,0.9456979541
C,8.2567815868,0.3647706521,-0.7663424965
H,6.3454864107,1.0479597491,-1.4783376067
C,8.2007904736,-1.3219073196,0.9558909001
H,6.2470774692,-1.9118263253,1.6335771611
C,8.9363547489,-0.4955393614,0.1014082607
H,8.8142743545,1.0093904286,-1.441239786
H,8.714183424,-1.9920712023,1.6408770786
H,10.0226500443,-0.5213771861,0.111612289
C,-6.101123843,-0.423311662,0.0533434663
C,-6.8513015751,-1.2564249836,-0.8000988822
C,-6.8119625661,0.3759911072,0.9708343524
C,-8.2455052691,-1.2958740139,-0.734948622
H,-6.3325969296,-1.8649958422,-1.5344344491
C,-8.2063484235,0.3460057042,1.0302217099
H,-6.2594343824,1.0125895903,1.6547709731
C,-8.9330102262,-0.4926155786,0.1794489713
H,-8.7957727507,-1.9483226021,-1.4083199206
H,-8.7257747194,0.9730889206,1.7504999448
H,-10.0182549412,-0.5189303552,0.2279187146
Cl,0.0003787844,-3.1937870393,-0.1283659528

Cartesian Coordination of 4b·Cl⁻ at DFT

–2218.1510306 hartree

F,0.0116512426,4.2659564762,0.7905041694
H,1.7018713918,-1.6476839972,-0.1325662102
H,-1.7007163723,-1.6488870725,-0.0853385617
H,-0.0045867515,-0.6457653905,-0.4879937209
N,2.5103472482,-1.0034861994,-0.1221414057
N,-2.5094050558,-1.0051714188,-0.0720227379
O,1.2320228802,2.3866066675,0.1155101799
O,-1.2281479982,2.3840258928,0.1556965853
F,-0.0255815961,3.644872253,-1.4297604761
B,-0.0025421252,3.2069058233,-0.1022121002
C,-1.2072490444,1.085287198,-0.0696833773
C,2.4627580101,0.3839890333,-0.0761053381
C,-2.4615329823,0.3821621938,-0.0240107392
C,3.7929066692,-1.4279996791,-0.1010886021
C,4.629403269,-0.2954386762,-0.0525527057
C,3.7866182082,0.8529504398,-0.0285191553
C,-3.7834274755,0.8504580678,0.0578340892
C,-4.6266563719,-0.2985662302,0.0560758089
C,1.2070725888,1.0861879336,-0.0969287652
C,-3.791261909,-1.4301548063,-0.0245707193
C,-0.0022989103,0.4153763782,-0.2876068791
C,-6.1010288425,-0.3249161484,0.1269982098
C,-6.8644856887,-1.1238658219,-0.7380228351
C,-6.8085887757,0.445125844,1.0745894378
C,-8.2623033228,-1.1706385981,-0.6706959294
H,-6.3600891374,-1.7143216035,-1.4968632521
C,-8.1971015966,0.4195351721,1.1490159342
H,-6.2539989217,1.062635835,1.7742541223
C,-8.9347898498,-0.3918659683,0.2762320296
H,-8.8030276783,-1.8037962052,-1.3649266717
H,-8.7296248618,1.0150689943,1.8843293504
C,6.1063462665,-0.3210967674,-0.0431806139

C,6.8622281275,0.4792713813,-0.9260002106
C,6.8231120351,-1.1500421678,0.832891415
C,8.2527443977,0.4544750727,-0.9283480863
H,6.3442462754,1.1203917818,-1.6326351911
C,8.2227787433,-1.1961309912,0.8378258712
H,6.2796259407,-1.7661225579,1.5429277135
C,8.9437395622,-0.3867858897,-0.0456879358
H,8.8229960765,1.0731796804,-1.6145954583
H,8.7264146493,-1.8535025684,1.5375485047
Cl,0.001269429,-3.1001732814,-0.1669200998
C,4.225161609,2.2875437966,0.0602046534
H,4.1313407336,2.8015021957,-0.9050859095
H,3.6058295943,2.844699254,0.765918585
H,5.2706005913,2.3523341952,0.3749275266
C,4.1175695724,-2.8892696206,-0.1436119613
H,5.0471630885,-3.0638230745,-0.6936267363
H,4.2443589917,-3.3075064947,0.8633732113
H,3.3065555077,-3.4456591146,-0.622085551
C,-4.1124040492,-2.8928995955,-0.030471533
H,-5.0026798832,-3.0971488613,0.5717496606
H,-4.3060315356,-3.2634110826,-1.0455078705
H,-3.2704126792,-3.4680734601,0.3654944095
C,-4.221964686,2.2871431564,0.0780230463
H,-4.1676647394,2.7151473227,1.0872384875
H,-3.5760688171,2.9033550911,-0.5506373166
H,-5.2550882933,2.3806230934,-0.2700216691
O,-10.3019132892,-0.3536653273,0.427810237
O,10.3167409828,-0.3458122486,-0.1246248277
C,11.0617592427,-1.1807208533,0.7460067021
H,12.1122990945,-0.9922456012,0.51711358
H,10.8714327424,-0.9373796476,1.7998752459
H,10.8386777117,-2.2426021152,0.5761103744
C,-11.0925648877,-1.1533941653,-0.4355545522
H,-12.1296608481,-0.9722625664,-0.1471517831
H,-10.9542557036,-0.8699856967,-1.4875564025
H,-10.8649707945,-2.2213976592,-0.3179692495

Cartesian Coordination of 4c·Cl⁻ at DFT

–2676.24071 hartree

F,0.0090581563,4.3587926017,0.7823302076
H,1.694185255,-1.553769305,-0.1339098483
H,-1.6934412196,-1.5529880297,-0.1115580148
H,-0.0011996386,-0.5478192162,-0.5156772634
N,2.5050325737,-0.912296093,-0.1170284668
N,-2.5037264043,-0.9107215885,-0.1089599021
O,1.2328922184,2.4797880903,0.1129150154
O,-1.2275516442,2.4783673455,0.1365783683
F,-0.0139279028,3.740498794,-1.4390827873
B,0.0001666046,3.3023155602,-0.1122531498
C,-1.205578568,1.1813517995,-0.0944891411
C,2.462939695,0.4754918772,-0.07458317
C,-2.4599580882,0.4766357518,-0.0588432524
C,3.7847079994,-1.3428139865,-0.0813641175
C,4.6255317133,-0.2133444684,-0.0286678487
C,3.7877818577,0.9394998992,-0.0174041675
C,-3.7831875313,0.9420049709,0.0100237852
C,-4.6234659381,-0.2098643557,-0.0049010992
C,1.2086375475,1.180980509,-0.1049818498
C,-3.7842051393,-1.3395826144,-0.0780669346
C,0.0003407738,0.5119509097,-0.3088524669
C,-6.0983718661,-0.2408501906,0.0445979659
C,-6.8240958379,-1.0613290722,-0.84293129
C,-6.8133673396,0.5361057574,0.9682709926
C,-8.2192717217,-1.1141012818,-0.7985196442
H,-6.2799626178,-1.6342835281,-1.5824928522
C,-8.2090150524,0.4902683389,1.0120598875
H,-6.2964430092,1.1630416978,1.6858118802
C,-8.9291369339,-0.3387765005,0.1411756864
C,6.1019883231,-0.2464323896,-0.0009596587
C,6.8631409173,0.5534212886,-0.8660615449
C,6.7801149807,-1.0927607164,0.899214371
C,8.2592817143,0.5061331069,-0.8400919648
H,6.3826277445,1.2000185928,-1.5916117568
C,8.1759408169,-1.1466784886,0.9249392944
H,6.1978667701,-1.6860849365,1.5923855611
C,8.9331619959,-0.3470262573,0.0443137904
C,-4.0966098995,-2.8045685916,-0.0838586995
H,-4.9897410104,-3.0142994952,0.5119051146
H,-4.2780951314,-3.1788043346,-1.0998951705
H,-3.2535539371,-3.3728633058,0.3195985461
C,-4.2232350917,2.3780611783,0.0292250076
H,-4.1988678091,2.7961601741,1.0436455348
H,-3.5597488854,2.9993514928,-0.5753547681
H,-5.2464468044,2.473609747,-0.3459186716
C,4.2302552407,2.3729297499,0.0685844169
H,4.1666188853,2.8753362585,-0.9051793563
H,3.5938277511,2.9398916931,0.7505314388
H,5.2672893296,2.4360800374,0.4097267842
C,4.0997488201,-2.8065382363,-0.1215301627
H,5.0325467701,-2.988114583,-0.6634280221
H,4.2126843085,-3.2266964049,0.8864241819
H,3.2886849362,-3.3562739912,-0.6074584411
O,-10.3078319859,-0.3435074784,0.1724978477
O,-8.9908341202,-1.8862475646,-1.6291747333
O,-8.8673814762,1.2262559609,1.9772528905
O,8.9662735024,1.2648737593,-1.7516412505
O,10.3116112498,-0.3543666625,0.0830262974
O,8.9037673642,-1.9435070525,1.7714558106
C,-8.3373970795,-2.6557662099,-2.62936292
H,-9.1317957534,-3.1680289059,-3.1749425124
H,-7.7739696756,-2.0174779918,-3.3213497003
H,-7.660097901,-3.3984880046,-2.1891376094
C,-10.886155496,-1.4843257672,0.8152842111
H,-11.9687813258,-1.3410724732,0.7769354621
H,-10.6205708212,-2.4070626205,0.287862815
H,-10.561060292,-1.5444186102,1.8613533012
C,-9.6020965219,2.3519484022,1.4840753524
H,-10.3911472005,2.0362751233,0.7940478309
H,-10.0453015026,2.8323116242,2.3595190058
H,-8.9297934848,3.0602888295,0.9824968722
C,9.6786349976,2.3749371146,-1.1944927987
H,8.9843742592,3.072293348,-0.7076978704
H,10.4329387281,2.0389563332,-0.475774105
H,10.1643778591,2.8763177573,-2.0348630249
C,10.9205094189,-1.477617879,-0.5626441413
H,10.6249708223,-2.4147882173,-0.0784140449
H,10.6513042157,-1.5046501026,-1.6258218564
H,11.9999163127,-1.3401074952,-0.4625056475
C,8.1992778326,-2.7451822773,2.7099661948
H,8.9642679955,-3.2771467787,3.2782232831

H,7.6008694516,-2.1296083771,3.3931197561
H,7.5454829249,-3.4710001166,2.2101259938
Cl,0.0004410252,-3.0054599285,-0.178831057

Cartesian Coordination of 4d at AM1

–1.2156606 hartree

F,-0.3640478569,6.0859347867,0.4676888681
H,3.3400945146,4.3771189203,-0.2143638356
H,-4.0553445592,4.4551909354,-0.779775146
H,-0.4034590136,1.5666063191,0.013235959
N,3.3069427136,3.3871303828,-0.2254714517
N,-4.0636223633,3.4843750988,-0.5810639473
O,0.8697881304,4.6100643503,-0.6213958809
O,-1.5831842313,4.6383445745,-0.6773725832
F,-0.3171504029,6.1032046454,-1.7097534108
B,-0.3478991749,5.4385677421,-0.6280900903
C,-1.5857970217,3.339861582,-0.4168037873
C,2.1115316513,2.6504819961,-0.3089846316
C,-2.896692206,2.7266297297,-0.366883348
C,4.3786734723,2.5225671504,-0.1688411571
C,3.8803441905,1.1912243549,-0.222959668
C,2.4519301471,1.2713415584,-0.313334594
C,-3.2940237901,1.3826633472,-0.1273717863
C,-4.7238714308,1.3463853285,-0.2073906562
C,0.8234497952,3.308351077,-0.3879627399
C,-5.1690720408,2.6686558906,-0.488135694
C,-0.3919134907,2.6300410613,-0.2399246274
C,-5.5816387374,0.1936823091,-0.0404270785
C,-6.6748663205,0.2541741245,0.8337677545
C,-5.3331133743,-0.9834821044,-0.7583931269
C,-7.5252693676,-0.8487746447,0.9791262421
H,-6.8827620757,1.1715942673,1.4046664596
C,-6.1693549478,-2.0935507911,-0.5985543019
H,-4.4881678659,-1.033701875,-1.4612823572
C,-7.2748613279,-2.0426169127,0.2741599749
C,4.6817124224,-0.0127379703,-0.1921051862
C,4.331092325,-1.0678855891,0.6516260038
C,5.8131950247,-0.1212646396,-1.0169950104
C,5.1160835663,-2.2352447876,0.6904644925
H,3.4513605156,-0.9951382236,1.3079821974
C,6.58684826,-1.2828970058,-0.9898833012
H,6.0692735474,0.7126084714,-1.6854478436
C,6.2512716249,-2.3560125119,-0.1286708212
C,-6.5541618644,3.1455147522,-0.6651956792
H,-7.2410401177,2.2652282058,-0.7466359617
H,-6.8701764901,3.7626869764,0.2140433932
H,-6.6554179649,3.7668965512,-1.590076563
C,-2.4379759956,0.234766193,0.1786506177
H,-1.7350980264,0.0247161676,-0.668577736
H,-1.834329955,0.4275454096,1.1028666214
H,-3.0576629708,-0.6812048591,0.3549270296
C,1.5474404794,0.1259044805,-0.4310748406
H,1.0020307026,-0.0457238114,0.5330601862
H,0.7926596357,0.2938177575,-1.2413800613
H,2.1242186442,-0.8033500772,-0.6732305414
C,5.7809066934,2.967705178,-0.0568244687
H,6.4189552691,2.102861548,0.2562375447
H,6.1493552006,3.3437878917,-1.0450531672
H,5.8916414269,3.7864328303,0.697597234
O,-8.0510564739,-3.1589579689,0.5260192082
O,-8.6568377752,-0.6760675783,1.7580010451
O,-6.0062890964,-3.2233653222,-1.3870484024
O,4.7047520209,-3.1697734311,1.6164939397
O,6.9585476513,-3.5447952533,-0.170226733
O,7.7321464878,-1.4657866918,-1.7372456419
C,-8.6945285533,-1.5153338637,2.9277784892
H,-8.7137181301,-2.5912279091,2.6119595136
H,-7.7831012463,-1.3200719413,3.5504626862
C,-8.9138636748,-3.5148541731,-0.5732837086
H,-9.6205155834,-2.6675027207,-0.7707074817
H,-8.2889171144,-3.7100331818,-1.4837251074
C,-4.7700632144,-3.9200352997,-1.1890475767
H,-4.7310013339,-4.6125586659,-2.0732129188
H,-3.9086657274,-3.2040464983,-1.2294271882
C,4.9787688416,-4.5459289475,1.3039721211
H,4.8660208195,-4.7269427444,0.2042909632
H,6.0356141711,-4.7693465517,1.6097438602
C,8.2689519616,-3.4479290044,0.4216141816
H,8.8801536902,-2.7097873948,-0.1604546506
H,8.170129941,-3.1044617837,1.4840470092
C,7.9388164746,-0.5272611164,-2.8029532047
H,7.0147184153,-0.4550217112,-3.4336283807
H,8.1775693301,0.4776534466,-2.3652589316
C,9.1104859119,-1.0665761322,-3.6049406352
H,10.0002807931,-1.1820834891,-2.9327274947
H,8.8552594455,-2.0860123167,-3.9957643976
C,9.4354908127,-0.1318367688,-4.7491661193
H,9.6834095658,0.8862347198,-4.3477135906
H,8.5366316325,-0.0176741627,-5.4111306721
C,10.600938622,-0.6538810069,-5.5621440761
H,11.4996613659,-0.7688130967,-4.9003920587
H,10.3532884451,-1.6720057883,-5.9633541081
C,10.9300212863,0.2778697603,-6.7087873183
H,10.0310966205,0.3926439164,-7.3703349028
H,11.1771363702,1.2960764353,-6.3074848745
C,12.0952267047,-0.243397044,-7.5221000411
H,12.9943712018,-0.3582809547,-6.8609521042
H,11.8483601936,-1.2615083979,-7.9237205477
C,12.4259424959,0.687181608,-8.6696334275
H,11.5251225814,0.8019568957,-9.3289057958
H,12.6709542575,1.7052709817,-8.2662234145
C,13.5856154401,0.172202478,-9.4823043708
H,13.3506413992,-0.8310584821,-9.9133041868
H,13.8124444248,0.8724393563,-10.3221014936
H,14.499592558,0.0746292352,-8.8477776279
C,8.8623670631,-4.8427518991,0.3461677797
H,8.2020241461,-5.5590019018,0.9017033067
H,8.88968897,-5.1774125484,-0.7235320081
C,10.2561657194,-4.8528340735,0.9341950182
H,10.9066116974,-4.1295479161,0.3748509621
H,10.2187979329,-4.5080738838,2.0013591957
C,10.8644151884,-6.2375010964,0.8691747891
H,10.9013067977,-6.5821803537,-0.1979121294
H,10.213644632,-6.9608477504,1.4278164101
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Cartesian Coordination of 4e at AM1

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Cartesian Coordination of 4f at AM1

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Cartesian Coordination of 4f·Cl⁻ at AM1

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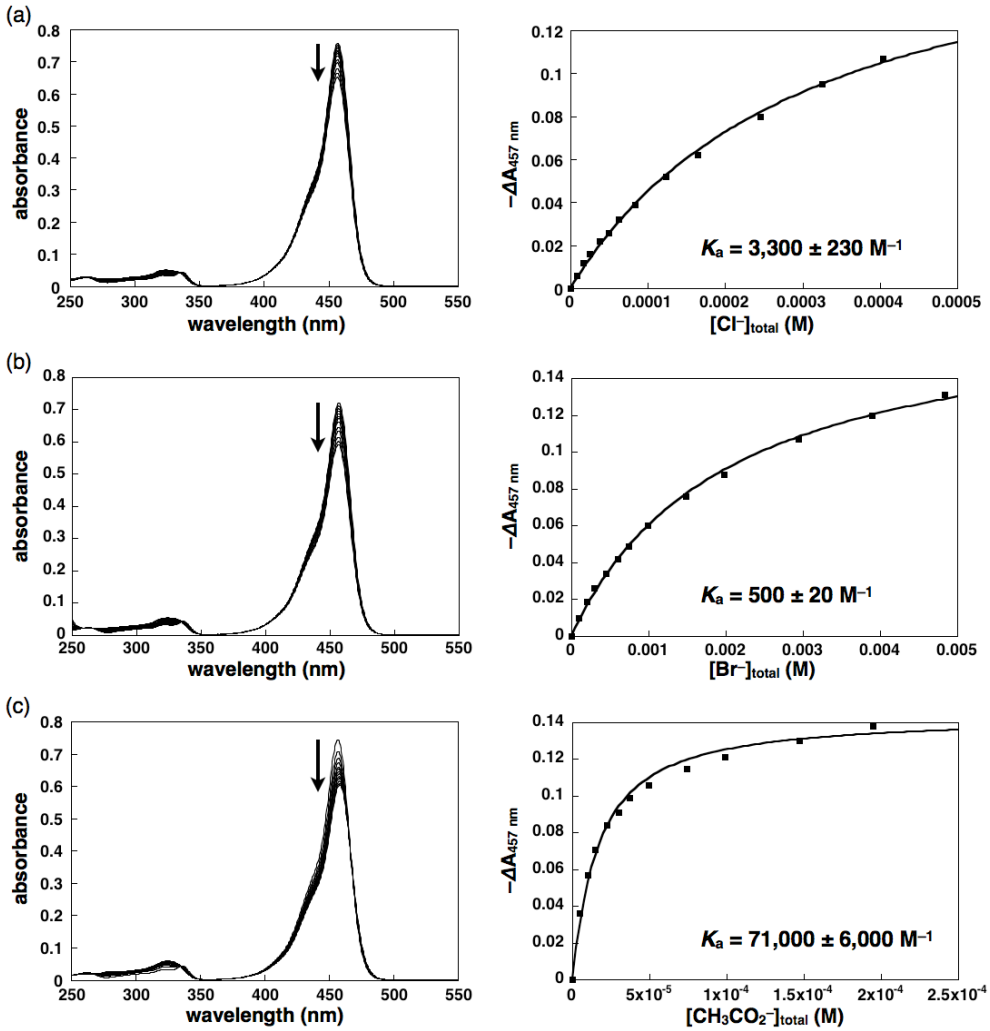
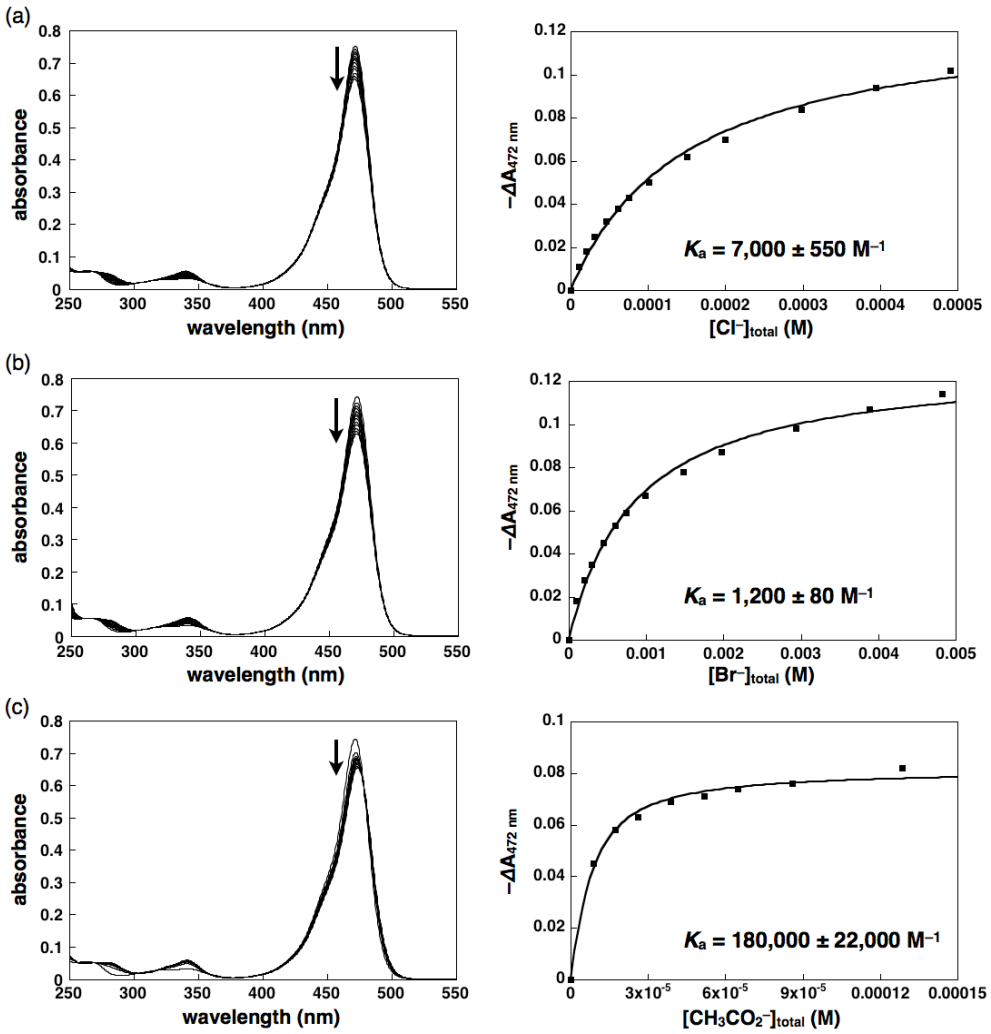
[S8] (Complete ref. 9)] *Gaussian 09* (Revision D.01), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, 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. Fox, Gaussian, Inc., Wallingford CT, 2009.

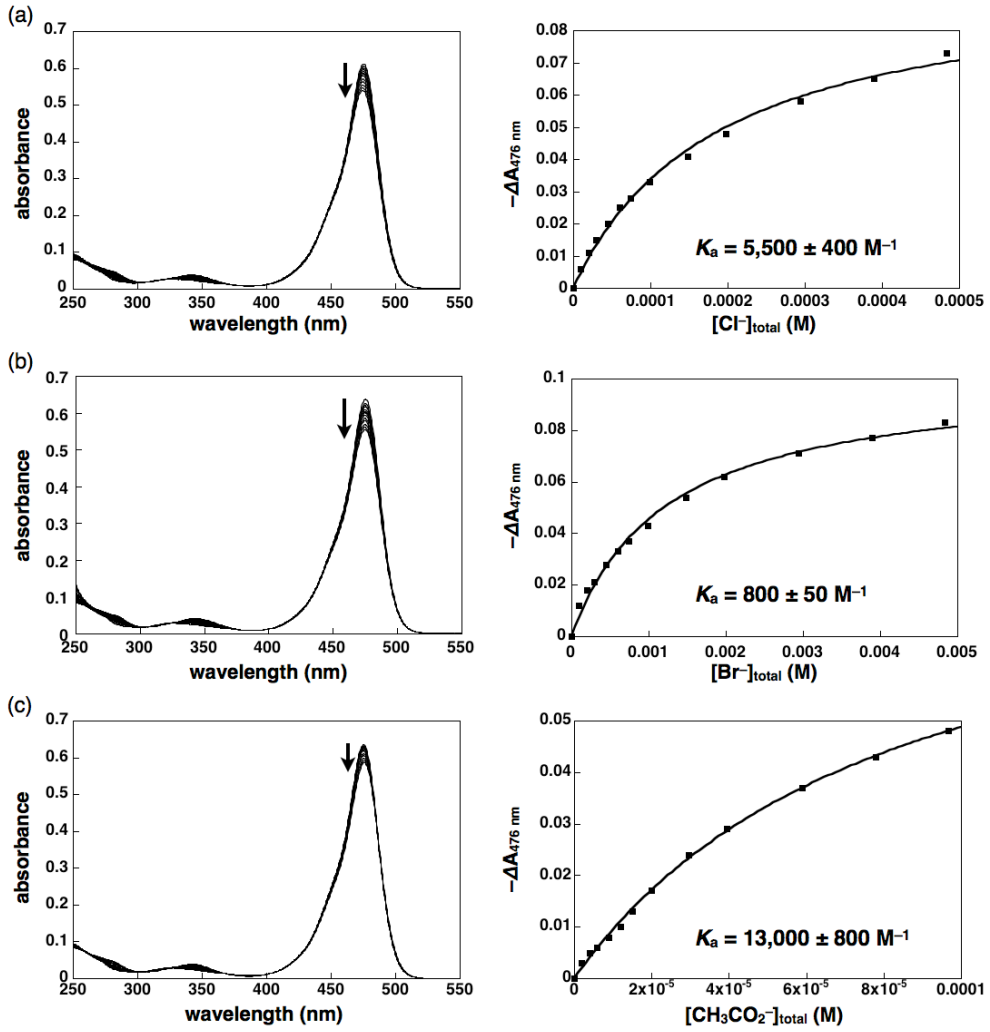
4. Anion-binding behaviors



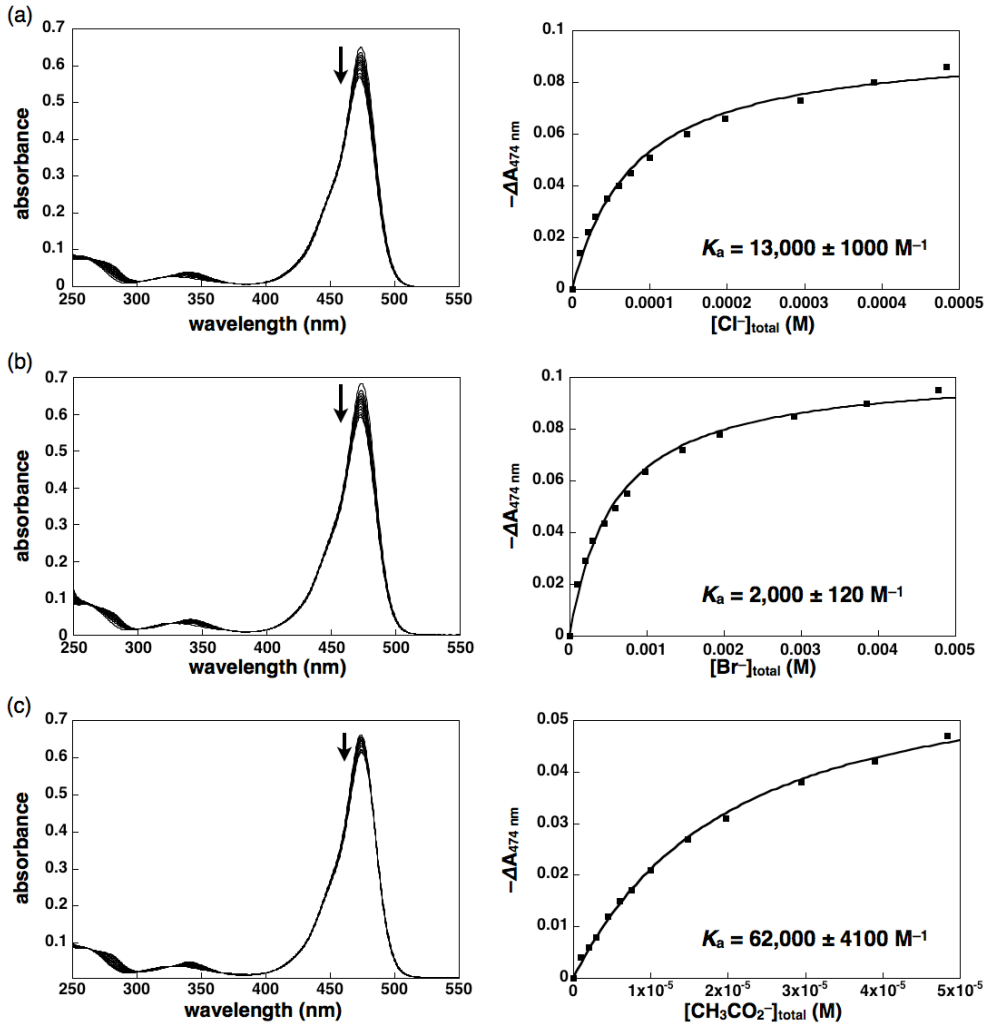
Supporting Figure 19 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **3a** (5.0×10^{-6} M) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as tetrabutylammonium (TBA) salts in CH_2Cl_2.



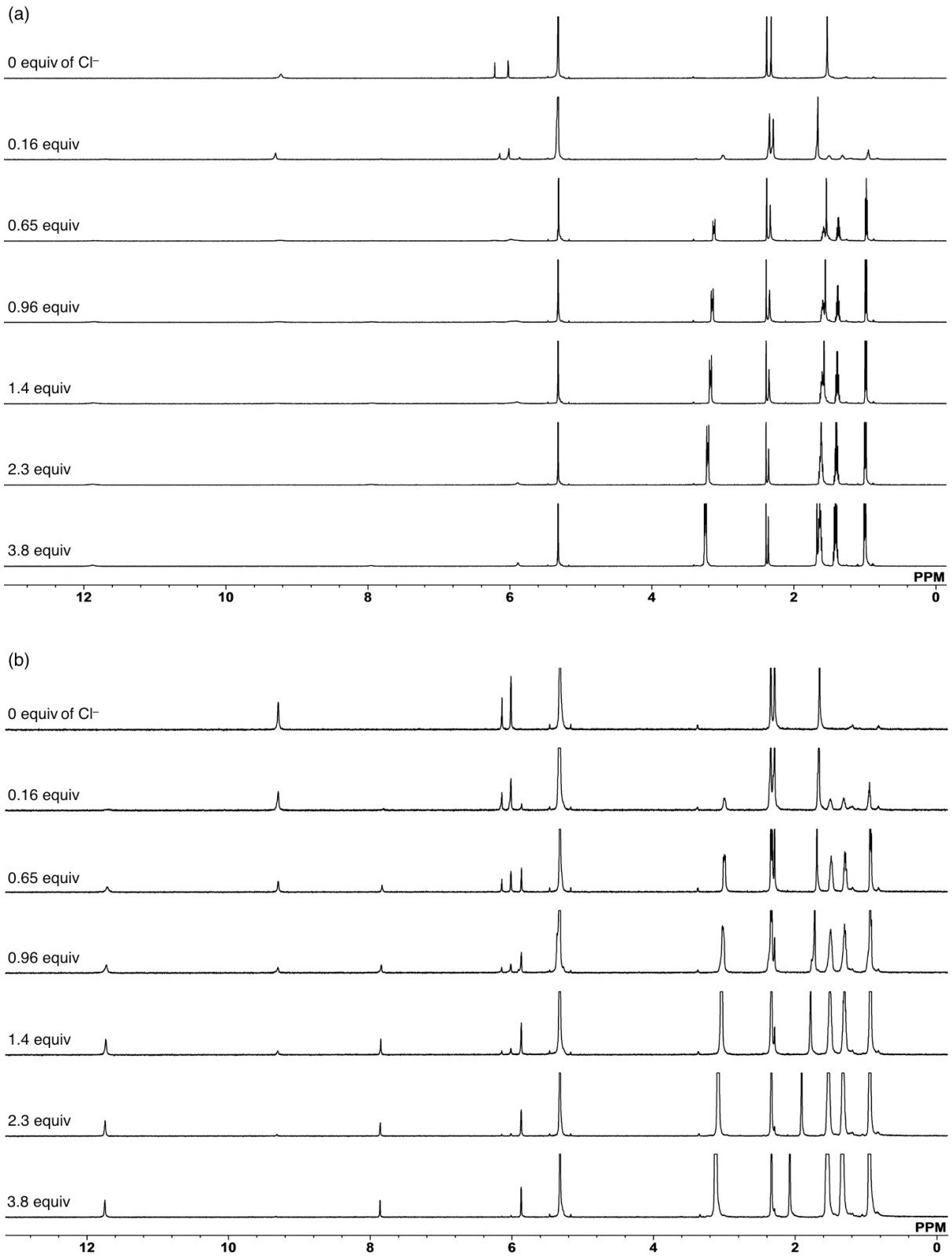
Supporting Figure 20 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **4a** (5.0×10^{-6} M) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2.



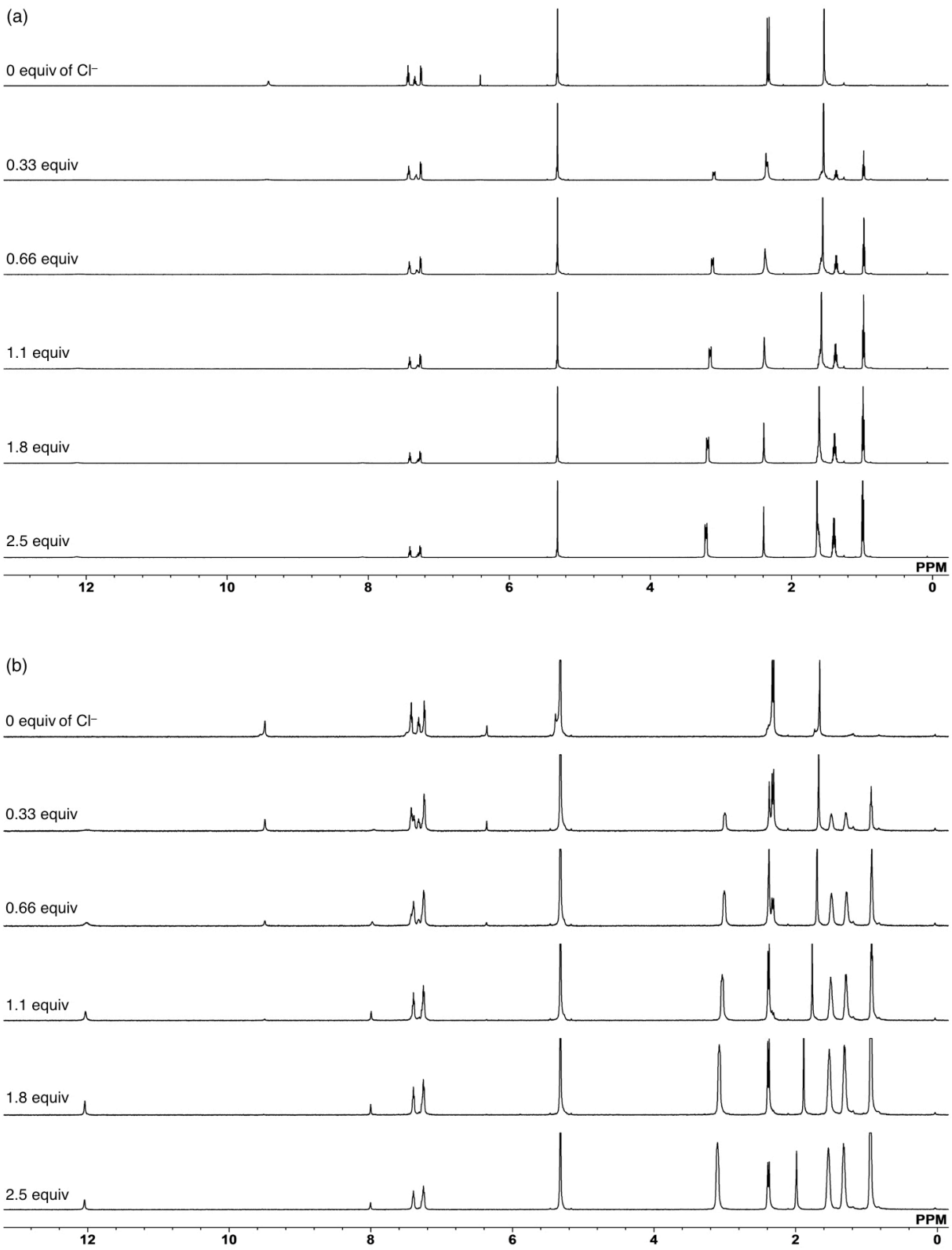
Supporting Figure 21 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **4b** (5.0×10^{-6} M) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2.



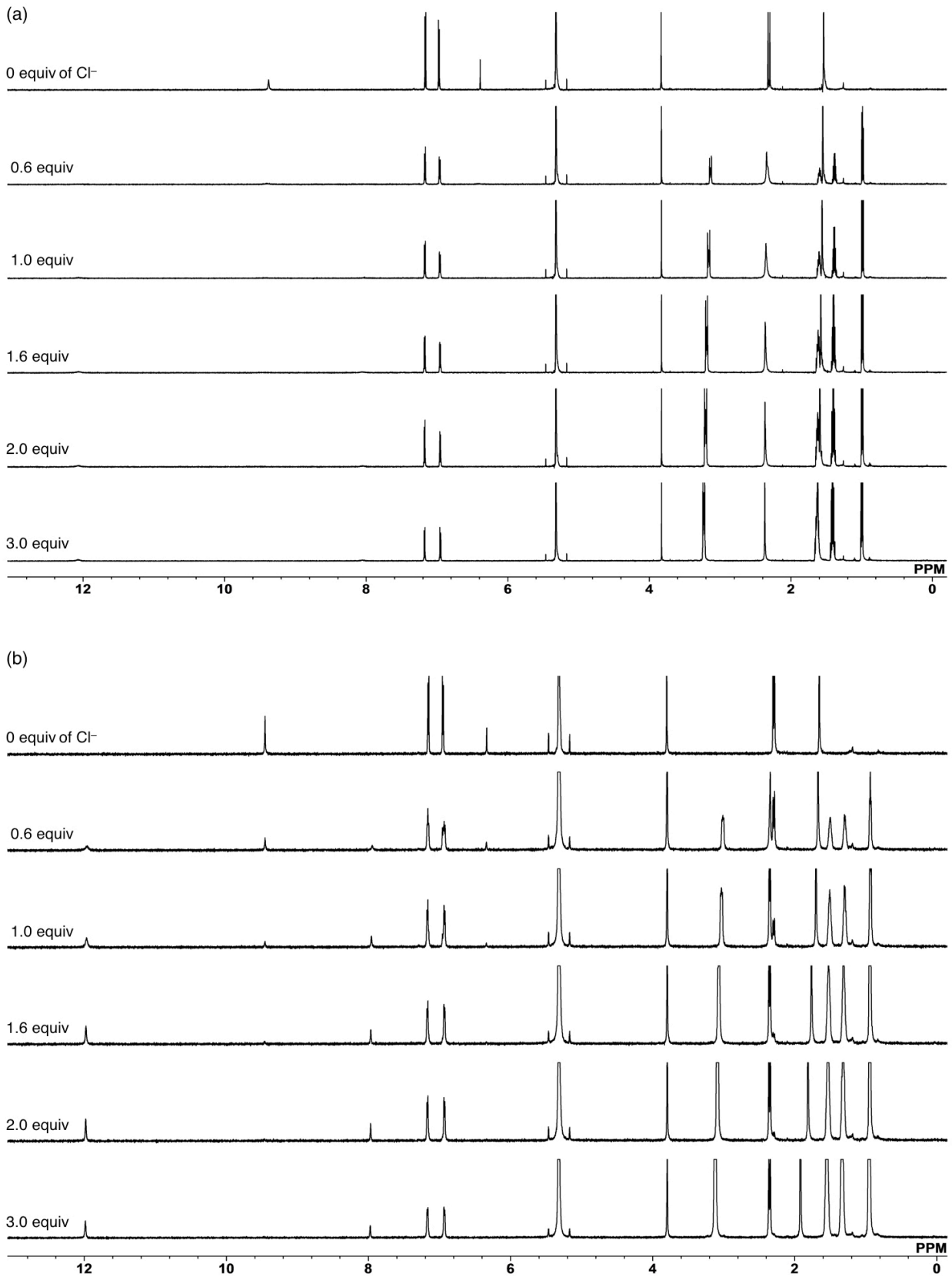
Supporting Figure 22 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **4c** (5.0×10^{-6} M) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2.



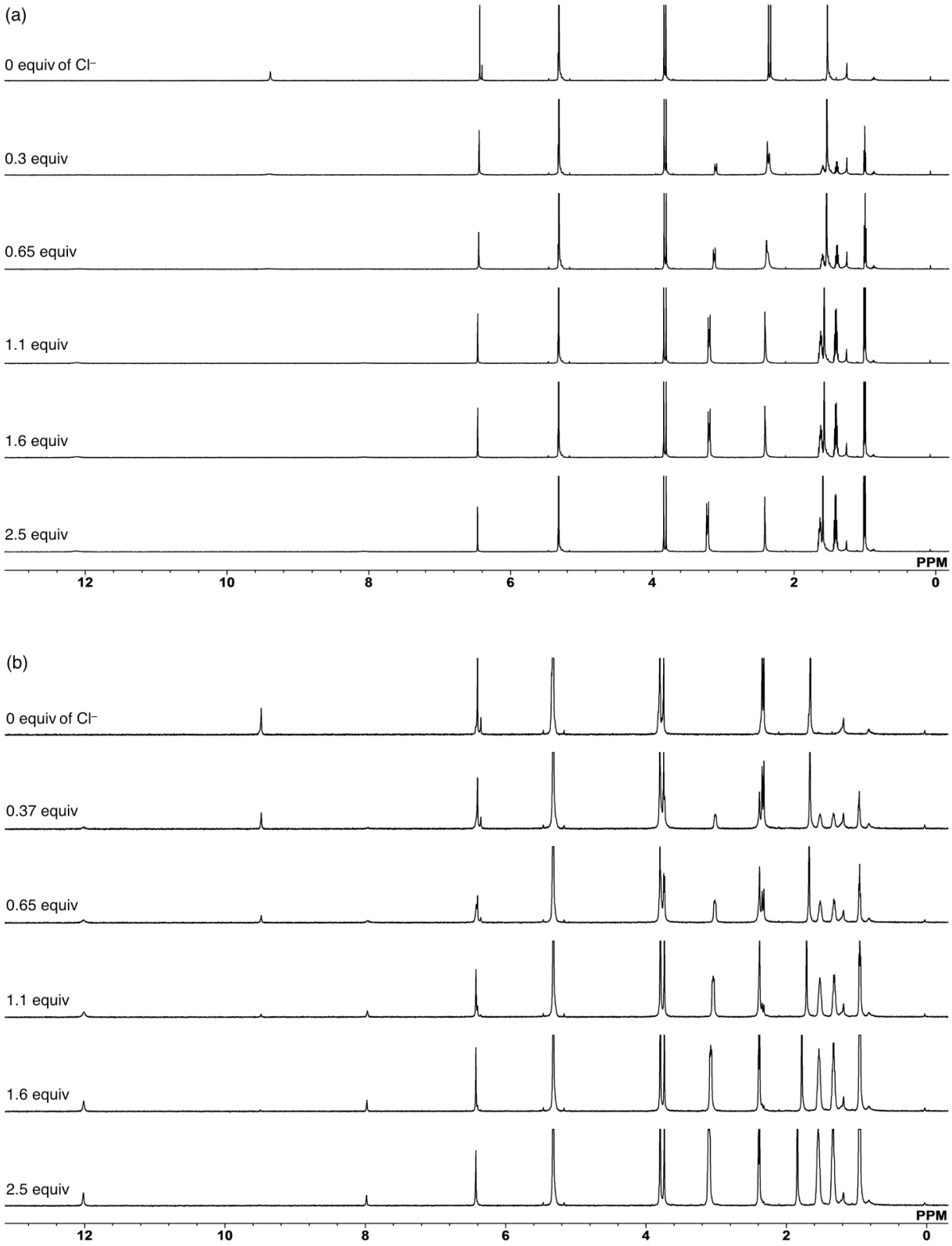
Supporting Figure 23 ^{1}H NMR spectral changes of **3a** (1×10^{-3} M) upon the addition of Cl^- (0–3.8 equiv) added as a TBA salt in CD_2Cl_2 at (a) 20 °C and (b) –50 °C. Pyrrole β-H of **3a** was shifted to upfield upon the addition of Cl^- due to the shielding effect caused by π–π stacking.



Supporting Figure 24 ^{1}H NMR spectral changes of **4a** (1×10^{-3} M) upon the addition of Cl^- (0–2.5 equiv) added as a TBA salt in CD_2Cl_2 at (a) 20 °C and (b) –50 °C. The pyrrole NH signals by the interaction with Cl^- suggested the existence of a [1+1]-type binding mode in solution.

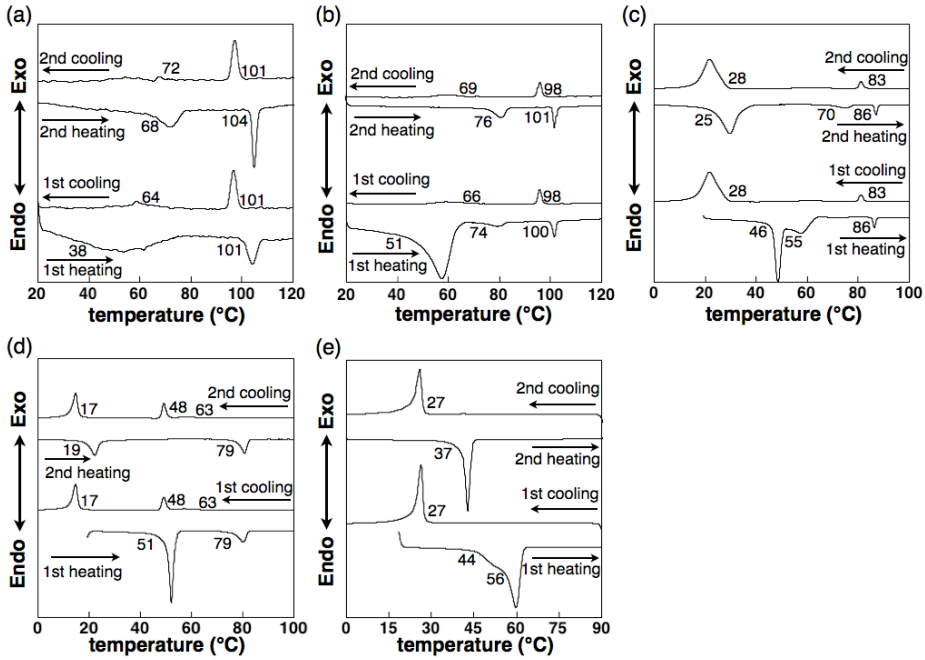


Supporting Figure 25 ^{1}H NMR spectral changes of **4b** (1×10^{-3} M) upon the addition of Cl^- (0–3.0 equiv) added as a TBA salt in CD_2Cl_2 at (a) 20 °C and (b) –50 °C. The pyrrole NH signals by the interaction with Cl^- suggested the existence of a [1+1]-type binding mode in solution.

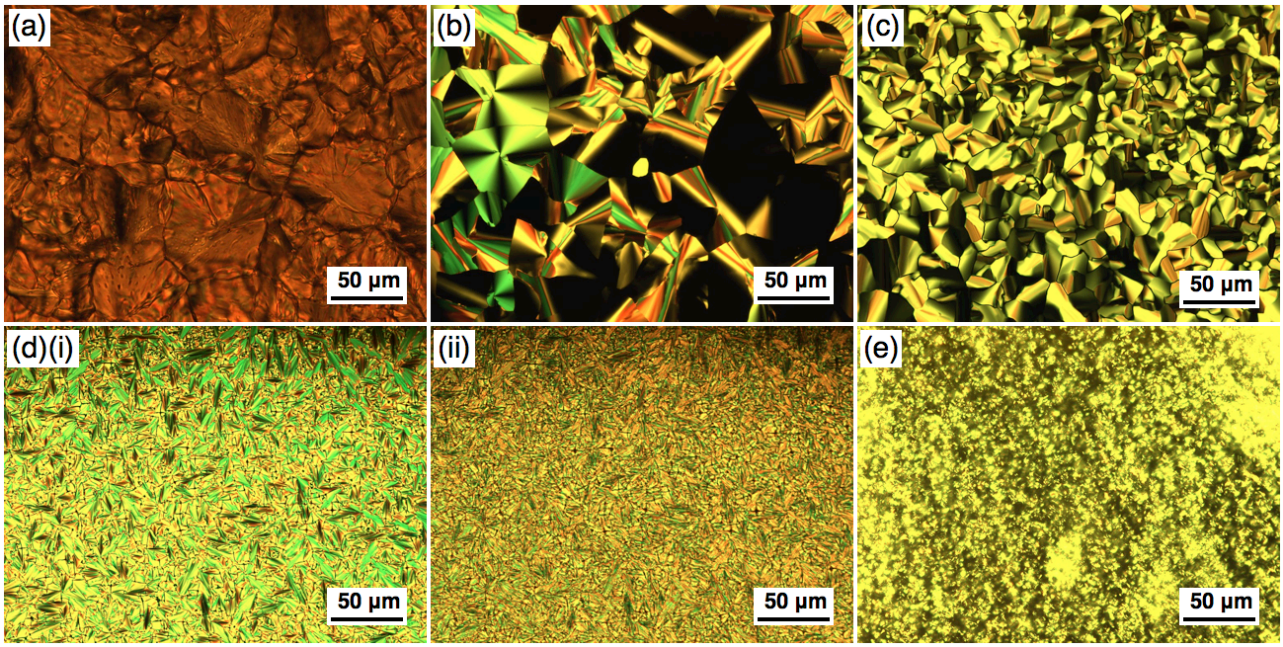


Supporting Figure 26 ^{1}H NMR spectral changes of **4c** (1×10^{-3} M) upon the addition of TBA salt of Cl^- (0–2.5 equiv) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C. The pyrrole NH signals by the interaction with Cl^- suggested the existence of a [1+1]-type binding mode in solution.

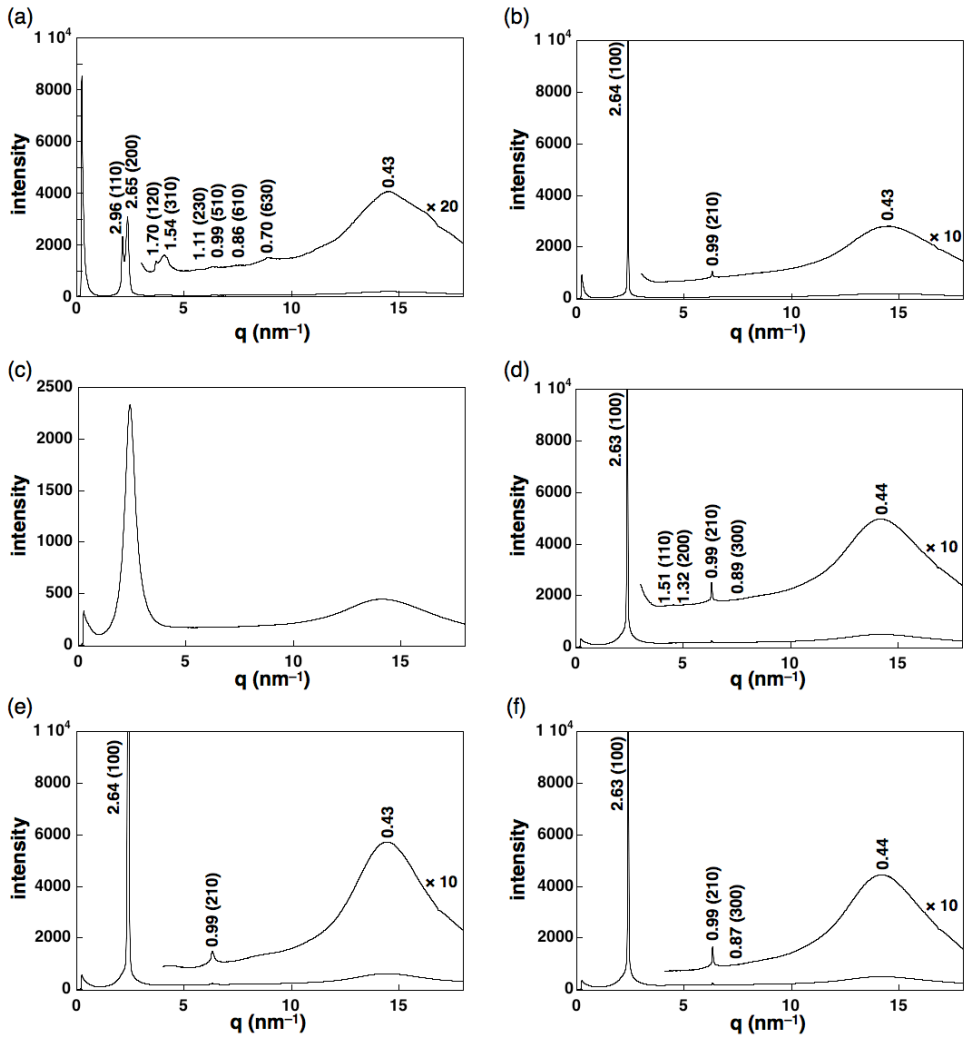
5. Assembled behaviors



Supporting Figure 27 DSC thermograms of (a) **4d**, (b) **4e**, (c) **4f**, (d) **4f**·Cl^--TBA^+, and (e) **4f**·Cl^--$C_8H_{17}Me_3N^+$. Onset temperatures (°C) of phase transitions are labeled although some peaks are weak. Although only a single peak was observed in the thermal process of (e) **4f**·Cl^--$C_8H_{17}Me_3N^+$, the mesophase was revealed by POM measurement.



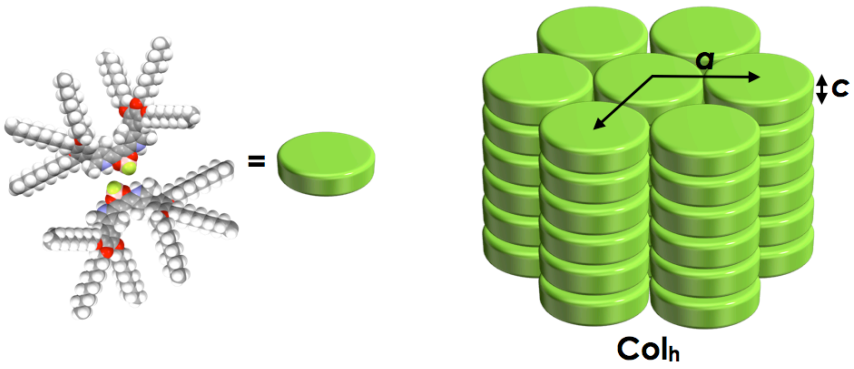
Supporting Figure 28 POM textures of (a) **4d** at 100 °C, (b) **4e** at 95 °C, (c) **4f** at 80 °C, (d) **4f**·Cl^--TBA^+ at (i) 63 °C and (ii) 46 °C, and (e) **4f**·Cl^--$C_8H_{17}Me_3N^+$ at 32 °C upon 1st cooling.



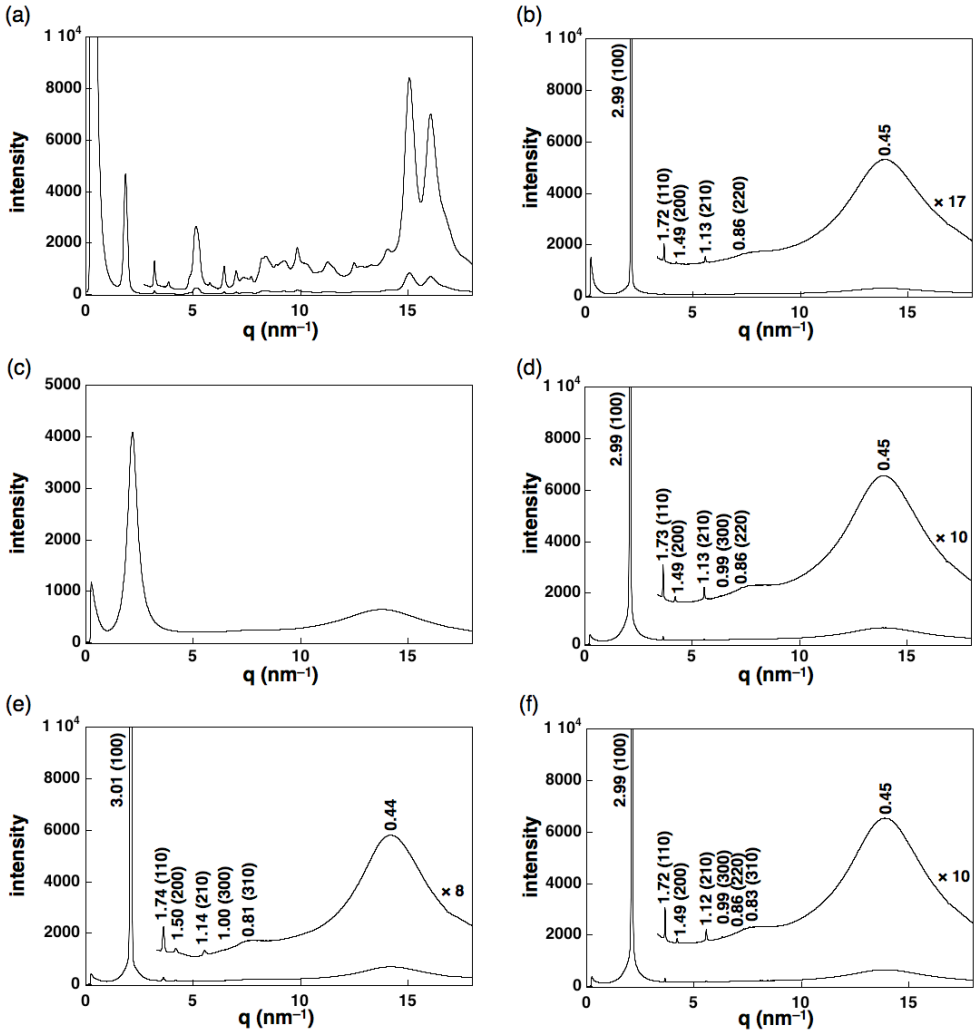
Supporting Figure 29 Synchrotron XRD patterns of (a) **4d** as a solid prepared by recrystallization from CH_2Cl_2/MeOH at 25 °C, (b) 85 °C, (c) 120 °C, (d) 87 °C, (e) 25 °C, and (f) 90 °C upon (a,b) 1st heating, (c–e) 1st cooling, and (f) 2nd heating.

Supporting Table 2 XRD peaks of **4d** at (a) 25 °C, (b) 85 °C, (d) 87 °C, (e) 25 °C, and (f) 90 °C upon (a,b) 1st heating, (d,e) 1st cooling, and (f) 2nd heating.

	q (nm^{-1})	*d*-spacing (nm)	ratio	ratio (calc.)	*hkl*
	2.12	2.96	1.00	1.000	110
	2.37	2.65	0.90	0.895	200
(a) **4d**	3.69	1.70	0.57	0.571	120
25 °C (1st heating), Col_r	4.08	1.54	0.52	0.534	310
a = 5.30 nm, b = 3.57 nm, c = 0.43 nm	5.66	1.11	0.38	0.402	230
M = 1227.61, Z = 4 for ρ = 1.0	6.32	0.99	0.33	0.333	330
	7.33	0.86	0.29	0.289	610
	14.49	0.43	–	–	001
(b) **4d**	2.38	2.64	1.00	1.000	100
85 °C (1st heating), Col_h	6.31	0.99	0.38	0.378	210
a = 3.05 nm, c = 0.43 nm	14.59	0.43	–	–	001
M = 1227.61, Z = 2 for ρ = 1.18					
	2.39	2.63	1.00	1.000	100
(d) **4d**	4.15	1.51	0.57	0.577	110
87 °C (1st cooling), Col_h	4.77	1.32	0.50	0.500	200
a = 3.04 nm, c = 0.44 nm	6.32	0.99	0.38	0.377	210
M = 1227.61, Z = 2 for ρ = 1.16	7.06	0.89	0.34	0.333	300
	14.23	0.44	–	–	001
(e) **4d**	2.38	2.64	1.00	1.000	100
25 °C (1st cooling), Col_h	6.31	0.99	0.38	0.377	210
a = 3.05 nm, c = 0.43 nm	14.45	0.43	–	–	001
M = 1227.61, Z = 2 for ρ = 1.18					
(f) **4d**	2.39	2.64	1.00	1.000	100
90 °C (2nd heating), Col_h	6.32	0.99	0.38	0.377	210
a = 3.05 nm, c = 0.44 nm	7.19	0.87	0.33	0.333	300
M = 1227.61, Z = 2 for ρ = 1.15	14.20	0.44	–	–	001



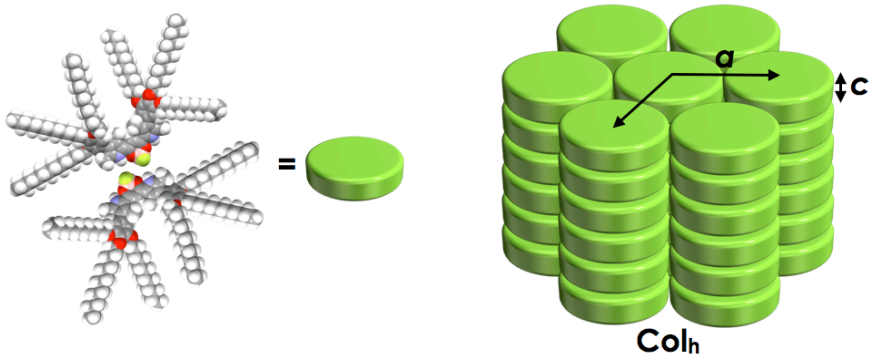
Supporting Figure 30 Possible packing model of **4d** in a Col_h structure.



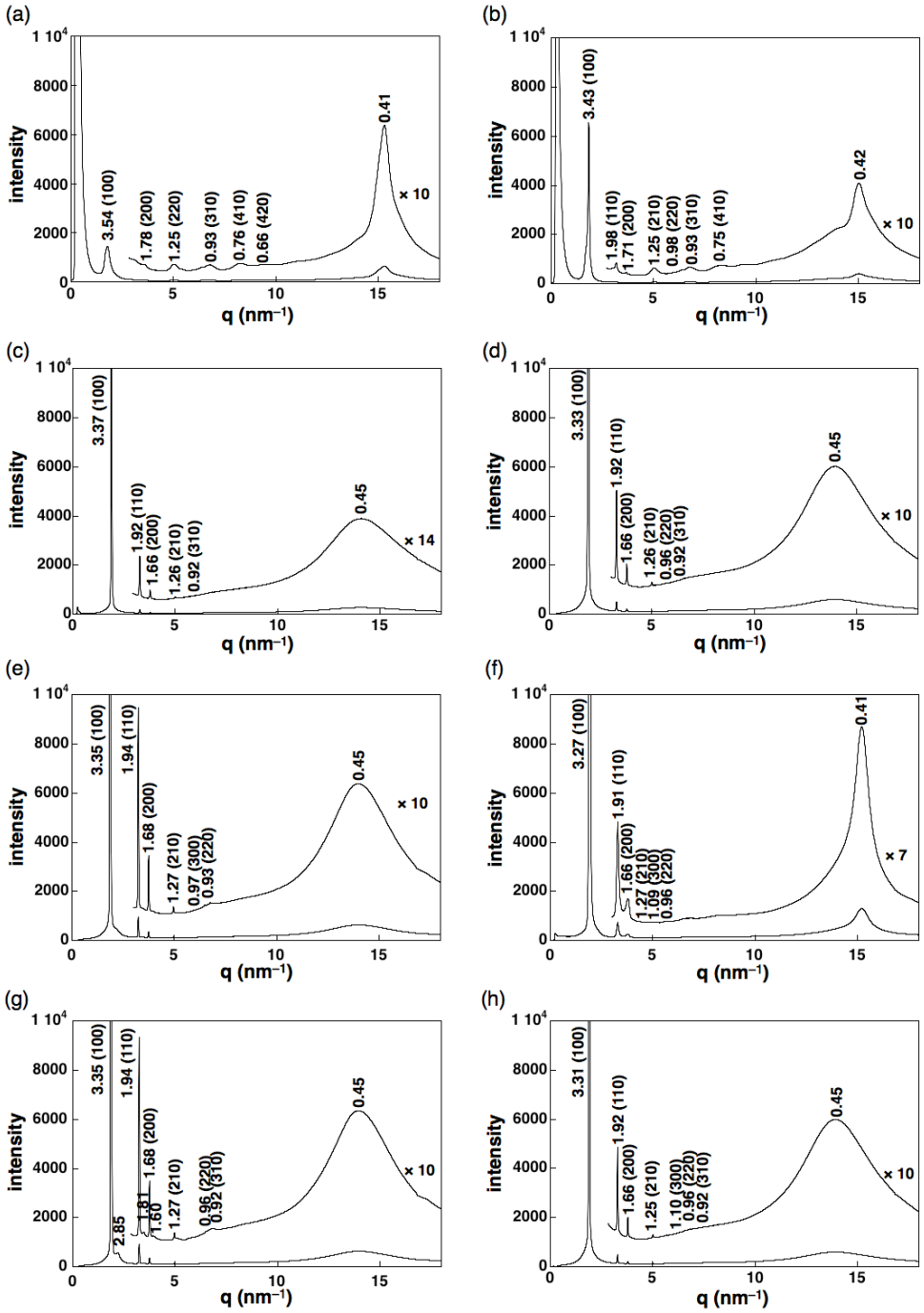
Supporting Figure 31 Synchrotron XRD patterns of (a) **4e** as a solid prepared by recrystallization from CH_2Cl_2/MeOH at 25 °C, (b) 88 °C, (c) 120 °C, (d) 84 °C, (e) 25 °C, and (f) 88 °C upon (a,b) 1st heating, (c–e) 1st cooling, and (f) 2nd heating.

Supporting Table 3 XRD peaks of **4e** at (b) 88 °C, (d) 84 °C, (e) 25 °C, and (f) 88 °C upon (b) 1st heating, (d) 1st cooling, and (f) 2nd heating. The peaks which can be indexed are represented.

	q (nm^{-1})	*d*-spacing (nm)	ratio	ratio (calc.)	*hkl*
	2.10	2.99	1.00	1.000	100
(b) **4e**	3.65	1.72	0.58	0.577	110
88 °C (1st heating), Col_h	4.22	1.49	0.50	0.500	200
a = 3.45 nm, c = 0.45 nm	5.56	1.13	0.38	0.378	210
M = 1564.25, Z = 2 for ρ = 1.12	7.31	0.86	0.29	0.289	220
	13.91	0.45	–	–	001
	2.10	2.99	1.00	1.000	100
	3.63	1.73	0.58	0.577	110
(d) **4e**	4.21	1.49	0.50	0.500	200
84 °C (1st cooling), Col_h	5.56	1.13	0.38	0.378	210
a = 3.45 nm, c = 0.45 nm	6.31	0.99	0.33	0.333	300
M = 1564.25, Z = 2 for ρ = 1.12	7.30	0.86	0.29	0.289	220
	7.56	0.83	0.28	0.277	310
	13.94	0.45	–	–	001
	2.09	3.01	1.00	1.000	100
	3.61	1.74	0.58	0.577	110
(e) **4e**	4.18	1.50	0.50	0.500	200
25 °C (1st cooling), Col_h	5.53	1.14	0.38	0.378	210
a = 3.47 nm, c = 0.44 nm	6.26	1.00	0.34	0.333	300
M = 1564.25, Z = 2 for ρ = 1.11	7.69	0.82	0.27	0.277	310
	14.20	0.44	–	–	001
	2.10	2.99	1.00	1.000	100
	3.65	1.72	0.58	0.577	110
(f) **4e**	4.21	1.49	0.50	0.500	200
88 °C (2nd heating), Col_h	5.58	1.12	0.38	0.378	210
a = 3.45 nm, c = 0.45 nm	6.31	0.99	0.33	0.333	300
M = 1564.25, Z = 2 for ρ = 1.12	7.32	0.86	0.29	0.289	220
	7.59	0.83	0.28	0.277	310
	13.90	0.45	–	–	001



Supporting Figure 32 Possible packing model of **4e** in a Col_h structure.



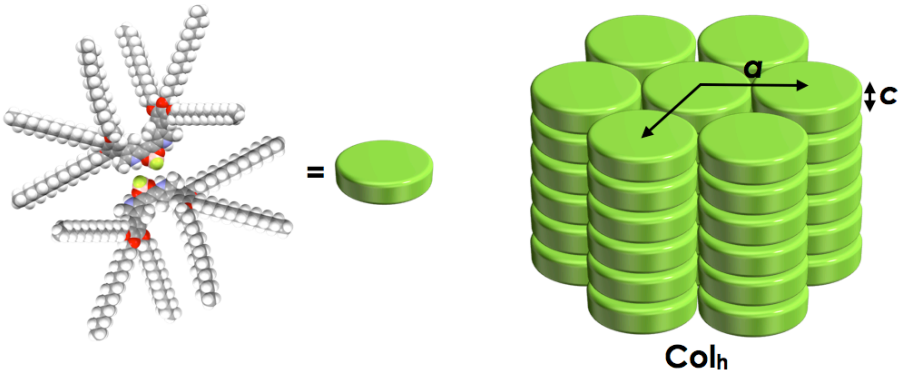
Supporting Figure 33 Synchrotron XRD patterns of (a) **4f** as a solid prepared by recrystallization from CH_2Cl_2/MeOH at 25 °C, (b) 50 °C, (c) 75 °C, (d) 75 °C (e) 54 °C, (f) 15 °C, (g) 58 °C, and (h) 78 °C upon (a–c) 1st heating, (d–f) 1st cooling, and (g,h) 2nd heating.

Supporting Table 4 XRD peaks of **4f** at (a) 25 °C, (b) 50 °C, (c) 75 °C, (d) 75 °C (e) 54 °C, (f) 15 °C, (g) 58 °C, and (h) 78 °C upon (a–c) 1st heating, (d–f) 1st cooling, and (g,h) 2nd heating.

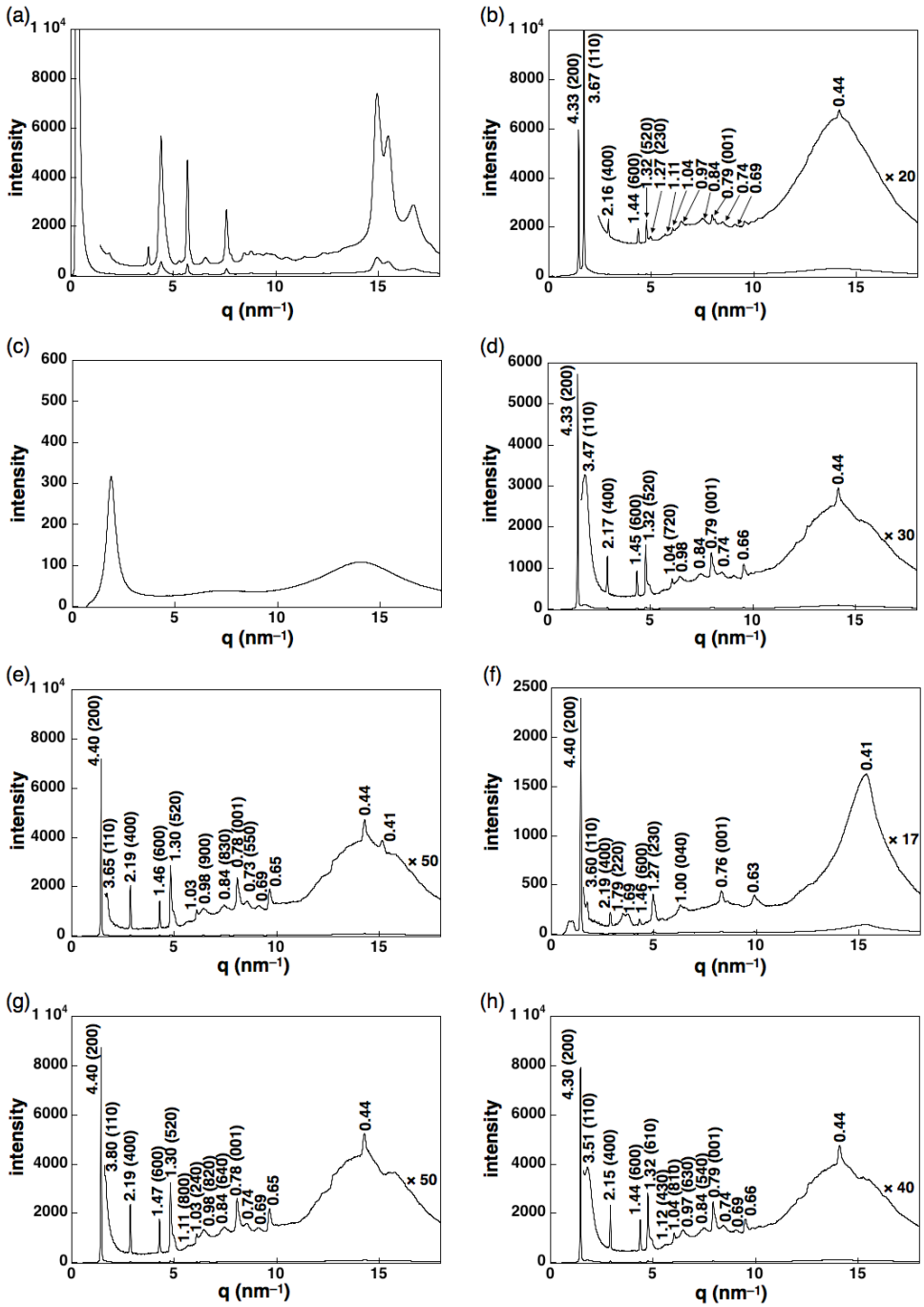
	q (nm^{-1})	*d*-spacing (nm)	ratio	ratio (calc.)	*hkl*
(a) **4f** 25 °C (1st heating), Col_h a = 4.09 nm, c = 0.41 nm M = 1900.90, Z = 2 for ρ = 1.07	1.78	3.54	1.00	1.000	100
	3.53	1.78	0.50	0.500	200
	5.02	1.25	0.35	0.333	300
	6.77	0.93	0.26	0.277	310
	8.27	0.76	0.22	0.218	410
	9.48	0.66	0.19	0.189	420
	15.29	0.41	–	–	001
(b) **4f** 50 °C (1st heating), Col_h a = 3.96 nm, c = 0.42 nm M = 1900.90, Z = 2 for ρ = 1.11	1.83	3.43	1.00	1.000	100
	3.17	1.98	0.58	0.577	110
	3.67	1.71	0.50	0.500	200
	5.02	1.25	0.36	0.378	210
	6.43	0.98	0.29	0.289	220
	6.75	0.93	0.27	0.277	310
	8.34	0.75	0.22	0.218	410
	15.04	0.42	–	–	001
(c) **4f** 75 °C (1st heating), Col_h a = 3.83 nm, c = 0.45 nm M = 1900.90, Z = 2 for ρ = 1.10	1.86	3.37	1.00	1.000	100
	3.26	1.92	0.57	0.577	110
	3.78	1.66	0.49	0.500	200
	4.99	1.26	0.37	0.378	210
	6.82	0.92	0.27	0.277	310
	14.01	0.45	–	–	001
(d) **4f** 75 °C (1st cooling), Col_h a = 3.84 nm, c = 0.45 nm M = 1900.90, Z = 2 for ρ = 1.10	1.89	3.33	1.00	1.000	100
	3.28	1.92	0.58	0.577	110
	3.78	1.66	0.50	0.500	200
	4.99	1.26	0.38	0.378	210
	6.57	0.96	0.29	0.289	220
	6.82	0.92	0.28	0.277	310
	13.94	0.45	–	–	001
(e) **4f** 54 °C (1st cooling), Col_h a = 3.87 nm, c = 0.45 nm, M = 1900.90, Z = 2 for ρ = 1.08	1.91	3.35	1.00	1.000	100
	3.24	1.94	0.58	0.577	110
	3.75	1.68	0.50	0.500	200
	4.96	1.27	0.38	0.378	210
	6.49	0.97	0.29	0.289	220
	6.76	0.93	0.28	0.277	310
	13.98	0.45	–	–	001
(f) **4f** 15 °C (1st cooling), Col_h a = 3.78 nm, c = 0.41 nm M = 1900.90, Z = 2 for ρ = 1.25	1.92	3.27	1.00	1.000	100
	3.29	1.91	0.58	0.577	110
	3.79	1.66	0.50	0.500	200
	4.95	1.27	0.39	0.378	210
	5.75	1.09	0.33	0.333	300
	6.56	0.96	0.29	0.289	220
	15.20	0.41	–	–	001
(g) **4f** 58 °C (2nd heating), Col_h a = 3.87 nm, c = 0.45 nm M = 1900.90, Z = 2 for ρ = 1.08	1.88	3.35	1.00	1.000	100
	3.24	1.94	0.58	0.577	110
	3.75	1.68	0.5	0.500	200
	4.96	1.27	0.38	0.378	210
	6.51	0.96	0.29	0.289	220
	6.81	0.92	0.27	0.277	310
	13.93	0.45	–	–	001

Supporting Table 4 (continued)

	q (nm^{-1})	*d*-spacing (nm)	ratio	ratio (calc.)	*hkl*
	1.90	3.31	1.00	1.000	100
	3.28	1.92	0.58	0.577	110
(h) **4f**	3.79	1.66	0.5	0.500	200
78 °C (2nd heating), Col_h	5.01	1.25	0.38	0.378	210
a = 3.82 nm, c = 0.45 nm	5.69	1.10	0.33	0.333	300
M = 1900.90, Z = 2 for ρ = 1.11	6.57	0.96	0.29	0.289	220
	6.83	0.92	0.27	0.277	310
	13.95	0.45	–	–	001



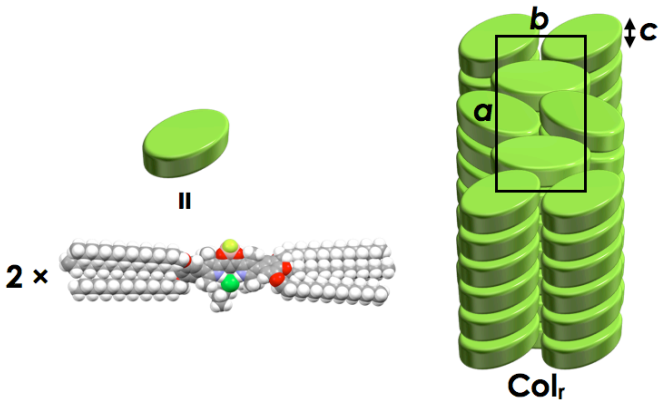
Supporting Figure 34 Possible packing model of **4f** in a Col_h structure.



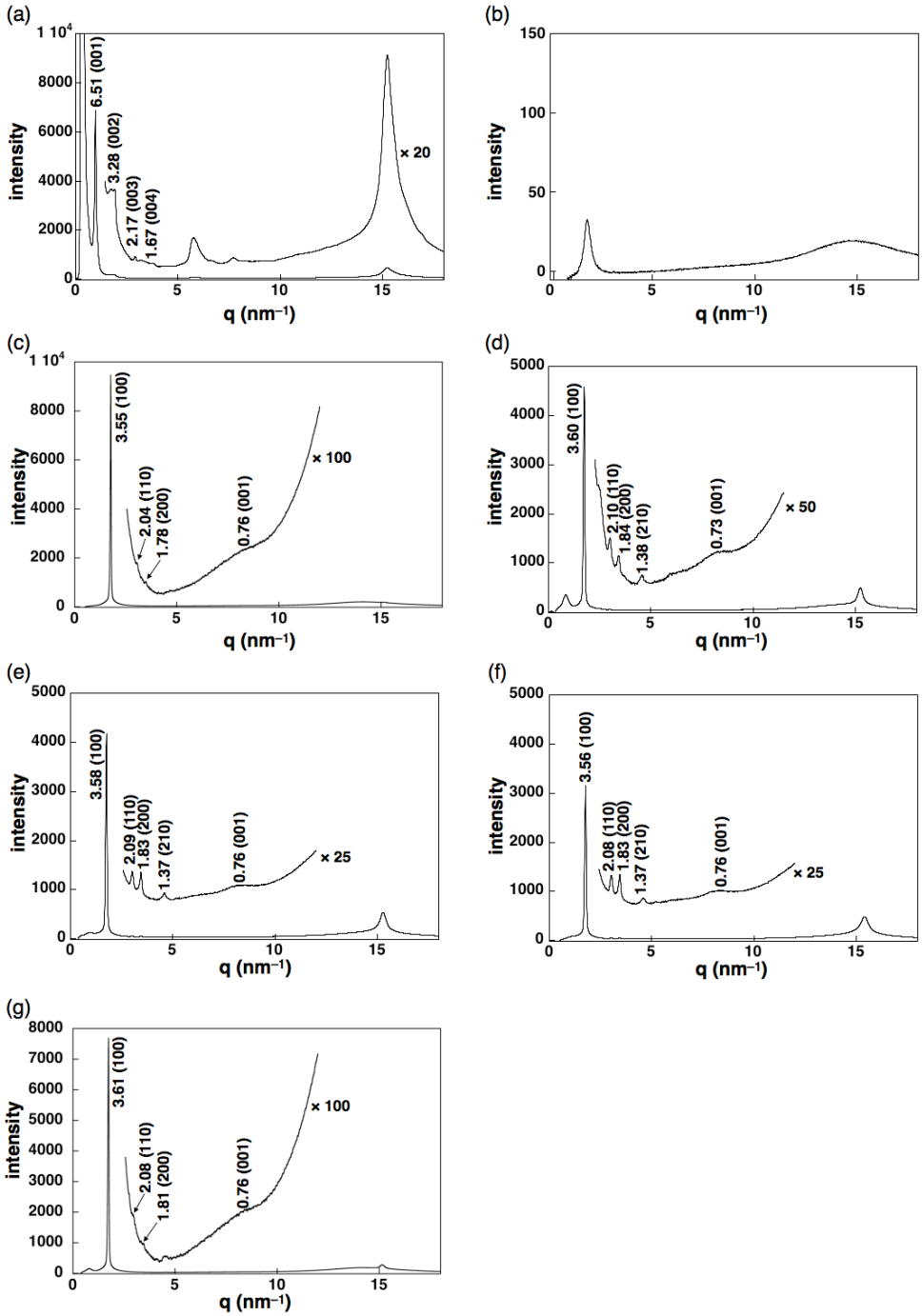
Supporting Figure 35 Synchrotron XRD patterns of **4f**·Cl^--TBA^+, whose sample was prepared by the precipitation from 1,4-dioxane at (a) 25 °C, (b) 65 °C, (c) 90 °C, (d) 63 °C, (e) 46 °C, (f) 0 °C (g) 55 °C, and (h) 73 °C upon (a,b) 1st heating, (c–f) 1st cooling, and (g,h) 2nd heating.

Supporting Table 5 XRD peaks of **4f**·Cl^--TBA^+ at (b) 65 °C, (d) 63 °C, (e) 46 °C, (f) 0 °C, (g) 55 °C, and (h) 73 °C upon (a) 1st heating, (d–f) 1st cooling, and (g,h) 2nd heating. The peaks which can be indexed are represented.

	q (nm^{-1})	*d*-spacing (nm)	ratio	ratio (calc.)	*hkl*
(b) **4f**·Cl^--TBA^+ 65 °C (1st heating), Col_r a = 8.66 nm, b = 4.06 nm, c = 0.79 nm M = 2178.82, Z = 8 for ρ = 1.04	1.45	4.33	1.00	1.000	200
	1.71	3.67	0.85	0.850	110
	2.91	2.16	0.50	0.500	400
	4.35	1.44	0.33	0.333	600
	4.77	1.32	0.30	0.305	520
	4.96	1.27	0.29	0.298	230
	6.04	1.04	0.24	0.242	810
	6.46	0.97	0.22	0.228	240
	7.97	0.79	–	–	001
(d) **4f**·Cl^--TBA^+ 63 °C (1st cooling), Col_r a = 8.66 nm, b = 3.79 nm, c = 0.79 nm M = 2178.82, Z = 8 for ρ = 1.12	1.45	4.33	1.00	1.000	200
	1.81	3.47	0.80	0.802	110
	2.90	2.17	0.50	0.500	400
	4.34	1.45	0.33	0.333	600
	4.77	1.32	0.31	0.295	520
	6.06	1.04	0.24	0.239	720
	7.97	0.79	–	–	001
(e) **4f**·Cl^--TBA^+ 46 °C (1st cooling), Col_r a = 8.79 nm, b = 4.01 nm, c = 0.78 nm M = 2178.82, Z = 8 for ρ = 1.06	1.43	4.40	1.00	1.000	200
	1.72	3.65	0.83	0.828	110
	2.86	2.19	0.50	0.500	400
	4.29	1.46	0.33	0.333	600
	4.83	1.30	0.30	0.300	520
	6.44	0.98	0.22	0.298	900
	7.44	0.84	0.19	0.196	830
	8.08	0.78	–	–	001
	8.57	0.73	0.17	0.166	550
(f) **4f**·Cl^--TBA^+ 0 °C (1st cooling), Col_r a = 8.80 nm, b = 3.94 nm, c = 0.76 nm M = 2178.82, Z = 8 for ρ = 1.10	1.43	4.40	1.00	1.000	200
	1.74	3.60	0.82	0.817	110
	2.87	2.19	0.50	0.500	400
	3.52	1.79	0.41	0.408	220
	4.31	1.46	0.33	0.333	600
	4.96	1.27	0.29	0.286	230
	6.29	1.00	0.23	0.224	040
	8.29	0.76	–	–	001
(g) **4f**·Cl^--TBA^+ 55 °C (2nd heating), Col_r a = 8.80 nm, b = 4.21 nm, c = 0.78 nm M = 2178.82, Z = 8 for ρ = 1.00	1.43	4.40	1.00	1.000	200
	1.65	3.80	0.86	0.863	110
	2.86	2.19	0.50	0.500	400
	4.28	1.47	0.33	0.333	600
	4.81	1.31	0.30	0.307	520
	5.67	1.11	0.25	0.250	800
	6.09	1.09	0.23	0.233	240
	6.44	0.98	0.22	0.221	820
	7.44	0.84	0.19	0.194	640
	8.06	0.78	–	–	001
(h) **4f**·Cl^--TBA^+ 73 °C (2nd heating), Col_r a = 8.59 nm, b = 3.84 nm, c = 0.79 nm, M = 2178.82, Z = 8 for ρ = 1.11	1.46	4.30	1.00	1.000	200
	1.79	3.51	0.82	0.816	110
	2.92	2.15	0.50	0.496	400
	4.36	1.44	0.33	0.333	600
	4.75	1.32	0.31	0.309	610
	6.02	1.04	0.24	0.240	810
	6.46	0.97	0.23	0.222	630
	7.49	0.84	0.20	1.194	540
	7.94	0.79	–	–	001



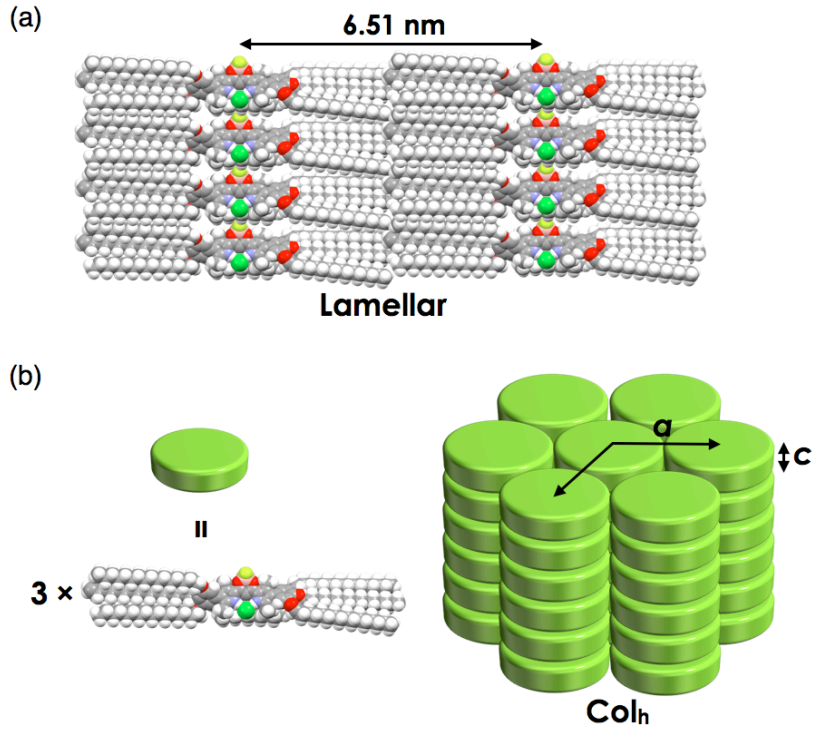
Supporting Figure 36 Possible packing model of **4f**·Cl^--TBA^+ in a Col_r structure.



Supporting Figure 37 Synchrotron XRD patterns of **4f**·Cl^{-}-$C_8H_{17}Me_3N^{+}$, whose sample was prepared by the precipitation from 1,4-dioxane at (a) 25 °C, (b) 75 °C, (c) 45 °C, (d) 32 °C, (e) 27 °C, (f) 0 °C, and (g) 45 °C upon (a) 1st heating, (b–f) 1st cooling, and (g) 2nd heating.

Supporting Table 6 XRD peaks of **4f**·Cl^--$C_8H_{17}Me_3N^+$ at (a) 25 °C, (c) 45 °C, (d) 32 °C, (e) 27 °C, (f) 0 °C, and (g) 45 °C upon (a) 1st heating, (c–f) 1st cooling, and (g) 2nd heating. The peaks which can be indexed are represented.

	q (nm^{-1})	*d*-spacing (nm)	ratio	ratio (calc.)	*hkl*
	0.96	6.51	1.00	1.000	001
(a) **4f**·Cl^--$C_8H_{17}Me_3N^+$	1.91	3.28	0.51	0.500	002
25 °C (1st heating), Lamellar	2.90	2.17	0.33	0.333	003
	3.76	1.67	0.26	0.250	004
(c) **4f**·Cl^--$C_8H_{17}Me_3N^+$	1.77	3.55	1.00	1.000	100
45 °C (1st cooling), Col_h	3.08	2.04	0.57	0.577	110
a = 4.09 nm, c = 0.76 nm	3.53	1.78	0.50	0.500	200
M = 2108.69, Z = 3 for ρ = 0.96	8.30	0.76	–	–	001
	1.74	3.60	1.00	1.000	100
(d) **4f**·Cl^--$C_8H_{17}Me_3N^+$	3.00	2.10	0.58	0.577	110
32 °C (1st cooling), Col_h	3.41	1.84	0.51	0.500	200
a = 4.16 nm, c = 0.73 nm	4.57	1.38	0.38	0.378	210
M = 2108.69, Z = 3 for ρ = 0.96	8.55	0.73	–	–	001
	1.76	3.58	1.00	1.000	100
(e) **4f**·Cl^--$C_8H_{17}Me_3N^+$	3.01	2.09	0.58	0.577	110
27 °C (1st cooling), Col_h	3.44	1.83	0.51	0.500	200
a = 4.13 nm, c = 0.76 nm	4.58	1.37	0.38	0.378	210
M = 2108.69, Z = 3 for ρ = 0.94	8.22	0.76	–	–	001
	1.77	3.56	1.00	1.000	100
(f) **4f**·Cl^--$C_8H_{17}Me_3N^+$	3.02	2.08	0.58	0.577	110
0 °C (1st cooling), Col_h	3.44	1.83	0.51	0.500	200
a = 4.11 nm, c = 0.76 nm	4.58	1.37	0.38	0.378	210
M = 2108.69, Z = 3 for ρ = 0.95	8.30	0.76	–	–	001
(g) **4f**·Cl^--$C_8H_{17}Me_3N^+$	1.74	3.61	1.00	1.000	100
45 °C (2nd heating), Col_h	3.02	2.08	0.58	0.577	110
a = 4.17 nm, c = 0.76 nm	3.47	1.81	0.50	0.500	200
M = 2108.69, Z = 3 for ρ = 0.92	8.30	0.76	–	–	001



Supporting Figure 38 Possible packing models of **4f**·Cl^--$C_8H_{17}Me_3N^+$ in (a) lamellar and (b) Col_h structures.