Electronic Supplementary Information

Anion-driven structures of radially arranged π-conjugated acyclic anion receptors

Hiromitsu Maeda,* Tomohiro Shirai and Shinobu Uemura

College of Pharmaceutical Sciences, Ritsumeikan University, Kusatsu 525–8577, Japan and Department of Applied Chemistry and Biochemistry, Graduate School of Science and Technology, Kumamoto University, Kumamoto 860–8555, Japan

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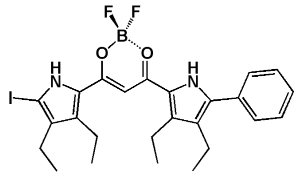
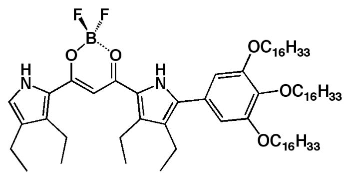
1. Synthetic procedures and spectroscopic data for anion receptors

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. UV-visible spectra were recorded on a Hitachi U-3500 spectrometer. Fluorescence spectra were recorded on a Hitachi F-4500 fluorescence spectrometer for ordinary solution. 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. Matrix-assisted laser desorption ionization time-of-flight mass spectrometries (MALDI-TOF-MS) were recorded on a Shimadzu Axima-CFRplus using positive and negative mode. Fourier transform ion cyclotron resonance mass spectrometries (FT-ICR-MS) were recorded on a Bruker solariX (Qh-FT-ICR-MS) and were carried out in the Joint Usage/Research Center (JURC) at Institute for Chemical Research (ICR), Kyoto University with the help of Prof. Hikaru Takaya and Dr. Katsuhiro Isozaki, Kyoto University. Electrospray ionization mass spectrometric (ESI-MS) studies were recorded on a BRUKER microTOF using negative mode ESI-TOF method. Fast atom bombardment mass spectrometric (FAB-MS) studies were made using a JEOL-HX110 instrument in the positive ion mode with a 3-nitrobenzylalcohol matrix with the help of Prof. Tomohiro Miyatake, Ryukoku University. TLC analyses were carried out on aluminum sheets coated with silica gel 60 (Merck 5554). Column chromatography was performed on Sumitomo alumina KCG-1525, Wakogel C-200 and C-300, and Merck silica gel 60 and 60H.

BF$_2$ complex of 1-(3,4-diethyl-5-iodopyrrol-2-yl)-3-(3,4-diethyl-5-phenylpyrrol-2-yl)-1,3-propanedione, 2b.[S1] To a CH_2Cl_2 (50 mL) solution of BF$_2$ complex of 1-(3,4-diethyl-5-phenylpyrrol-2-yl)-3-(3,4-diethylpyrrol-2-yl)-1,3-propanedione[S2] (219 mg, 0.500 mmol) at r.t. was added *N*-iodosuccinimide (115 mg, 0.511 mmol). The mixture was stirred at r.t. for 3 h. After confirming the consumption of the starting material by TLC analysis, the mixture was washed with water and extracted with CH_2Cl_2, dried over anhydrous $MgSO_4$, and evaporated to dryness. The residue was then chromatographed over silica gel flash column (eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **2b** (218 mg, 0.390 mmol, 78%). R_f = 0.42 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.37 (s, 1H, NH), 9.33 (s, 1H, NH), 7.52–7.47 (m, 4H, Ar-H), 7.42 (m, 1H, Ar-H), 6.46 (s, 1H, CH), 2.82 (m, 4H, CH_2CH$_3$), 2.63 (q, J = 7.8 Hz, 2H, CH_2CH$_3$), 2.42 (q, J = 7.8 Hz, 2H, CH_2CH$_3$), 1.33 (t, J = 7.8 Hz, 3H, CH$_2$$CH_3$), 1.28 (t, J = 7.8 Hz, 3H, CH$_2$$CH_3$), 1.18 (t, J = 7.8 Hz, 3H, CH$_2$$CH_3$), 1.11 (t, J = 7.8 Hz, 3H, CH$_2$$CH_3$). MALDI-TOF-MS: *m/z* (% intensity): 563.1 (100), 564.1 (70). Calcd for $C_{25}H_{28}BF_2IN_2O_2$ ([M]$^-$): 564.13.

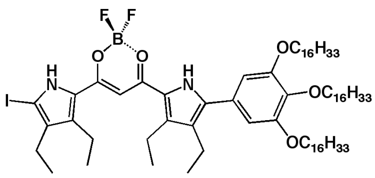


BF$_2$ complex of 1-(3,4-diethyl-5-(3,4,5-trihexadecyloxyphenyl)pyrrol-2-yl)-3-(3,4-diethylpyrrol-2-yl)-1,3-propanedione, 2c′.[S1] A round-bottomed flask placed with BF$_2$ complex of 1-(3,4-diethyl-5-iodopyrrol-2-yl)-3-(3,4-diethylpyrrol-2-yl)-1,3-propanedione **2a**[S2] (200 mg, 0.410 mmol), 3,4,5-trihexadecyloxyphenylboronic acid pinacol ester[S3] (453 mg, 0.490 mmol), Pd(PPh$_3$)$_4$ (47.4 mg, 0.0410 mmol), and Na_2CO_3 (130 mg, 1.23 mmol) was flushed with N_2 and charged with a mixture of degassed DME (20 mL) and water (2 mL). The mixture was heated at 80 °C for 12 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over flash silica gel column (eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to give **2c′** (261 mg, 0.226 mmol, 55%) as an orange solid. R_f = 0.50 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.31 (s, 1H, NH), 9.29 (s, 1H, NH), 6.94 (m, 1H, pyrrole-H), 6.66 (s, 2H, Ar-H), 6.50 (s, 1H, CH), 4.04 (q, J = 6.6 Hz, 6H, OCH$_2$), 2.85–2.78 (m, 4H, CH_2CH$_3$), 2.61 (q, J = 7.8 Hz, 2H, CH_2CH$_3$), 2.48 (q, J = 7.8 Hz, 2H, CH_2CH$_3$), 1.85–1.78 (m, 6H, OCH$_2$$CH_2C_{14}H_{29}$), 1.51–1.47 (m, 6H, OC$_2H_4$$CH_2C_{13}H_{27}$), 1.36–1.20 (m, 84H, OC$_2H_4$$C_{12}H_{24}CH_3$ + CH$_2$$CH_3$), 0.92–0.86 (m, 9H, OC$_{15}H_{30}$$CH_3$). MALDI-TOF-MS: *m/z* (% intensity): 1159.0 (100), 1160.0 (36). Calcd for $C_{73}H_{125}BF_2N_2O_5$ ([M]$^-$): 1158.96.

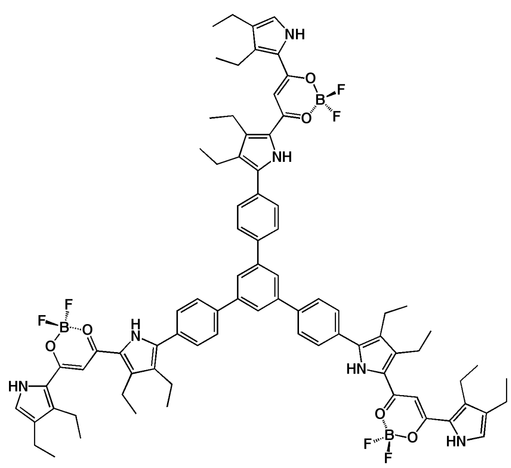


BF$_2$ complex of 1-(3,4-diethyl-5-iodopyrrol-2-yl)-3-(3,4-diethyl-5-(3,4,5-trihexadecyloxyphenyl)pyrrol-2-yl)-1,3-propanedione, 2c. To a CH_2Cl_2 (50 mL) solution of **2c′**[S1] (211 mg, 0.182 mmol) at r.t. was added *N*-iodosuccinimide (50.0 mg, 0.222 mmol). The mixture was stirred at r.t. for 3 h. After confirming the consumption of the starting material by TLC analysis, the mixture was washed with water and extracted with CH_2Cl_2, dried over anhydrous $MgSO_4$, and evaporated to dryness. The residue was then chromatographed over silica gel flash column (eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to afford **2c** (149 mg, 0.116 mmol, 64%) as an orange solid. R_f = 0.49 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm)

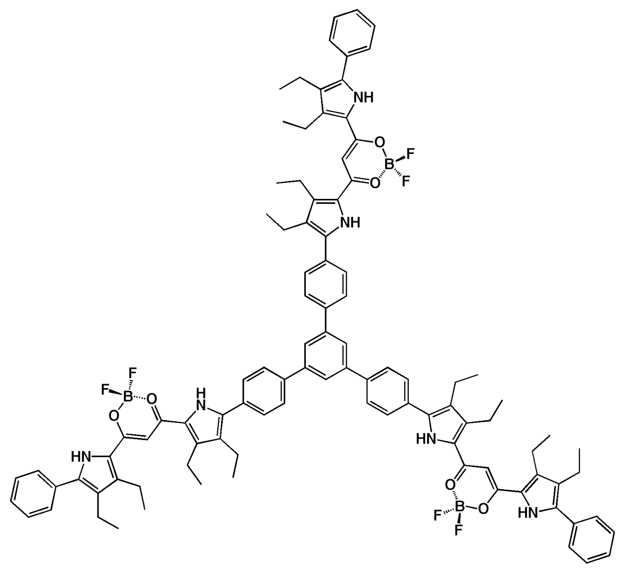
9.37 (s, 1H, NH), 9.27 (s, 1H, NH), 6.65 (s, 2H, Ar-H), 6.44 (s, 1H, CH), 4.04 (t, J = 6.6 Hz, 6H, OCH_2), 2.83 (m, 4H, CH_2CH_3), 2.61 (q, J = 7.8 Hz, 2H, CH_2CH_3), 2.44 (q, J = 7.8 Hz, 2H, CH_2CH_3), 1.82 (m, 6H, $OCH_2CH_2C_{14}H_{29}$), 1.53–1.46 (m, 6H, $OC_2H_4CH_2C_{13}H_{27}$), 1.39–1.25 (m, 84H, $OC_2H_4C_{12}H_{24}CH_3$ + CH_2CH_3), 0.89–0.86 (m, 9H, $OC_{15}H_{30}CH_3$). MALDI-TOF-MS: *m/z* (% intensity): 1283.8 (100), 1284.8 (80). Calcd for $C_{73}H_{124}BF_2IN_2O_5$ ($[M-H]^-$): 1284.49.



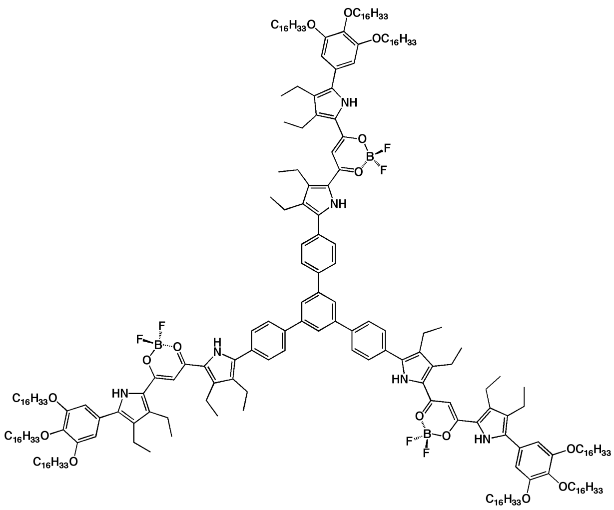
α-H-*p*-3mer, 3a. A round-bottomed flask placed with **2a**[S2] (100 mg, 0.177 mmol), 1,3,5-tri[*p*-(boronic acid)phenyl]benzene[S4] (25.8 mg, 0.0590 mmol), $Pd(PPh_3)_4$ (20.5 mg, 0.0177 mmol), and Na_2CO_3 (37.5 mg, 0.354 mmol) was flushed with N_2 and charged with a mixture of degassed DME (10 mL) and water (1 mL). The mixture was heated at 80 °C for 18 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over flash silica gel column (eluent: $CHCl_3$) and recrystallized from CH_2Cl_2/hexane to give **3a** (3.8 mg, 3.0 μmol, 5%) as an orange solid. R_f = 0.24 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.42 (br, 3H, NH), 9.31 (br, 3H, NH), 7.92 (s, 3H, Ar-H), 7.86 (d, J = 8.4 Hz, 6H, Ar-H), 7.67 (d, J = 8.4 Hz, 6H, Ar-H), 6.95 (m, 3H, pyrrole-H), 6.55 (s, 3H, CH), 2.87 (q, J = 7.8 Hz, 6H, CH_2CH_3), 2.82 (q, J = 7.8 Hz, 6H, CH_2CH_3), 2.69 (q, J = 7.8 Hz, 6H, CH_2CH_3), 2.51 (q, J = 7.8 Hz, 6H, CH_2CH_3), 1.35 (t, J = 7.8 Hz, 9H, CH_2CH_3), 1.29 (t, J = 7.8 Hz, 9H, CH_2CH_3), 1.27–1.22 (m, 18H, CH_2CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 489 (3.2). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 522 (489). MALDI-TOF-MS: *m/z* (% intensity): 1386.6 (100), 1387.6 (68). Calcd for $C_{81}H_{87}B_3F_6N_6O_6$ ($[M]^-$): 1386.69. This compound was further characterized by single-crystal X-ray diffraction analysis.



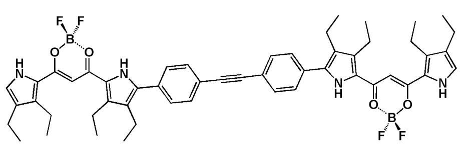
α-Ph-*p*-3mer, 3b. A round-bottomed flask placed with **2b**[S1] (100 mg, 0.177 mmol), 1,3,5-tri[*p*-(boronic acid)phenyl]benzene[S4] (25.8 mg, 0.0590 mmol), $Pd(PPh_3)_4$ (20.5 mg, 0.0177 mmol), and Na_2CO_3 (37.5 mg, 0.354 mmol) was flushed with N_2 and charged with a mixture of degassed DME (10 mL) and water (1 mL). The mixture was heated at 80 °C for 18 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over flash silica gel column (eluent: $CHCl_3$) and recrystallized from CH_2Cl_2/hexane to give **3b** (6.7 mg, 4.1 μmol, 7%) as an orange solid. R_f = 0.24 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.42 (br, 3H, NH), 9.31 (br, 3H, NH), 7.92 (s, 3H, Ar-H), 7.86 (d, J = 8.4 Hz, 6H, Ar-H), 7.67 (d, J = 8.4 Hz, 6H, Ar-H), 6.95 (m, 3H, pyrrole-H), 6.55 (s, 3H, CH), 2.87 (q, J = 7.8 Hz, 6H, CH_2CH_3), 2.82 (q, J = 7.8 Hz, 6H, CH_2CH_3), 2.69 (q, J = 7.8 Hz, 6H, CH_2CH_3), 2.51 (q, J = 7.8 Hz, 6H, CH_2CH_3), 1.35 (t, J = 7.8 Hz, 9H, CH_2CH_3), 1.29 (t, J = 7.8 Hz, 9H, CH_2CH_3), 1.27–1.22 (m, 18H, CH_2CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 512 (3.0). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 548 (512). MALDI-TOF-MS: *m/z* (% intensity): 1614.7 (100), 1615.7 (88). Calcd for $C_{81}H_{87}B_3F_6N_6O_6$ ($[M]^-$): 1614.78.



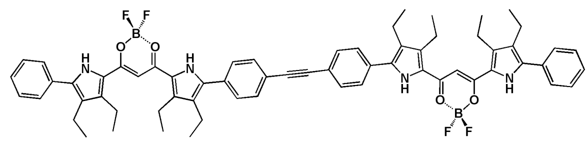
α-C$_{16}$Ph-*p*-3mer, 3c. A round-bottomed flask placed with **2c**[S1] (60.7 mg, 0.0472 mmol), 1,3,5-tri[*p*-(boronic acid)phenyl]benzene[S4] (7.00 mg, 0.0160 mmol), $Pd(PPh_3)_4$ (5.4 mg, 4.67 μmol), and Na_2CO_3 (10.1 mg, 0.096 mmol) was flushed with N_2 and charged with a mixture of degassed DME (10 mL) and water (1 mL). The mixture was heated at 80 °C for 18 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over flash silica gel column (eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to give **3c** (7.3 mg, 1.9 μmol, 12%) as a red solid. R_f = 0.23 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.41 (br, 3H, NH), 9.27 (br, 3H, NH), 7.93 (s, 3H, Ar-H), 7.87–7.81 (m, 6H, Ar-H), 7.69–7.64 (m, 6H, Ar-H), 6.67 (s, 6H, Ar-H), 6.58 (s, 3H, CH), 4.03 (t, J = 6.6 Hz, 18H, OCH_2), 2.87 (m, 12H, *CH_2*CH_3), 2.70 (q, *J* = 7.8 Hz, 6H, *CH_2*CH_3), 2.62 (q, *J* = 7.8 Hz, 6H, *CH_2*CH_3), 1.85–1.77 (m, 18H, OCH_2*CH_2*$C_{14}H_{29}$), 1.55–1.45 (m, 18H, OC_2H_4*CH_2*$C_{13}H_{27}$), 1.36–1.25 (m, 252H, OC_2H_4*$C_{12}H_{24}$*CH_3 + CH_2*CH_3*), 0.87–0.86 (m, 27H, $OC_{15}H_{30}$*CH_3*). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 519 (3.8). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 563 (519). MALDI-TOF-MS: *m/z* (% intensity): 3777.0 (100), 3777.9 (77). Calcd for $C_{243}H_{387}B_3F_6N_6O_{15}$ ($[M]^-$): 3776.99.



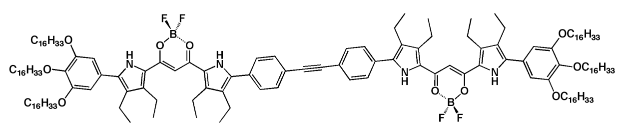
α-H-*p*-2mer, 4a. A round-bottomed flask placed with **2a**[S2] (200 mg, 0.410 mmol), 4,4′-diphenylacetylene boronic acid[S5] (49.5 mg, 0.186 mmol), $Pd(PPh_3)_4$ (43.0 mg, 0.0372 mmol), and Na_2CO_3 (119 mg, 1.12 mmol) was flushed with N_2 and charged with a mixture of degassed DME (10 mL) and water (1 mL). The mixture was heated at 80 °C for 18 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over flash silica gel column (eluent: 2% $MeOH/CH_2Cl_2$) and recrystallized from THF/hexane to give **4a** (22.8 mg, 0.026 mmol, 14%) as a red solid. R_f = 0.31 (2% $MeOH/CH_2Cl_2$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): *δ* (ppm) 9.35 (s, 2H, NH), 9.31 (s, 2H, NH), 7.66 (d, *J* = 8.4 Hz, 4H, Ar-H), 7.53 (d, *J* = 8.4 Hz, 4H, Ar-H), 6.95 (m, 2H, pyrrole-H), 6.54 (s, 2H, CH), 2.86–2.80 (m, 4H, *CH_2*CH_3), 2.65 (q, *J* = 7.8 Hz, 2H, *CH_2*CH_3), 2.50 (q, *J* = 7.8 Hz, 2H, *CH_2*CH_3), 1.34 (t, *J* = 7.2 Hz, 6H, CH_2*CH_3*), 1.28 (t, *J* = 7.2 Hz, 6H, CH_2*CH_3*), 1.24–1.20 (m, 12H, *CH_2*CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 496 (2.1). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 532 (496). MALDI-TOF-MS: *m/z* (% intensity): 897.4 (55), 898.4 (100). Calcd for $C_{52}H_{56}B_2F_4N_4O_4$ ($[M]^-$): 898.44.



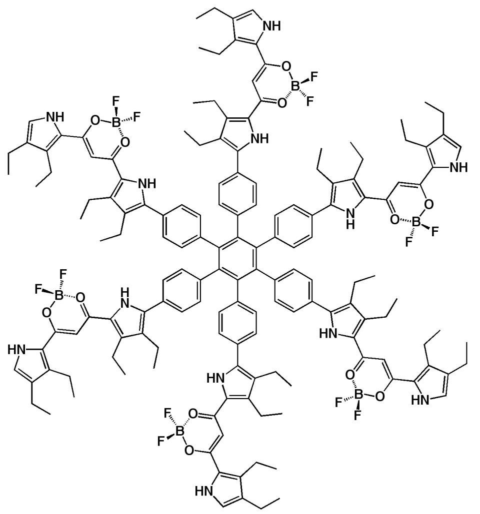
α-Ph-*p*-2mer, 4b. A round-bottomed flask placed with **2b**[S1] (100 mg, 0.177 mmol), 4,4′-diphenylacetylenediboronic acid[S5] (23.5 mg, 0.0885 mmol), $Pd(PPh_3)_4$ (20.5 mg, 0.0177 mmol), and Na_2CO_3 (56.3 mg, 0.531 mmol) was flushed with N_2 and charged with a mixture of degassed DME (10 mL) and water (1 mL). The mixture was heated at 80 °C for 18 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over flash silica gel column (eluent: 0.5% $MeOH/CH_2Cl_2$) and recrystallized from CH_2Cl_2/hexane to give **4b** (14.0 mg, 0.013 mmol, 15%) as a red solid. R_f = 0.23 (0.5% $MeOH/CH_2Cl_2$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): *δ* (ppm) 9.39 (s, 2H, NH), 9.38 (s, 2H, NH), 7.66 (d, *J* = 7.8 Hz, 4H, Ar-H), 7.55–7.48 (m, 12H, Ar-H), 7.42 (m, 2H, Ar-H), 6.58 (s, 2H, CH), 2.87 (m, 8H, *CH_2*CH_3), 2.68–2.61 (m, 8H, *CH_2*CH_3), 1.37–1.34 (m, 12H, CH_2*CH_3*), 1.22–1.19 (m, 12H, CH_2*CH_3*). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 520 (2.3). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 558 (520). MALDI-TOF-MS: *m/z* (% intensity): 1048.5 (64), 1049.5 (100). Calcd for $C_{64}H_{64}B_2F_4N_4O_4$ ($[M]^-$): 1050.50. This compound was further characterized by single-crystal X-ray diffraction analysis.



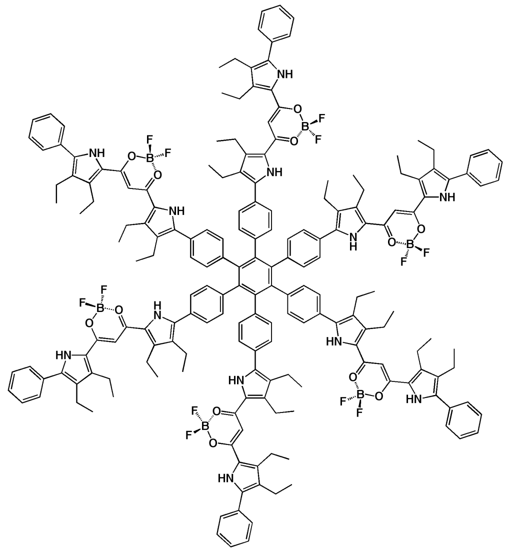
α-C_{16}Ph-*p*-2mer, 4c. A round-bottomed flask placed with **2c**[S1] (100 mg, 0.0780 mmol), 4,4′-diphenylacetylenediboronic acid[S5] (10.4 mg, 0.0390 mmol), $Pd(PPh_3)_4$ (9.0 mg, 0.00780 mmol), and Na_2CO_3 (33.1 mg, 0.312 mmol) was flushed with N_2 and charged with a mixture of degassed DME (10 mL) and water (1 mL). The mixture was heated at 80 °C for 18 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over flash silica gel column (eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to give **4c** (30.2 mg, 0.012 mmol, 31%) as a red solid. R_f = 0.37 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): *δ* (ppm) 9.38 (s, 2H, NH), 9.30 (s, 2H, NH), 7.66 (d, *J* = 8.4 Hz, 4H, Ar-H), 7.54 (d, *J* = 8.4 Hz, 4H, Ar-H), 6.66 (s, 4H, Ar-H), 6.57 (s, 2H, CH), 4.02 (t, *J* = 6.6 Hz, 12H, OCH_2), 2.86 (m, 8H, *CH_2*CH_3), 2.67–2.61 (m, 8H, *CH_2*CH_3), 1.83 (m, 12H, OCH_2*CH_2*$C_{14}H_{29}$), 1.53–1.46 (m, 12H, OC_2H_4*CH_2*$C_{13}H_{27}$), 1.37–1.25 (m, 168H, OC_2H_4*$C_{12}H_{24}$*CH_3 + CH_2*CH_3*), 0.89–0.86 (m, 18H, $OC_{15}H_{30}$*CH_3*). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 526 (2.1). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 568 (526). MALDI-TOF-MS (FT-ICR-MS): *m/z* (% intensity): 2492.0 (100), 2493.0 (60). Calcd for $C_{160}H_{256}B_2F_4N_4O_{10}$ ($[M]^-$): 2491.98.



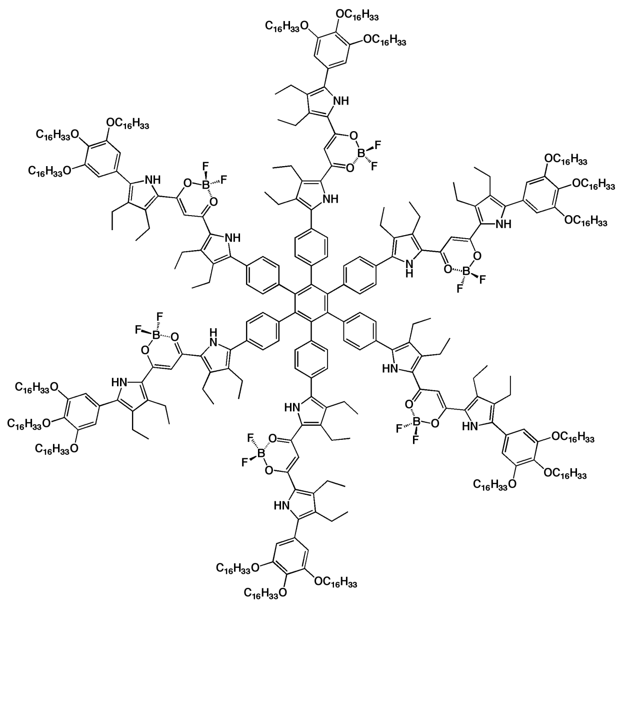
α-H-*p*-6mer, 5a. $Co_2(CO)_8$ (2.0 mg, 5.76 μmol) was added to a solution of **4a** (20.8 mg, 0.0231 mmol) in 1,4-dioxane (5 mL). The mixture was refluxed for 20 h under a N_2 atmosphere. After removing the solvent under reduced pressure, the residue was purified by flash silica gel column chromatography (eluent: 2% MeOH/CH_2Cl_2) and crystallization from CH_2Cl_2/hexane to afford **5a** (8.3 mg, 0.090 mmol, 39%) as an orange solid. R_f = 0.34 (2% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C): δ (ppm) 9.25 (s, 6H, NH), 9.14 (s, 6H, NH), 7.14 (d, J = 8.4 Hz, 12H, Ar-H), 7.05 (d, J = 8.4 Hz, 12H, Ar-H), 6.90 (m, 6H, pyrrole-H), 6.49 (s, 6H, CH), 2.76–2.72 (m, 24H, CH_2CH$_3$), 2.48–2.44 (m, 24H, CH_2CH$_3$), 1.25–1.18 (m, 54H, CH$_2$$CH_3$), 1.01 (t, J = 7.2 Hz, 18H, CH$_2$$CH_3$). UV/vis ($CH_2Cl_2$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 482 (5.7). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 525 (482). MALDI-TOF-MS: *m/z* (% intensity): 2694.3 (100), 2695.3 (85). Calcd for $C_{156}H_{168}B_6F_{12}N_{12}O_{12}$ ([M]$^-$): 2695.33.



α-Ph-*p*-6mer, 5b. $Co_2(CO)_8$ (3.9 mg, 0.0113 mmol) was added to a solution of **4b** (47.6 mg, 0.0453 mmol) in 1,4-dioxane (15 mL). The mixture was refluxed for 20 h under a N_2 atmosphere. After removing the solvent under reduced pressure, the residue was purified by flash silica gel column chromatography (eluent: 0.5% MeOH/CH_2Cl_2) and crystallization from CH_2Cl_2/hexane to afford **5b** (21.3 mg, 0.020 mmol, 45%) as a red solid. R_f = 0.28 (0.5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.31 (s, 6H, NH), 9.16 (s, 6H, NH), 7.52–7.37 (m, 30H, Ar-H), 7.25 (d, J = 8.4 Hz, 12H, Ar-H), 7.07 (d, J = 8.4 Hz, 12H, Ar-H), 6.49 (s, 6H, CH), 2.82–2.76 (m, 24H, CH_2CH$_3$), 2.60 (q, J = 7.8 Hz, 12H, CH_2CH$_3$), 2.49 (q, J = 7.8 Hz, 12H, CH_2CH$_3$), 1.30–1.27 (m, 36H, CH$_2$$CH_3$), 1.18 (t, J = 7.2 Hz, 18H, CH$_2$$CH_3$), 1.02 (t, J = 7.2 Hz, 18H, CH$_2$$CH_3$). UV/vis ($CH_2Cl_2$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 506 (5.0). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 551 (506). MALDI-TOF-MS: *m/z* (% intensity): 3150.5 (94), 3151.5 (100). Calcd for $C_{192}H_{192}B_6F_{12}N_{12}O_{12}$ ([M]$^-$): 3151.51.



α-C$_{16}$Ph-*p*-6mer, 5c. $Co_2(CO)_8$ (1.4 mg, 4.2 μmol) was added to a solution of **4c** (42.0 mg, 0.0168 mmol) in 1,4-dioxane (15 mL). The mixture was refluxed for 20 h under a N_2 atmosphere. After removing the solvent under reduced pressure, the residue was purified by GPC-HPLC (JAIGEL 2.5H; eluent: $CHCl_3$) and crystallization from CH_2Cl_2/MeOH to afford **5c** (15.0 mg, 6.0 μmol, 36%) as a red solid. R_f = 0.21 (CH_2Cl_2). ^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C): δ (ppm) 9.22 (s, 6H, NH), 9.14 (s, 6H, NH), 7.15 (d, J = 8.4 Hz, 12H, Ar-H), 7.06 (d, J = 8.4 Hz, 12H, Ar-H), 6.63 (s, 12H, Ar-H), 6.48 (s, 6H, CH), 4.02 (t, J = 6.6 Hz, 36H, OCH$_2$), 2.78 (m, 24H, CH_2CH$_3$), 2.59 (m, 12H, CH_2CH$_3$), 2.50 (m, 12H, CH_2CH$_3$), 1.83–1.76 (m, 36H, OCH$_2$$CH_2C_{14}H_{29}$), 1.55–1.46 (m, 36H, OC$_2H_4$$CH_2C_{13}H_{27}$), 1.35–1.25 (m, 504H, OC$_2$H$_4$$C_{12}H_{24}CH_3$ + CH$_2$$CH_3$), 0.88–0.86 (m, 54H, OC$_{15}H_{30}$$CH_3$). UV/vis ($CH_2Cl_2$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 513 (6.4). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 565 (513). MALDI-TOF-MS: *m/z* (% intensity): 7480.9 (100), 7481.9 (95). Calcd for $C_{480}H_{769}B_6F_{12}N_{12}O_{30}$ ([M + H]$^+$): 7480.95.



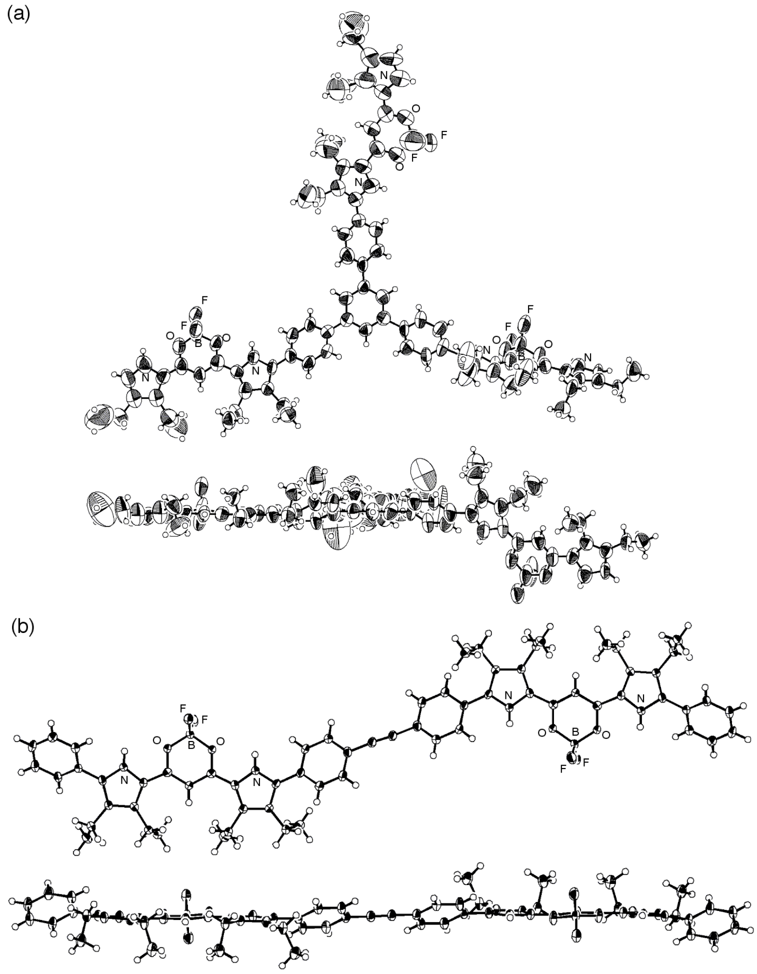
[S1] Y. Haketa and H. Maeda, manuscript in preparation.
[S2] H. Maeda and Y. Haketa, *Org. Biomol. Chem.*, 2008, **6**, 3091–3095.
[S3] Y. Haketa, S. Sakamoto, K. Chigusa, N. Nakanishi and H. Maeda, *J. Org. Chem.*, 2011, **76**, 5177–5184.
[S4] H. Noguchi, T. Sioda, C. Chou and M. Suginome, *Org. Lett.*, 2008, **10**, 377–380.
[S5] K. E. Maly, T. Maris and J. D. Wuest, *CrystEngComm*, 2005, **38**, 33–35.

2. X-ray crystallographic data for anion receptors.

Method for single-crystal X-ray analysis. Crystallographic data for anion receptors are summarized in Supporting Table 1. A single crystal of **3a** was obtained by vapor diffusion of heptane into a chlorobenzene solution. The data crystal was a red prism of approximate dimensions 0.50 mm × 0.10 mm × 0.10 mm. Data were collected at 93 K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Cu-Kα radiation (λ = 1.54187 Å), and structure was solved by direct method. A single crystal of **4b** was obtained by vapor diffusion of hexane into a CH_2Cl_2 solution. The data crystal was a red prism of approximate dimensions 0.20 mm × 0.20 mm × 0.10 mm. Data were collected at 93 K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Cu-Kα radiation (λ = 1.54187 Å), and structure was solved by direct method. In each compound, the non-hydrogen atoms were refined anisotropically. The calculations were performed using the Crystal Structure crystallographic software package of Molecular Structure Corporation.[S6] The scattering arising from the presence of disordered solvents in the crystal **3a** was removed by use of the utility SQUEEZE in the PLATON software package.[S7] CIF files (CCDC-904788 and 904789) can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

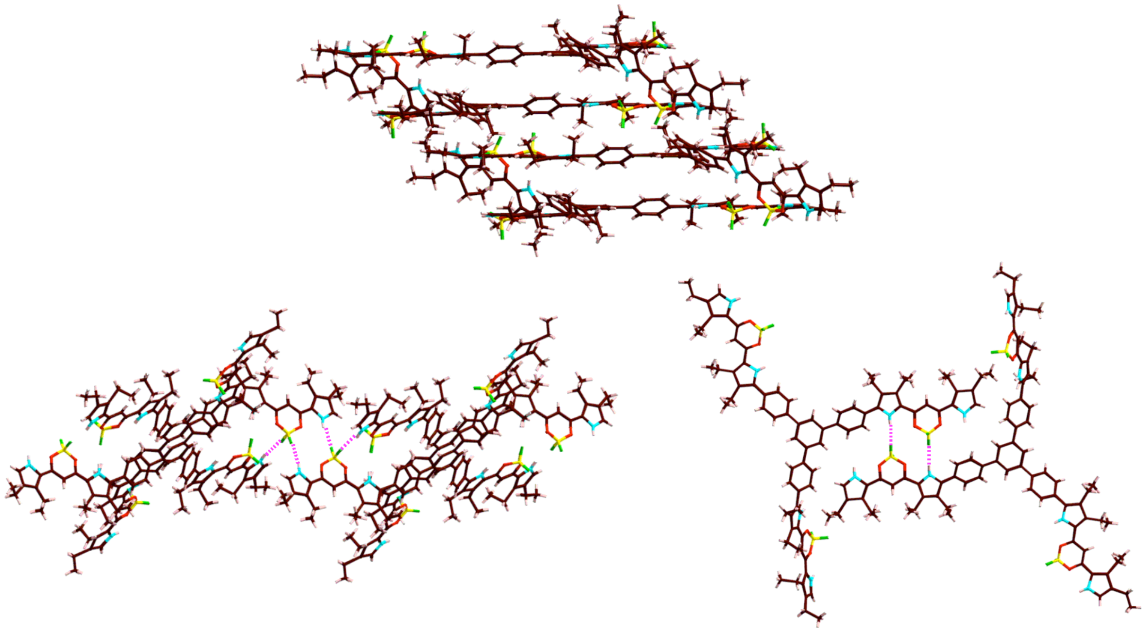
Supporting Table 1 Crystallographic details for compounds **3a** and **4b**.

	3a	**4b**
formula	$C_{81}H_{87}B_3F_6N_6O_6$	$C_{64}H_{64}B_2F_4N_4O_4 \cdot 2CH_2Cl_2$
fw	1387.00	1220.66
crystal size, mm	0.50 × 0.10 × 0.10	0.20 × 0.20 × 0.10
crystal system	triclinic	triclinic
space group	*P*-1 (no. 2)	*P*-1 (no. 2)
a, Å	11.7587(6)	10.5826(4)
b, Å	19.9823(9)	10.9562(4)
c, Å	20.7892(11)	13.5953(4)
α, °	87.324(2)	94.776(2)
β, °	87.101(2)	95.113(2)
γ, °	84.7857(19)	107.929(2)
V, Å^3	4854.0(4)	1483.56(9)
ρ_{calcd}, gcm^{-3}	0.949	1.366
Z	2	1
T, K	93(2)	93(2)
μ, mm^{-1} (Cu-Kα)	0.549	2.354
no. of reflns	13932	5238
no. of unique reflns	2952	3516
variables	896	383
λ, Å (Cu-Kα)	1.54187	1.54187
R_1 ($I > 2\sigma(I)$)	0.1014	0.0596
wR_2 ($I > 2\sigma(I)$)	0.1901	0.1503
GOF	1.036	1.097

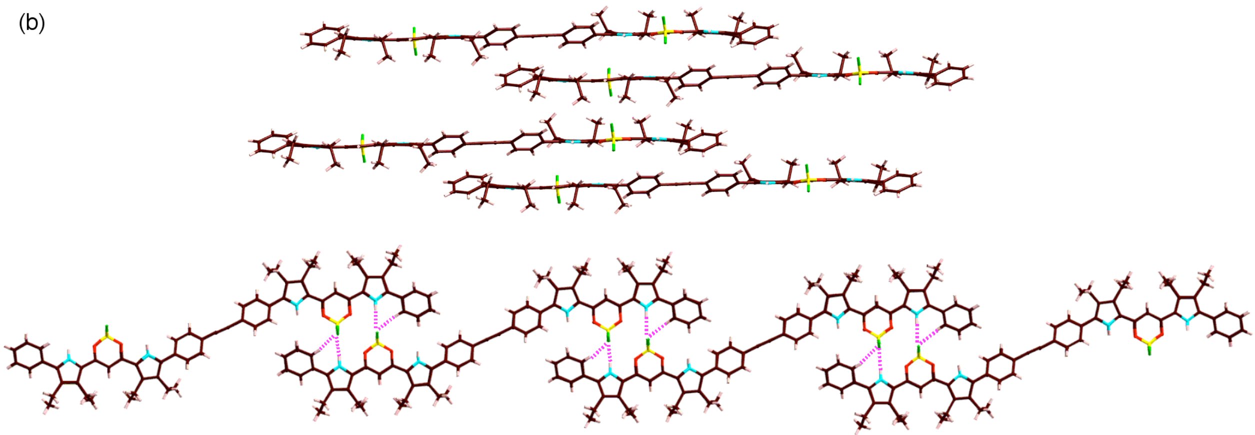


Supporting Figure 1 Ortep drawings of single-crystal X-ray structures (top and side view) of (a) **3a** and (b) **4b**. Thermal ellipsoids are scaled to the 50% probability level. The dimer **4b** has crystallographically imposed inversion symmetry. Solvent molecules are omitted for clarity.

(a)



(b)



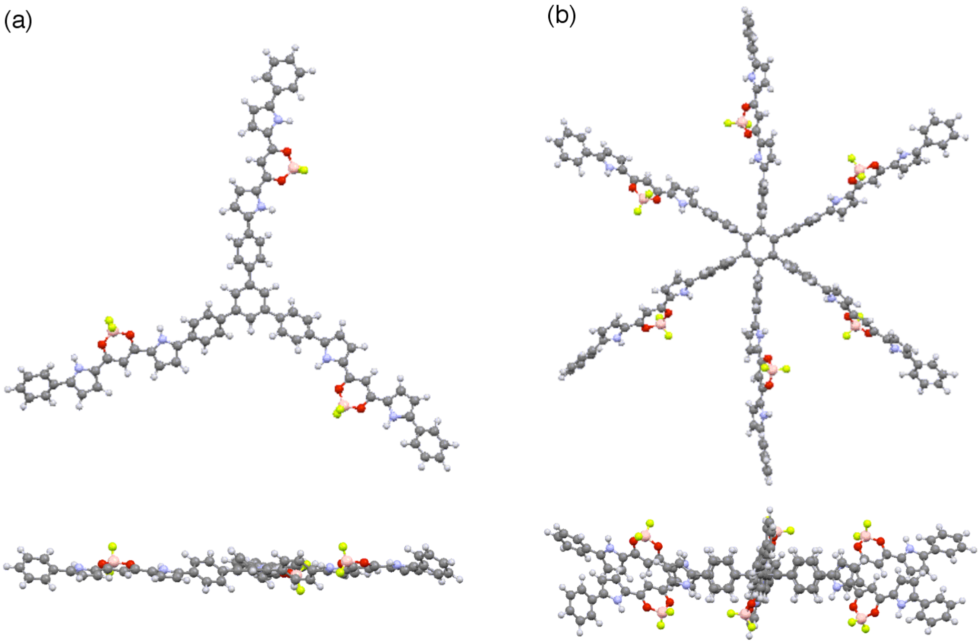
Supporting Figure 2 Packing diagrams of (a) **3a** and (b) **4b** (hydrogen-bonding and stacking assemblies). Solvent molecules are omitted for clarity. Atom color code: brown, pink, yellow, green, blue, and red refer to carbon, hydrogen, boron, fluorine, nitrogen, and oxygen, respectively.

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

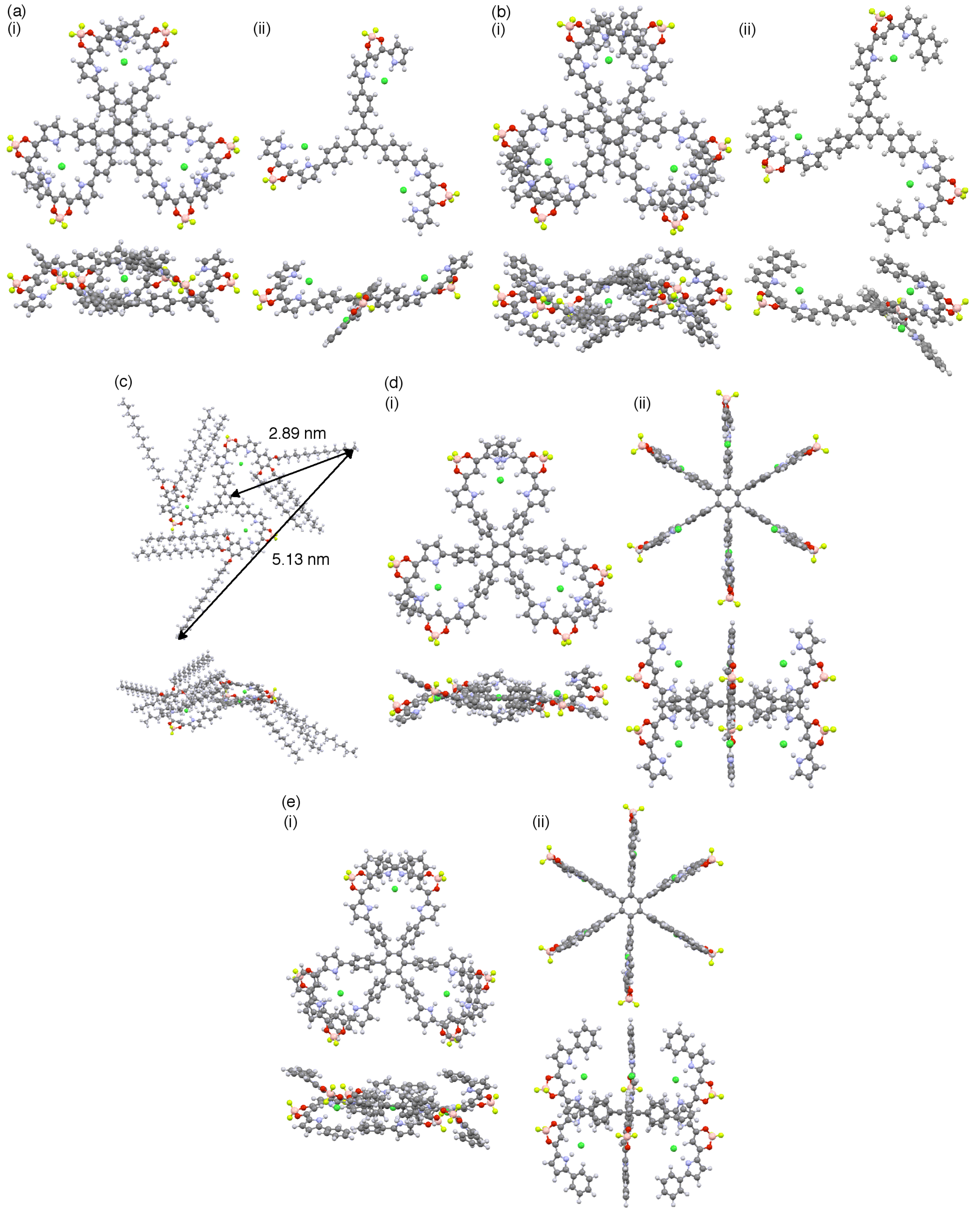
[S8] (a) A. L. Spek, *PLATON, A Multipurpose Crystallographic Tool*; Utrecht University: Utrecht, 2005; (b) P. van der Sluis and A. L. Spek, *Acta Crystallogr. Sect. A*, 1990, **46**, 194–201.

3. Optimization of anion receptors by AM1 calculations

DFT and semi-empirical calculations. Semi-empirical calculations for anion receptors and their receptor–anion complexes were carried out by using Gaussian 03 program[S8] and 2.4 GHz MacBook Pro computers. The structures were optimized, and the total electronic energies were calculated at the AM1 level.



Supporting Figure 3 Optimized structures of (a) **3b** and (b) **5b** at AM1 level. β-Ethyl-substituents are omitted for concise calculations.



Supporting Figure 4 Optimized structures of (a)(i) **3a**$_2$·Cl^-_3 and (ii) **3a**·Cl^-_3 (see also Supporting Figure 5), (b)(i) **3b**$_2$·Cl^-_3 and (ii) **3b**·Cl^-_3 (see also Supporting Figure 9), (c) **3c**·Cl^-_3, (d)(i) **5a**·Cl^-_3 and (ii) **5a**·Cl^-_6 (see also Supporting Figure 14), and (e)(i) **5b**·Cl^-_3 and (ii) **5b**·Cl^-_6 (see also Supporting Figure 18) at AM1 level.

Cartesian Coordination of 3b (AM1)

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Cartesian Coordination of 5b (AM1)

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Cartesian Coordination of $3a_2 \cdot Cl^-_3$ (AM1)

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C,4.140357038,-7.3971415035,-4.0754148888
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C,0.6248995969,-6.5471902176,-9.5949878319
C,-1.5361811153,8.7890026442,-4.9395127283
C,-6.0334006528,9.7224324122,-1.5865825272
C,-6.7524332612,10.5455123877,-2.4929611209
C,4.4422835511,-3.9084274395,-0.9320058977
C,3.8732098556,-4.287465669,-2.1593747436
C,3.0002910766,-3.3960921614,-2.8017735239
C,2.6674400356,-2.183489603,-2.2033291576
C,-2.7341466387,-4.4957734326,11.8805153812
C,-1.4465285698,-2.3581020029,11.2402448994
C,-1.2477905178,-3.5360243028,3.7043254021
C,-2.1957819783,-0.8162249704,-1.6707248402
C,-2.9205723893,0.6416238301,0.1373693126
C,-2.0098357261,11.6177638301,0.36610957
C,-2.3012493053,-1.6631076784,0.6076073079
C,-2.0947168649,-5.1176938414,2.0859998424
C,-2.6450918293,0.4321132521,-1.2191592609
C,5.9531999215,-5.4635398834,-8.1800500695
C,6.710781288,-5.367213019,-9.3769166819
C,-4.6582644185,3.3118448652,2.1410536094
C,0.6537636106,1.7675332251,9.4153409993
C,4.8052333562,-7.7951197285,-2.8868962818
C,1.1250718618,5.1271268602,-2.8584729903
C,1.8076124074,2.9315529663,-1.2219916823
C,2.2454265234,4.3319500963,-3.1533263807
C,2.5813838477,3.2506643609,-2.3472475537
C,-4.7482512114,9.9578965353,-3.4167254851
C,-3.6262533219,9.8025833319,-4.3051024457
C,1.9465618569,1.7661778753,0.9698697444
C,2.6152827433,-0.5559907459,1.0929467627
C,2.7911928691,-0.5859965138,-0.297339904
C,-4.076923253,9.3801951128,2.5253165575
C,2.1126930171,1.7476698043,-0.4199566794
C,2.5422148673,0.5700875857,-1.0467863496
C,2.0773068623,1.8244404797,5.2925252901
C,1.4469364496,0.751764531,5.945513057
C,1.1283729461,-0.3961381257,5.203824354
C,0.7498829292,6.1868711668,-3.7774324668
C,1.3778354931,6.5188157934,-5.0116258375
C,0.6212251941,7.555947488,-5.6104237559
C,4.1605124712,-5.6058186711,-2.6961554446
C,-0.4547741482,7.8491750905,-4.7360577079
C,1.3904645299,-0.4459399198,3.8367065398
C,1.9807196859,0.6411871324,3.1780456912
C,2.3385747289,1.7705092388,3.9285865964
C,-2.2911446526,-5.6559009889,9.968491092
C,-5.9427380887,10.6958680848,-3.6446721649
C,1.0981264343,0.8857829616,7.3488872638
C,4.8222497331,-6.6752155883,-2.0231215189
C,-0.6419441721,-1.7166121115,10.2936637725
C,-0.3533054485,-0.3617701589,10.4516515496
C,1.166587438,2.0750731,8.1338701631
C,-1.9344662377,-3.6974619,11.0218717563
C,-2.9583407386,-5.729098955,11.216958942
C,4.1095150002,-2.6960108892,-0.3392950381
C,2.1932442545,0.6159552726,1.7315060566
C,-1.5067534539,-4.8656333746,3.3369337685
C,3.6750345306,-3.4078402118,-10.1230371648
C,-2.7489509647,-0.41138828,1.0461510129
Cl,2.4403951866,-4.5484378764,-6.4202337177
Cl,0.173460521,-3.2234362533,7.5956816573
Cl,-2.5457434703,7.8262176101,-0.9204964374
F,4.9531214031,-10.5557905317,-6.8896145484
F,-5.2593433004,12.1772925544,3.1162867208
F,-2.3032018837,0.2796363077,13.041800066
F,0.7027665042,-9.5278000195,9.3755804611
F,2.5216636838,-9.7928100928,8.2158911895
F,2.1401424671,-3.0195635119,-12.8109783315
F,-3.6217060341,11.9724257166,4.5302343253
F,3.2559427328,-1.1777223276,-12.5179523471
F,-1.9999573325,11.5605504638,-6.3047713251
F,-0.3748607515,-0.587624299,13.5442686546
F,-3.0585600581,10.1195961994,-7.5400761521
F,3.2545729026,-11.4097077404,-5.8365300238
H,-3.4653096317,7.1641539546,0.9141898964
H,-0.8143009749,-3.2894201033,4.6885794788
H,-2.3230988324,-6.1513128726,1.7857485206
H,-2.7691996186,1.2599288086,-1.9348278468
H,6.1933911857,-5.9949837845,-7.2566914241
H,7.6795099139,-5.8211724207,-9.5518714076
H,-5.3998118605,3.3761857357,2.9513853019
H,-3.2030762571,9.1782992111,0.5443422344
H,-1.6264236223,13.7552330696,0.8539595414
H,-4.7639592933,1.1578917418,2.0549250492
H,2.4524586537,-3.5014594347,-8.3215336116
H,0.4721804646,-2.5478862309,-5.0433505713
H,-0.1738029608,-2.3120759312,-2.6847114251
H,-0.6391829059,-0.391102235,-10.4199866732
H,-2.1488924868,0.1185160399,-8.2013390015
H,-2.0598485072,3.0627181669,-0.7362986539
H,1.1106131163,-1.3457628268,3.2653495482
H,-0.2828685443,-2.2639357121,9.4004942496
H,5.2413412772,-6.633720806,-1.0232843421
H,1.5292785867,3.0398619683,7.7954180678
H,-2.7010417728,5.2776647396,0.1263929856
H,-5.5514394116,7.8739006952,4.5762195289
H,-5.5511986811,5.1863883788,4.0814893048
H,-0.2439931224,11.1175457973,-2.3641085911
H,-0.0577479708,13.6733819541,-1.395325963
H,4.327276018,-4.2023832272,12.1509391196
H,0.6953551312,-5.3169963351,7.7079152502
H,3.7375084456,-6.7184929043,11.2268563009
H,-1.8368348696,-7.7886783079,3.049894658
H,-3.4943641326,0.2240151877,-3.814019334
H,-2.8416595538,0.0191631799,-6.1914523084
H,-6.3194436525,9.3902083934,-0.5863279574
H,0.1927747513,-5.5864700759,-9.8827802749
H,-0.0517046689,-8.0071156054,-11.1421330059
H,3.0163343038,-6.5660020034,-6.4103149193
H,1.4135072967,-9.7917396618,-9.6604152142
H,4.5615709314,-2.4195599252,0.6253499688
H,-2.4625336405,8.5146136614,-2.9868764878

H,-0.4920214398,5.4511187961,-1.4203291881
H,0.1024368511,3.5236454872,-0.0156144421
H,5.2051407944,-8.7889777096,-2.7028519848
H,0.7976603288,8.0478896116,-6.5637786977
H,2.2665561728,6.0493253809,-5.4203464052
H,2.3597397113,2.7228068502,5.8615422375
H,2.672208971,0.5504887142,-2.1401990238
H,1.6747665108,-5.9363583738,-7.8299586493
H,1.6074306193,2.6876975045,1.4684297374
H,3.4593354177,2.6362315995,-2.598706113
H,2.8592893074,4.555929238,-4.0386031031
H,-2.2217089259,-6.4085731488,9.1803016744
H,-6.157946121,11.2592274811,-4.5485705002
H,2.8263701846,2.6232276146,3.4324552186
H,0.5394928491,2.4314750895,10.2683751949
H,-3.523745438,-6.5778241589,11.5847816358
H,2.7987356687,-1.4646516847,1.6875100713
H,-1.1260481067,-4.1031612617,9.065232768
H,-0.9709302109,7.028443331,-2.8333131471
H,0.4222856446,-1.091114171,7.8518855642
H,-3.0900518614,-4.187470827,12.859708994
H,1.9613074238,-1.5076098719,-2.7125126234
H,2.5590429142,-3.6412581702,-3.7839938585
H,5.1518938416,-4.5805548531,-0.4265850287
H,-7.7321114755,10.9753359269,-2.3180542375
H,0.6611768565,-1.2728221984,5.6863924754
H,-2.8326257054,-4.2933369439,0.2331609507
H,-1.2921925947,-1.4591273697,3.1185316765
H,-0.6852458436,-9.1775566817,5.100411276
H,6.2112058469,-4.2945523598,-11.2974043902
H,2.8836620776,-2.4642104889,10.6012351384
H,-2.9551062034,-0.248654342,2.1156468492
H,-1.6754619673,-2.8432527915,-1.1011151608
H,0.9632981084,-2.5928125969,-7.1523172357
H,4.0318048841,-4.6778112261,-7.626097174
H,-1.7903067201,9.8164070943,-0.7999094275
H,1.5573809141,-3.8480098041,8.9075035685
H,3.2848165923,-5.5098098512,-4.6550676038
H,-4.0992376945,8.7939147744,-1.7087727936
H,-0.2123290799,-5.0159814298,5.8447028273
N,0.3793670895,-1.9718995286,-7.673630941
N,0.5749709842,-0.1275652089,8.1333875986
N,-0.3524373946,7.0131434741,-3.6167648888
N,-1.677651014,-4.434004362,9.8511527655
N,-4.8333381838,9.3676243514,-2.1440875114
N,1.4173453239,-6.6738926362,-8.4822263109
N,3.7659585823,-6.0520894375,-3.9457641992
N,-3.9850792907,6.9918432566,1.7698212294
N,-0.464275753,-5.8690187928,5.3886123542
N,2.1972726661,-4.245782946,9.6056906931
N,-1.5448357859,10.7955440921,-0.676478026
N,4.7817326475,-4.7676029476,-8.3229533337
O,2.9031137959,-9.8148033935,-7.3026308447
O,4.0867072463,-9.4996507152,-5.1426253141
O,-3.7094243927,10.4291031041,-5.4664467126
O,-1.5498482772,9.4017870232,-6.113747455
O,-3.1724848015,12.0037748159,2.3822576803
O,-4.3977273076,10.1764101319,3.5331682651
B,2.7161106126,-2.2125582673,-12.0054411991
B,-4.1482686647,11.6255502427,3.4225917917
B,1.5654420118,-9.0304835576,8.5753790999
B,3.8329333676,-10.3738733452,-6.3025444965
B,-1.2989996603,-0.4163960579,12.6787074726
B,-2.5707840485,10.4218097576,-6.4017305328

Cartesian Coordination of 3a·Cl^-_3 (AM1)

-1.5145189 hartree
C,-2.8277472415,1.9052481267,-11.5738271391
H,-2.7596168283,1.8628183387,9.6961715105
H,-0.5109520187,1.886084412,5.4971332217
H,-3.1897973547,-1.4753876153,4.8461888599
H,-3.1983134003,0.9917535947,-9.6345694593
H,-5.8029878576,-3.7345309863,7.6432189706
H,-3.6575386106,-1.3464437738,6.9769310264
H,-3.9491682433,-0.6562739524,-6.8994549056
H,7.6419508616,1.9664865513,0.0652543763
H,8.9521462706,4.2576656699,2.0114957688
H,-5.2393116982,0.4902119921,-13.3978895072
H,-5.7564271589,-3.5723474787,-4.2887964406
H,-7.0288704678,-3.6527192822,-6.7033860873
H,-4.5205639999,-2.8856552554,-2.7367585073
H,-2.9517013478,-2.2963572941,-0.9204871665
N,7.8547838487,1.3173754699,-0.7278653348
N,-3.4619878304,1.1233337329,-10.647371757
N,-6.4449846888,-4.1183315507,8.3874624821
N,-3.2187402388,-0.4799390395,7.3660071273
N,-4.5865131713,-1.3888334318,-6.508467359
N,9.8465469022,4.7666710061,2.2439079456
O,-6.1231819747,-1.2837351484,-11.338444351
O,-6.6724207719,-2.539361932,-9.2818380436
O,12.3409515127,3.6122848603,-0.164068744
O,-6.2945667517,-1.770893176,11.183329481
O,11.3425862784,1.9116793447,-1.6531927049
O,-4.7015270411,0.0462174019,10.6666021217
C,-3.4681828747,1.7664465221,-12.8347452716
C,-5.9189433885,-1.6867109458,-8.600272375
C,-3.6040421584,-1.5658337804,-4.2016696312
C,-1.8186122513,-0.8876259599,-2.1206611563
C,-1.7024093728,-0.2975008033,-3.3863845772
C,-2.5814856116,-0.6281948251,-4.4158112342
C,-5.37349412,-0.5508887688,-9.2055042046
C,-0.9640184302,-0.0128360311,2.6930264358
C,-0.4572870856,0.9801403866,3.5438210088
C,-7.5840145718,-4.3175653778,10.3670145359
C,-5.8501483602,-2.4155248125,10.1124452127
C,-4.7554233173,-1.9519501742,9.3814739849
C,-4.3028914068,-0.6488393302,9.609762112
C,-6.5986503197,-3.5684631501,9.6703347138
C,-3.4565084027,0.0209293657,8.6536352739
C,-8.0245011761,-5.3389285116,9.4891811599
C,-7.302582855,-5.1786190963,8.2758105503
C,-2.0805586162,1.4875201482,7.5840191274
C,-2.3882968783,0.4013156288,6.7043703075
C,-2.7551896977,1.248897931,8.8002695992
C,-0.925796023,1.1016580095,4.8469481152
C,-1.9154381799,0.2345811364,5.3399315534
C,-2.4184807588,-0.7646736151,4.4920912348
C,-1.9472746318,-0.8813928959,3.1862845295
C,7.6578597826,-0.1349657497,-2.4788341219
C,12.0348057324,5.4442604819,2.1522080461

C,11.255490093,3.5326633234,0.5943468024
C,10.2685541532,2.5738161241,0.3604817089
C,10.285162945,1.8801005898,-0.8531439892
C,11.0822820102,4.5359757063,1.6180305481
C,9.1165808422,1.1775552937,-1.3224518046
C,11.3605288794,6.2289917812,3.1202861226
C,10.0109292168,5.7846655543,3.1431198729
C,-4.5325163486,0.8483877527,-12.6559100109
C,6.9592084143,0.5286842414,-1.4205959437
C,9.005871641,0.2778970566,-2.4176841752
Cl,-2.8630859936,0.6769701244,-7.7893190332
Cl,-4.5796105727,-2.9569035404,6.4147017692
Cl,7.4273399522,3.2395635725,1.5092245709
F,13.0498651531,3.1793015017,-2.1943324308
F,13.3193392654,1.6736181165,-0.6553386437
F,-8.2019881163,-1.6302396167,-10.6210903332
F,-4.7321144682,-1.0584407264,12.6002346546
F,-6.3859252347,0.2380756903,12.059472626
F,-6.9969328958,-3.2956816403,-11.3157121661
H,-7.3662241806,-5.7631622249,7.3572283216
H,-1.9632703619,2.5143058418,-11.3065763295
H,-0.910456375,0.4445620442,-3.5721688009
H,-2.457059287,-0.1368136739,-5.4001724273
H,-4.8454605574,0.209057217,-8.5980757659
H,0.3142303831,1.6726790493,3.1748772035
H,-7.9147913136,-4.1183288836,11.3815310259
H,2.850214382,-1.5026556064,-2.0197721567
H,7.219388341,-0.8195301635,-3.1962044594
H,9.8268135014,-0.0146014136,-3.0657782771
H,9.179746715,6.1464836294,3.7496357275
H,-3.1847171687,2.2708041943,-13.7504876827
H,0.8390882766,-0.4498650961,-2.3416194029
H,1.5918270499,0.2646596703,1.8586498574
H,-2.4273438238,-0.5669839418,0.4921919463
H,5.2618118398,-1.2402758867,-2.5022828268
H,5.4775508797,2.0070299286,0.37964138
H,3.0719321346,1.7329810989,0.8418070495
H,9.4283545292,2.444440497,1.0689855889
H,13.0767323695,5.5003064658,1.8528471108
H,11.7799217009,7.0193801876,3.7307786834
H,-2.3497295465,-1.674561999,2.5375934444
H,-4.3254407719,-2.5593779989,8.5625086949
H,-8.7687884452,-6.0997707255,9.6902920944
H,-1.4491623419,2.3362434827,7.3461245618
C,-5.6062483843,-2.0215593185,-7.2328483043
C,3.5528796026,1.0729682696,0.1035687578
C,2.7924572165,0.0980640526,-0.5563164445
C,3.4281266713,-0.7259587199,-1.4966499278
C,-3.7234048646,-2.1528673055,-2.9304817033
C,-2.8449596867,-1.8194432808,-1.906488873
C,-4.5197262699,0.4595579367,-11.2897605466
C,-5.385952578,-0.4658567157,-10.598640337
C,0.4705252642,-0.3645035096,-1.3075320029
C,0.8891753211,0.0455443375,1.0396148848
C,-0.4715361658,-0.1351720048,1.321006107
C,1.3674164306,-0.0701700403,-0.2717780037
C,-0.8911617278,-0.5534543283,-1.039863631
C,-1.3555472612,-0.4352190076,0.2769503851
C,4.7835949116,-0.5776556911,-1.7659155273
C,5.5455514021,0.401740965,-1.1067390321
C,4.9113894633,1.2269922197,-0.1648800904
C,-4.5367836104,-1.9496927668,-5.248588473
C,-5.5480209791,-2.9587034715,-5.1579875062
C,-6.2106597271,-3.0048097232,-6.4029549857
B,-7.0555150028,-2.1998192386,-10.6617689354
B,12.5700414197,2.5710117442,-1.1787566385
B,-5.5207221549,-0.6254578442,11.6886220527

Cartesian Coordination of $3b_2{\cdot}Cl^-_3$ (AM1)

-2.5365406 hartree
C,2.030169959,-1.624458178,-4.5374018346
C,1.3479093076,-1.8749484541,1.5291728936
C,2.1143387301,-1.6698641497,-0.7695007344
C,2.9117755558,-0.1136829044,0.9231045918
Cl,-5.6339062312,-6.500674096,2.3796921792
Cl,1.8125239172,0.8424061875,-7.9552430208
Cl,3.3353828489,5.9580056337,5.8319908118
F,8.4661193514,9.9389618517,4.8225802129
F,7.4911418179,11.0050959992,3.2013336953
F,-6.338732904,-7.6425148252,8.9600918128
F,-0.1716906025,-4.0946446068,-12.5106792826
F,0.1836998145,6.2213955301,11.7665321637
F,-7.4078204423,-11.0886709399,-2.7051634933
F,0.6891987492,4.1914356392,12.3478818968
F,4.7578175232,5.5718322051,-11.465076851
F,-9.158400361,-10.1928235684,-1.7841687651
F,6.5955388158,5.7062163237,-10.31538367
F,1.9519585339,-3.702541014,-12.740515229
F,-7.1928589924,-5.6981679415,9.4120543732
H,1.887442617,-4.9957521897,-3.9997768214
H,2.0383206884,-0.8628248924,-5.3356750418
H,-0.9050234156,-3.5530497285,7.4369741493
H,1.6021594459,-1.6657949479,-7.3173314236
H,-7.305364217,-6.372332031,3.33444316
H,3.1875524288,7.9011092514,6.1489946777
H,4.9003394264,5.5635849658,3.65765043
H,-3.6609060159,-4.993723285,4.5349459832
H,0.9189539143,1.1611250247,-9.7107758664
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Cartesian Coordination of 3b·Cl$^-_3$ (AM1)

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Cartesian Coordination of 3c·Cl$^-$$_3$ (AM1)

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C,-1.023223148,-1.9240597124,10.4950160247
C,-0.3171948972,-0.7167620994,10.4781352945
C,-2.8485639168,-3.2244888817,11.531096937
C,0.2047368651,-0.1822826016,9.2451314192
C,-4.5118106319,-4.7204990469,11.9684241527
C,-4.2750060774,-4.6739818885,10.5608705175
C,1.340830285,1.0175737909,7.6774356998
C,0.4977852047,0.0648870911,7.0233265057
C,1.147983585,0.8661174328,9.0674390195
C,0.891871139,0.849540526,4.7205134533
C,0.3718051163,-0.1256008505,5.5881188827
C,-0.2384101278,-1.2627054428,5.0372660296
C,-0.2975990598,-1.4282154408,3.6553279159
C,6.3745028035,0.2125365635,-5.0909866006
C,10.5476212301,7.2814996988,-2.9697745128
C,9.7830834882,4.9994382036,-3.9375480241
C,9.0088075924,3.8629065469,-3.6990579288
Cl,-2.156558014,-2.8930296327,7.696492914
Cl,-5.5216101466,-1.5328782031,-6.1168013411
Cl,6.4311944658,4.3471275452,-1.8827657411
F,-1.1374132353,0.4471985212,13.4964302827
F,0.3663606902,-1.1159951365,13.41708257
F,-10.4458962402,-5.7237558977,-6.8300825563
F,11.7316870173,3.3005582907,-5.5501047122
F,10.6861440899,4.4162172779,-7.0914509867
F,-9.0662913741,-7.0174902802,-7.8961326792
B,10.6838622327,3.9429714742,-5.9051042059

Cartesian Coordination of 5a·Cl$^-_3$ (AM1)

-2.7724307 hartree
C,-3.1922475809,0.8188206142,1.8477595442
Cl,-2.6220741301,0.5910676506,8.6999995768
Cl,8.4345729932,0.9839754823,-1.753471172
Cl,-5.7816191065,-0.8935525946,-6.1363563636
F,-3.9138014095,-3.8443513849,-12.3960419959
F,10.3328118986,2.2166383472,-8.4351367133
F,13.1555151605,2.1437592157,2.4389604676
F,-12.2965040179,-0.9114157201,-5.3720761924
F,2.1482742212,3.8435241396,12.7379450982
F,-8.9200293509,-2.2931667119,9.9239503114
F,-11.8361390007,-2.8696444255,-6.2014783397
F,-4.8120906009,-1.8821196461,-12.6423468257
F,11.1180189033,0.3971218755,-7.5433458092
F,-8.7898418573,-0.1608122562,10.3198777762
F,13.0251834832,0.2103100473,3.4226133384
F,1.7163635696,1.782930112,13.2752019527
H,8.8439930316,1.1811329283,-3.8608877191
H,-7.6644146983,-2.3580344164,-0.322400111
H,-9.8873295806,-2.4663997953,-1.9250653117
H,3.8780149616,1.3776813892,9.3609255133
H,-2.9820539027,1.2544226888,-1.9487277247
H,-5.2589943376,0.6873304296,-2.7635171967
H,-8.0148181691,0.1050493347,-5.5097634824

H,1.9510369507,-1.3786320173,2.7720499757
H,-2.1721592431,4.0898966177,13.6929793388
H,-0.9622289465,1.5144892166,9.7394592805
H,-4.8798426092,4.131862509,13.2438716133
H,-5.2896480215,2.7141945175,10.9351041284
H,-2.836750191,-2.460696047,0.2611023886
H,4.4653122252,2.0082906523,-3.3430012078
H,3.4857742586,-1.3157712781,-0.1162952419
H,3.4661744173,-2.0834429305,-4.3478405821
H,2.6263744293,2.0482041681,-1.6721388675
H,1.6298551318,-2.0423017571,-2.6612800078
H,-5.1338186791,-3.0203724447,-0.5295917661
H,-5.8288671615,-2.1827370208,13.1070382538
H,11.8726996319,-1.2111182716,-4.1029930936
H,6.6618112424,-0.4138676621,-7.8988851823
H,-3.2436749634,1.5070449979,0.9898254604
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H,6.7726508185,0.7539192027,-3.8088197981
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H,-4.284321089,-0.2266458599,6.6988793895
H,-3.0099617762,1.894417556,10.100245742
H,-1.2153099267,-1.3766940486,-10.1358894824
H,13.23568258,4.8359991017,-2.546033211
H,11.3390871147,3.7354314208,-0.9041355504
H,-10.741216177,0.5061909829,-9.3948704006
H,-10.0436454457,-3.60989839,-7.6685467804
H,-10.3990922813,-5.0496192374,-9.9758443824
H,14.4280390962,-1.7331084103,-3.2565421974
H,9.9519488288,0.6721220015,-0.3446567635
H,14.5645929438,-0.8696932587,-0.6563292399
H,6.2901086371,1.9761201892,4.0451777469
H,0.1269058792,-0.6053173712,-7.8656139285
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H,-1.6663055249,-1.0621676665,12.3100291196
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H,-8.4467168102,-0.4030808274,5.8455982024
H,-7.0754961281,-0.05278204,3.4949338531

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N,-7.156587843,-1.267060123,-3.4238733895
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N,-8.0851805786,-3.1971733057,-8.4924853289
N,-3.4583878376,-0.9302179393,11.1249824452
N,-5.136194113,-0.2826831075,6.1833836711
N,-3.1499427837,2.4806265007,10.9416076763
N,6.4215668613,0.4442456844,-4.6910258528
O,8.9941060689,0.9649988942,-7.2276153577
O,0.0957350975,3.100022834,12.5253301313
O,10.9024930059,2.2366641844,-6.3171683609
O,-7.8781169008,-1.0072089705,8.4823187682
O,-7.0633279491,-1.4819334465,10.7642318844
O,-5.758055063,-3.3713684771,-11.3050388091
O,11.1792276346,1.1927251129,2.751282769
O,12.9199754297,0.2987695087,1.2327202504
O,-3.5780478596,-2.3117779964,-10.8585369025
O,-10.4923446512,-2.0202350484,-4.6932645146
O,-10.7760009793,-1.1208860474,-6.9814513746
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C,-6.413211197,-0.40954327,6.7477523746
C,-4.1654068623,-0.0761416866,3.8769677579
C,-6.6410292811,-0.6621146694,8.1546943202
C,-7.3712754044,-0.3264253035,5.706993846
C,-6.6598399802,-0.1463615696,4.4931081265
C,-5.2757607238,-0.1356129309,4.8126154313
C,-1.3614610593,-1.5985296102,-3.2266973791
C,-1.7622256102,-1.7532583475,-4.550492687
C,-5.853792922,-1.1002268135,10.3843701999
C,5.3382823666,1.1024828596,1.4370918544
C,4.3124128098,2.0170344164,1.7119483114
C,-1.3748043449,-0.2753249278,-0.4022809019
C,3.1081289854,0.8957195645,7.2960917372
C,9.2162960674,1.35357046,-4.8901391995
C,4.0883017723,-0.0459662664,-3.9462802829
C,5.0332625423,-0.0881464337,0.7631690755
C,-1.045066481,-0.0567479403,0.9473132854
C,1.2967504387,0.2292573771,0.3230848043
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C,-8.8911504062,-2.1220872487,-2.1893506326
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C,-3.4569913504,0.3127691805,-1.6342899382
C,-4.7322423667,-0.0062724617,-2.0901792689
C,-8.9169293721,-0.5089768144,-5.6338992641
C,0.6518921257,0.3569813723,2.7262328225
C,-2.7218273803,3.6395234798,12.8711133781
C,1.527391108,-0.5435798428,3.3505163554
C,-0.7294638051,2.6312984491,11.6021265019
C,-4.8020966034,-1.2731198041,11.3514844434
C,10.3064227682,1.0812579751,1.7626031883
C,-8.5169303863,-1.6115323958,-3.4600284811
C,6.3527092607,-0.2298164975,-6.8731844825
C,12.3177227462,-1.0246885369,-3.1230316517
C,-4.9056214564,-1.8264716231,12.6585826829
C,6.682447215,1.3472246967,1.9356398112
C,-4.6548943593,-2.0818442955,-0.8466616228
C,2.2604132732,-1.1524164372,-2.8093955317
C,2.0180867815,0.0014491391,-2.0502654454
C,2.8100609353,1.138068374,-2.2633453738
C,3.2837396334,-1.1758709807,-3.7531751672
C,-9.6112129997,-0.506427857,-6.8465900762
C,3.7181935989,-0.3754865627,0.4068399714
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C,3.8418174627,1.1131336731,-3.1967270736
C,0.295256399,0.17964095,1.3117399387
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C,-3.3723296145,-1.7678466057,-0.404919828
C,0.9634822044,0.0068352436,-1.0281257151
C,-9.3440385516,-1.3672962552,-4.615559366
C,-4.3442431567,2.9308505511,11.437243563
C,-4.1171012489,3.6603995576,12.63496943
C,1.6862525842,1.4666876851,8.9894005993
C,-2.1279982903,2.9014001801,11.8090346212
C,1.1221136429,1.9166638848,10.244226167
C,-0.253214469,1.9687811506,10.4604272013
C,-7.4246252035,0.8973791844,-9.3710710886
C,-8.6592942673,1.072962863,-10.0485596522
C,-2.7403536145,-1.2501042016,12.2459700677
C,-3.6067640648,-1.8142983239,13.220440188
C,1.8797002464,-0.3768397943,4.6868467387
C,1.3526015735,0.6894615132,5.4274962785
C,0.461559402,1.5798289334,4.8123501958
C,0.1221368399,1.4191344983,3.4717138063
C,5.0920066043,-0.5024218156,-6.2817932565
C,12.179768395,3.6632294047,-4.1425866587
C,10.3848887245,2.0990051772,-5.1058699524
C,-0.9136689218,0.4541535358,-5.0627223695
C,-2.9497717555,-1.5573051142,-8.7477310679
C,-7.4438181805,-3.5200901067,-9.6995720124
C,-3.9712298716,-2.0908112463,-9.6131779707
C,-5.2658081051,-2.4112887742,-9.180760847
C,-6.1206765055,-3.071788676,-10.0659328806
C,-8.3245379882,-4.3310066236,-10.4584627612
C,-0.5281401184,0.6127727723,-3.7337745573
C,-0.7466435111,-0.411897449,-2.8024916527
C,-5.6096727195,-0.6171354758,9.0896639145
C,-3.0691550631,-0.9396601508,4.0092849558
C,-2.0534112076,-0.9358382337,3.0569338305
C,-2.1048376449,-0.0597570804,1.964302613
B,10.3746553113,1.4317616088,-7.4315623438
B,1.5275179911,2.7612624633,12.474352096
B,12.6155465203,0.9867434579,2.4976250172
B,-4.5058664156,-2.8474428344,-11.8627582407
C,-0.3735279325,-0.2296905106,-1.3927451221
C,-1.5329552948,-0.7302573845,-5.4805899784
C,-1.605266327,-1.2768272446,-9.1260115182
C,8.5104189355,0.884229793,-5.9967172267

C,11.0438433085,2.8116769768,-4.0442999417
C,7.1682376461,0.3586737739,-5.8745336068
C,12.4408194818,4.1619025126,-2.8442040167
C,11.4616465031,3.6008284588,-1.9813537076
C,-9.6730597121,0.55459039,-9.2040032515
C,5.1556398477,-0.063079806,-4.9329988998
C,1.7770257329,0.900673663,6.8016925505
C,-9.3383925209,-3.7670945693,-8.4938579944
C,-9.5134515952,-4.4897590573,-9.6968776316
C,2.686654766,0.5288504932,0.6954991552
C,13.6333842857,-1.2836107264,-2.6718185994
C,8.9278069935,1.3328748133,2.1030910657
C,12.4357065943,-0.316762375,-0.9837467918
C,10.6949812244,0.6761784975,0.4801989
C,12.0065413193,0.2509254453,0.2740169089
C,13.7090434308,-0.8362602784,-1.3253400023
C,7.0088153708,1.7369477561,3.2683030155
C,-1.8551485027,-0.9370323756,-6.8847953141
C,-0.917805803,-0.8826410871,-7.9582702033
C,8.4174487352,1.7209019676,3.3728009926
B,-11.4180392847,-1.7304758623,-5.8024367173
B,-8.2234511739,-1.2252441913,9.8949105177

Cartesian Coordination of 5a·Cl^-_6 (AM1)
-2.6972353 hartree
Cl,-0.1393509058,0.0113480302,-8.3917566284
Cl,-0.0235214988,0.1346042721,8.3915972578
Cl,8.3852019443,0.2091591881,-0.2319129541
F,3.8706827734,-12.2412087362,4.7289263107
F,12.5668838677,-3.8096609933,-3.0488521616
F,-12.5460485429,3.811290741,3.0998262569
F,4.0630198647,2.9658080529,-12.7203350473
F,-5.2099973416,12.0351138464,-3.0907263748
F,-12.568170072,2.4579051071,4.790745637
F,-3.9532187401,-2.7987243799,12.5769099854
F,5.2103710719,-12.0563271614,3.0370568807
F,-3.8700764591,12.2104392516,-4.7834238466
F,12.5988273816,-2.4532983439,-4.737234143
F,-2.4780964647,-4.3782490748,12.7198548731
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H,14.2259140271,1.9422739238,0.6978263652
H,9.7085566875,-1.3118445793,-0.9113307053
H,14.3756246397,-0.095849482,-1.1303558122
H,5.6081661232,-3.7095616181,-4.2659565977
H,-3.5484686188,-4.2902434992,5.6837889494
H,8.2955712943,-4.014740459,-4.6595663538
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H,-14.224241153,-1.9473805682,-0.6274204205
H,0.9502865649,11.7426033923,1.1987022973
H,1.6405900982,-2.5924255068,-2.3059350523
H,3.6020993989,0.5297420309,-0.0464936188
H,3.7592095079,-3.4310344962,3.162359065
H,0.8517065788,-5.7383703914,0.9022369708
H,-5.5814648878,3.7193610518,4.2771616547
H,-8.2661839736,4.0237084341,4.6842994159
H,4.1161436101,4.4079740437,-8.376083914
H,-3.6036266675,-0.4910767461,0.0065571968
H,-5.7944440134,0.2406130693,0.8703977989
H,-9.6980355093,1.3093512531,0.9520044981
H,2.1244245859,2.7170097193,-1.6668044421
H,0.4756301543,0.5120881903,-14.4044374176
H,0.418178018,1.5932122748,-9.6995053048
H,-1.2616954732,-1.6023517997,-14.2328391549
H,-1.683298888,-2.0193810481,-11.5539550658
H,-1.6157013007,2.546956874,2.3559824965
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H,3.8324164849,-3.3391462099,-3.1729257734
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H,-0.9511600485,-11.7403560396,-1.2490247915
H,-14.3639869443,0.0934286535,1.1985711924
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H,-3.2042881913,-3.2490599767,3.8740073001
H,-1.5311704911,-0.5997370469,9.6998206055
H,-0.448325063,-0.5351688111,14.404244194
H,-2.4580023339,-2.4190789963,1.6670319594
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Cartesian Coordination of 5b·Cl$^-$$_3$ (AM1)

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Cartesian Coordination of 5b·Cl$^{-}_{6}$ (AM1)

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[S8] **Complete form of reference 8b:** *Gaussian 03* (Revision C.01), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.

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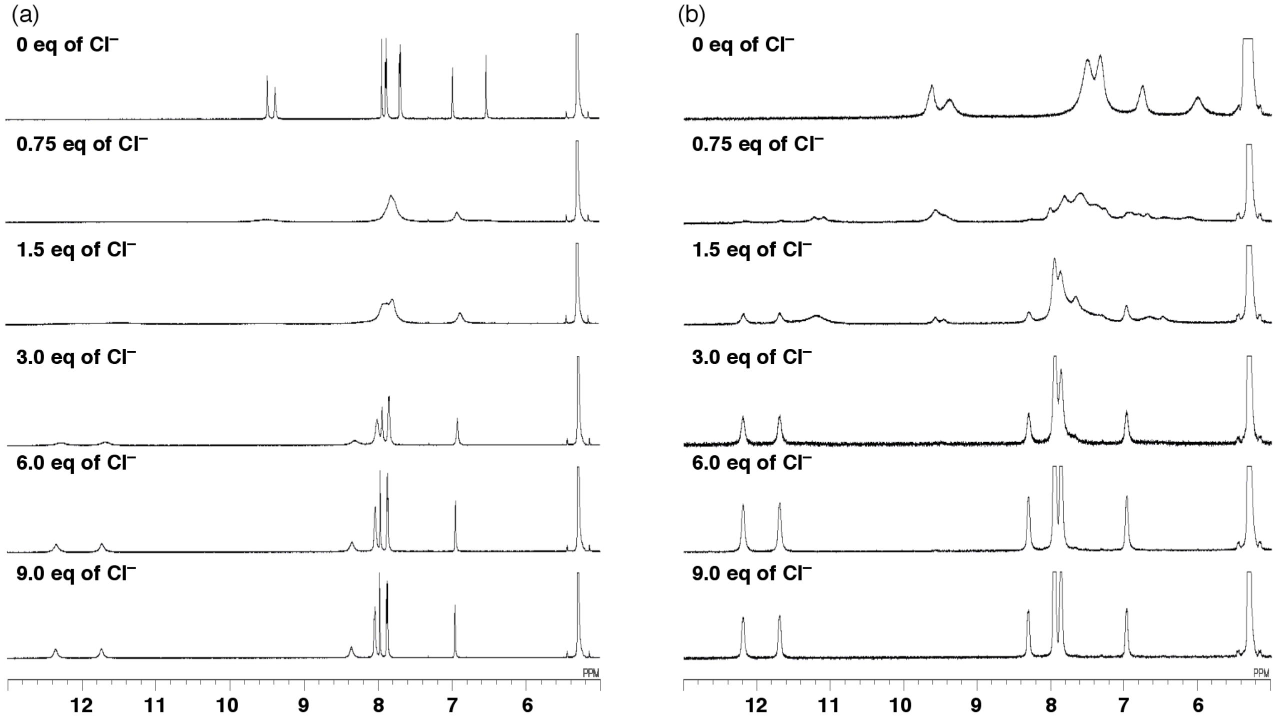
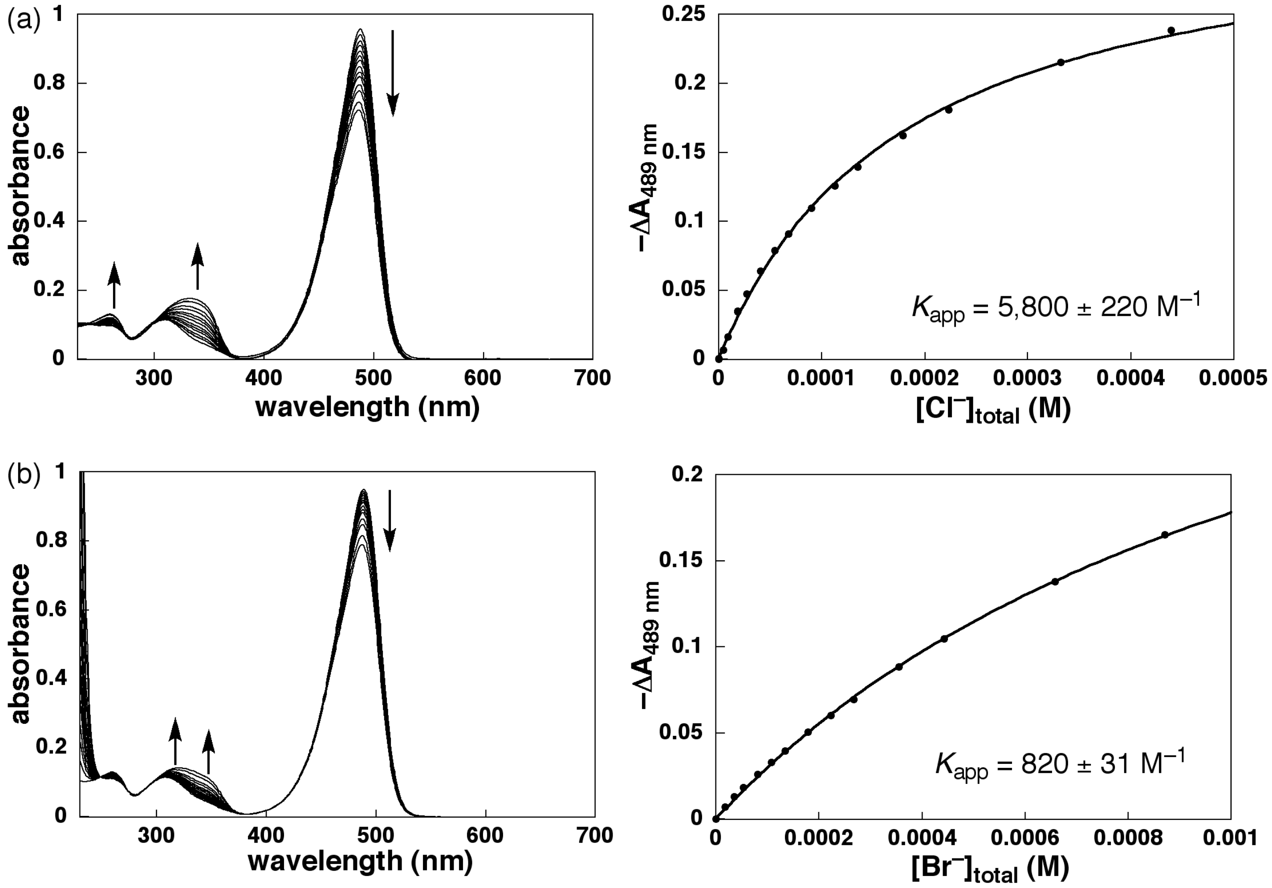
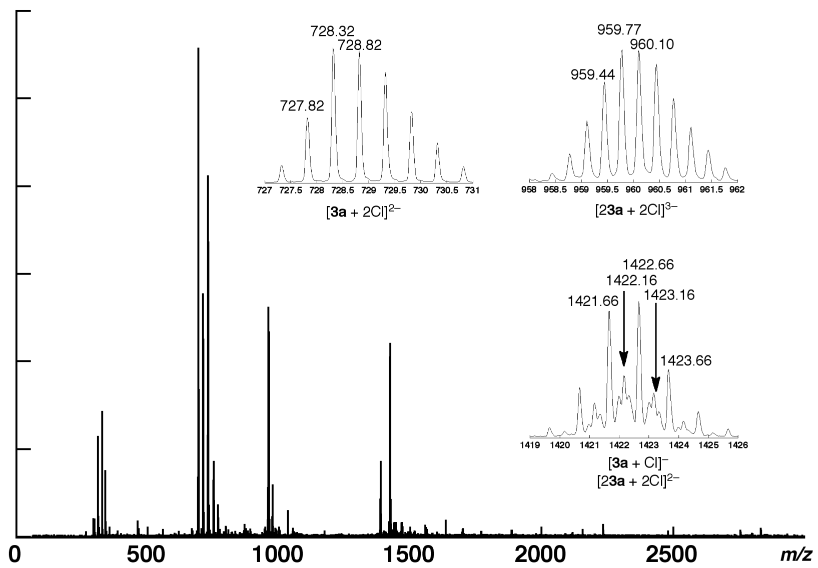
4. Anion-binding properties



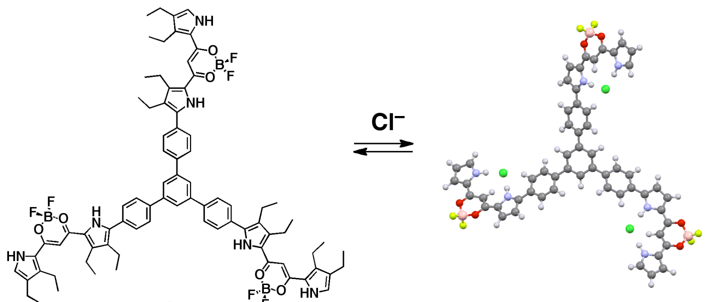
Supporting Figure 5 ^{1}H NMR spectral changes of **3a** (1.0×10^{-3} M) in CD_2Cl_2 at (a) r.t. and (b) –50 °C upon the addition of Cl^- (0–9.0 equiv) added as a TBA salt. In the presence of 0.75–1.5 equiv of Cl^-, NH signals are shifted to downfield around 11 ppm at –50 °C, suggesting the formation of complicated intermediates. Upon the addition of 3.0 equiv of Cl^-, **3a** formed a [1 + 3]-type complex **3a**·Cl^-_3 as suggested by the pair of signals around 12 ppm (see also Supporting Figure 8).



Supporting Figure 6 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 binding fitting curves (right) of **3a** (3.0×10^{-6} M) upon the addition of (a) Cl^- and (b) Br^- as TBA salts in CH_2Cl_2.

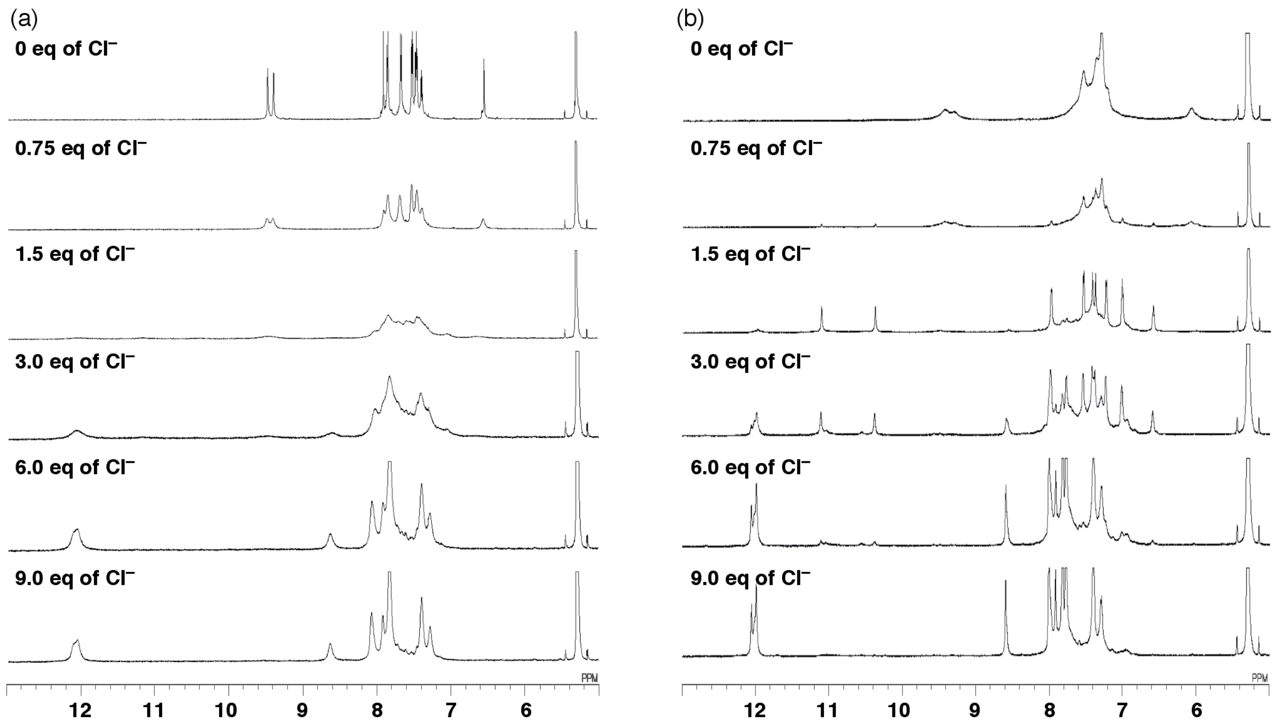


Supporting Figure 7 ESI-TOF-MS at the negative mode of **3a** with 1.5 equiv of Cl^- as a TBA salt from CH_3CN solution (1.0×10^{-5} M).

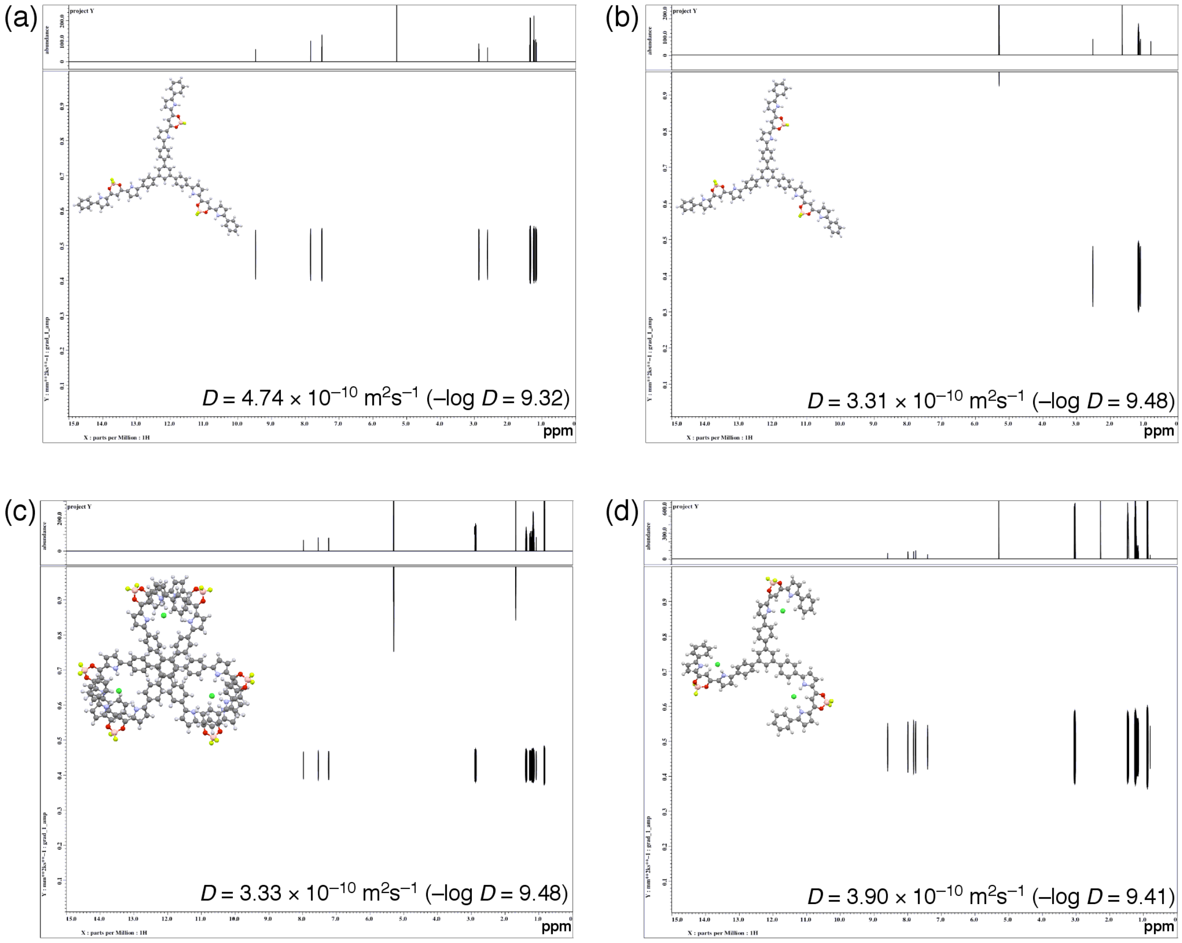


3a $\rightleftarrows$ **3a**·Cl^-_3

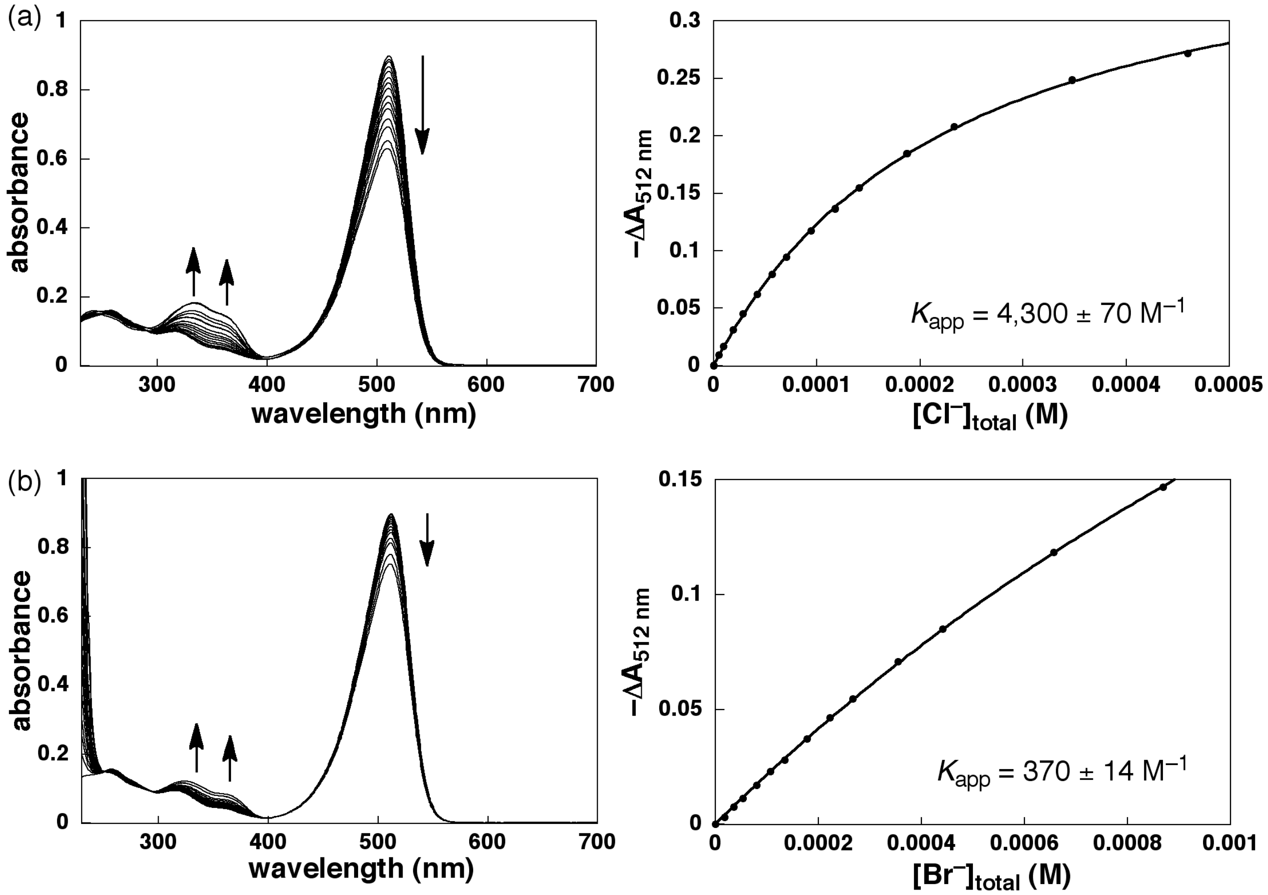
Supporting Figure 8 Optimized structure of Cl^- complex of **3a** at AM1 level (see also Supporting Figure 4a). Upon the addition of 3 equiv of Cl^-, the trimer **3a** gave a [1 + 3]-type complex **3a**·Cl^-_3 by following the formation of complicated intermediates possibly including **3a**$_2$·Cl^-_3 (see also Supporting Figure 5). The optimized structures between **3a** and **3a**·Cl^-_3 are omitted in this figure.



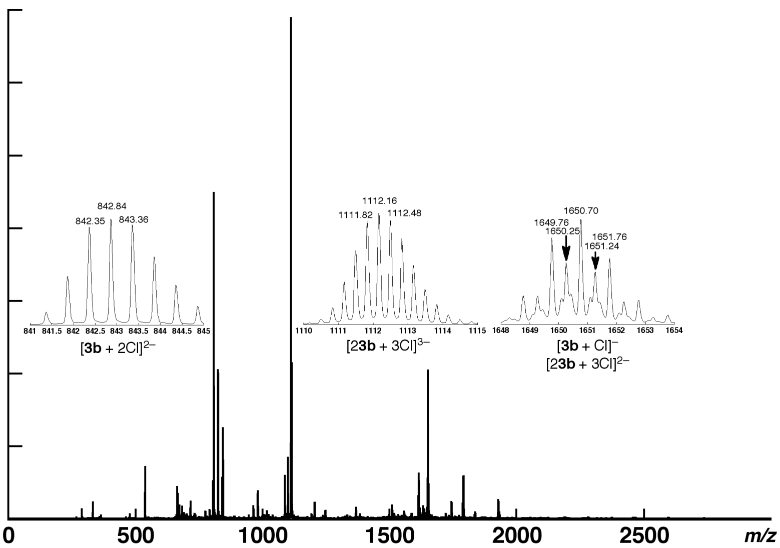
Supporting Figure 9 ^{1}H NMR spectral changes of **3b** (1.0×10^{-3} M) in CD_2Cl_2 at (a) r.t. and (b) –50 °C upon the addition of Cl^- (0–9.0 equiv) added as a TBA salt. Broad and complicated signals at –50 °C in the absence of Cl^- suggested the formation of the aggregate of **3b**. Upon the addition of Cl^-, fairly sharp signals at 10–11 ppm corresponding to a [2 + 3]-type complex **3b**$_2$·Cl^-_3 were emerged. Upon the addition of an excess amount of Cl^-, NH signals were observed at 12 ppm due to the formation of a [1 + 3]-type complex **3b**·Cl^-_3 (see also Supporting Figure 13).



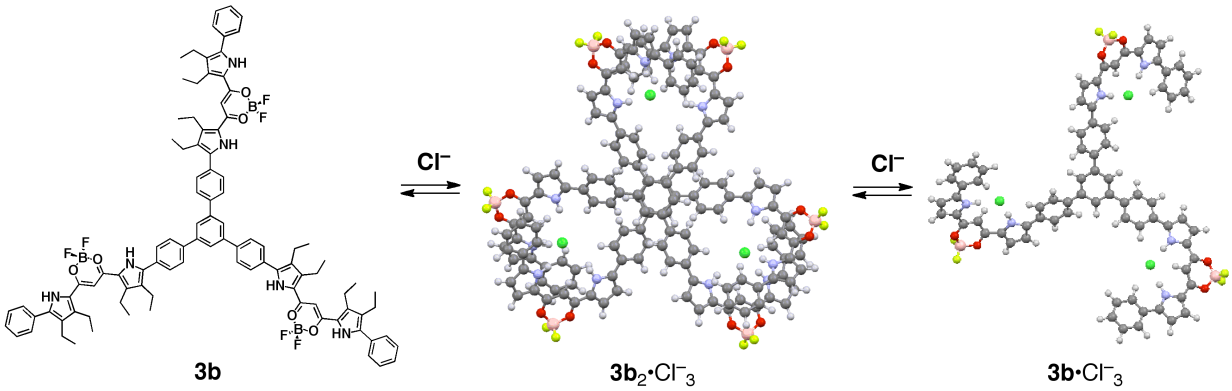
Supporting Figure 10 ^{1}H DOSY of **3b** with (a) 0 (at r.t.), (b) 0, (c) 1.5, and (d) 6.0 equiv of Cl^- added as a TBA salt in CD_2Cl_2 (1.0 × 10^{-3} M) at –50 °C. The smaller D value in the absence of TBACl at –50 °C is ascribable to the formation of assemblies of **3b**.



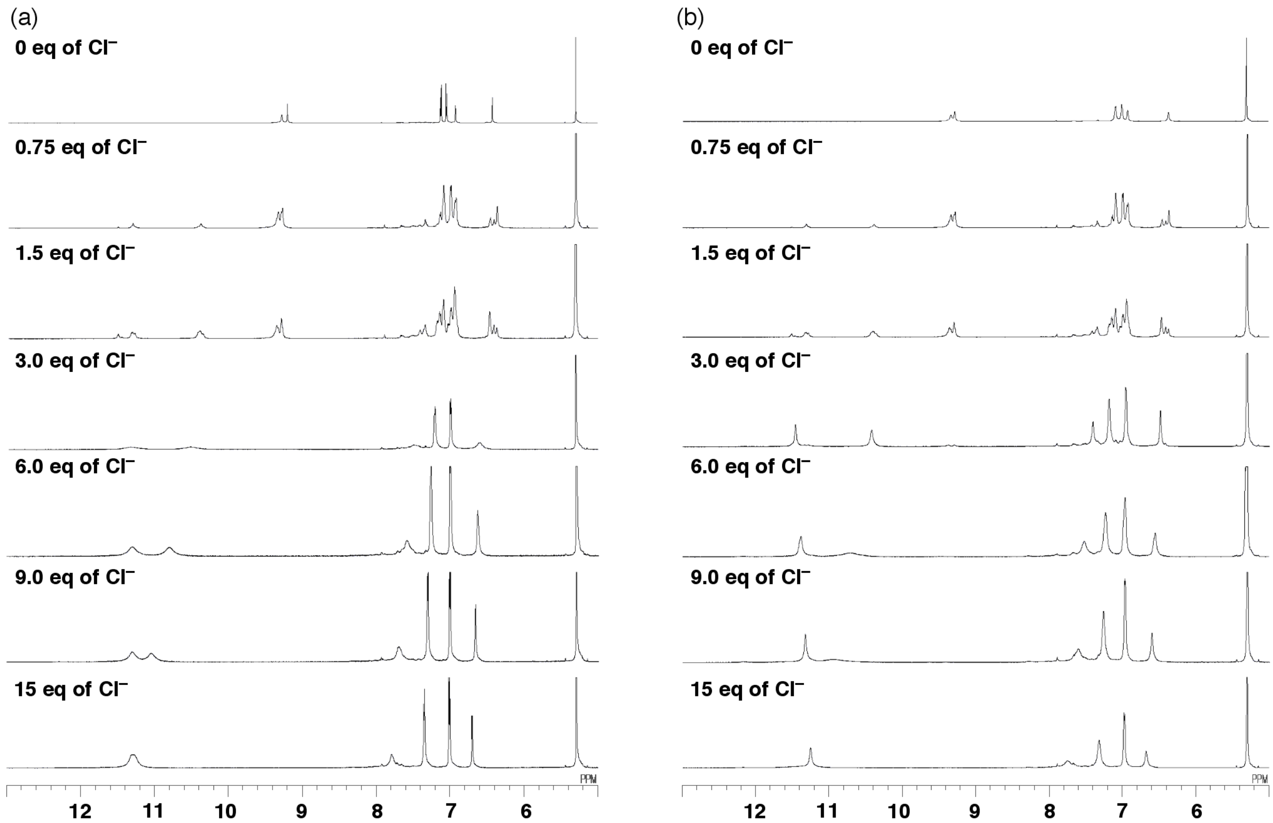
Supporting Figure 11 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 binding fitting curves (right) of **3b** (3.0×10^{-6} M) upon the addition of (a) Cl^- and (b) Br^- as TBA salts in CH_2Cl_2.



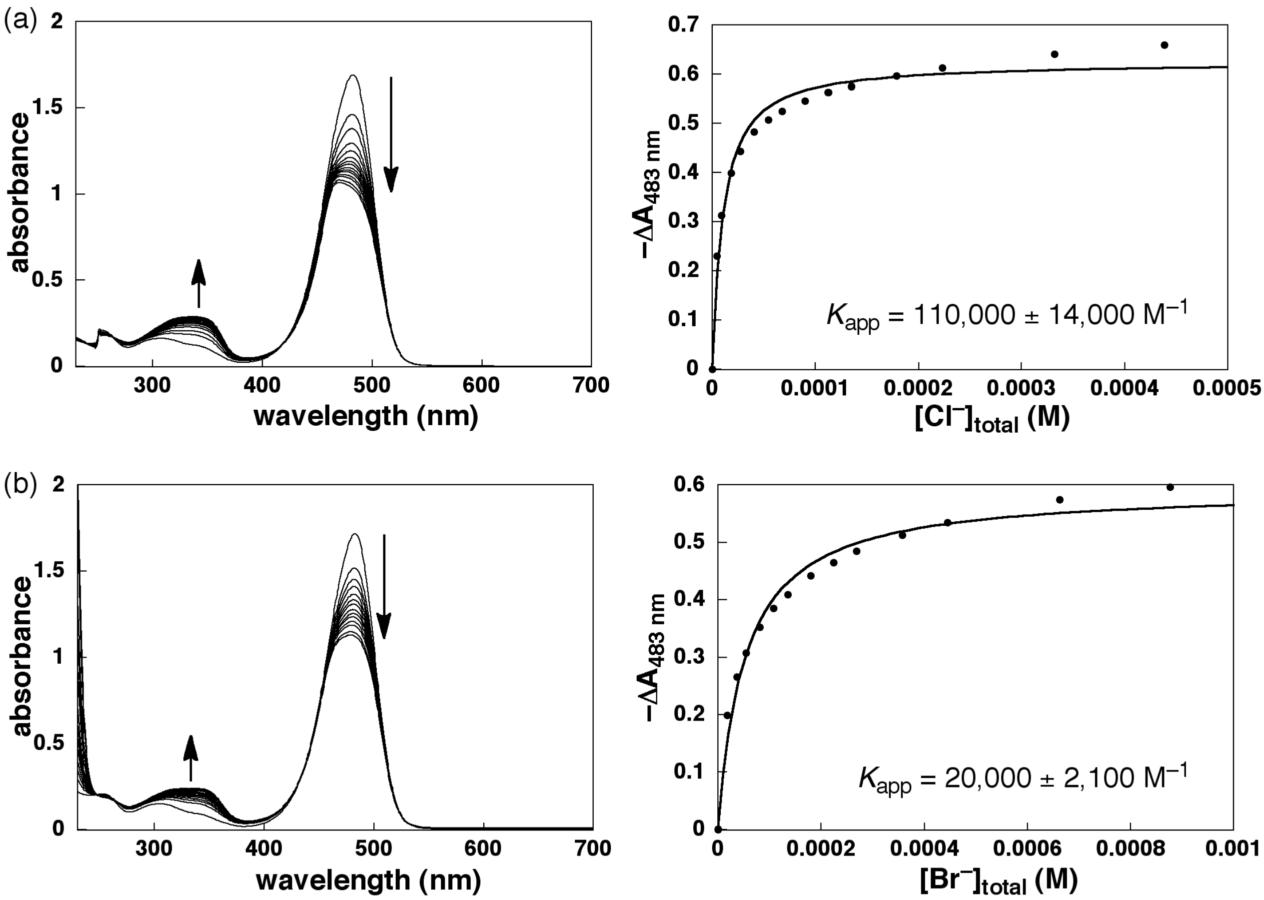
Supporting Figure 12 ESI-TOF-MS at the negative mode of **3b** with 1.5 equiv of Cl^- as a TBA salt from CH_3CN solution (1.0×10^{-5} M).



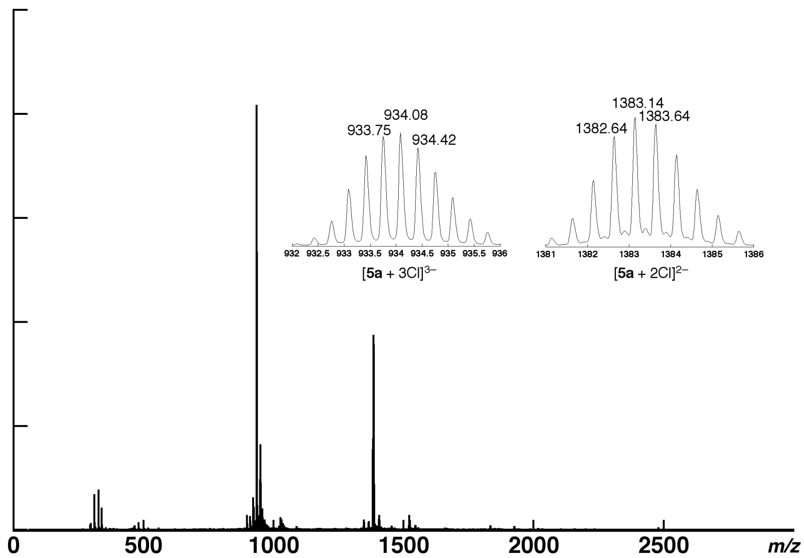
Supporting Figure 13 Optimized structures of Cl⁻ complexes of **3b** at AM1 level (see also Supporting Figure 4b). The trimer **3b** gave a [2 + 3]-type cage-like cluster $\mathbf{3b}_2\cdot Cl^-_3$ prior to the formation of a [1 + 3]-type complex $\mathbf{3b}\cdot Cl^-_3$. The optimized structures between **3b** and $\mathbf{3b}_2\cdot Cl^-_3$ and those between $\mathbf{3b}_2\cdot Cl^-_3$ and $\mathbf{3b}\cdot Cl^-_3$ are omitted in this figure.



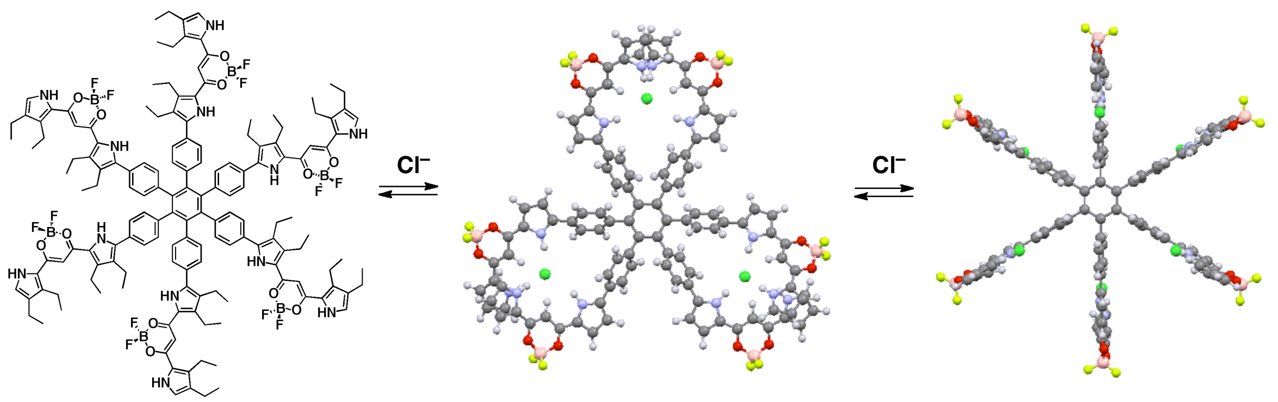
Supporting Figure 14 ^{1}H NMR spectral changes of **5a** (1.0×10^{-3} M) in CD_2Cl_2 at (a) r.t. and (b) –50 °C upon the addition of Cl⁻ (0–15 equiv) added as a TBA salt. Upon the addition of 3.0 equiv of Cl⁻, fairly sharp NH signals at 10.5 ppm and 11.4 ppm at –50 °C suggest that **5a** provided an intramolecular "[2 (receptor units) + 1 (anion)]-type" complexing, resulting in the formation of a [1 (receptor) + 3 (anion)]-type complex $\mathbf{5a}\cdot Cl^-_3$. In the presence of 6.0–9.0 equiv of Cl⁻, the intramolecular "[2 (receptor units) + 1 (anion)]"-type complexing and "[1 (receptor unit) + 1 (anion)]"-type complexing states were in the fast equilibrium. Furthermore, upon the addition of 15 equiv of Cl⁻, **5a** formed a [1 (receptor) + 6 (anion)]-type complex $\mathbf{5a}\cdot Cl^-_6$ (see also Supporting Figure 17).



Supporting Figure 15 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 binding fitting curves (right) of **5a** (3.0×10^{-6} M) upon the addition of (a) Cl^- and (b) Br^- as TBA salts in CH_2Cl_2. Titration plots do not fit the 1:1 binding curves, due to the formation of an intramolecular "[2 + 1]-type" complex (see also Supporting Figure 14 and 17). Estimated K_a values include large errors, because these values are calculated on the assumption that each receptor unit independently binds anions. The hexamer **5a** did not clearly exhibit stepwise spectral changes, and it was difficult to determine the individual binding constants ($K_1 \sim K_6$ values) from these data even by spectral analysis program.

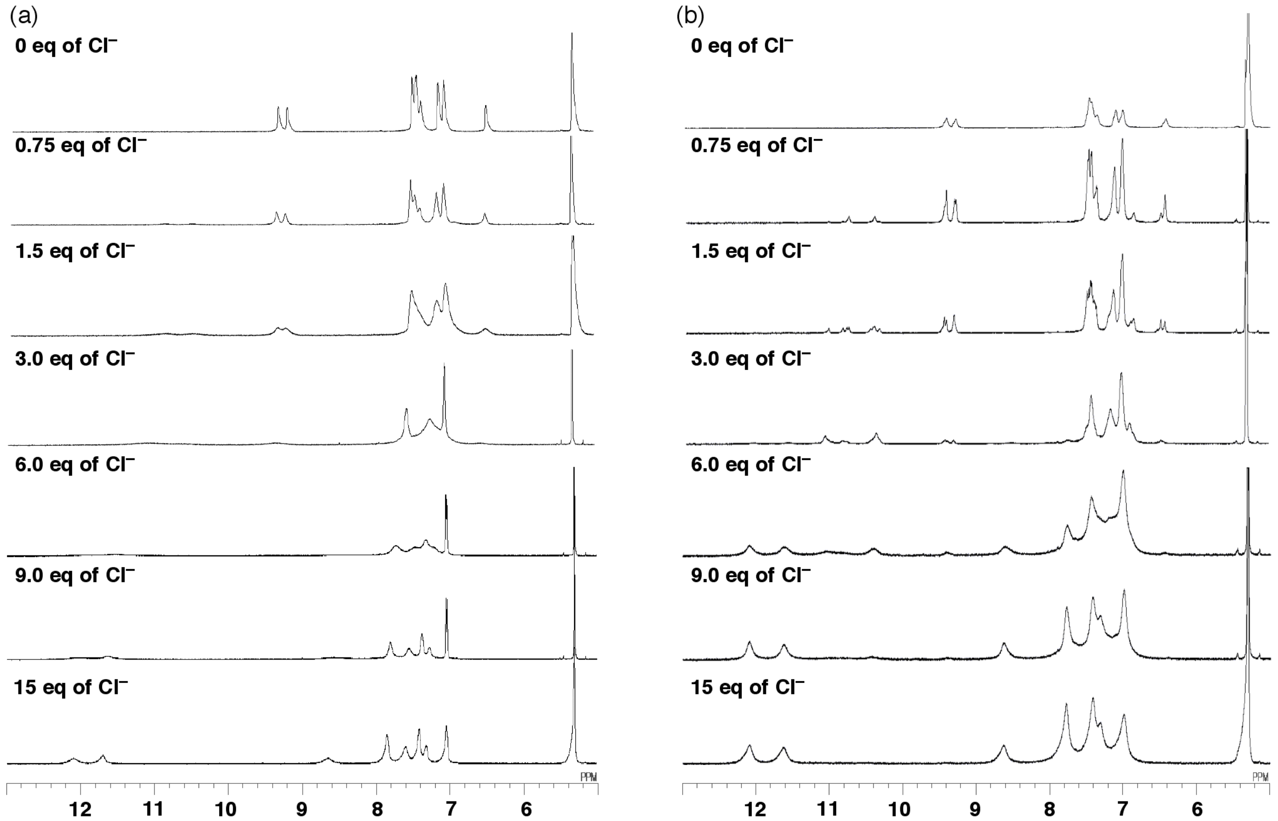


Supporting Figure 16 ESI-TOF-MS at negative mode of **5a** with 3.0 equiv of Cl^- as a TBA salt from CH_3CN solution (1.0×10^{-5} M).

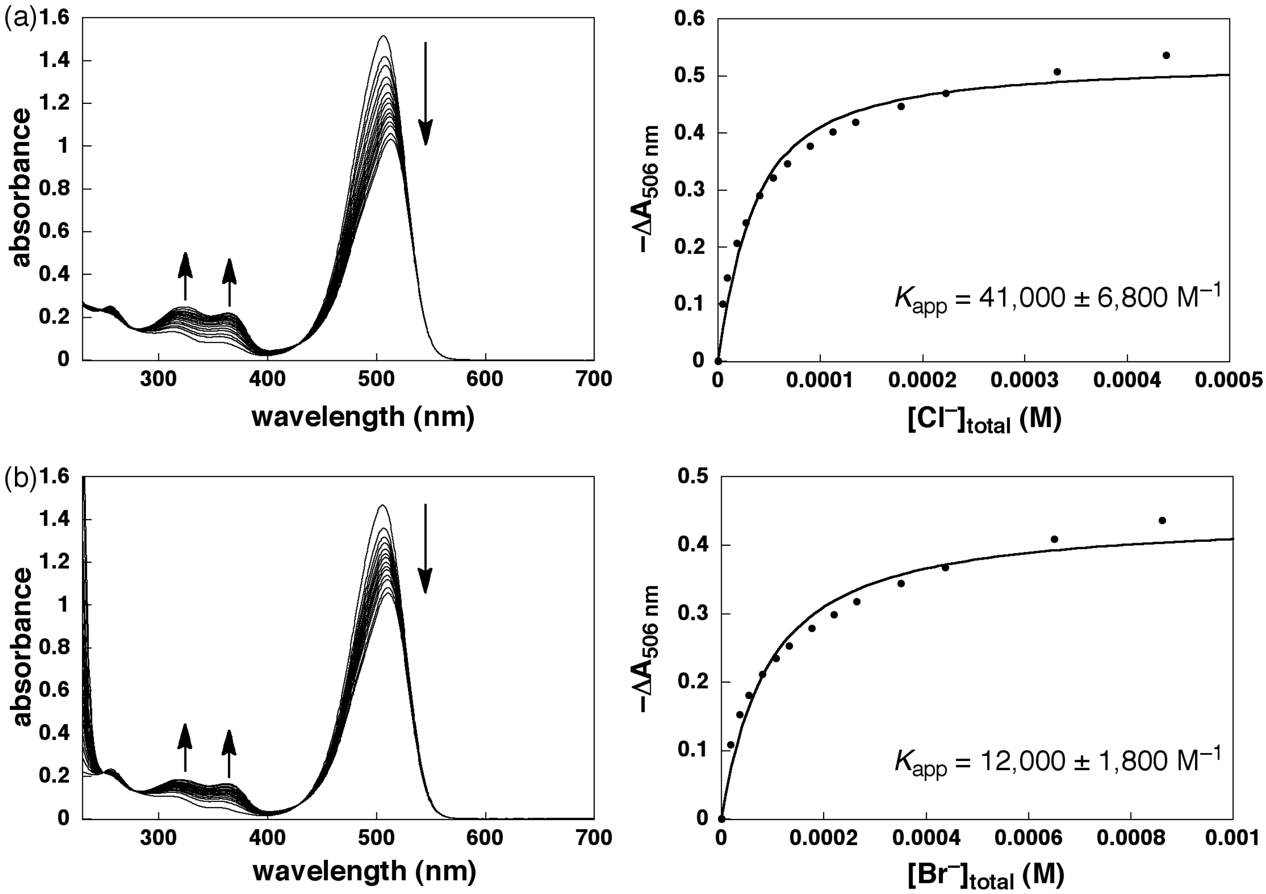


5a $\quad$ **5a**•Cl⁻$_3$ $\quad$ **5a**•Cl⁻$_6$

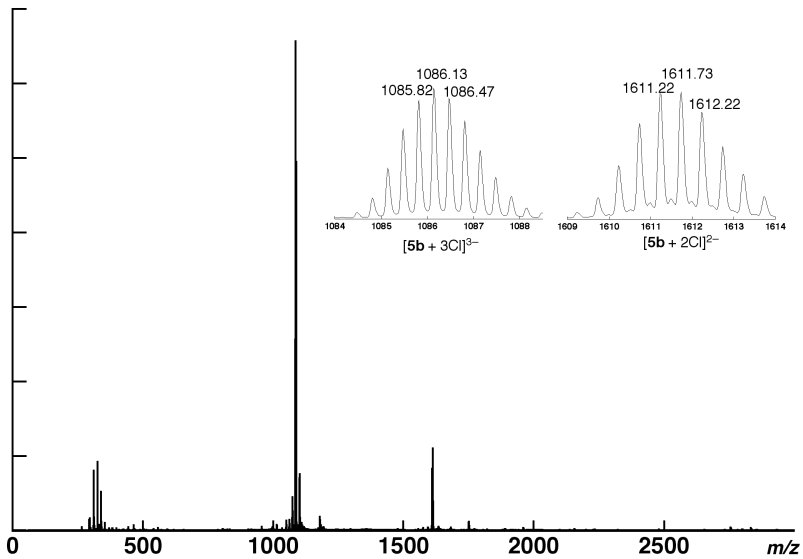
Supporting Figure 17 Optimized structures of Cl^- complexes of **5a** at AM1 level (see also Supporting Figure 4d). The hexamer **5a** gave an intramolecular [1 + 3]-type complex **5a**·Cl^-_3 prior to the formation of a [1 + 6]-type complex **5a**·Cl^-_6 due to the arrangement of the receptor units at all the positions of the core benzene unit. The optimized structures between **5a** and **5a**·Cl^-_3 and those between **5a**·Cl^-_3 and **5a**·Cl^-_6 are omitted in this figure.



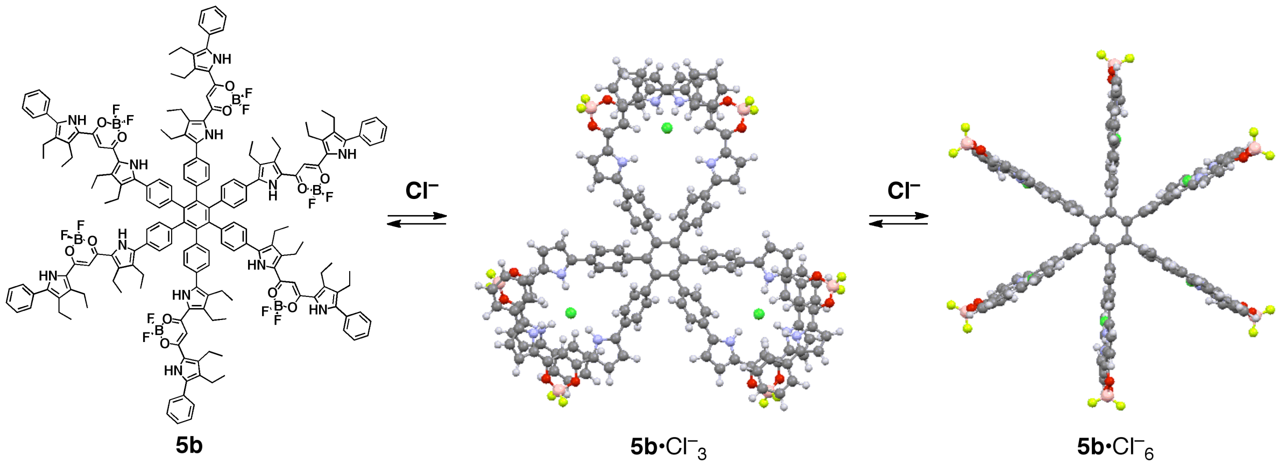
Supporting Figure 18 ^{1}H NMR spectral changes of **5b** (1.0×10^{-3} M) in CD_2Cl_2 at (a) r.t. and (b) –50 °C upon the addition of Cl^- (0–15 equiv) added as a TBA salt. The NH signals at 10–11 ppm in the presence of Cl^- suggest the intramolecular complexing, resulting in the formation of a [1 + 3]-type complex **5b**·Cl^-_3. Upon the addition of an excess amount of Cl^-, NH signals were shifted to downfield at 12 ppm, due to the formation of a [1 + 6]-type complex **5b**·Cl^-_6 (see also Supporting Figure 21).



Supporting Figure 19 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 binding fitting curves (right) of **5b** (3.0×10^{-6} M) upon the addition of (a) Cl^- and (b) Br^- as TBA salts in CH_2Cl_2. Titration plots do not fit the 1:1 binding curves, due to the formation of intramolecular complexes (see also Supporting Figure 18 and 21). Estimated K_a values include large errors, because these values are calculated on the assumption that each receptor unit independently binds anions. The hexamer **5b** did not clearly exhibit stepwise spectral changes, and it was difficult to determine the individual binding constants ($K_1 \sim K_6$ values) from these data even by spectral analyses program.



Supporting Figure 20 ESI-TOF-MS at the negative mode of **5b** with 3.0 equiv of Cl^- as a TBA salt from CH_3CN solution (1.0×10^{-5} M).

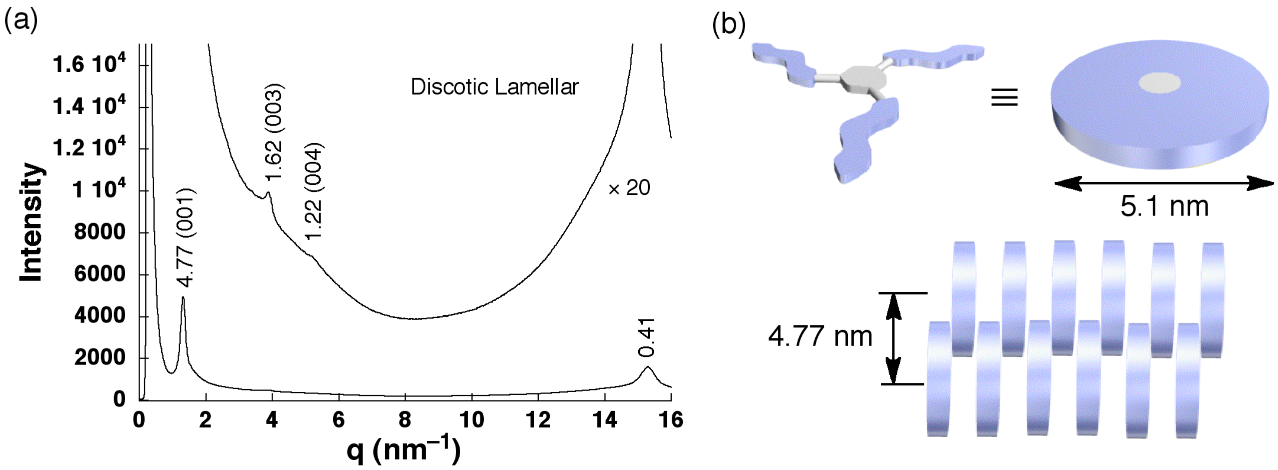


Supporting Figure 21 Optimized structures of Cl^- complexes of **5b** at AM1 level (see also Supporting Figure 4e). Upon the addition of Cl^-, an intramolecular [1 + 3]-type complex was formed prior to the formation of a [1 + 6]-type complex **5b**·Cl^-_6 (see also Supporting Figure 18). The optimized structures between **5b** and **5b**·Cl^-_3 and those between **5b**·Cl^-_3 and **5b**·Cl^-_6 are omitted in this figure.

5. Formation of assembled structures of anion receptors and receptor–anion complexes

Synchrotron X-ray diffraction (XRD) analysis. High-resolution XRD analyses were 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 530.403 mm for and **3c** (a Cl^- complex as a $TATA^+$ salt), 531.034 mm for **5c**, 532.704 mm for **3c**, and 540.180 mm for **5c** (a Cl^- complex as a $TATA^+$ salt) were used with an imaging plate as a detector. The sample was sealed in a quartz capillary where the diffraction pattern was obtained with a 0.01° step in 2θ. The exposure time to the X-ray beam was 10 s for **3c**, **3c** (a Cl^- complex as a $TATA^+$ salt), and **5c** and 30 s for **5c** (a Cl^- complex as a $TATA^+$ salt).

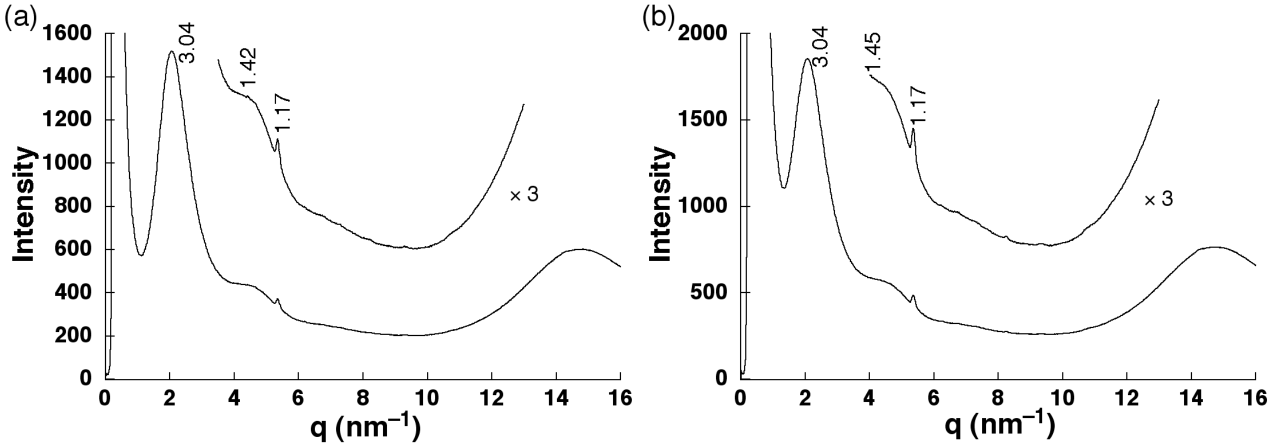
STM Investigations. STM investigations were carried out using Nanoscope IIIa systems (Veeco Instruments, Santa Barbara, CA). Mechanical cut Pt/Ir (80/20) wires (0.25 mm) were used as STM tips. 1,2,4-Trichlorobenzene (TCB, Aldrich) was used as solvents for STM experiments. The TCB solutions of trimer **3c** (5×10^{-4} M), hexamer **5c** (2.5×10^{-3} M), and **3c**·Cl^- complex (1×10^{-3} to 3×10^{-3} M) were prepared for STM investigation. A droplet of the solutions was placed onto fresh cleaved highly oriented pyrolitic graphite (HOPG, Optigraph GmbH) surface for STM investigation at the TCB solution–HOPG interfaces. The scales of the images were calibrated using the visualized lattice of the underlying HOPG.



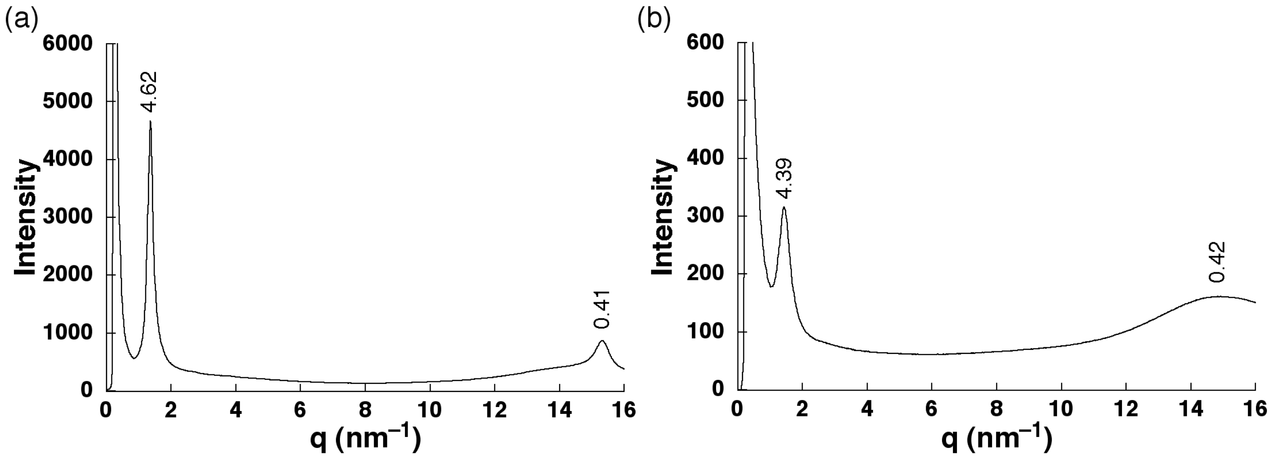
Supporting Figure 22 (a) XRD patterns of the precipitates of **3c** obtained from CH_2Cl_2/MeOH by drying at r.t., and (b) a possible packing structure of **3c**. The measurements were conducted to the dried precipitates in quartz capillary prepared from CH_2Cl_2/MeOH.

Supporting Table 2 Summary of XRD data of **3c**.

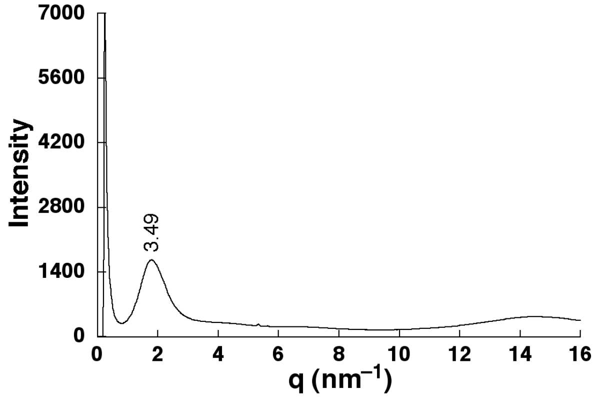
	q (nm^{-1})	*d*-spacing (nm)	ratio	*hkl*
	1.3168	4.77	1.0000	001
r.t. (Lamellar)	3.8808	1.62	0.33931	003
	5.1454	1.22	0.25592	004



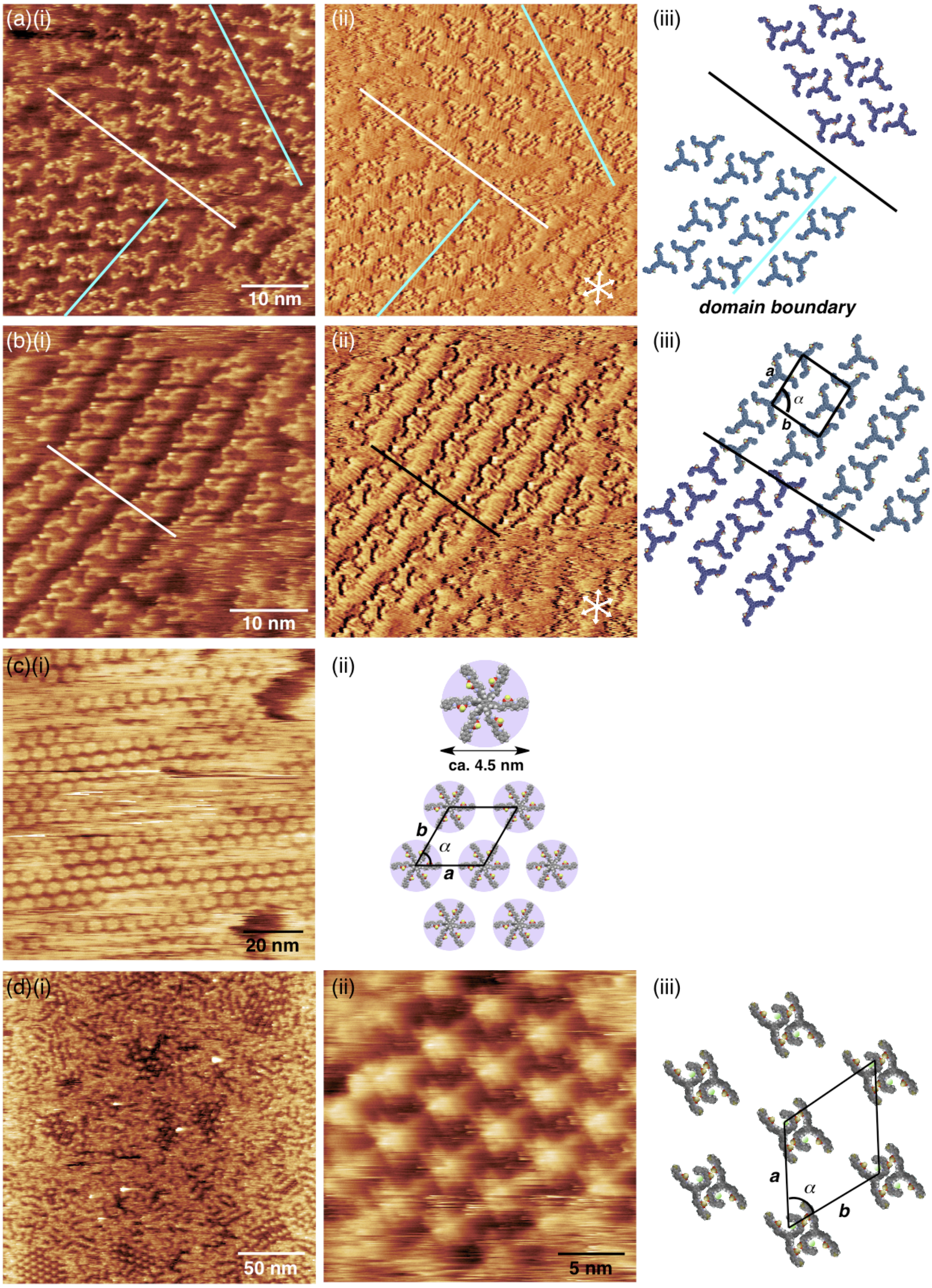
Supporting Figure 23 XRD patterns of the precipitates of **3c** (a Cl^- complex as a $TATA^+$ salt) (a) at r.t. obtained from octane (**3c**: 20 mg/mL with 3 equiv of salt) by drying at r.t. and (b) at r.t. (1st rapid cooling). The measurements were conducted to the dried precipitates in quartz capillary prepared from octane solution at r.t. Broad peaks suggest the formation of fairly less ordered packing of **3c** (a Cl^- complex as a $TATA^+$ salt).



Supporting Figure 24 XRD patterns of (a) the precipitates of **5c** at r.t. obtained from CH_2Cl_2/MeOH by drying at r.t. and (b) at r.t. (1st rapid cooling). The measurements were conducted to the dried precipitates in quartz capillary prepared from CH_2Cl_2/MeOH.



Supporting Figure 25 XRD patterns of the precipitates of **7c** (a Cl^- complex as a $TATA^+$ salt) at r.t. obtained from octane (**5c**: 20 mg/mL with 6 equiv of salt) by drying at r.t. The measurements were conducted to the dried precipitates in quartz capillary prepared from octane solution at r.t. Broad peaks suggest the formation of fairly less ordered packing of **5c** (a Cl^- complex as a $TATA^+$ salt)



Supporting Figure 26 STM images and the molecular models of self-assembled structures at the TCB–HOPG interfaces: (a)(i) topographic image of **3c** (E_{bias} = 0.80 V, I_t = 115 pA), (ii) current image of (i), and (iii) the corresponding molecular model; (b)(i) topographic image of **3c** (another observed region) (E_{bias} = 0.80 V, I_t = 100 pA), (ii) current image of (i), and (iii) the corresponding molecular model; (c)(i) topographic image of **5c** (E_{bias} = 0.80 V, I_t = 65 pA) and (ii) the corresponding molecular model; (d)(i) topographic image of **3c**·Cl^- (as a TBA salt) (E_{bias} = 0.90 V, I_t = 205 pA), (ii) high resolution topographic image (E_{bias} = 0.90 V, I_t = 185 pA), and (iii) the tentative molecular model of the 2D self-assembly of [1 + 1]-type complex. In the current images of (a)(ii) and (b)(ii), the alkyl chains as lines between three-leg-cores were clearly observed. The black lines in (a) and (b) are the domain boundaries between the ordered structures with the different molecular conformations of **3c**. The light blue lines in (a) are the domain boundaries between the ordered structures with the same molecular conformations. In (c), in comparison with the trimer **3c**, no legs of the hexamer **5c** were identified at the similar interface. The reason should be the bulky molecule with highly polar moieties. The tunneling current was not changed for the observation of the hexamer because of the higher leak current and the scratching of molecules by the tip. In the images in (d)(i) and (ii), the four-legs features packed hexagonally, and the unit cell was smaller than that of self-assembled structures of the anion-free trimer **3c**.