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Supplementary Information

Ion-based materials of boron-modified dipyrrolyldiketones as anion receptors

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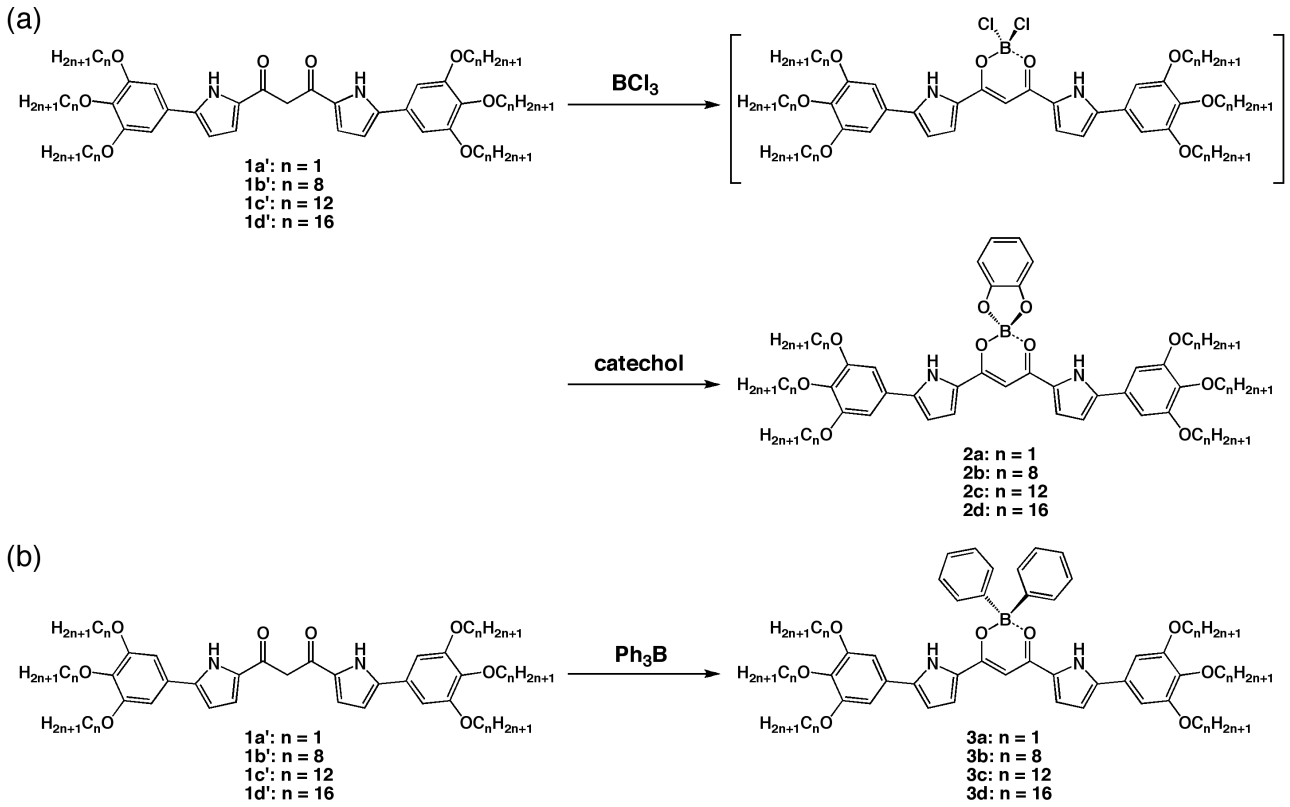
1. Synthetic procedures and spectroscopic data for anion receptors

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 for the solution state and a System Instruments surface and interface spectrometer SIS-50 for the solid (gel) state. Fluorescence spectra were recorded on a Hitachi F-4500 fluorescence spectrometer for ordinary solution and a Hamamatsu Quantum Yields Measurements System for Organic LED Materials C9920-02 for gelated materials, respectively. 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 modes. TLC analyses were carried out on aluminum sheets coated with silica gel 60 (Merck 5554). Column chromatography was performed on Wakogel C-300 and Merck silica gel 60H.



Supporting Figure 1 Synthesis of dipyrrolyldiketone boron complexes (a) **2a**–**d** and (b) **3a**–**d**.

Catechol-substituted boron complex of 1,3-bis(5-(3,4,5-trimethoxyphenyl)pyrrol-2-yl)-1,3-propanedione, 2a. Following the literature procedure,[S1] a CH_2Cl_2 solution (30 mL) of 1,3-bis(5-(3,4,5-trimethoxyphenyl)pyrrol-2-yl)-1,3-propanedione **1a**′[S2] (53.5 mg, 0.10 mmol) was treated with a CH_2Cl_2 solution (0.40 mL) of BCl_3 (0.42 mg, 0.40 mmol) at r.t. under nitrogen, and stirred for 2 h at the same temperature. The reaction mixture was changed to red. After the consumption of the starting diketone was confirmed by TLC analysis, catechol (22.1 mg, 0.20 mmol) was added. The mixture was heated at reflux for 10 h, cooled then washed with Na_2CO_3 aq. and water, dried over anhydrous Na_2SO_4, filtered, and evaporated to dryness. The residue was then chromatographed over silica gel column chromatography (Wakogel C-300, eluent: 3% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **2a** (54.8 mg, 0.084 mmol, 84%) as a red brown solid. R_f = 0.65 (3.5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.50 (br, 2H, NH), 7.25–7.23 (m, 2H, pyrrole-H), 6.91–6.89 (m, 2H, Ar-H), 6.84–6.81 (m, 2H, Ar-H), 6.78 (s, 4H, Ar-H), 6.69–6.67 (m, 2H, pyrrole-H), 6.62 (s, 1H, CH), 3.93 (s, 12H, OCH_3), 3.85 (s, 6H, OCH_3). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 166.55, 154.06, 150.77, 141.37, 139.27, 126.83, 125.78, 120.22, 119.81, 111.23, 109.84, 102.80, 90.37, 61.18, 56.63. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 521.0 (1.2). MALDI-TOF-MS: *m/z* (% intensity): 653.4 (100), 654.3 (83). Calcd for $C_{35}H_{33}BN_2O_{10}$ ($[M]^+$): 652.22. This compound was further characterized by single-crystal X-ray diffraction analysis.

Catechol-substituted boron complex of 1,3-bis(5-(3,4,5-trioctyloxyphenyl)pyrrol-2-yl)-1,3-propanedion

e, 2b. A dry CH_2Cl_2 solution (90 mL) of 1,3-bis(5-(3,4,5-trioctyloxyphenyl)pyrrol-2-yl)-1,3-propanedione **1b′**[S2] (163.5 mg, 0.15 mmol) was treated with a CH_2Cl_2 solution (0.70 mL) of BCl_3 (0.73 mg, 0.70 mmol) at r.t. under nitrogen. The reaction mixture was changed to red and was stirred for 1 h at the same temperature. After the consumption of the starting diketone was confirmed by TLC analysis, catechol (80.4 mg, 0.73 mmol) was added. The mixture was heated at reflux for 12 h, cooled then washed with Na_2CO_3 aq. and water, dried over anhydrous Na_2SO_4, filtrated, and evaporated to dryness. The residue was then chromatographed over a silica gel column (Wakogel C-300, eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to afford **2b** (127.4 mg, 0.102 mmol, 70%) as a red solid. R_f = 0.73 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.50 (br, 2H, NH), 7.22–7.21 (m, 2H, pyrrole-H), 6.90–6.88 (m, 2H, catechol-H), 6.84–6.82 (m, 2H, catechol-H), 6.75 (s, 4H, Ar-H), 6.65–6.63 (m, 2H, pyrrole-H), 6.59 (s, 1H, CH), 4.02 (t, J = 6.6 Hz, 8H, OCH_2), 3.97 (t, J = 6.6 Hz, 4H, OCH_2), 1.84–1.79 (m, 8H, OCH_2CH_2), 1.75–1.71 (m, 4H, OCH_2CH_2), 1.49–1.44 (m, 12H, $OC_2H_4CH_2$), 1.35–1.28 (m, 48H, $OC_3H_6(CH_2)_4$), 0.89–0.86 (m, 18H, $OC_7H_{14}CH_3$). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 166.34, 153.96, 150.77, 141.70, 139.50, 126.68, 125.24, 120.17, 119.77, 111.07, 109.82, 90.27, 73.76, 69.62, 32.05, 31.98, 30.49, 29.69, 29.52, 29.43, 26.25, 22.85, 22.83, 14.26 (some of the signals for octyl chains were overlapped). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 526.0 (0.94). MALDI-TOF-MS: *m/z* (% intensity): 1241.6 (92), 1242.6 (100). Calcd for $C_{77}H_{118}BNO_2O_{10}$ ($[M]^+$): 1241.88.

Catechol-substituted boron complex of 1,3-bis(5-(3,4,5-tridodecyloxyphenyl)pyrrol-2-yl)-1,3-propanedione, 2c. A dry CH_2Cl_2 solution (45 mL) of 1,3-bis(5-(3,4,5-tridodecyloxyphenyl)pyrrol-2-yl)-1,3-propanedione **1c′**[S2] (101.8 mg, 0.07 mmol) was treated with a CH_2Cl_2 solution (0.34 mL) of BCl_3 (0.342 mg, 0.34 mmol) at r.t. under nitrogen. The reaction mixture was changed to red and was stirred for 1 h at the same temperature. After the consumption of the starting diketone was confirmed by TLC analysis, catechol (38.1 mg, 0.35 mmol) was added. The mixture was heated at reflux for 12 h, cooled then washed with Na_2CO_3 aq. and water, dried over anhydrous Na_2SO_4, filtrated, and evaporated to dryness. The residue was then chromatographed over a silica gel column (Wakogel C-300, eluent: CH_2Cl_2/hexane = 3:4) and recrystallized from CH_2Cl_2/MeOH to afford **2c** (72.2 mg, 0.045 mmol, 68%) as a red solid. R_f = 0.82 (CH_2Cl_2/hexane = 3:4). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.45 (br, 2H, NH), 7.23–7.22 (m, 2H, pyrrole-H), 6.90–6.89 (m, 2H, catechol-H), 6.83–6.82 (m, 2H, catechol-H), 6.75 (s, 4H, Ar-H), 6.65–6.64 (m, 2H, pyrrole-H), 6.59 (s, 1H, CH), 4.02 (t, J = 6.6 Hz, 8H, OCH_2), 3.97 (t, J = 6.6 Hz, 4H, OCH_2), 1.84–1.79 (m, 8H, OCH_2CH_2), 1.75–1.71 (m, 4H, OCH_2CH_2), 1.49–1.44 (m, 12H, $OC_2H_4CH_2$), 1.35–1.28 (m, 96H, $OC_3H_6(CH_2)_8$), 0.89–0.86 (m, 18H, $OC_{11}H_{22}CH_3$). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 166.33, 153.96, 150.77, 141.70, 139.49, 126.67, 125.24, 120.16, 119.76, 111.06, 109.82, 104.15, 90.27, 73.76, 69.62, 32.09, 30.50, 29.91, 29.86, 29.82, 29.79, 29.57, 29.54, 26.25, 22.85, 14.28 (some of the signals for dodecyl chains were overlapped). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 526.0 (0.89). MALDI-TOF-MS: *m/z* (% intensity): 1578.1 (88), 1579.1 (100). Calcd for $C_{101}H_{166}BNO_2O_{10}$ ($[M]^+$): 1578.26.

Catechol-substituted boron complex of 1,3-bis(5-(3,4,5-trihexadecyloxyphenyl)pyrrol-2-yl)-1,3-propanedione, 2d. A dry CH_2Cl_2 solution (25 mL) of 1,3-bis(5-(3,4,5-trihexadecyloxyphenyl)pyrrol-2-yl)-1,3-propanedione **1d′**[S2] (67.1 mg, 0.037 mmol) was treated with a CH_2Cl_2 solution (0.20 mL) of BCl_3 (0.204 mg, 0.20 mmol) at r.t. under nitrogen. The reaction mixture was changed to red, and was stirred for 1 h at the same temperature. After the consumption of the starting diketone was confirmed by TLC analysis, catechol (22.1 mg, 0.20 mmol) was added. The mixture was heated at reflux for 12 h, cooled then washed with Na_2CO_3 aq. and water, dried over anhydrous Na_2SO_4, filtrated, and evaporated to dryness. The residue was then chromatographed over a silica gel column (Wakogel C-300, eluent: CH_2Cl_2/hexane = 3:4) and recrystallized from CH_2Cl_2/MeOH to afford **2d** (57.3 mg, 0.030 mmol, 80%) as a red solid. R_f = 0.70 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.44 (br, 2H, NH), 7.23–7.22 (m, 2H, pyrrole-H), 6.90–6.89 (m, 2H, catechol-H), 6.84–6.83 (m, 2H, catechol-H), 6.75 (s, 4H, Ar-H), 6.65–6.64 (m, 2H, pyrrole-H), 6.60 (s, 1H, CH), 4.02 (t, J = 6.6 Hz, 8H, OCH_2), 3.98 (t, J = 6.6 Hz, 4H, OCH_2), 1.87–1.80 (m, 8H, OCH_2CH_2), 1.79–1.74 (m, 4H, OCH_2CH_2), 1.52–1.45 (m, 12H, $OC_2H_4CH_2$), 1.44–1.22 (m, 144H, $OC_3H_6CH(CH_2)_{12}$), 0.89–0.86 (m, 18H, $OC_{15}H_{30}CH_3$). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 166.33, 153.96, 150.78, 141.70, 139.49, 126.67, 125.23, 120.17, 119.76, 111.06, 109.82, 104.15, 90.27, 73.76, 69.62, 32.09, 30.50, 29.88, 29.83, 29.80, 29.58, 29.53, 26.26, 22.85, 14.28 (some of the signals for hexadecyl chains were overlapped). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 525.5 (0.91). MALDI-TOF-MS: *m/z* (% intensity): 1914.8 (100), 1915.8 (87). Calcd for $C_{125}H_{213}BNO_2O_{10}$ ($[M]^+$): 1914.63.

Diphenyl-substituted boron complex of 1,3-bis(5-(3,4,5-methoxyphenyl)pyrrol-2-yl)-1,3-propanedione, 3a. Following the literature procedure,[S3] BPh_3 (79.5 mg, 0.33 mmol) was added to a solution of **1a′**[S2] (53.4 mg, 0.10 mmol) in dry toluene (3.0 mL) under nitrogen and the reaction mixture was refluxed for 12 h. The solvent was evaporated to dryness. The residue was the chromatographed over flash silica gel column (Merck silica gel 60H, eluent: 1% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **3a** (43.1 mg, 0.062 mmol, 62%) as an orange solid. R_f = 0.20 (1% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C):

δ (ppm) 9.55 (m, 2H, NH), 7.58 (d, J = 6.6 Hz, 4H, phenyl-H), 7.33–7.28 (m, 6H, phenyl-H), 7.13–7.12 (m, 2H, pyrrole-H), 6.82 (s, 4H, Ar-H), 6.63–6.62 (m, 2H, pyrrole-H), 6.48 (s, 1H, CH), 3.96 (s, 12H, OCH_3), 3.89 (s, 6H, OCH_3). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 169.16, 154.04, 140.12, 139.02, 132.91, 128.12, 127.36, 127.03, 126.48, 118.70, 110.62, 103.06, 92.08, 61.20, 56.71 (a signal of the core unit is missing presumably due to the $^{10/11}$B–^{13}C coupling[S4]). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 503.5 (0.89). MALDI-TOF-MS: *m/z* (% intensity): 697.7 (100), 698.7 (60). Calcd for $C_{41}H_{39}BN_2O_8$ ($[M]^+$): 698.28.

Diphenyl-substituted boron complex of 1,3-bis(5-(3,4,5-trioctyloxyphenyl)pyrrol-2-yl)-1,3-propanedione, 3b. BPh_3 (84.9 mg, 0.35 mmol) was added to a solution of **1b′**[S2] (171.8 mg, 0.15 mmol) in dry toluene (3.0 mL) under nitrogen and the reaction mixture was refluxed for 12 h. The solvent was evaporated to dryness. The residue was the chromatographed over silica gel column (Wakogel C-300, eluent: 50% hexane/CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to afford **3a** (78.6 mg, 0.061 mmol, 40%) as a dark red solid. R_f = 0.46 (1.5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.46 (m, 2H, NH), 7.58 (d, J = 6.6 Hz, 4H, phenyl-H), 7.35–7.30 (m, 6H, phenyl-H), 7.10–7.09 (m, 2H, pyrrole-H), 6.78 (s, 4H, Ar-H), 6.59–6.58 (m, 2H, pyrrole-H), 6.45 (s, 1H, CH), 4.05 (t, J = 6.6 Hz, 8H, OCH_2), 3.99 (t, J = 6.6 Hz, 4H, OCH_2), 1.83 (quin, J = 7.8 Hz, 8H, $OCH_2C\underline{H}_2$), 1.76 (quin, J = 7.8 Hz, 4H, $OCH_2C\underline{H}_2$), 1.49 (m, 12H, $OC_2H_4C\underline{H}_2$), 1.31 (m, 48H, $OC_3H_6(C\underline{H}_2)_4$), 0.88 (t, J = 7.2 Hz, 18H, $OC_7H_{14}C\underline{H}_3$). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 167.00, 153.97, 140.37, 139.30, 132.89, 127.96, 127.33, 126.97, 125.94, 118.67, 110.43, 104.50, 91.07, 73.78, 69.75, 32.06, 31.98, 30.50, 29.70, 29.58, 29.52, 29.44, 26.27, 26.25, 22.83, 14.26 (some of the signals for octyl chains were overlapped and a signal of the core unit is missing presumably due to the $^{10/11}$B–^{13}C coupling[S4]). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 507.5 (0.64). MALDI-TOF-MS: *m/z* (% intensity): 1285.9 (86), 1286.9 (100), 1287.9 (30). Calcd for $C_{83}H_{123}BN_2O_8$ ($[M]^+$): 1286.94.

Diphenyl-substituted boron complex of 1,3-bis(5-(3,4,5-tridodecyloxyphenyl)pyrrol-2-yl)-1,3-propanedione, 3c. BPh_3 (80.6 mg, 0.33 mmol) was added to a solution of **1c′**[S2] (150.1 mg, 0.103 mmol) in dry toluene (3.0 mL) under nitrogen and the reaction mixture was refluxed for 12 h. The solvent was evaporated to dryness. The residue was the chromatographed over silica gel column (Wakogel C-300, eluent: 50% hexane/CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to afford **3c** (65.1 mg, 0.040 mmol, 40%) as an orange solid. R_f = 0.23 (50% hexane/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.45 (m, 2H, NH), 7.58 (d, J = 6.6 Hz, 4H, phenyl-H), 7.30–7.25 (m, 6H, phenyl-H), 7.10–7.09 (m, 2H, pyrrole-H), 6.78 (s, 4H, Ar-H), 6.59–6.58 (m, 2H, pyrrole-H), 6.45 (s, 1H, CH), 4.05 (t, J = 6.6 Hz, 8H, OCH_2), 3.98 (t, J = 6.6 Hz, 4H, OCH_2), 1.83 (quin, J = 7.8 Hz, 8H, $OCH_2C\underline{H}_2$), 1.75 (quin, J = 7.8 Hz, 4H, $OCH_2C\underline{H}_2$), 1.49 (m, 12H, $OC_2H_4C\underline{H}_2$), 1.31 (m, 96H, $OC_3H_6(C\underline{H}_2)_8$), 0.88 (t, J = 7.2 Hz, 18H, $OC_{11}H_{22}C\underline{H}_3$). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 168.99, 153.96, 140.37, 139.30, 132.89, 127.95, 127.33, 126.97, 125.93, 118.66, 110.42, 104.48, 91.98, 73.77, 69.75, 32.08, 30.51, 29.92, 29.86, 29.82, 29.79, 29.58, 29.55, 29.52, 26.26, 22.85, 14.28 (some of the signals for dodecyl chains were overlapped and a signal of the core unit is missing presumably due to the $^{10/11}$B–^{13}C coupling[S4]). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 507.0 (1.16). MALDI-TOF-MS: *m/z* (% intensity): 1623.3 (65), 1624.3 (100), 1625.3 (41). Calcd for $C_{107}H_{171}BN_2O_8$ ($[M]^+$): 1623.31.

Diphenyl-substituted boron complex of 1,3-bis(5-(3,4,5-trihexadecyloxyphenyl)pyrrol-2-yl)-1,3-propanedione, 3d. BPh_3 (60.3 mg, 0.25 mmol) was added to a solution of **1d′**[S2] (179.4 mg, 0.10 mmol) in dry toluene (3.0 mL) under nitrogen and was refluxed for 12 h. The solvent was evaporated to dryness. The residue was the chromatographed over silica gel column (Wakogel C-300, eluent: 50% hexane/CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to afford **3d** (127.7 mg, 0.065 mmol, 65%) as an orange solid. R_f = 0.52 (50% hexane/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.53 (m, 2H, NH), 7.59 (d, J = 6.6 Hz, 4H, phenyl-H), 7.31–7.26 (m, 6H, phenyl-H), 7.11–7.10 (m, 2H, pyrrole-H), 6.80 (s, 4H, Ar-H), 6.61–6.60 (m, 2H, pyrrole-H), 6.47 (s, 1H, CH), 4.07 (t, J = 6.6 Hz, 8H, OCH_2), 4.00 (t, J = 6.6 Hz, 4H, OCH_2), 1.84 (quin, J = 7.8 Hz, 8H, $OCH_2C\underline{H}_2$), 1.77 (quin, J = 7.8 Hz, 4H, $OCH_2C\underline{H}_2$), 1.50 (m, 12H, $OC_2H_4C\underline{H}_2$), 1.29 (m, 144H, $OC_3H_6(C\underline{H}_2)_{12}$), 0.89 (t, J = 7.2 Hz, 18H, $OC_{15}H_{30}C\underline{H}_3$). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 168.99, 153.96, 140.37, 139.29, 132.88, 127.95, 127.34, 126.97, 125.93, 118.66, 110.42, 104.48, 91.98, 73.77, 69.75, 32.09, 30.51, 29.88, 29.83, 29.80, 29.59, 29.53, 26.26, 22.85, 14.28 (some of the signals for hexadecyl chains were overlapped and a signal of the core unit is missing presumably due to the $^{10/11}$B–^{13}C coupling[S4]). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 507.5 (1.05). MALDI-TOF-MS: *m/z* (% intensity): 1960.2 (69), 1961.2 (100), 1962.2 (87). Calcd for $C_{131}H_{219}BN_2O_8$ ($[M]^+$): 1959.69.

[S1] H. Maeda, Y. Fujii and Y. Mihashi, *Chem. Commun.*, 2008, 4285–4287.
[S2] H. Maeda, Y. Haketa and T. Nakanishi, *J. Am. Chem. Soc.*, 2007, **129**, 13661–13674.
[S3] H. Maeda, M. Takayama, K. Kobayashi and H. Shinmori, *Org. Biomol. Chem.*, 2010, **8**, 4308–4315.
[S4] Similar trends were observed in the boron-dipyrromethene complexes (BODIPY) possessing aryl moieties on the boron: C. Goze, G. Ulrich, L. J. Mallon, B. D. Allen, A. Harriman and R. Ziessel, *J. Am. Chem. Soc.*, 2006, **128**, 10231–130239.

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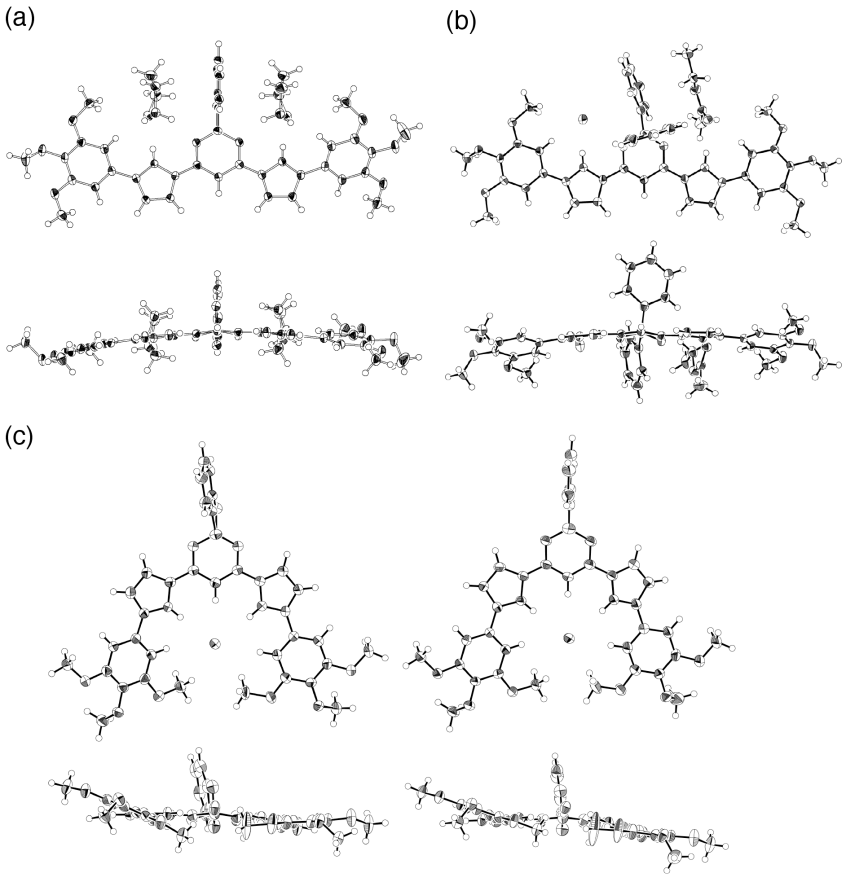
2. Single-crystal X-ray crystallographic data

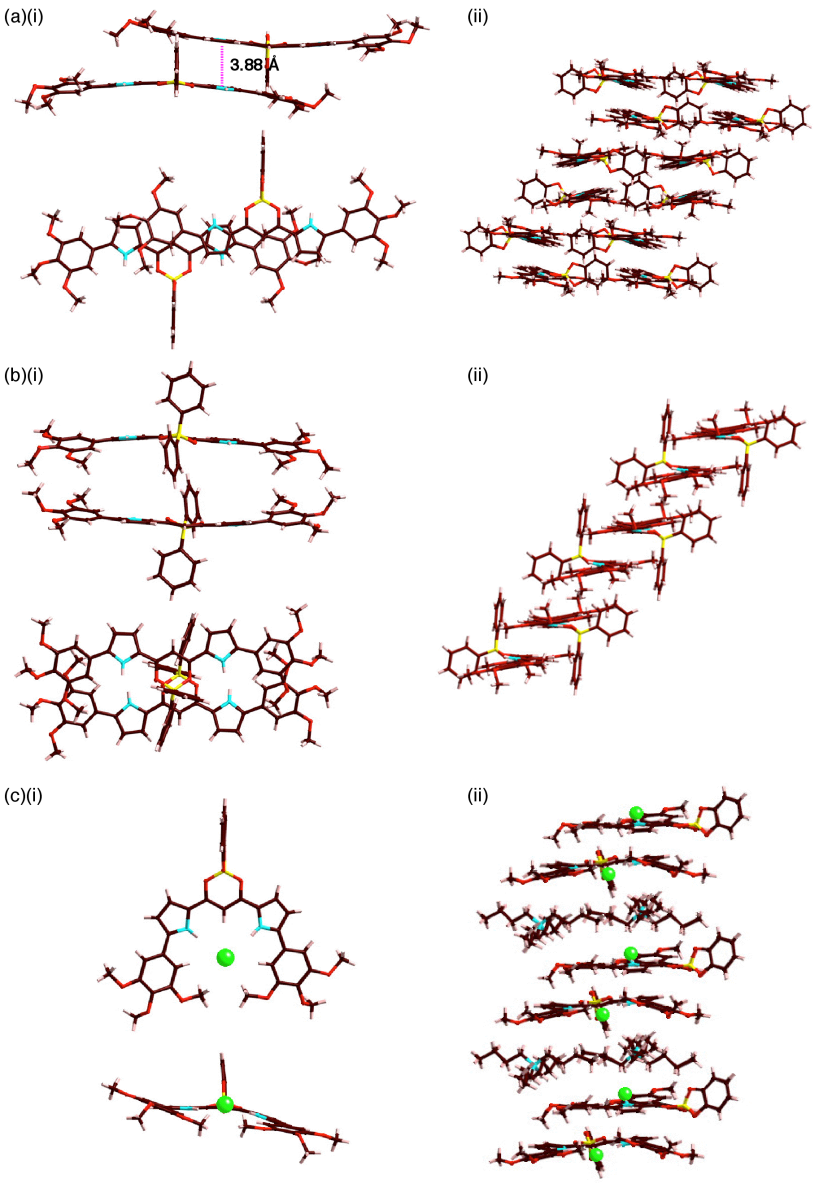
Single-crystal X-ray analysis. Crystallographic data for **2a**, **3a**, and **2a**·TBACl are summarized in Supporting Table 1. A single crystal of **2a** was obtained by vapor diffusion of heptane into a THF solution of **2a**. The data crystal was a red-colored prism of approximate dimensions 0.50 mm × 0.20 mm × 0.20 mm. Data was collected at 123 K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Mo-Kα radiation (λ = 0.71075 Å), structure was solved by direct method. A single crystal of **3a** was obtained by vapor diffusion of octane into an EtOAc solution of **3a**. The data crystal was a red-colored prism of approximate dimensions 0.20 mm × 0.20 mm × 0.05 mm. Data was collected at 93 K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Cu-Kα radiation (λ = 1.54187 Å), structure was solved by direct method. A single crystal of **2a**·TBACl was obtained by vapor diffusion of octane into an EtOAc solution of **2a** in the presence of 1 equiv of TBACl. The data crystal was a red-colored prism of approximate dimensions 0.50 mm × 0.30 mm × 0.30 mm. Data was collected at 93 K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Cu-Kα radiation (λ = 1.54187 Å), structure was solved by direct method. In each case, the non-hydrogen atoms were refined anisotropically. The calculations were performed using the Crystal Structure crystallographic software package of Molecular Structure Corporation.[S5] CIF files (CCDC-894126, 921412, and 894127) 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 **2a**, **3a**, and **2a**·TBACl.

	2a	**3a**	**2a**·TBACl
formula	$C_{35}H_{33}BF_2N_2O_{10}\cdot 2C_4H_8O$	$C_{41}H_{39}BN_2O_8\cdot C_4H_8O_2\cdot$water	$C_{35}H_{33}BN_2O_{10}\cdot C_{16}H_{36}NCl$
fw	796.65	801.65	930.35
crystal size, mm	0.50 × 0.20 × 0.20	0.20 × 0.20 × 0.05	0.50 × 0.30 × 0.30
crystal system	monoclinic	triclinic	triclinic
space group	$P2_1/c$ (no. 14)	P-1 (no. 2)	P-1 (no. 2)
a, Å	18.372(5)	11.2288(2)	12.1540(2)
b, Å	11.078(4)	12.3482(3)	19.3011(4)
c, Å	19.847(5)	16.4083(3)	21.6869(4)
α, °	90	71.0113(13)	88.2974(9)
β, °	97.849(9)	70.5677(11)	78.0546(10)
γ, °	90	80.8212(12)	82.5905(10)
V, Å^3	4002(2)	2025(7)	4935.68(16)
ρ_{calcd}, gcm^{-3}	1.322	1.314	1.252
Z	4	2	4
T, K	123(2)	93(2)	93(2)
μ, mm^{-1}	0.096 (Mo-Kα)	0.771 (Cu-Kα)	1.173 (Cu-Kα)
no. of reflns	36795	20067	52386
no. of unique reflns	9024	6583	17410
variables	529	540	1211
λ, Å	0.71075 (Mo-Kα)	1.54187 (Cu-Kα)	1.54187 (Cu-Kα)
R_1 ($I > 2\sigma(I)$)	0.0486	0.0518	0.0837
wR_2 ($I > 2\sigma(I)$)	0.1115	0.1588	0.2251
GOF	1.046	1.051	1.004



Supporting Figure 2 ORTEP drawing (top and side view) of single-crystal X-ray structures of (a) **2a**, (b) **3a**, and (c) **2a**·TBACl (two independent structures). TBA cations in (c) are omitted for clarity. Thermal ellipsoids are scaled to the 50% probability level.

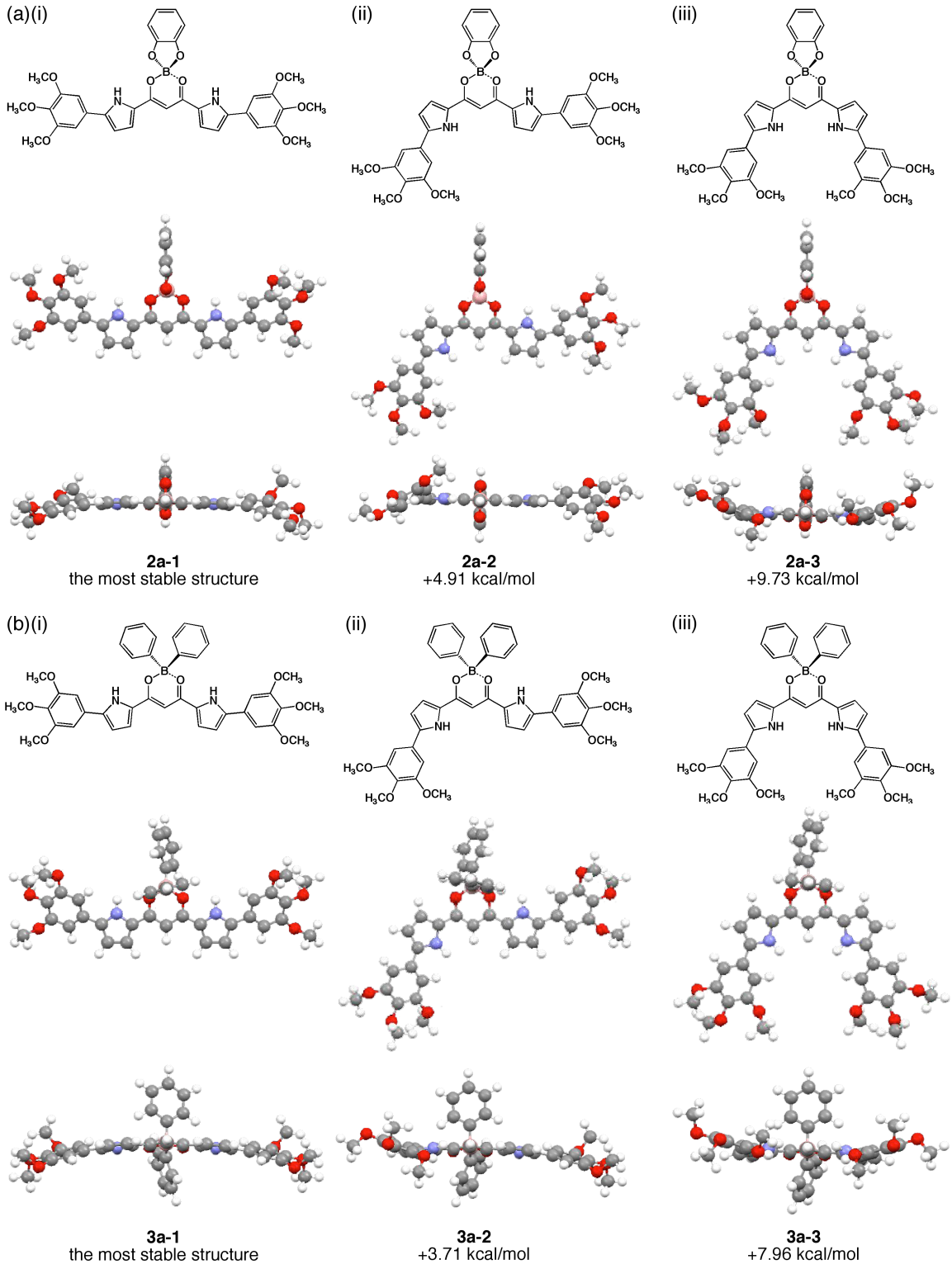


Supporting Figure 3 Assembled structures of (a) **2a** ((i) a stacking dimer (top and side views) and (ii) a columnar structure), (b) **3a** ((i) a stacking dimer (top and side views) and (ii) a columnar structure), and (c) **2a**·TBACl ((i) a Cl^- complex of **2a** (one of the two conformations; top and side view) and (ii) a columnar structure) in the solid state. Atom color code: brown, pink, yellow, yellow green, blue, and red represent carbon, hydrogen, boron, chlorine, nitrogen, and oxygen, respectively.

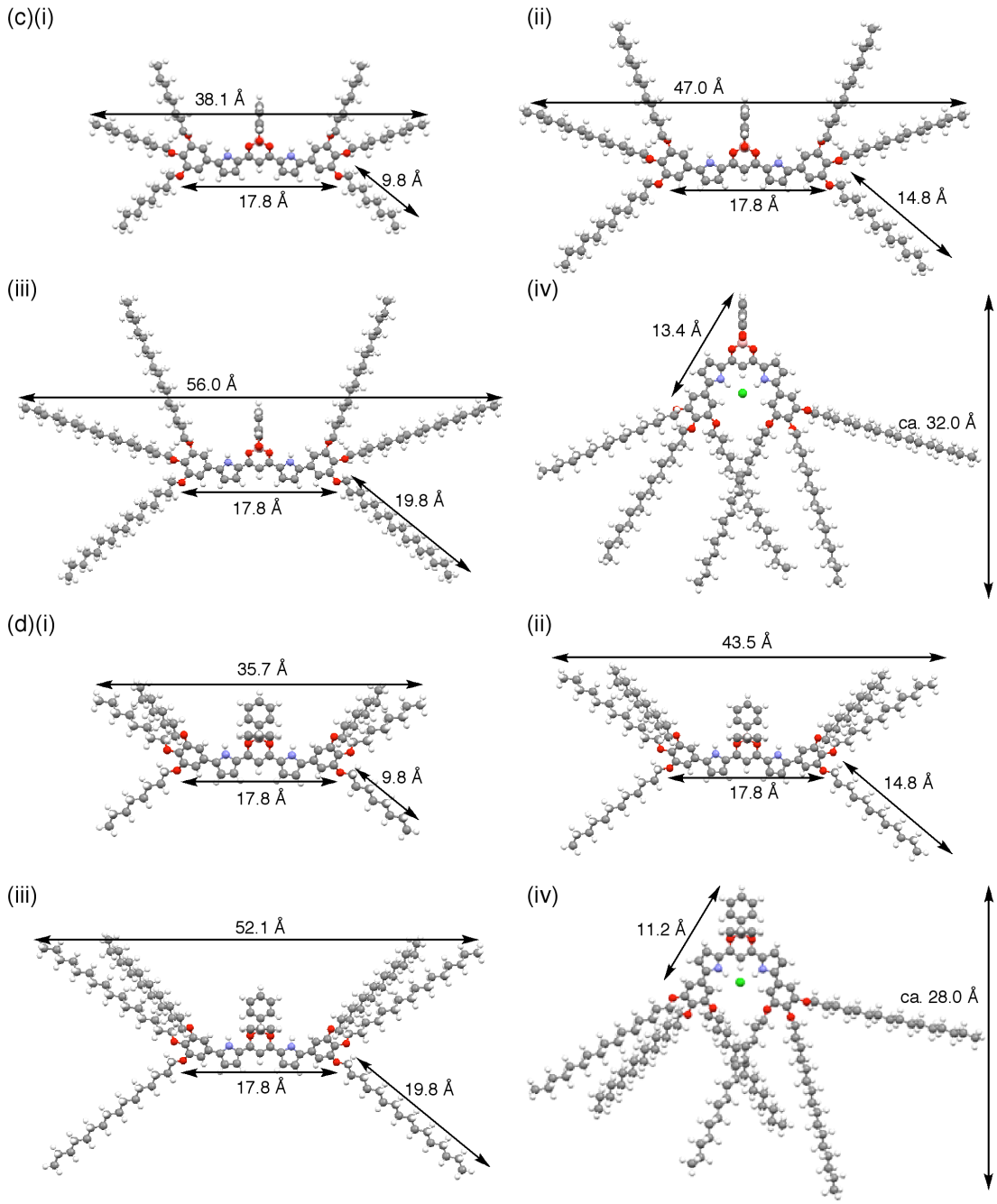
[S5] *CrystalStructure (Ver. 3.8), Single Crystal Structure Analysis Software,* Rigaku/MSC and Rigaku Corporation, 2006.

3. Optimization of anion receptors and receptor–anion complexes

DFT and AM1 calculation. Ab initio and semi-empirical calculations of anion receptors and their Cl^- complexes were carried out by using Gaussian 03 program[S6] and an HP Compaq dc5100 SFF computer. The structures were optimized, and the total electronic energies were calculated at the B3LYP level using a 6-31G(d,p) basis set for **2a** and **3a** and at AM1 level for **2b**–**d**, **2d**·Cl^-, **3b**–**d**, and **3d**·Cl^-.



Supporting Figure 4 Optimized structures of (a) **2a** (three conformations) and (b) **3a** (three conformations) at B3LYP/6-31G(d,p) level and (c)(i) **2b**, (ii) **2c**, (iii) **2d**, and (iv) **2d**·Cl^-, and (d)(i) **3b**, (ii) **3c**, (iii) **3d**, and (iv) **3d**·Cl^- at AM1 level.



Supporting Figure 4 (Continued)

Cartesian Coordination of 2a-1

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Cartesian Coordination of 2a-2

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Cartesian Coordination of 2a-3

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Cartesian Coordination of 3a-1

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O,9.3462868857,-2.6035774675,-0.980523058
O,-9.3199069345,-2.667462731,-1.0916449047
O,1.2254734776,0.2334543859,0.0201134208
O,-1.2395313506,0.2360406204,0.0416487799
O,-9.9637917601,0.0642558468,-0.9304149093
O,9.9694205132,0.1308852291,-0.7872402184
O,-7.92335859,1.8907827724,-0.2673218079
C,7.1092083562,-2.1444268941,-0.3274803643
C,-10.4482510011,-2.8421385334,-0.2261607136
C,-2.8879454939,-2.981805253,0.732072047
C,8.7807157388,2.3935135374,0.8983157684
C,7.6738230778,0.5849681549,-0.1724698426
C,10.1345778705,0.6402050534,-2.1200114566
C,-6.3937003913,0.0885129415,0.0002104325
C,2.8878367251,-2.9710171936,0.7435341459
C,4.7283757795,-1.7394790984,0.246911448
C,-2.4864779901,-1.6744646341,0.4431185093
C,4.2839478508,-3.0174291365,0.6157393988
C,-7.6820226127,0.5383170537,-0.2810020613
H,11.0285980545,-1.8498216377,0.0162260156
H,10.1264638988,-3.1290123426,0.8860871357
H,5.6387180429,0.858671733,0.3705927551
H,-9.4462650353,1.4038979168,-2.4515492492
H,-3.5877814771,-0.0048149396,-0.1852202675
H,3.5839006198,0.0164843008,-0.1426244272
C,-0.0162443529,2.2235196208,-0.972829878
C,8.4021717616,-1.6910182649,-0.5810714159
C,-0.0021494178,-1.6768619414,0.6877962611
C,-1.2050267552,-1.0212995797,0.4073023976
C,2.4824980428,-1.6648163533,0.453499332
B,-0.0047768961,1.1408530208,0.2187263967
C,-8.3885048526,-1.7457016191,-0.6834319529
C,10.4614512358,-2.7772259156,-0.0978933839
C,6.0807564046,-1.2443225454,-0.005411395
C,-6.0800946283,-1.2789372921,-0.0728687732
C,6.3840424445,0.1245363768,0.0834340928
C,-8.6918760299,-0.3731224102,-0.6365057285
C,-10.1112791719,0.5529020157,-2.2730103482
C,-7.0970530995,-2.1884758135,-0.404900665
C,1.1979095971,-1.01938789,0.4043809286
C,-8.819472546,2.3487400064,0.754224945
C,-4.7288279372,-1.7633572621,0.2048268393
C,-0.574171976,4.4423373543,-1.8411536835
C,-0.5211062171,3.5216710601,-0.7920776309
C,1.2032372301,2.2716963513,2.2556186715
C,1.2557568728,2.8123617385,3.5402041578
C,0.1092869052,2.8297821511,4.3380577724
C,-1.0806419465,2.3033100792,3.8360340366
C,-1.117881171,1.7616003592,2.5483653192
C,0.0194034514,1.7272952399,1.7246028082
C,0.4420392012,1.8904030309,-2.259849319
C,0.4004411365,2.8025335061,-3.3151355873
C,-0.1115886436,4.0851213345,-3.1082223211
C,-4.2820496882,-3.0368564414,0.5854755647
C,8.6955553562,-0.3168609609,-0.5184894906
H,-8.891800491,3.430523164,0.6286899852
H,-11.1507733582,0.8718137314,-2.3700950681
H,-11.0657565227,-3.6140028126,-0.6893904636
H,11.0915082301,-3.5417107636,-0.5564346112
H,11.1736124824,0.9661618346,-2.1963867067
H,8.8485445113,3.4767588417,0.7833292781

Cartesian Coordination of 3a-2

-2322.0524971 hartree

H,9.1539922831,-4.6931268541,0.3661534865
H,0.7778219903,4.7963293466,-4.488950084
H,2.2742411097,2.1167583495,2.0142129452
H,2.3682675484,2.9630571382,4.3282487549
H,0.7440647632,4.6831255239,5.097712778
H,-0.9703519861,5.5457699379,3.5132616955
H,-1.0530942464,4.7028124059,1.1965737352
H,2.6967125466,4.6214225033,0.0752515047
H,3.7230638094,6.0793671487,-1.6316875416
H,8.5206918235,-6.2342894028,-0.2802690696
H,5.4757801488,0.1046079554,0.4396729862
H,-9.2811444575,-3.1561477901,2.4026135748
H,-8.2010671546,-4.4353023588,1.7606162698
H,-9.9740875569,-4.5944183602,1.6009946276
H,-7.618876758,1.0245825954,0.3650846245
H,-8.2355122494,-4.711808691,-1.3725912551
H,-6.8417586416,-4.2606461677,-2.4016482855
H,-6.7848983772,-5.7557012399,-1.4291079891
H,-0.2293012538,3.3230852365,-2.7823078411
H,2.7659042087,6.1817922177,-3.9259570527
H,-5.99508213,2.4753222211,-0.8538639126
H,7.709573734,-5.4528666893,1.1032566907
N,2.9029686087,-0.6257559537,-0.0140669602
N,-3.6985322485,0.2678589632,-0.1269478799
O,-9.6392127218,-0.516321269,0.7413352916
O,1.290652262,1.4922175194,-0.2469879966
O,-0.9200879222,2.5585165677,-0.4974265941
O,8.0255572444,0.0826717548,0.1662518659
O,9.141314624,-2.4396211557,-0.4079868225
O,-6.5282129373,-4.0607292699,-0.3449041537
O,-9.1468926707,-3.2514771572,0.3183028295
O,7.4074429518,-4.6198401551,-0.7896260394
C,-10.7169201276,-0.7109339957,-0.1831532582
C,0.705595072,4.3111234526,4.0772526663
C,-0.2559661705,4.7941412867,3.1862836028
C,-0.2990565307,4.3144401523,1.8773739975
C,0.6030290262,3.3392386667,1.4134298813
C,2.2787248379,4.6414428285,-0.9284104709
C,2.8586174603,5.4721253184,-1.8890585177
C,2.322223807,5.5315602324,-3.1763590118
C,-5.0894597313,1.9344960867,-0.6210756562
C,7.7812524071,-2.284812101,-0.2634693637
H,2.7269822034,-3.8355210577,0.5508952004
H,-1.1750955744,-0.650672915,0.3858293611

C,0.6412877217,3.9205686359,-2.5232237817
C,1.5590712678,2.8724675625,2.3306201866
H,3.3172351943,0.2576458229,-0.2749761567
H,-3.3681068106,-0.6222323124,0.2094337901
H,4.9175573333,-4.0978405922,-0.4624654314
H,-10.5236225933,-0.176310623,-1.121575114
H,-10.8782975195,-1.7719848,-0.3896885134
H,-11.6024202208,-0.2880461483,0.2948104666
H,8.3298834884,0.0576621758,2.233678525
H,9.6077224336,-0.7419571709,1.2671616382
H,9.4484988825,1.0389425672,1.249355974
H,9.1876382276,-2.6174904153,-2.4903585992
H,9.4393595517,-0.9593457006,-1.8560374859
H,10.7170481671,-2.19559088,-1.6691520899
H,-4.852388135,-2.1462817799,-0.6650443701
H,0.3433017032,-2.5870246782,0.5662905064
C,1.1611607506,3.8410623649,-1.2199635938
C,1.6157655348,3.3474843961,3.6438094838
C,-3.7799901117,2.4392092651,-0.6386959718
C,8.9040417337,0.0943735464,1.2997933541
C,7.228278368,-1.0299622025,0.0473880897
C,9.6394305702,-2.0224775146,-1.6890947824
C,-5.8284038908,-1.7873041696,-0.3551058747
C,1.3067415962,-2.1331689364,0.3836487445
C,3.5386481436,-1.8278401769,0.1092188242
C,-2.9146876582,1.3924860693,-0.3184911763
C,2.5481613305,-2.7864140259,0.3663482571
C,-6.8427049121,-2.7304036259,-0.2021579441
C,6.9247714529,-3.3896085505,-0.4198023863
C,-0.7126470815,0.2981510937,0.1517015951
C,-1.4788497427,1.416725235,-0.2006368582
C,1.5415716924,-0.7771249356,0.1399434361
C,-8.4070020525,-0.9551934685,0.3285553385
C,8.2508423678,-5.2750145664,0.165400958
C,4.9887852161,-1.974348038,-0.008046332
C,-6.0827551113,-0.4207207584,-0.150865273
C,5.8492675744,-0.8791943307,0.1758411694
C,-8.1414860199,-2.3255767309,0.1523915842
C,-9.1385094378,-3.891983364,1.6037048371
C,-7.3864046532,-0.0178018381,0.1791813157
C,0.6797011883,0.3704700888,0.0279874049
C,-7.1456068966,-4.7258818767,-1.4559114085
C,-5.0227574554,0.5763561248,-0.2942041506
C,1.2068043968,4.7532426256,-3.4906325289
C,5.5461701846,-3.2310884773,-0.2932870644
B,0.5410329989,2.8406226347,-0.1227565527
H,-3.461358346,3.4452864697,-0.8655846733

Cartesian Coordination of 3a-3

-2322.0457311 hartree
H,-6.5597937205,-0.6780612132,0.3401743296
H,-2.6837238939,-5.2049283703,1.3112894991
H,-4.0847419811,-6.2025363589,0.8137225071
H,-0.8421241157,6.6482894495,-4.2917198381
H,-0.9487740913,4.7314711539,-2.7404875193
H,2.1269942316,4.5238883532,1.770808739
H,2.0727206687,5.078485022,4.1749699404
H,-0.0842750339,5.6421326861,5.2794667483
H,-2.1819803376,5.6487907817,3.940750048
H,-2.1199374859,5.1023941576,1.5356697986
H,1.0638606507,7.0402159873,0.2648695457
H,1.1890064813,8.9562542094,-1.2862106718
H,0.2314499806,8.7754626409,-3.5753674236
H,-5.7407214047,1.3408955841,-0.8499249789
H,0.0017293615,0.5295079593,-0.0733584403
H,8.2120224727,-4.6922403303,-0.4927223524
H,8.6432694859,-3.0477131404,-1.0544151198
H,6.642276441,-5.1592749772,2.1811766146
H,4.9778270212,-5.797604273,1.9906237534
H,-2.7143745291,-2.3534565597,-0.7441640558
H,3.9351458977,3.2443704858,-0.7911759721
H,5.7706210433,1.2459322335,-0.7616380707
H,-3.8693535021,3.3046162106,-0.8782029356
H,-7.6295363336,-4.5197587853,1.9453361186
H,-7.6611354541,-2.8732074031,2.6483009738
H,2.6848408165,-2.3825014764,-0.8443607605
N,-2.6980685384,0.3182386627,-0.2377867822
N,2.6981584312,0.2687201869,-0.2302105436
O,7.6220150836,-3.1245846161,0.7678286343
O,3.2981181196,-4.8483429464,-0.5547948424
O,-7.7590551289,-2.9490879187,0.562226552
O,1.2667769792,3.5855495645,-0.4481078328
O,-1.2015859154,3.6050585711,-0.4853022903
O,-6.1203748149,-5.2037169663,0.1504416965
O,5.9664242831,-5.3294824498,0.2083991381
O,-3.4355732558,-4.7934351274,-0.5953489872
C,3.7020570826,-2.5095002969,-0.4885428798
C,6.339690106,-2.9403894411,0.3086948579
C,5.9891365526,-5.7891716296,1.5690686146
C,-3.7463651878,-2.4481072407,-0.4220230222
C,3.7628674884,2.1948429704,-0.6059550113
C,4.0299331935,-0.0387955905,-0.3352852861
C,-2.4796468516,1.6755508522,-0.4040431945
C,4.70905174,1.157617448,-0.5823567226
C,-8.0494316578,-3.514644983,1.8477672832
C,-4.2588158767,-3.7390788284,-0.2923631704
C,-3.7193855484,2.2556992802,-0.6715865303
H,-7.7816670631,-4.9511648356,-1.0969134384
H,-6.3171591275,-5.6133270994,-1.8906812748
H,-2.0176643147,-0.3405819959,0.1046347164
H,1.999262277,-0.3858973402,0.0819783776
H,3.6283262884,-5.1780062537,-2.5920399491
H,4.5688652246,-6.2291489021,-1.4884568607
H,6.5206641814,-0.8194809256,0.4237544407
B,0.0311225653,4.4549181729,-0.1295874892
C,-6.4234527392,-2.8035659198,0.2709836846
C,3.6101040324,-5.7282526122,-1.6430981595
C,4.52727133,-1.4080062062,-0.2090544642
C,-4.5613231987,-1.3226157576,-0.2188483867
C,5.8559236277,-1.6409113202,0.1817355234
C,-5.6107604658,-3.9298857642,0.0430323941
C,-6.9172852679,-5.6108079361,-0.9740756475
C,-5.9043136081,-1.5184200676,0.1423636898
C,1.2272137472,2.2933833922,-0.3045884225
C,-3.1695868005,-5.7147461834,0.4696681688
C,-4.0331886812,0.0329571299,-0.3630077725
C,-0.4166882716,6.7351879796,-3.2946986058
C,-0.4731726464,5.6534529969,-2.4145857164
C,1.1768365336,4.7736204933,2.2368675908
C,1.1504203056,5.084630184,3.5989143914

C,-0.0581564101,5.4002811514,4.2201338947
C,-1.2344034417,5.4037894659,3.4669551481
C,-1.1944577783,5.0950030063,2.1068650775
C,0.0087710445,4.7683542721,1.4554733458
C,0.6537003618,6.9413079011,-0.7370064971
C,0.7226588063,8.0289827495,-1.6100986617
C,0.1853785945,7.9295323255,-2.8942526234
C,-4.6848113519,1.236595411,-0.6473203474
C,0.0598211908,5.7260724378,-1.1158760154
C,4.174939073,-3.8139569895,-0.3466351061
C,0.0115733893,1.6089228776,-0.147427718
C,-1.1883333939,2.3123665673,-0.3250590963
C,2.5078090931,1.6327666685,-0.3734077356
C,8.5367711346,-3.6970308585,-0.1767851515
C,5.5001563323,-4.0425504583,0.0624911138
H,9.4969732893,-3.7669789102,0.337393574
H,6.380897028,-6.8076367067,1.5409311573
H,2.8067371248,-6.4666674358,-1.6717409333
H,-2.4849641808,-6.4587048598,0.0582153108
H,-7.2552114709,-6.6256336571,-0.7564155273
H,-9.1375902988,-3.5600396682,1.9189151061

Cartesian Coordination of 2b (AM1)

-0.9823198 hartree
H,-2.0363701449,-3.5530499169,-2.08488
H,19.6241701212,2.9701491995,-4.44925
H,-6.7462001458,-3.5730797248,-0.98988
H,9.1390802467,6.0463796272,0.86565
H,10.7870302299,5.63658956,0.25253
H,16.036349606,-9.6573706542,2.79838
H,15.1120896117,-9.5198406165,4.34833
H,16.8587096311,-9.0420706877,4.29083
H,0.0000898913,-2.66355,-1.58509
H,2.0365498551,-3.5530700831,-2.08486
H,4.7467998456,-3.7844501936,-2.22519
H,0.000090093,2.28096,4.04244
H,-0.0000498047,4.78715,4.02794
H,11.6569102284,5.5998495245,2.61703
H,10.0089802452,6.0107095917,3.22913
H,11.254909887,-2.7702604591,-0.64859
H,10.2692298916,-2.6581404189,0.88761
H,5.8828200283,0.69449976,-1.04826
H,-17.1551998659,3.2874506998,-4.29038
H,-17.5640399338,1.6225007165,-4.85503
H,-15.3252099667,0.8160306252,-4.09802
H,-14.9164098988,2.4812206085,-3.5332
H,-11.7050202699,-6.6156895225,2.0566
H,-12.6267302755,-6.7528594849,0.51029
H,-14.6295299341,1.6144005968,-1.1853
H,-15.0380800021,-0.0509393865,-1.75035
H,-12.3820099672,0.8035805051,-0.42261
H,-12.7888900352,-0.8619294783,-0.9893
H,-12.6765699317,1.6752405171,-2.77516
H,-13.0853399996,0.0093205338,-3.34057
H,-16.036090394,-9.6572593458,2.79869
H,-15.1120303883,-9.5193293835,4.34872
H,-16.8586703688,-9.0417493123,4.29093
H,-11.254700113,-2.7701895409,-0.64859
H,-10.2690501084,-2.6579995811,0.88762
H,-10.9578095817,10.253480447,2.93659
H,-12.6099195986,9.8409405144,2.32348
H,-12.3487095865,10.1371405037,4.09161
H,-16.3211202919,-7.1558193342,2.74888
H,-15.3995102863,-7.0182893718,4.29478
H,-14.6343602327,-5.705419403,1.61421
H,-13.7125802271,-5.5678994406,3.16031
H,-13.3937603291,-8.0663794536,3.19238
H,-14.3153703347,-8.203939416,1.64636
H,-5.8826399717,0.69456024,-1.04841
H,-10.7880997701,5.6359204401,0.25244
H,-9.1400397533,6.0465103729,0.86474
H,-12.023630168,-4.1174095095,2.02564
H,-12.9467501736,-4.2544594719,0.4794
H,-10.0112602107,-5.1659195916,0.9135
H,-10.933860216,-5.294589554,-0.63227
H,-10.9104896694,8.1047704451,4.24842
H,-12.5582096862,7.6931205123,3.63714
H,-11.6905696846,7.7304504769,1.27412
H,-10.0428096679,8.1417704097,1.88587
H,-10.0088897548,6.0111104083,3.2286
H,-11.6569197716,5.5994404755,2.61734
H,-19.1298198676,3.2451807804,-2.72828
H,-19.5397699357,1.5757607971,-3.29448
H,-19.6243698789,2.9692408005,-4.44915
H,-9.8812198557,3.5369104031,-0.77496
H,-8.2337598391,3.9439503359,-0.16033
H,-10.756089857,3.5050304388,1.59599
H,-9.1072698402,3.9165503715,2.20783
H,-9.8600099438,1.3787104022,0.54161
H,-8.1886099267,1.795910334,1.17262
H,-10.4001999645,0.8702204243,-1.99489
H,-10.8169700336,-0.8242795587,-2.56569
H,-17.2786899691,0.7565807049,-2.50865
H,-16.8699099012,2.4216706882,-1.9439
H,10.756440143,3.5053495612,1.59556
H,9.1077301597,3.9160596285,2.20821
H,11.7051197301,-6.6159204775,2.05641
H,12.6269397245,-6.7529705151,0.51015
H,8.2331701609,3.9437196641,-0.15957
H,9.8805301443,3.5374795969,-0.77502
H,17.1549301341,3.2879693002,-4.29067
H,17.5640800662,1.6229892835,-4.85503
H,16.8696100988,2.4225393118,-1.94409
N,3.7069099597,-0.9869601512,-0.77122
N,-3.7067200403,-0.9869298488,-0.77126
O,8.3347600595,1.45971966,-0.89229
O,1.2175300061,0.1499799503,-0.17742
O,-1.2173299939,0.1499700497,-0.1774
O,9.2679598632,-3.3529603781,-0.83478
O,-10.2395700264,-0.6466495823,-0.55824
O,-8.3345899405,1.45977034,-0.89234
O,-9.2677501368,-3.3529096219,-0.83472
O,10.2397599736,-0.6466804177,-0.55827
O,0.0001100343,0.83997,1.6134
O,0.0001000836,2.04829,-0.41814
H,14.6344697673,-5.705560597,1.61429
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Cartesian Coordination of 2c (AM1)

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Cartesian Coordination of 2d (AM1)

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Cartesian Coordination of 2d·Cl⁻ (AM1)

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H,15.3745207919,-3.0885694697,6.6276977469
H,15.2241253902,-1.3797771833,6.0657372032
H,21.3788331541,0.4363754392,9.9403388631
H,21.5292583759,-1.2722244056,10.5022985971
H,-24.6417293178,2.9568220765,-2.4278248408
H,-25.2168643916,1.2765674137,-2.7498616572
H,-24.3854905099,0.5578476134,-0.4851559813
H,-23.8103328077,2.2381829548,-0.1630409621
H,-22.3054840845,2.1095430536,-2.1790578445
H,-22.8806788237,0.4291407708,-2.5011243342
H,-20.5429026866,-0.4188815195,-2.2517965302
H,-19.9677116674,1.2615470583,-1.9297406488
H,13.3223638615,-3.6939802653,5.3358383605
H,13.1720696626,-1.9851583319,4.7739456707
H,5.2642738726,13.093107321,3.1783724516
H,3.8709227737,13.8577602795,2.3230286891
H,-10.1327032344,10.2023675251,9.5313733995
H,-8.4313662036,10.1926085626,10.1344418314
H,-5.7650329036,2.0922868915,2.4823455744
H,-7.4662669725,2.1021961605,1.8787793079
H,4.3488992217,12.4535151818,0.2891415298
C,13.0798671837,-3.4654669406,3.1964924376
C,-12.3061937017,-2.7514704223,0.2699785907
C,-8.67491168,-3.8951017783,-0.2096737705
C,1.4882210413,5.4383768299,0.576996517
C,-1.8613561549,7.5685639438,-4.7651978052
C,-19.3197265625,-0.2080878848,-0.4776886886
C,21.288096668,-1.0433372469,8.3642823722
C,0.3800356132,3.2159520811,0.3153943162
C,0.5557425295,4.4258325976,1.2070898924
C,19.2361904041,-1.6490004309,7.0721638801
B,-0.9146601765,-12.3857909413,-1.2470574877
C,15.6758018055,-2.3757998139,5.8152917978
C,21.833185611,-0.5589483583,9.6910501453
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C,-23.9953414762,1.4879694318,-0.9764855818
C,-22.6954469709,1.1793397407,-1.6876670923
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C,4.8793650561,13.3908471091,2.1672089983
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C,-6.8024178479,1.7249433091,2.7008143693
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C,3.7219767421,-6.7753355541,-0.9763493397
C,-4.8035629607,-6.3016639482,-0.304800147
C,-2.8978026339,-2.1585122357,0.2556036464
C,5.8129109288,14.3977445074,1.5466550874
C,5.6753258728,-5.3592150138,-0.7498048705
C,-13.3440531684,-2.2121537892,-0.690825089
C,-14.6439568908,-1.9038683388,0.020736609
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C,15.3205697177,12.2190201993,-9.0256511421
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C,-0.8870966415,5.3220608827,-4.2647176176
C,-0.6591533735,6.8181170391,-4.2336006125
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C,-7.7262208355,4.3546528138,5.349232454
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C,-15.6819457792,-1.3645194672,-0.9398771485
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C,2.2006813546,0.1015528059,-2.5581863288
C,3.0833042649,-2.0972479025,-1.8051502892
C,-4.7801658302,14.309025822,-6.2620051464
C,-3.5854784576,13.5580008432,-5.733680105
C,3.1681292736,-8.1179294573,-1.0261972663
C,-2.8362039358,9.8149494848,-5.2651030158
C,3.9018567874,-9.3255804004,-1.2492671155
C,9.5192671321,-4.1905427335,1.9406873965
C,8.9794811398,-4.6751980922,0.6133610341
C,-2.6089947769,11.3110941992,-5.233370745
C,-3.8112705131,12.0613031083,-5.764854747
C,15.1320638197,-2.8601219771,4.488313535
C,-4.3014128753,-3.9311993218,-0.4216100816
C,-3.164956203,-9.5512356367,-0.6412532801
C,-9.9719255893,-3.5982094473,0.5206819223
C,-5.3171215889,-8.8116073882,-0.5638816363

Cartesian Coordination of 3b (AM1)

-0.7190711 hartree

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H,-16.2621909802,-2.1611383287,3.4848807422
H,-15.8858566034,-3.1007821993,5.7897071321
H,-16.0488271404,-1.4456524902,6.4911630949
H,12.352732411,-9.9638970076,-3.145620682
H,13.735529055,-9.5279059367,-2.0624274042
H,14.0146695912,-9.7598225153,-3.837414304
H,13.984000392,-7.3311116207,-3.2680525822
H,12.6049091386,-7.7660889962,-4.3483297413
H,-6.623037004,3.5606152525,-0.2057384398
H,-8.5913185367,-3.8692473962,-0.7959921775
H,-9.9694487699,-3.4374151145,0.2863648883
H,-11.4967024307,-3.2842074359,-1.7210188685
H,-10.1168722808,-3.7192918533,-2.8021228387
H,-10.2459352301,-1.2299552572,-0.9153518475
H,-8.8484629715,-1.6714349964,-2.0189495241
H,-2.158778109,-3.6722862019,3.3259822196
H,-2.1581087948,-2.2075301488,1.3108061312
H,2.1568045905,-2.1904789701,-1.4918905087
H,2.1586089996,-3.6255226426,-3.5283948672
H,-0.0002452688,-4.344427246,-4.5524656474
H,-2.1589519066,-3.6262551304,-3.5275704003
H,-2.1568480073,-2.1912072901,-1.4910554052
H,2.1581595001,-2.2068164256,1.3114696773
H,2.1586980605,-3.6715644264,3.3266375637
H,-0.0000719598,-4.4067519984,4.3383291383
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H,-12.5517226085,4.362169867,-1.5242230035
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H,-16.4047133422,10.0338108658,-0.9124204423
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H,16.3457947702,7.4311744415,-2.595173681
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N,3.6933161828,0.8389375647,-0.3818711682
N,-3.6932114126,0.8389806419,-0.3818829623
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O,-1.2040438354,-0.4147928608,-0.0308445045

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C,-11.7774825085,-5.8817868689,-2.5430456488
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C,16.5744458937,9.4442963518,-1.8463526878
C,14.6737744251,7.9157370357,-1.3099675602
C,16.1442916105,8.0126947081,-1.656827175
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C,16.3816269112,-2.1043430774,5.646150586
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C,4.1599554698,2.8934503513,-1.238865957
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C,11.7776571503,-5.8817610382,-2.5429996066
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C,10.4711452993,3.3998741922,-0.0575634812
C,6.1259134691,1.4488714636,-0.4008135564
C,-6.1258091275,1.4489124522,-0.4009024983
C,6.6149135754,0.1361785602,-0.3794094179
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C,-17.8782661684,-2.2720358511,5.6936725956
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C,-12.0322163957,0.0316317166,1.615229117
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C,-14.4279859966,-1.3364832569,4.2879394759
C,-15.9317252154,-1.5029731575,4.3312685153
C,-16.3815969067,-2.1043849734,5.6458202702
C,13.2959833473,-9.3697112621,-3.0769466256
C,13.0223475896,-7.9074303378,-3.3163216126
C,-6.9941128134,2.5246274853,-0.1882778521
C,1.1938159052,0.7782415219,-0.6083739082
C,-9.5607749157,-3.3079618339,-0.7496981318
C,-10.5335833022,-3.8578828946,-1.7695249789
C,-9.3054594841,-1.8345726217,-1.0089057068
C,-4.7229661546,1.7213147148,-0.6649079956
C,-1.2060475346,-3.3480651686,2.8836577635
C,-1.2045161946,-2.5278174053,1.7561024376
C,1.2032819218,-2.4987448102,-1.9462900713
C,1.2057088404,-3.304975533,-3.0836847991
C,-0.0001811181,-3.7085609541,-3.6561905918
C,-1.205991149,-3.3053848095,-3.0832234388
C,-1.2034011143,-2.499151708,-1.9458335972
C,-0.0000182015,-2.0824645402,-1.3672573356
C,1.2045322395,-2.527419979,1.7564628994
C,1.2059926017,-3.3476612874,2.8840262254
C,-0.0000437925,-3.7594328698,3.450312562
C,-4.1598305638,2.8934738923,-1.2389374791

C,-12.3492552313,4.9411890276,-0.584629314
C,8.8529793025,0.9764684714,0.1231928279

Cartesian Coordination of 3c (AM1)
-0.9816752 hartree
H,10.1708091211,1.1509616214,2.34906482
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H,-14.4499624714,6.2076410259,-2.055610977
H,-14.0640658232,8.6964441979,-2.0973694373
H,-14.4707865917,8.7890144316,-0.3410094839
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Cartesian Coordination of 3d (AM1)

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Cartesian Coordination of 3d·Cl⁻ (AM1)

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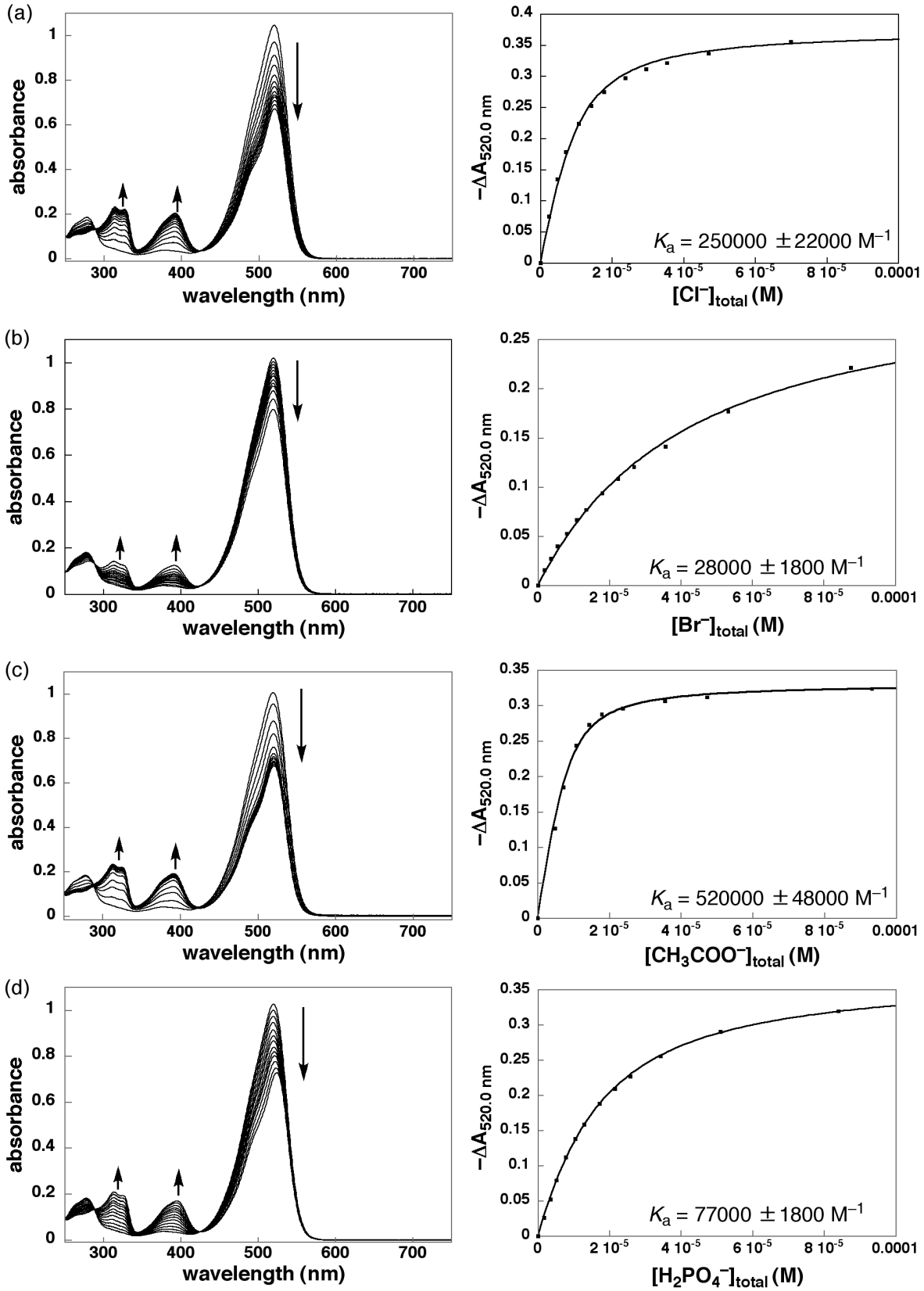
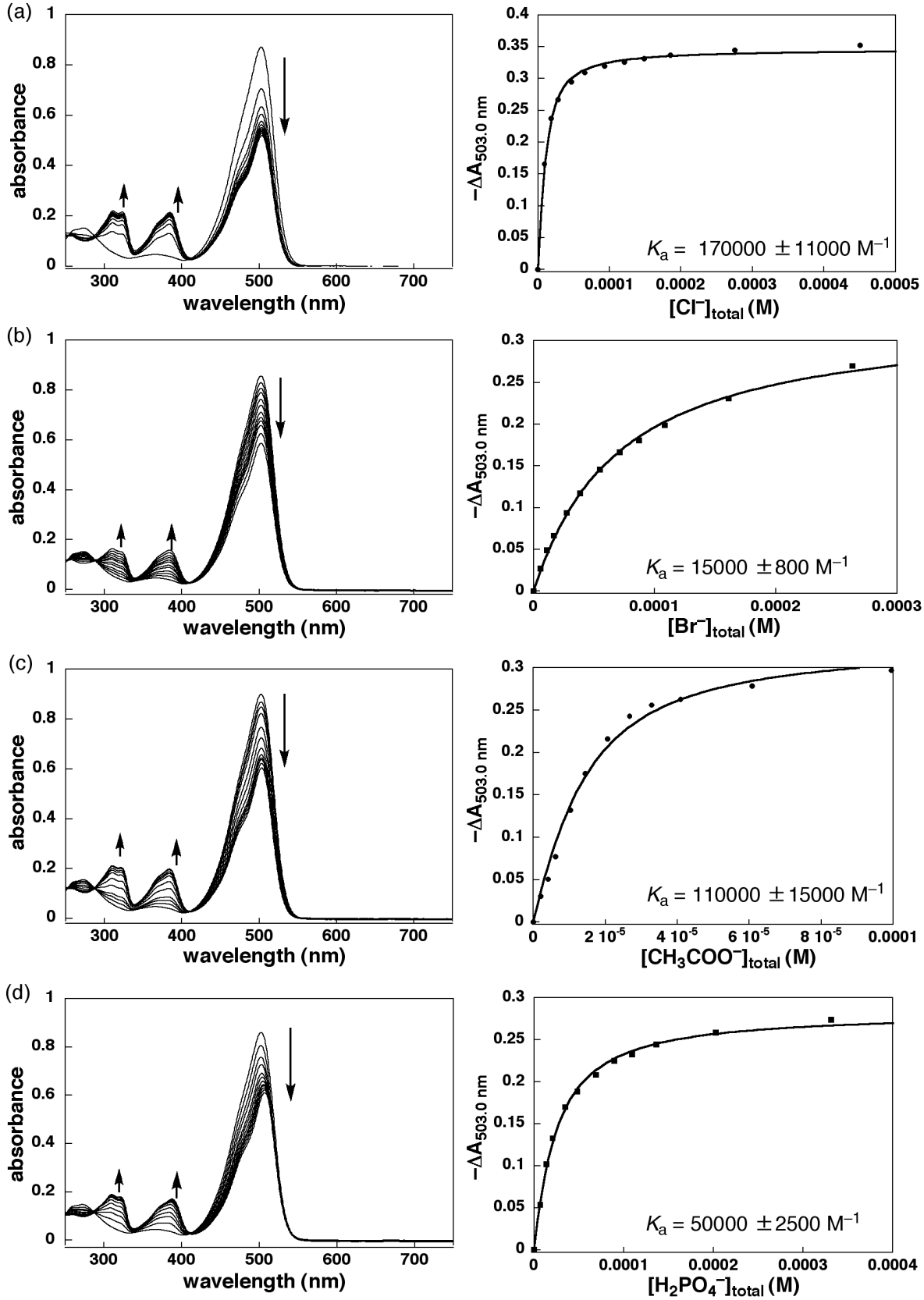
[S6 (as a complete ref. 10)] *Gaussian 03* (Revision C.01), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, 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. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

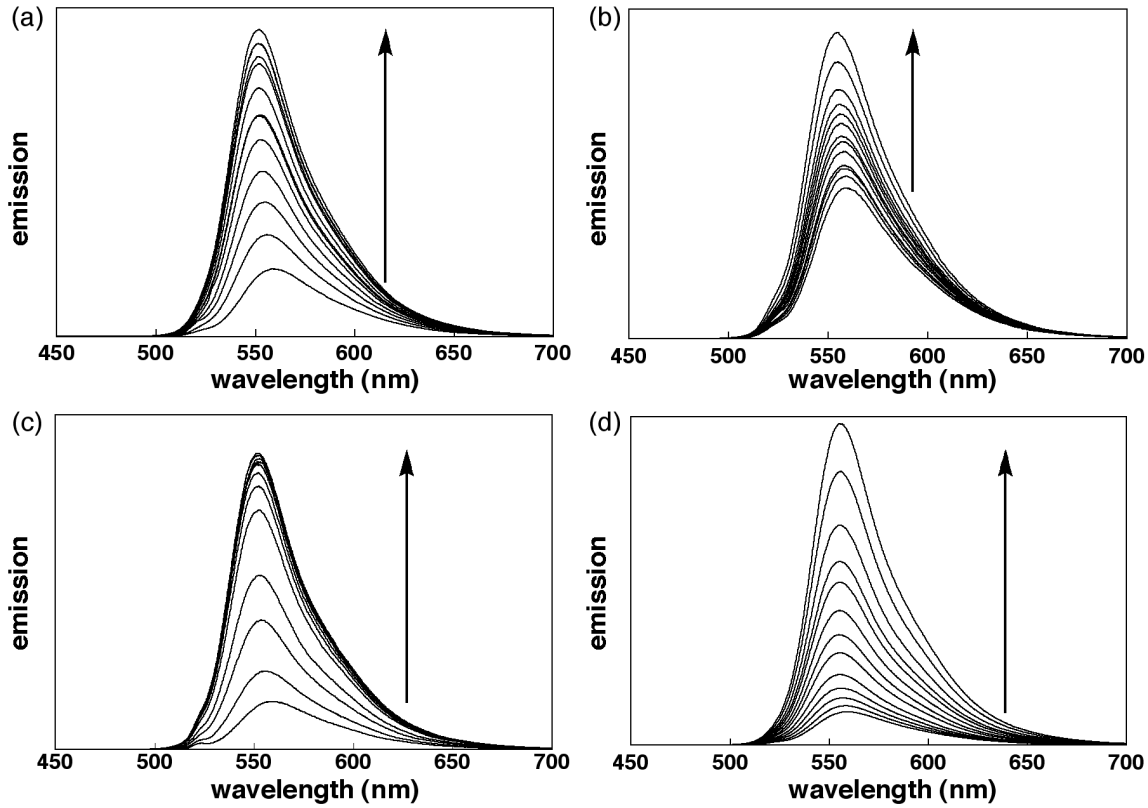
4. Anion-binding properties



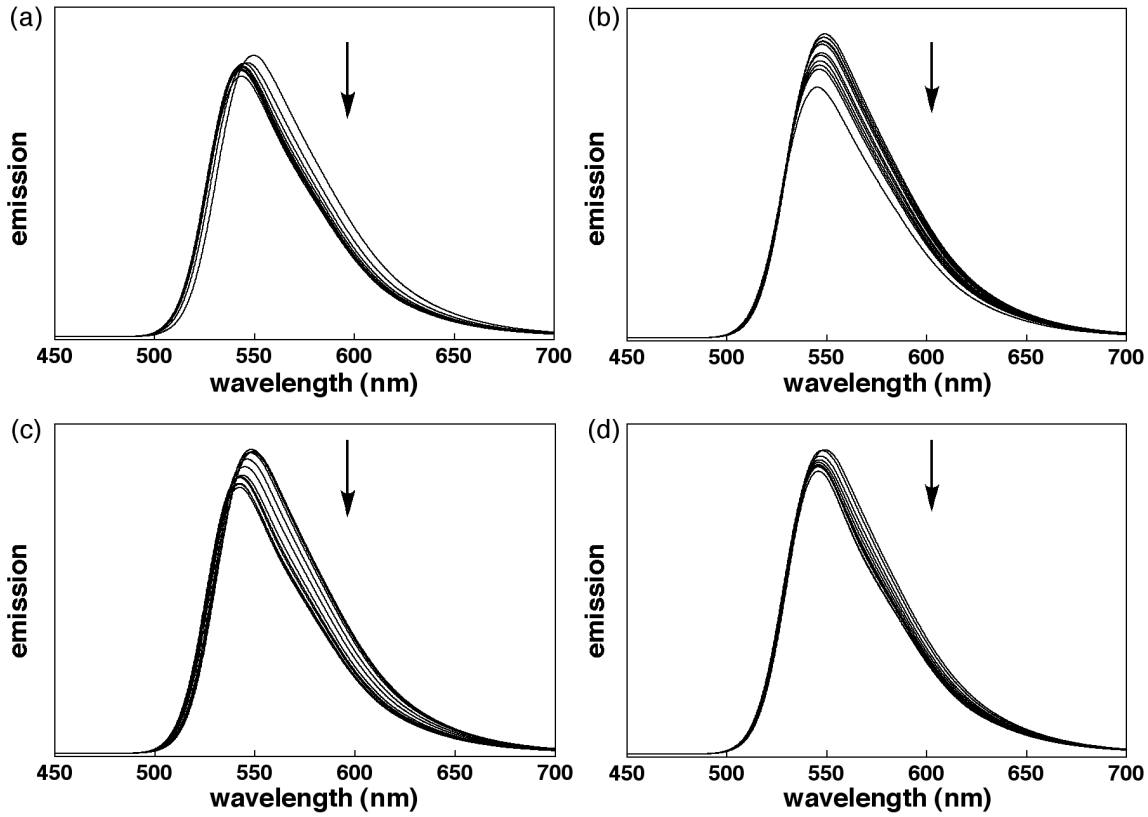
Supporting Figure 5 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **2a** (8.1–8.3 × 10^{-6} M) upon the addition of (a) Cl^-, (b) Br^-, (c) $CH_3CO_2^-$, and (d) $H_2PO_4^-$ as tetrabutylammonium (TBA) salts in CH_2Cl_2.



Supporting Figure 6 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **3a** (9.9×10^{-6} M) upon the addition of (a) Cl^-, (b) Br^-, (c) $CH_3CO_2^-$, and (d) $H_2PO_4^-$ as TBA salts in CH_2Cl_2.



Supporting Figure 7 Fluorescence emission spectral changes (excited at 520 nm) of **2a** ($8.1–8.3 \times 10^{-6}$ M) upon the addition of (a) Cl^- (0–30 equiv), (b) Br^- (0–20 equiv), (c) $CH_3CO_2^-$ (0–15 equiv), and (d) $H_2PO_4^-$ (0–7 equiv) as TBA salts in CH_2Cl_2.



Supporting Figure 8 Fluorescence emission spectral changes (excited at 503 nm) of **3a** (9.9×10^{-6} M) upon the addition of (a) Cl^- (0–25 equiv), (b) Br^- (0–18 equiv), (c) $CH_3CO_2^-$ (0–7 equiv), and (d) $H_2PO_4^-$ (0–20 equiv) as TBA salts in CH_2Cl_2.

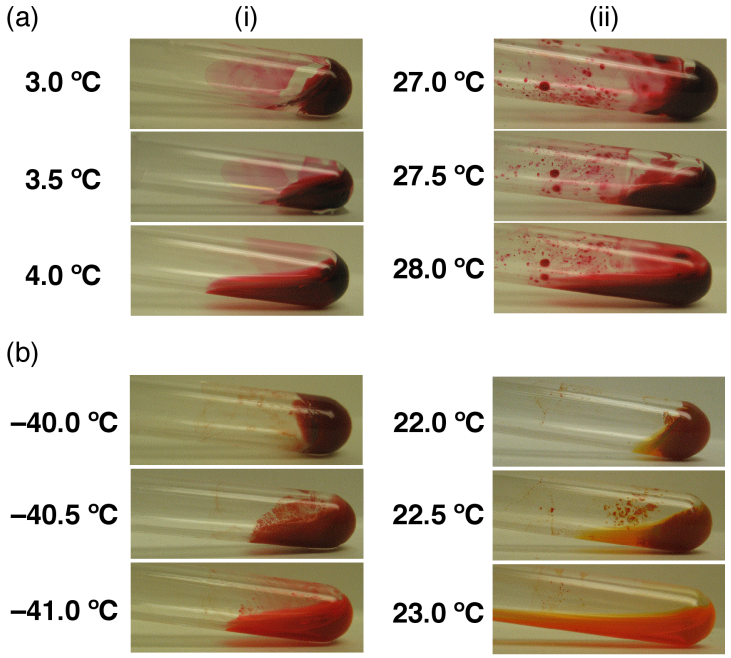
5. Formation of organized structures

Scanning electron microscopy (SEM). SEM images were obtained with a HITACHI S-4800 scanning electron microscope at acceleration voltages of 10 kV using a silicon (100) substrate. A platinum coating was applied using a HITACHI E-1030 ion sputter.

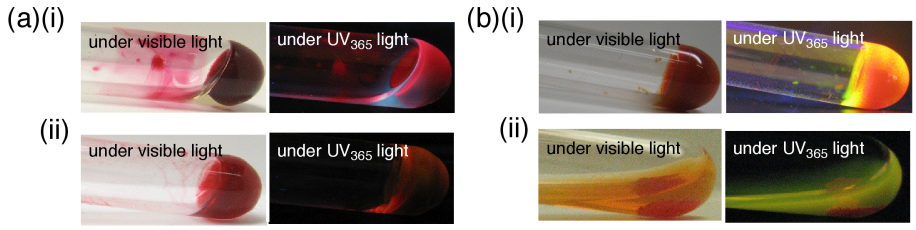
Differential Scanning Calorimetry (DSC). The phase transitions were measured on a differential scanning calorimetry (Perkin-Elmer Diamond DSC).

Polarized Optical Microscopy (POM). The textures were observed by using a polarization microscope (Nikon ECLIPSE E600 POL), equipped with a heating plate (Mettler FP-82 HT hot stage) controlled by a thermoregulator (Mettler FP-90 Central Processor).

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 543.0 mm (xerogels of **2d** and **3d** prepared from octane), 531.03 mm (**2b**–**d**), 530.40 mm (**3b**–**d** and **2d**·Cl^--$TATA^+$), and 540.18 mm (**3d**·Cl^--$TATA^+$) were used with an imaging plate as a detector, where the diffraction pattern was obtained with a 0.01° step in 2θ. The exposure time to the X-ray beam was 10 sec for the xeogels of **2d** and **3d** prepared from octane and 30 sec for the solid state of **2b**–**d** and **3b**–**d** and the precipitates of **2d**·Cl^--$TATA^+$ and **3d**·Cl^--$TATA^+$ prepared from 1,4-dioxane.



Supporting Figure 9 Phase transitions of (a)(i) **2c** and (ii) **2d** and (b)(i) **3c** and (ii) **3d** as supramolecular gels obtained from octane (10 mg/mL). Octyloxy-substituted **2b** was slightly dissolved in octane, whereas **3b** did not form gel.



Supporting Figure 10 Photographs of (a) **2d** and (b) **3d** as supramolecular gels or solutions ((i) receptors and (ii) those with 1 equiv of TATACl) obtained from octane (10 mg/mL).

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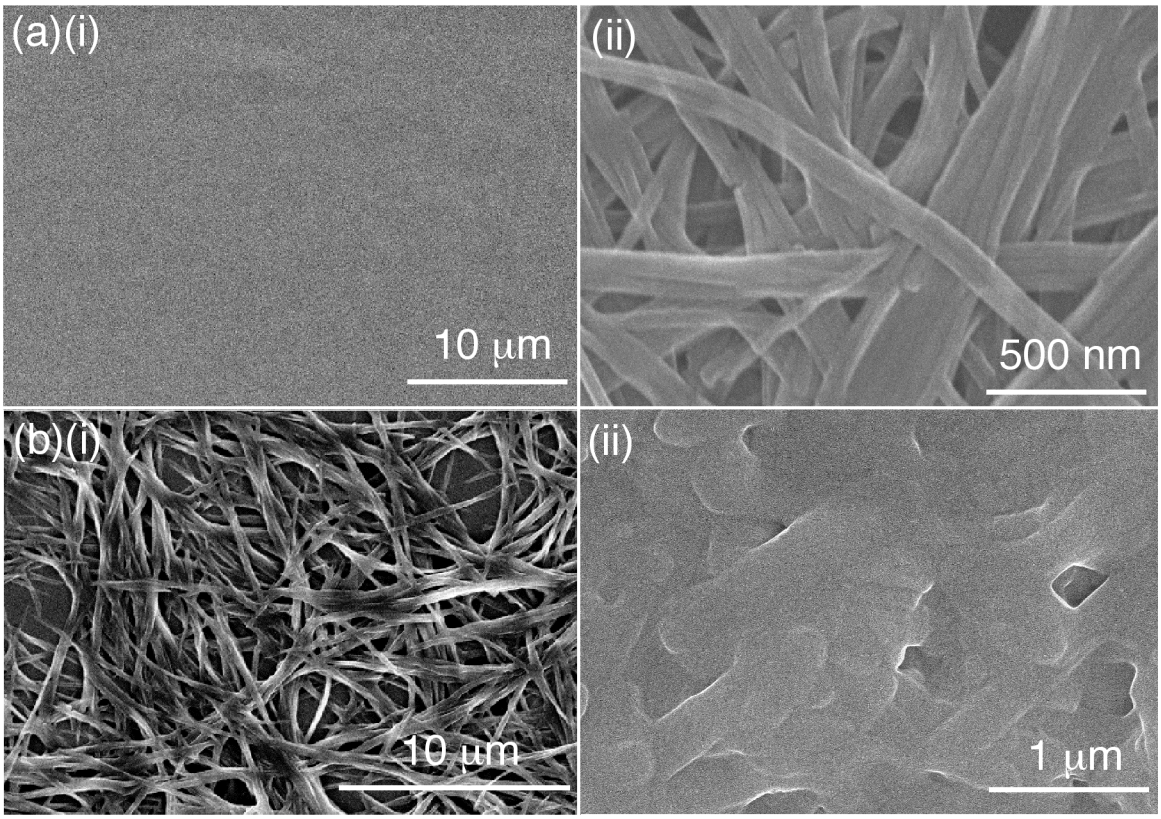
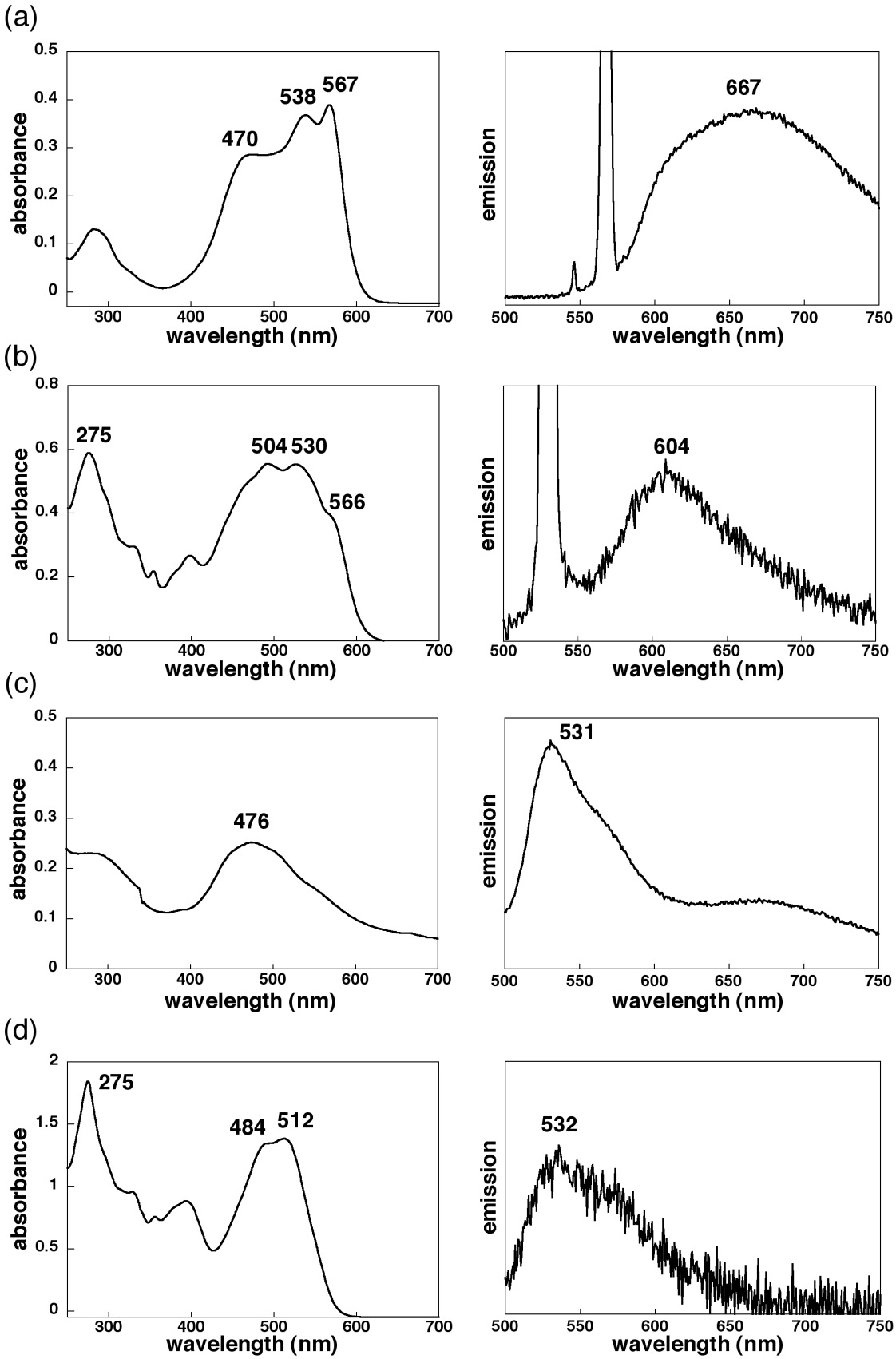
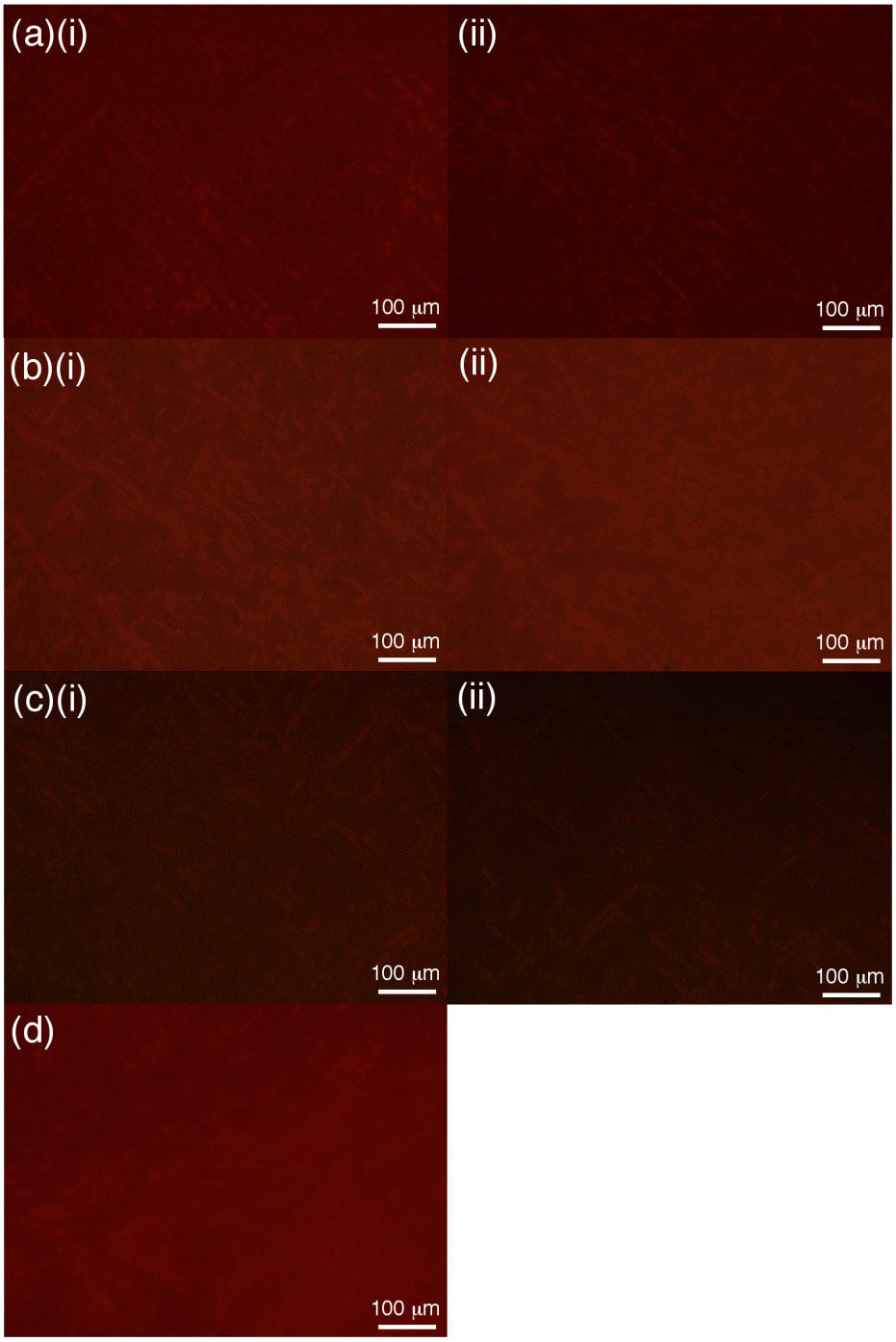


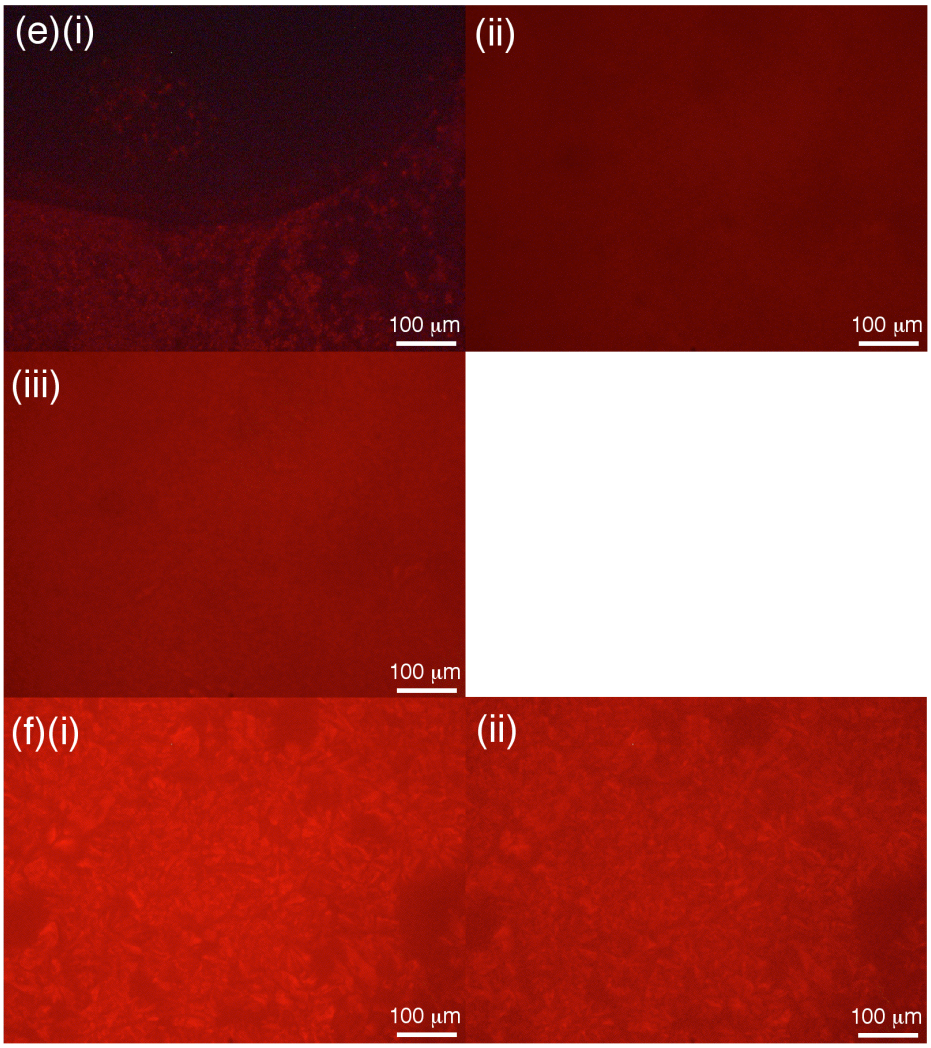
Supporting Figure 11 SEM images of xerogels prepared from octane (a) **2d** and (b) **3d** as (i) receptors and (ii) those with 1 equiv of TATACl obtained from octane (10 mg/mL).



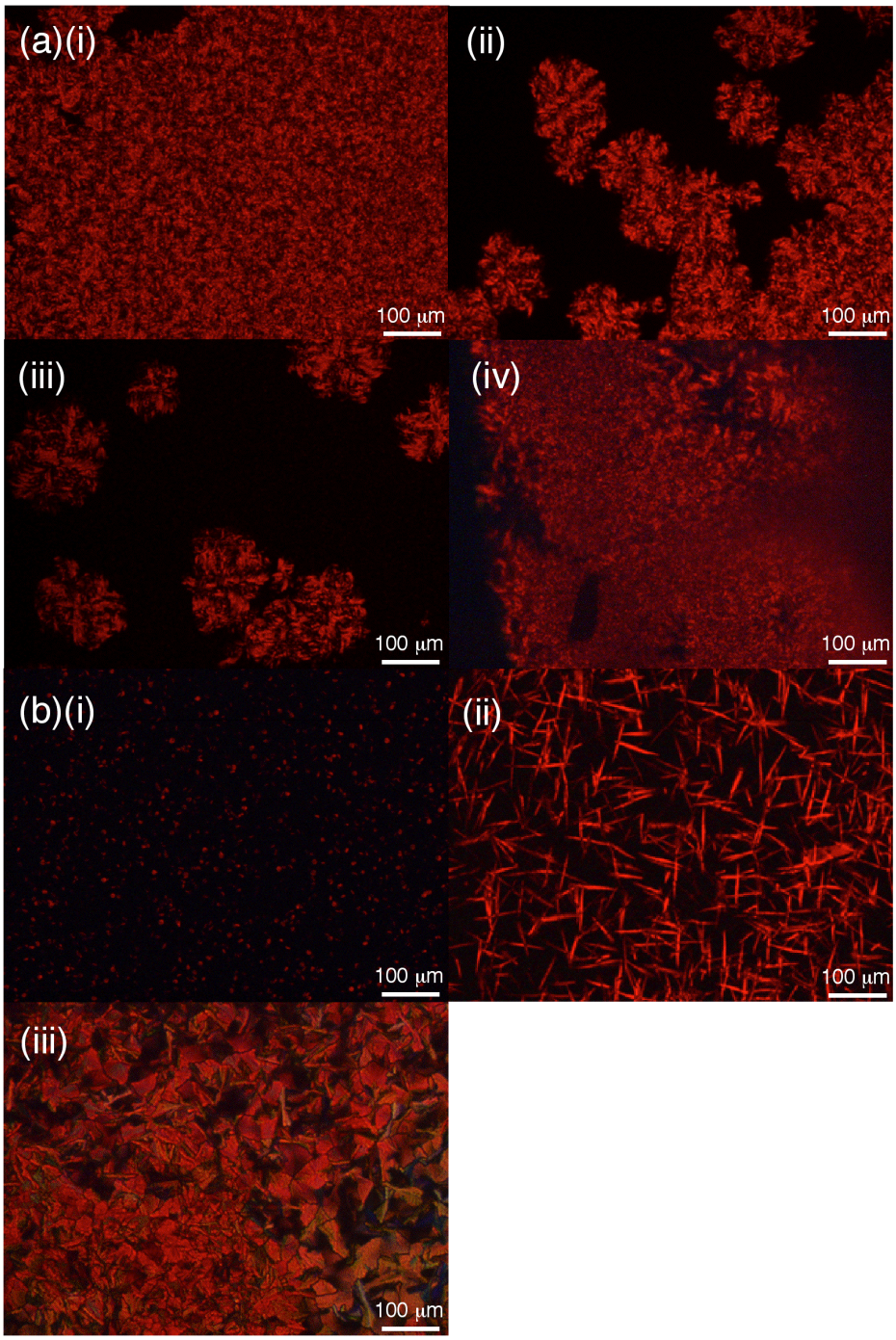
Supporting Figure 12 UV/vis absorption (left) and fluorescence emission (right) spectra of (a) **2d** (λ_{ex} = 567 nm), (b) **2d** with 1 equiv of TATACl (λ_{ex} = 547 nm), (c) **3d** (λ_{ex} = 476 nm), and (d) **3d** with 1 equiv of TATACl (λ_{ex} = 484 nm) in octane (10 mg/mL).



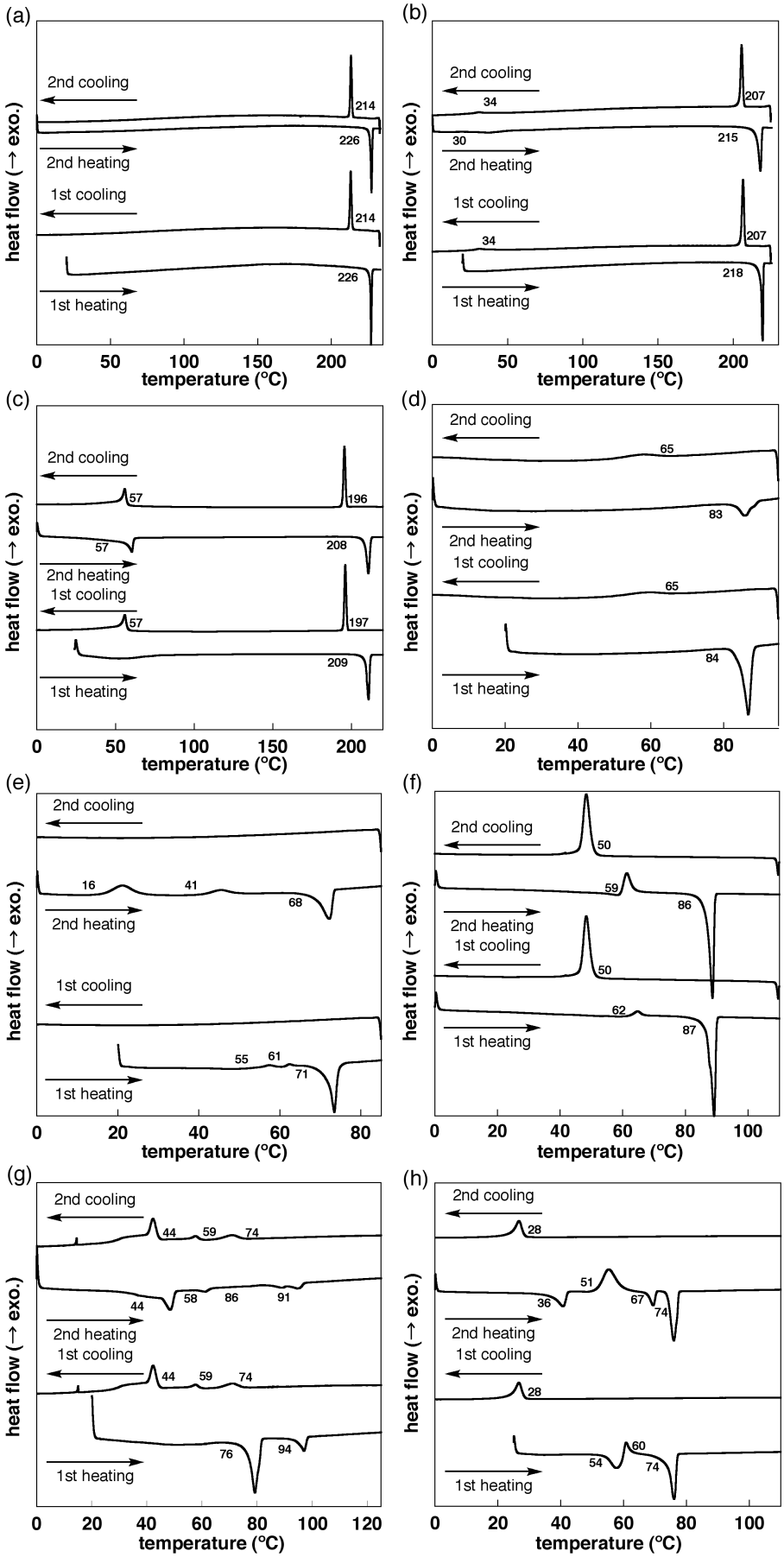
Supporting Figure 13 POM images of (a) **2b** at (i) 213 °C upon cooling from Iso and (ii) 213 °C upon heating, (b) **2c** at (i) 205 °C upon cooling from Iso and (ii) 205 °C upon heating, (c) **2d** at (i) 195 °C upon cooling from Iso and (ii) 195 °C upon heating, (d) **3b** at 25 °C upon cooling from Iso, (e) **3c** at (i) 15 °C upon cooling from Iso, (ii) 35 °C upon heating, and (iii) 55 °C upon heating, and (f) **3d** at (i) 25 °C upon cooling from Iso and (ii) 70 °C upon heating.



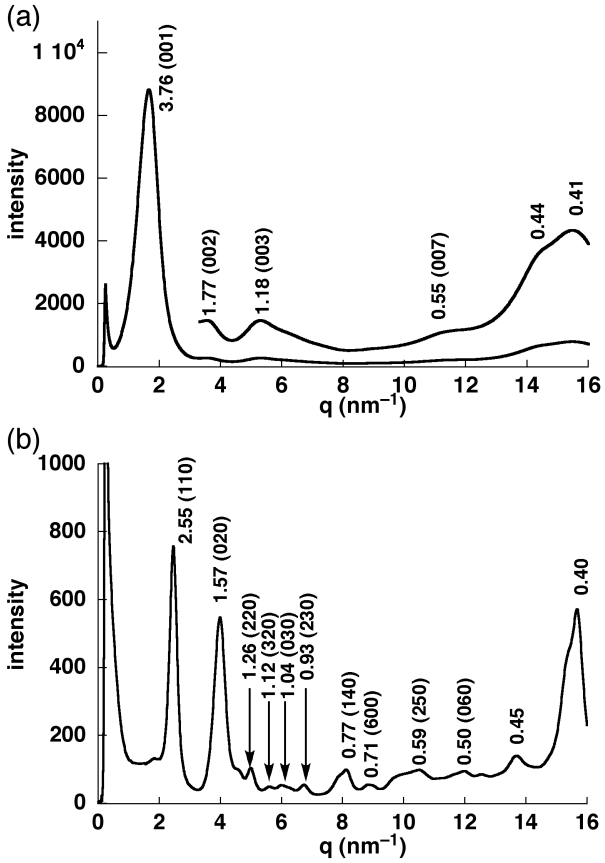
Supporting Figure 13 (Continued)



Supporting Figure 14 POM images of (a) **2d**·Cl^--$TATA^+$ at (i) 64 °C upon cooling from Iso, (ii) 52 °C upon cooling from Iso, (iii) 53 °C upon heating, and (iv) 66 °C upon heating and (b) **3d**·Cl^--$TATA^+$ at (i) 40 °C, (ii) 60 °C, and (iii) 70 °C upon heating.



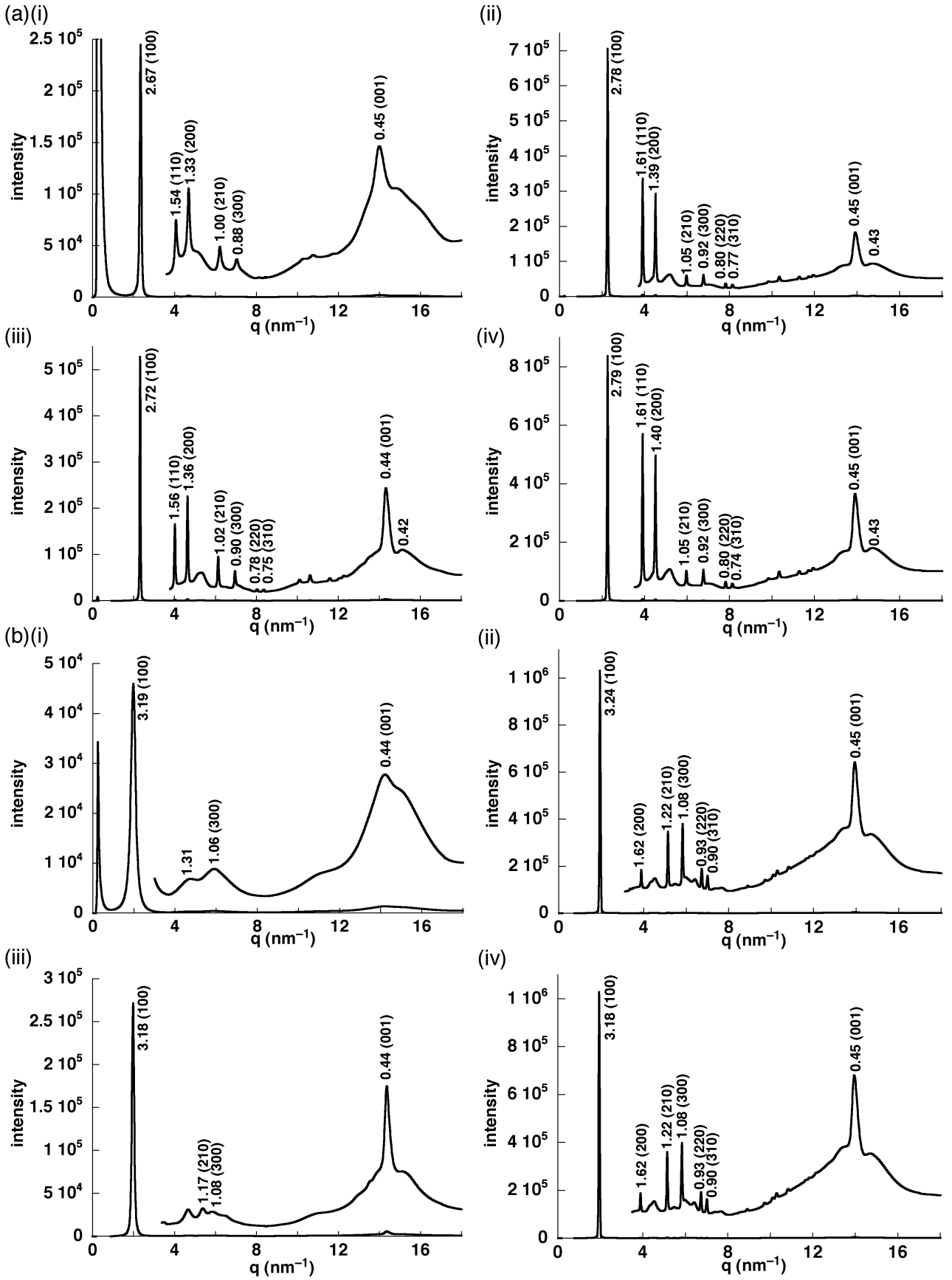
Supporting Figure 15 DSC thermograms of (a) **2b**, (b) **2c**, (c) **2d**, (d) **3b**, (e) **3c**, (f) **3d**, (g) **2d**·Cl^--$TATA^+$, and (h) **3d**·Cl^--$TATA^+$.



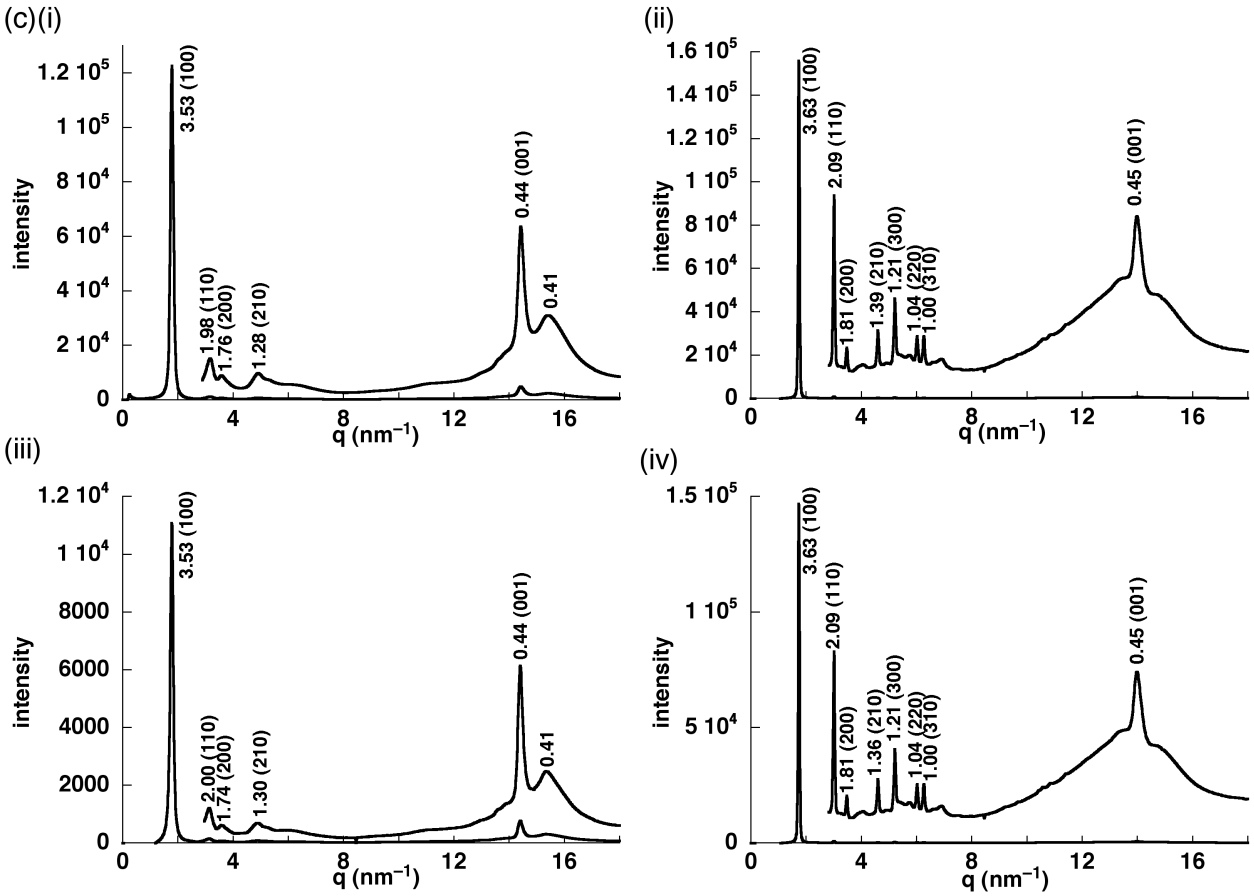
Supporting Figure 16 XRD patterns of (a) **2d** and (b) **3d** as xerogels prepared from octane (10 mg/mL). Only assignable peaks are indicated. The measurements were conducted to the xerogels in sample tubes frozen and pumped at –40 °C.

Supporting Table 2 Summary of XRD data of the xerogels of (a) **2d** and (b) **3d** prepared from octane.

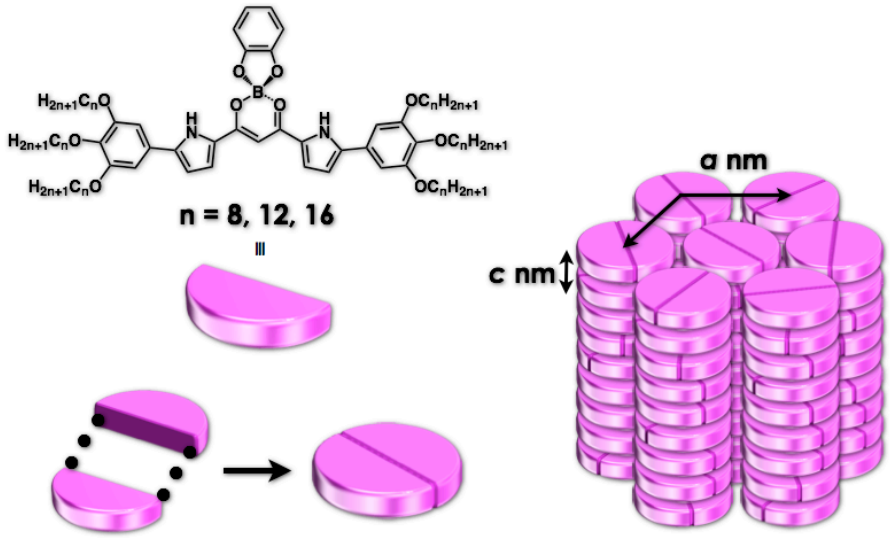
lattice parameters	q (nm^{-1})	d_{obs} (nm)	d_{cal} (nm)	hkl
(a)	1.67	3.76	3.77	001
2d	3.54	1.78	1.88	002
20 °C (lamellar)	5.31	1.18	1.26	003
M = 1914.85	11.33	0.55	0.53	007
	2.46	2.55	2.56	110
	3.99	1.57	1.58	020
	5.00	1.26	1.28	220
	5.60	1.12	1.07	320
(b)	5.99	1.05	1.05	030
3d	6.75	0.93	0.95	230
20 °C (Col_r)	8.12	0.77	0.78	140
a = 4.34 nm, b = 3.15 nm, c = 0.45 nm	8.84	0.71	0.72	600
M = 1960.96, Z = 1.8 ≈ 2 for ρ = 1.0	10.52	0.60	0.61	250
	12.50	0.50	0.52	060
	13.82	0.45	–	001
	15.65	0.40	–	–



Supporting Figure 17 XRD patterns of (a) **2b** at (i) 25 °C as a precipitate from CH_2Cl_2/MeOH, (ii) 210 °C upon cooling from Iso, (iii) 25 °C upon cooling from Iso, and (iv) 213 °C upon heating, (b) **2c** at (i) 25 °C as a precipitate from CH_2Cl_2/MeOH, (ii) 205 °C upon cooling from Iso, (iii) 25 °C upon cooling from Iso, and (iv) 205 °C upon heating, and (c) **2d** at (i) 25 °C as a precipitate from CH_2Cl_2/MeOH, (ii) 195 °C upon cooling from Iso, (iii) 25 °C upon cooling from Iso, and (iv) 195 °C upon heating.



Supporting Figure 17 (Continued)



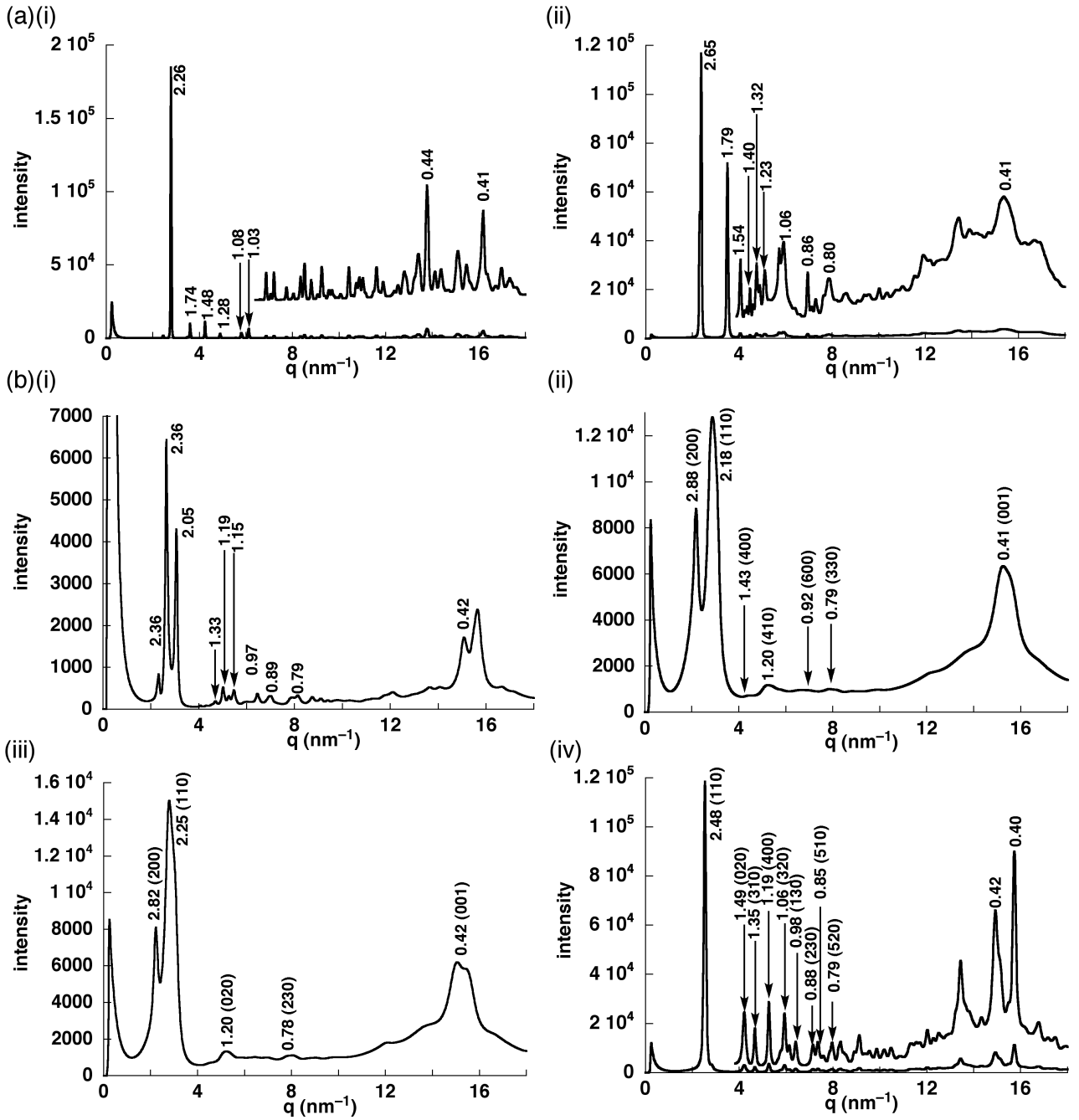
Supporting Figure 18 Packing model structure of Col_h phases of **2b**–**d**.

Supporting Table 3 Summary of XRD data of mesophases of **2b**–**d**.

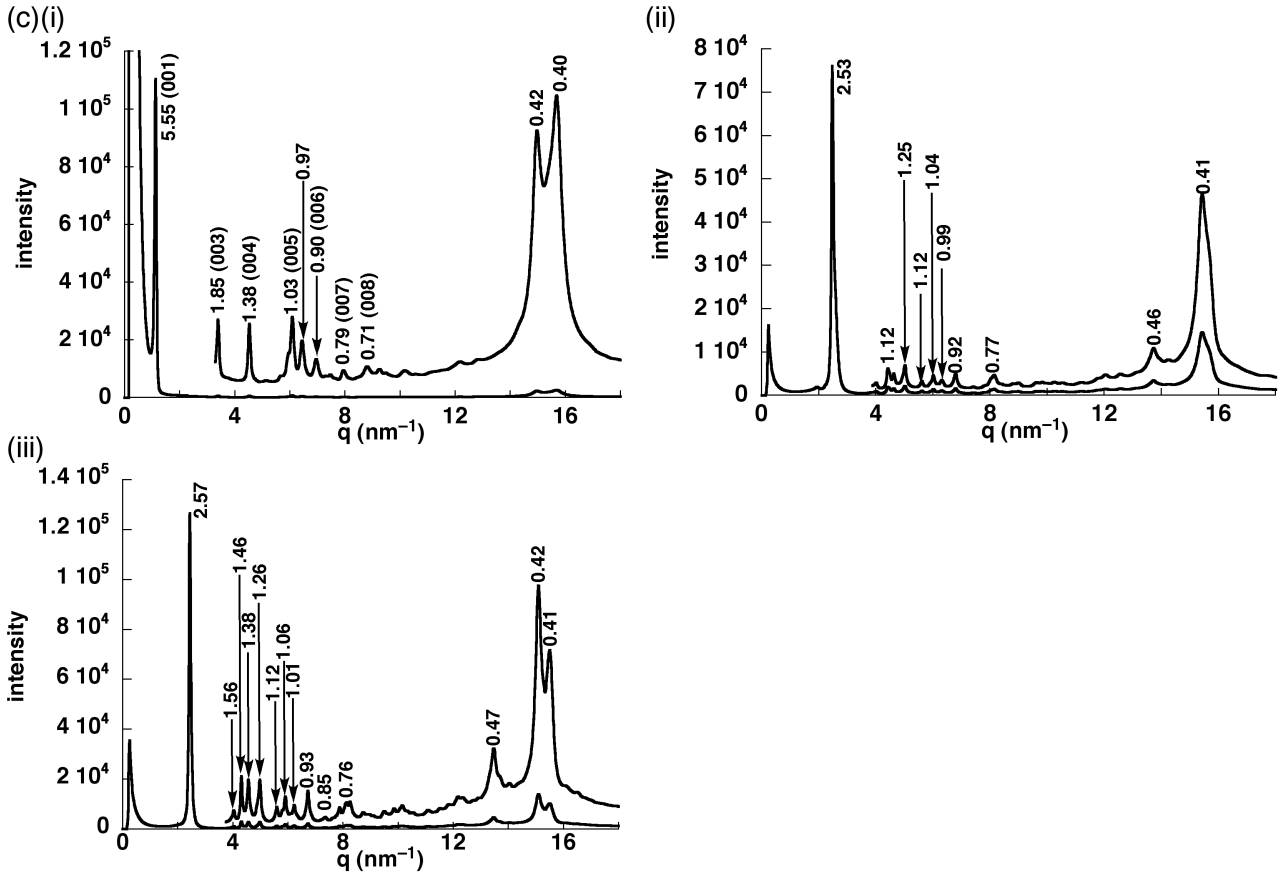
lattice parameters	q (nm^{-1})	d_{obs} (nm)	d_{cal} (nm)	hkl
(a)(i) **2b** at 25 °C (Cr, Col_h) a = 3.08 nm, c = 0.45 nm M = 1241.57, Z = 1.8 ≈ 2 for ρ = 1.0	2.34	2.67	2.67	100
	4.08	1.54	1.54	110
	4.07	1.33	1.34	200
	6.24	1.00	1.01	210
	7.06	0.88	0.89	300
	14.0	0.45	–	001
(a)(ii) **2b** at 210 °C (Col_h) a = 3.21 nm, c = 0.45 nm M = 1241.57, Z = 1.9 ≈ 2 for ρ = 1.0	2.25	2.78	2.78	100
	3.91	1.61	1.60	110
	4.51	1.39	1.39	200
	5.97	1.05	1.05	210
	6.77	0.92	0.92	300
	7.81	0.80	0.80	220
	8.13	0.77	0.77	310
	13.9	0.45	–	001
	14.7	0.43	–	–
(a)(iii) **2b** at 25 °C (Cr, Col_h) a = 3.21 nm, c = 0.45 nm M = 1241.57, Z = 1.9 ≈ 2 for ρ = 1.0	2.31	2.72	2.72	100
	4.01	1.56	1.57	110
	4.63	1.36	1.36	200
	6.13	1.02	1.03	210
	6.94	0.90	0.91	300
	8.02	0.78	0.78	220
	8.35	0.75	0.79	310
	14.3	0.44	–	001
	15.1	0.42	–	–
(a)(iv) **2b** at 213 °C (Col_h) a = 3.22 nm, c = 0.45 nm M = 1241.57, Z = 1.9 ≈ 2 for ρ = 1.0	2.25	2.79	2.79	100
	3.91	1.61	1.61	110
	4.50	1.40	1.39	200
	5.96	1.05	1.05	210
	6.76	0.92	0.93	300
	7.81	0.80	0.80	220
	8.45	0.74	0.77	310
	13.9	0.45	–	001
	14.7	0.43	–	–
(b)(i) **2c** at 25 °C (Cr, lamellar)	1.97	3.19	3.19	100
	4.81	1.31	1.60	200
	5.92	1.06	1.06	300
	14.2	0.44	–	001
(b)(ii) **2c** at 205 °C (Col_h) a = 3.74 nm, c = 0.45 nm M = 1578.21, Z = 2.0 ≈ 2 for ρ = 1.0	1.94	3.24	3.24	100
	3.89	1.62	1.62	200
	5.14	1.22	1.22	210
	5.82	1.08	1.08	300
	6.73	0.93	0.94	220
	7.01	0.90	0.89	310
	13.9	0.45	–	001

Supporting Table 3 (Continued)

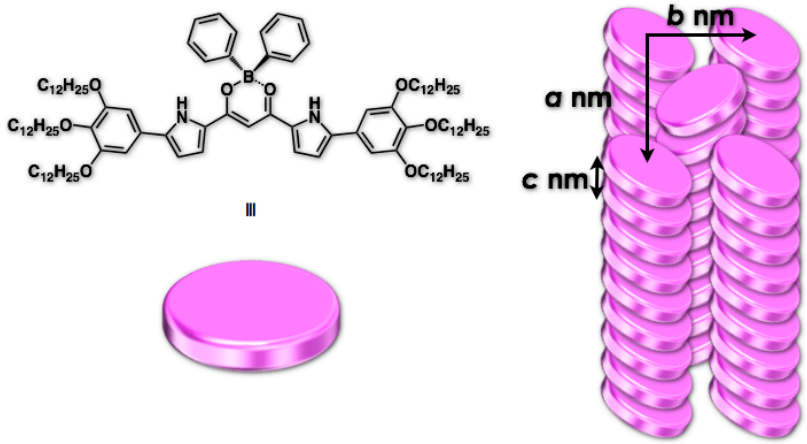
lattice parameters	q (nm^{-1})	d_{obs} (nm)	d_{cal} (nm)	hkl
(b)(iii)	1.98	3.18	3.18	100
2c	5.38	1.17	1.20	210
at 25 °C (Cr, Col_h)	5.82	1.08	1.06	300
a = 3.67 nm, c = 0.45 nm	14.3	0.44	–	001
M = 1578.21, Z = 2.0 ≈ 2 for ρ = 1.0				
	1.98	3.18	3.18	100
(b)(iv)	3.89	1.62	1.59	200
2c	5.14	1.22	1.20	210
at 205 °C (Col_h)	5.82	1.08	1.06	300
a = 3.67 nm, c = 0.45 nm	6.74	0.93	0.92	220
M = 1578.21, Z = 2.0 ≈ 2 for ρ = 1.0	7.01	0.90	0.88	310
	13.9	0.45	–	001
	1.78	3.53	3.53	100
(c)(i)	3.17	1.98	2.04	110
2d	3.60	1.76	1.77	200
at 25 °C (Cr, Col_h)	4.90	1.28	1.33	210
a = 4.07 nm, c = 0.44 nm	14.4	0.44	–	001
M = 1914.85, Z = 1.9 ≈ 2 for ρ = 1.0	15.4	0.41	–	–
	1.73	3.63	3.63	100
	3.01	2.09	2.09	110
(c)(ii)	3.47	1.81	1.82	200
2d	4.51	1.39	1.37	210
at 195 °C (Col_h)	5.18	1.21	1.21	300
a = 4.19 nm, c = 0.45 nm	6.02	1.04	1.05	220
M = 1914.85, Z = 2.1 ≈ 2 for ρ = 1.0	6.26	1.00	1.01	310
	13.9	0.45	–	001
	1.78	3.53	3.53	100
(c)(iii)	3.14	2.00	2.04	110
2d	3.61	1.74	1.77	200
at 25 °C (Cr, Col_h)	4.85	1.30	1.33	210
a = 4.07 nm, c = 0.44 nm	14.0	0.44	–	001
M = 1914.85, Z = 1.9 ≈ 2 for ρ = 1.0	15.3	0.41	–	–
	1.73	3.63	3.63	100
	3.01	2.09	2.10	110
(c)(iv)	3.47	1.81	1.82	200
2d	4.60	1.36	1.37	210
at 195 °C (Col_h)	5.21	1.21	1.21	300
a = 4.19 nm, c = 0.45 nm	6.02	1.04	1.05	220
M = 1914.85, Z = 2.1 ≈ 2 for ρ = 1.0	6.26	1.00	1.01	310
	14.3	0.45	–	001



Supporting Figure 19 XRD patterns of (a) **3b** at (i) 25 °C as a precipitate from CH_2Cl_2/MeOH and (ii) 20 °C upon cooling from Iso, (b) **3c** at (i) 25 °C as a precipitate from CH_2Cl_2/MeOH, (ii) 15 °C upon cooling from Iso, (iii) 35 °C upon heating, and (iv) 55 °C upon heating, and (c) **3d** at (i) 25 °C as a precipitate from CH_2Cl_2/MeOH, (ii) 25 °C upon cooling from Iso, and (iii) 75 °C upon heating. The XRD pattern in (a)(i) and (ii) were evidently derived from crystalline states, and those in (b)(i) and (c)(ii,iii) showed many unidentified peaks with highly ordered structures formed by cooling from Iso.



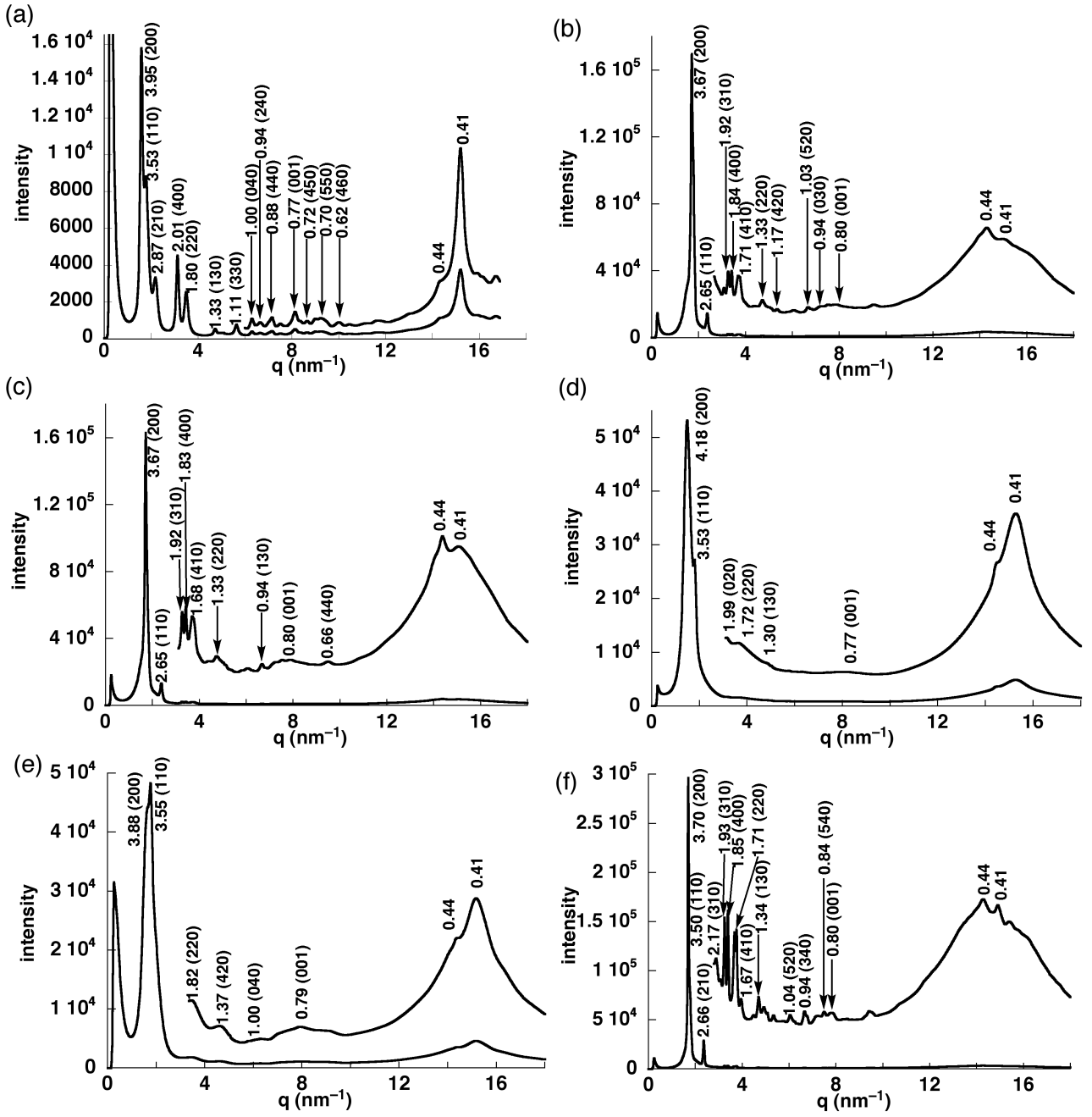
Supporting Figure 19 (Continued)



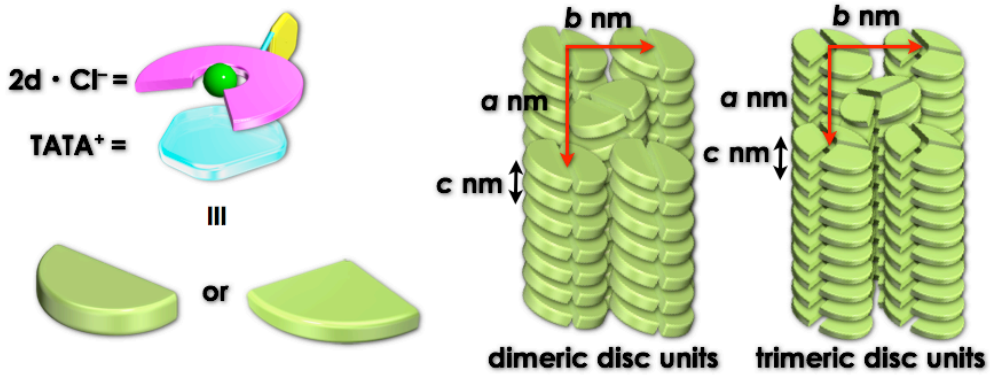
Supporting Figure 20 Packing model structures of Col_r phases of **3b** at 35 and 55 °C.

Supporting Table 4 Summary of XRD data of mesophases of **3c–d**.

lattice parameters	q (nm^{-1})	d_{obs} (nm)	d_{cal} (nm)	hkl
(b)(ii) **3c** at 15 °C (Cr, Col_r) a = 5.77 nm, b = 2.19 nm, c = 0.41 nm M = 1624.32, Z = 1.9 ≈ 2 for ρ = 1.0	2.18	2.88	2.89	200
	2.87	2.18	2.05	110
	4.40	1.43	1.45	400
	5.23	1.20	1.20	410
	6.80	0.92	0.97	600
	7.86	0.79	0.79	520
	15.3	0.41	–	001
(b)(iii) **3c** at 35 °C (Cr, Col_r) a = 5.62 nm, b = 2.46 nm, c = 0.42 nm M = 1624.32, Z = 2.1 ≈ 2 for ρ = 1.0	2.23	2.82	2.81	200
	2.79	2.25	2.26	110
	5.22	1.20	1.20	120
	8.04	0.78	0.80	230
	15.1	0.42	–	001
(b)(iv) **3c** at 55 °C (Cr, Col_r) a = 4.47 nm, b = 2.98 nm, c = 0.42 nm M = 1624.32, Z = 2.1 ≈ 2 for ρ = 1.0	2.54	2.48	2.48	110
	4.21	1.49	1.49	020
	4.67	1.35	1.33	310
	5.26	1.19	1.12	400
	5.92	1.06	1.05	320
	6.13	1.02	1.04	410
	6.41	0.98	0.97	130
	7.14	0.88	0.89	230
	7.35	0.85	0.86	510
	7.95	0.79	0.77	520
	14.9	0.42	–	001
	15.7	0.40	–	–
(c)(i) **3d** at 25 °C (Cr, lamellar) M = 1960.96	1.13	5.55	5.21	001
	2.23	1.88	1.74	003
	4.53	1.39	1.30	004
	6.09	1.03	1.04	005
	6.95	0.90	0.87	006
	7.94	0.79	0.74	007
	8.80	0.71	0.65	008
	14.9	0.42	–	–
	15.7	0.40	–	–



Supporting Figure 21 XRD patterns of **2d**·Cl⁻-TATA⁺ at (a) 25 °C as a precipitate from 1,4-dioxane, (b) 64 °C upon cooling from Iso, (c) 50 °C upon cooling from Iso, (d) 20 °C upon cooling from Iso, (e) 53 °C upon heating, and (f) 82 °C upon heating.



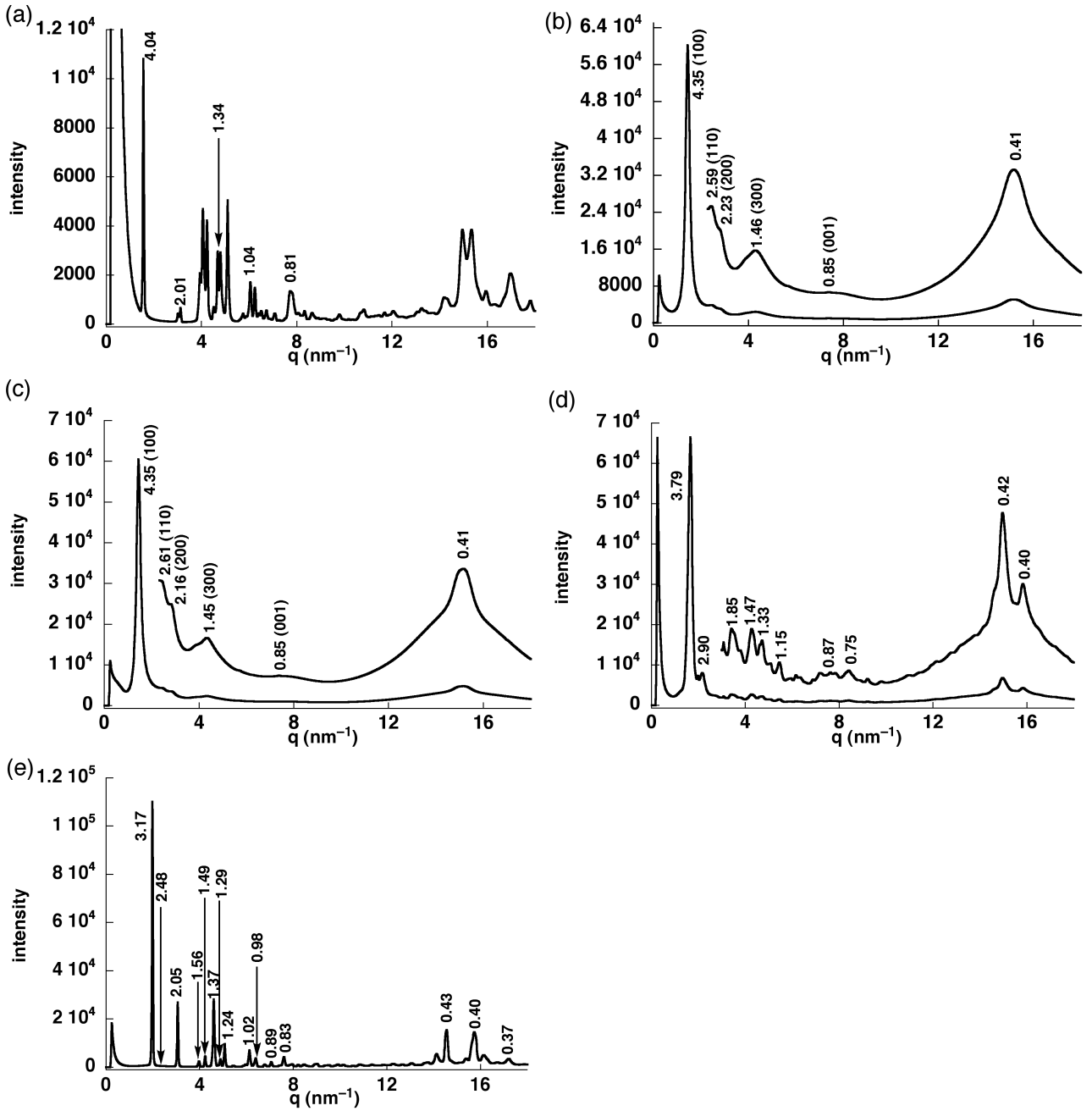
Supporting Figure 22 Packing model structure of a Col_r phase of **2d**·Cl⁻-TATA⁺.

Supporting Table 5 Summary of XRD data of mesophases of **2d**·Cl^--$TATA^+$.

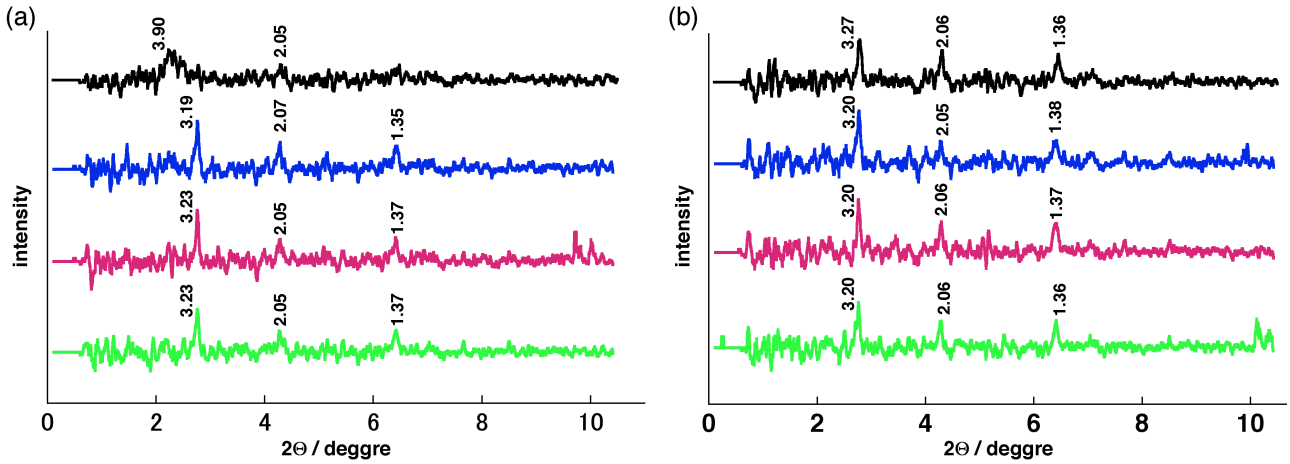
lattice parameters	q (nm^{-1})	d_{obs} (nm)	d_{cal} (nm)	hkl
(a) **2d**·Cl^--$TATA^+$ at 25 °C (Cr, Col_r) a = 7.90 nm, b = 3.95 nm, c = 0.77 nm M = 2357.85, Z = 6.1 ≈ 6 for ρ = 1.0	1.59	3.95	3.95	200
	1.77	3.53	3.53	110
	2.18	2.87	2.79	210
	3.13	2.01	1.98	400
	3.50	1.80	1.77	220
	4.73	1.33	1.30	130
	5.64	1.11	1.18	330
	6.30	1.00	0.99	040
	6.66	0.94	0.96	240
	7.15	0.88	0.88	440
	8.14	0.77	–	001
	8.66	0.73	0.73	450
	9.02	0.70	0.71	550
	10.0	0.62	0.62	460
	14.3	0.44	–	–
	15.2	0.41	–	–
(b) **2d**·Cl^--$TATA^+$ at 64 °C (Col_r) a = 7.34 nm, b = 2.84 nm, c = 0.80 nm M = 2357.85, Z = 4.3 ≈ 4 for ρ = 1.0	1.71	3.67	3.67	200
	2.37	2.65	2.65	110
	3.27	1.92	1.85	310
	3.40	1.84	1.84	400
	3.68	1.71	1.54	410
	4.72	1.33	1.33	220
	5.36	1.17	1.12	420
	6.05	1.03	1.02	520
	6.67	0.94	0.95	030
	7.86	0.80	–	001
	14.3	0.44	–	–
(c) **2d**·Cl^--$TATA^+$ at 50 °C (Col_r) a = 7.34 nm, b = 2.82 nm, c = 0.80 nm M = 2357.85, Z = 4.2 ≈ 4 for ρ = 1.0	1.71	3.67	3.67	200
	2.38	2.64	2.65	110
	3.26	1.92	1.85	310
	3.42	1.83	1.84	400
	3.73	1.68	1.54	410
	4.74	1.33	1.32	220
	6.68	0.94	0.94	130
	7.87	0.80	–	001
	9.47	0.66	0.66	440
	14.4	0.44	–	–
	15.1	0.41	–	–

Supporting Table 5 (Continued)

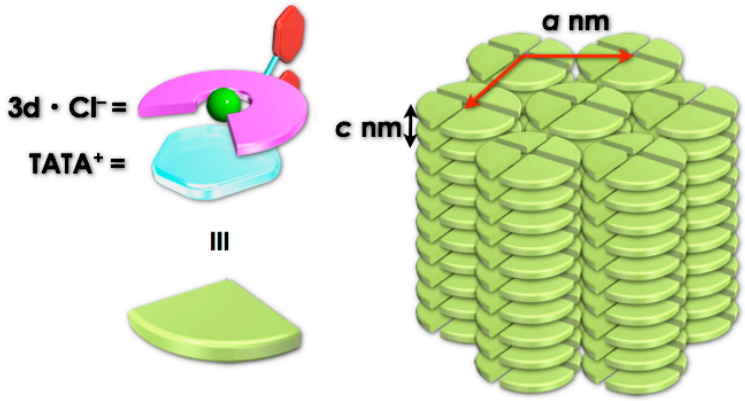
lattice parameters	q (nm^{-1})	d_{obs} (nm)	d_{cal} (nm)	hkl
(d) **2d**·Cl^--$TATA^+$ at 20 °C (Col_r) a = 8.36 nm, b = 3.89 nm, c = 0.77 nm M = 2357.85, Z = 6.4 ≈ 6 for ρ = 1.0	1.50	4.18	4.18	200
	1.78	3.53	3.53	110
	3.15	1.99	1.95	020
	3.64	1.72	1.76	220
	4.84	1.30	1.28	130
	8.16	0.77	–	001
	14.5	0.44	–	–
	15.3	0.41	–	–
(e) **2d**·Cl^--$TATA^+$ at 53 °C (Col_r) a = 7.76 nm, b = 3.99 nm, c = 0.79 nm M = 2357.85, Z = 6.1 ≈ 6 for ρ = 1.0	1.62	3.88	3.88	200
	1.77	3.55	3.55	110
	3.44	1.83	1.77	220
	4.60	1.37	1.39	420
	6.28	1.00	1.00	040
	7.94	0.79	–	001
	14.3	0.44	–	–
	15.2	0.41	–	–
(f) **2d**·Cl^--$TATA^+$ at 82 °C (Col_r) a = 7.40 nm, b = 3.97 nm, c = 0.80 nm M = 2357.85, Z = 6.0 ≈ 6 for ρ = 1.0	1.70	3.70	3.70	200
	1.79	3.50	3.50	110
	2.36	2.66	2.71	210
	2.90	2.17	2.10	310
	3.25	1.93	1.92	120
	3.39	1.85	1.85	400
	3.67	1.71	1.75	220
	3.75	1.67	1.68	410
	4.71	1.34	1.30	130
	6.04	1.04	1.08	430
	6.65	0.94	0.92	340
	7.50	0.84	0.82	540
	7.86	0.80	–	001
	14.3	0.44	–	–
	15.0	0.41	–	–



Supporting Figure 23 XRD patterns of **3d**·Cl^--$TATA^+$ at (a) 25 °C as a precipitate from 1,4-dixoane, (b) 25 °C upon cooling from Iso, (c) 40 °C upon heating, (d) 60 °C upon heating, and (e) 72 °C upon heating. The XRD pattern in (a) was evidently derived from crystalline peaks. Upon heating of a Col_h phase in (c), the diffraction in (d) showed many unidentified peaks of a crystal phase as a metastable state, which was converted to the mesophase in (e) showing unidentified peaks as a more stable state (see Supporting Figure 24).



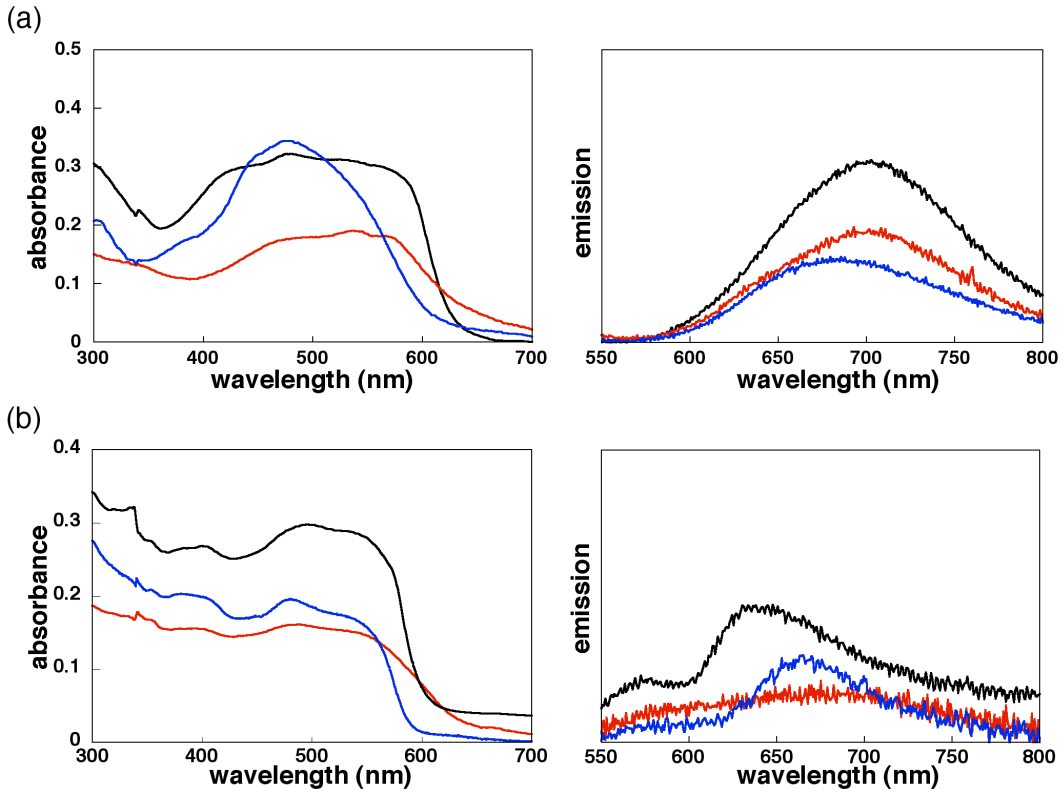
Supporting Figure 24 Time-dependent XRD patterns of **3d**·Cl⁻-TATA⁺ at (a) 60 °C and (b) 72 °C upon 2nd heating annealed for 0 min (black), 10 min (blue), 20 min (red), and 30 min (green). These observations were consistent with the metastable state in (d) in Supporting Figure 23 was converted to the more stable phase in (e) in Supporting Figure 23. The XRD measurements were carried out using a Rigaku NANO-Viewer in the Joint Usage/Research Center (JURC) at Institute for Chemical Research, Kyoto University.



Supporting Figure 25 Packing model structure of a mesophase of **3d**·Cl⁻-TATA⁺ at 25 °C upon cooling from Iso and 40 °C upon 2nd heating.

Supporting Table 6 Summary of XRD data of mesophases of **3d**·Cl⁻-TATA⁺.

lattice parameters	q (nm^{-1})	d_{obs} (nm)	d_{cal} (nm)	hkl
(b) **3d**·Cl⁻-TATA⁺ at 25 °C (Cr, Col_h) a = 5.02 nm, c = 0.85 nm M = 2404.97, Z = 4.2 ≈ 4 for ρ = 0.9	1.44	4.35	4.35	100
	2.42	2.59	2.51	110
	2.81	2.23	2.18	200
	4.31	1.46	1.45	300
	7.38	0.86	0.87	001
	15.1	0.41	–	–
(c) **3d**·Cl⁻-TATA⁺ at 40 °C (Col_h) a = 5.02, c = 0.85 nm M = 2404.97, Z = 4.2 ≈ 4 for ρ = 0.9	1.44	4.35	4.35	100
	2.40	2.62	2.51	110
	2.91	2.16	2.18	200
	4.33	1.45	1.45	300
	7.37	0.85	0.87	001
	15.2	–	–	–



Supporting Figure 26 UV/vis absorption (left) and fluorescence emission (right) spectra of (a) **1d** after annealing 160 °C for 10 min and then cooling to r.t. (black, λ_{max} = 480 nm with shoulders at ca. 425 and 573 nm and λ_{em} = 702 nm excited at 480 nm), **2d** after annealing 190 °C for 10 min and then cooling to r.t. (red, λ_{max} = 536 nm with shoulders at ca. 470 and 573 nm and λ_{em} = 693 nm excited at 536 nm), and **3d** after annealing at 45 °C on heating for 10 min and then cooling to r.t. (blue, λ_{max} = 480 nm and λ_{em} = 685 nm excited at 480 nm) and (b) **1d**·Cl^--$TATA^+$ after annealing 80 °C for 10 min and then cooling to r.t. (black, λ_{max} = ca. 498 nm with shoulders at ca. 560 nm and λ_{em} = 643 nm excited at λ_{ex} = 500 nm), **2d**·Cl^--$TATA^+$ upon annealing 65 °C for 10 min and then cooling to r.t. (red, λ_{max} = ca. 500 nm with shoulders at ca. 560 nm and λ_{em} = 680 nm excited at 500 nm), and **3d**·Cl^--$TATA^+$ after annealing 45 °C on heating for 10 min and then cooling to r.t. (blue, λ_{max} = 480 nm with shoulders at ca. 560 nm and λ_{em} = 662 nm excited at 480 nm). From these observations, although the further examinations are required, similar spectroscopic features were observed in BF_2 and BO_2 complexes. In addition, a smaller shoulder absorption peak of the BC_2 complex at ca. 560 nm than those of BF_2 and BO_2 complexes may suggest less effective stacking structures between π-conjugated moieties.