Electronic Supplementary Information

Solvent-dependent supramolecular assemblies of π-conjugated anion-responsive acyclic oligopyrroles

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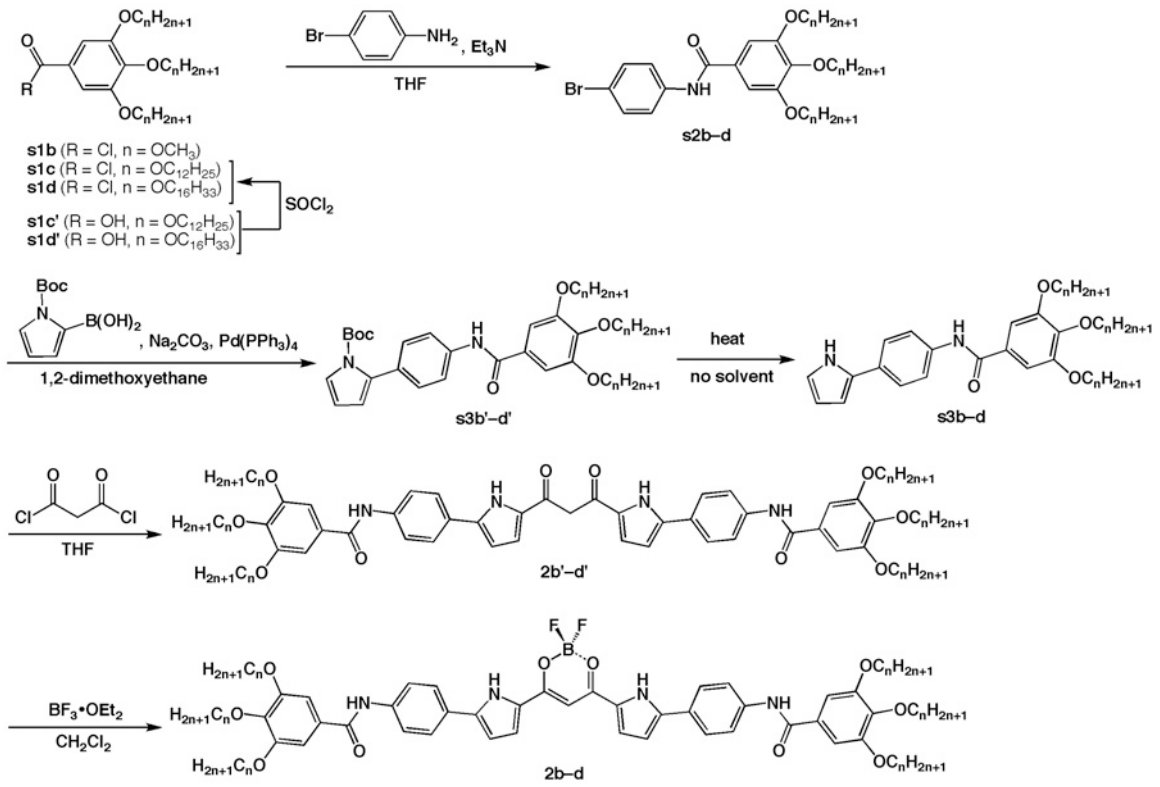
1. Synthetic procedures and spectroscopic data for anion receptors

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. Fast atom bombardment mass spectrometric studies (FAB-MS) 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-300, and Merck silica gel 60 and 60H.



Supporting Figure 1 Synthesis of dipyrrolyldiketone BF_2 complexes **2b–d**.

***N*-(4-Bromophenyl)-3,4,5-trimethoxybenzamide, s2b.** A mixture of 3,4,5-trimethoxybenzoyl chloride **s1b** (576.6 mg, 2.5 mmol) and triethylamine (505.9 mg, 5.0 mmol) in THF (14 mL) and 4-bromoaniline (430.0 mg, 2.5 mmol) in THF (14 mL) was stirred at room temperature for 2 days. The solvent was removed under reduced pressure and stirred the resulting residue triturated in chloroform (30 mL). The organic phase was washed with 0.5 M aqueous HCl (5 mL), saturated $NaHCO_3$ solution (10 mL), water (10 mL) and then dried over Na_2SO_4. Upon removal of the solvent under reduced pressure, the crude product was then added to ethanol (40 mL) and kept in the ice water bath for 12 h. The precipitate was filtered and dried to afford **s2b** (489.6 mg, 52%) as a white solid. R_f = 0.50 (50% EtOAc/hexane). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.69 (br, 1H, NH), 7.54 (d, J = 9.0 Hz, 2H, Ar-H), 7.50 (d, J = 9.0 Hz, 2H, Ar-H), 7.06 (s, 2H, Ar-H), 3.93 (s, 6H, OCH_3), 3.91 (s, 3H, OCH_3). MALDI-TOF-MS: m/z (% intensity): 364.6 (100), 365.6 (52). Calcd for $C_{16}H_{15}BrNO_4$ ([M – H]$^-$): 364.02.

***N*-(4-Bromophenyl)-3,4,5-tridodecyloxybenzamide, s2c.** A thionyl chloride (30 mL) solution of 3,4,5-tridodecyloxybenzoic acid **s1c′**[S1] (4.0 g, 5.9 mmol) was refluxed for 6 h, and the reaction mixture including 3,4,5-tridodecyloxybenzoyl chloride **s1c** was evaporated to dryness. To a dry CH_2Cl_2 (100 mL) solution of the residue were successively added triethylamine (3.0 g, 30.2 mmol) and 4-bromoaniline

(1.1 g, 6.7 mmol), and the mixture was stirred for 9 h at room temperature. The reaction mixture was washed twice with 1 M aqueous HCl (35 mL) and water (30 mL), then the organic phases dried over Na_2SO_4, and evaporated to dryness. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: $CHCl_3$/hexane = 3/4) and recrystallized from $CHCl_3$/MeOH to afford **s2c** (2.1 g, 43%) as a white solid. R_f = 0.54 ($CHCl_3$/hexane = 3/4). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.65 (br, 1H, NH), 7.53 (d, J = 9.0 Hz, 2H, Ar-H), 7.48 (d, J = 9.0 Hz, 2H, Ar-H), 7.02 (s, 2H, Ar-H), 4.04–4.00 (m, 6H, OCH_2), 1.82 (tt, J = 7.2 and 6.6 Hz, 4H, $OCH_2\underline{CH_2}$), 1.74 (tt, J = 7.2 and 6.6 Hz, 2H, $OCH_2\underline{CH_2}$), 1.49–1.44 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.35–1.26 (m, 48H, $OC_3H_6\underline{C_8H_{16}}CH_3$), 0.88–0.86 (m, 9H, $OC_{11}H_{22}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 828.5 (100), 829.4 (54). Calcd for $C_{49}H_{82}BrNO_4$ ($[M]^+$): 827.54.

***N*-(4-Bromophenyl)-3,4,5-trihexadecyloxybenzamide, s2d.** A thionyl chloride (12 mL) solution of 3,4,5-trihexadecyloxybenzoic acid **s1d**´[S1] (1.7 g, 1.74 mmol) was refluxed for 6 h, and the reaction mixture including 3,4,5-trihexadecyloxybenzoyl chloride **s1d** was evaporated to dryness. To a dry CH_2Cl_2 (26 mL) solution of the residue was successively added triethylamine (378.1 mg, 3.74 mmol) and 4-bromoaniline (335.7 mg, 1.95 mmol), and the mixture was stirred for 6 h at room temperature. The reaction mixture was washed twice with 1 M aqueous HCl (3 mL), dried over Na_2SO_4, and evaporated to dryness. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: $CHCl_3$) and recrystallized from $CHCl_3$/MeOH to afford **s2d** (822.6 mg, 46%) as a white solid. R_f = 0.26 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.65 (br, 1H, NH), 7.53 (d, J = 9.0 Hz, 2H, Ar-H), 7.48 (d, J = 9.0 Hz, 2H, Ar-H), 7.02 (s, 2H, Ar-H), 4.04–3.99 (m, 6H, OCH_2), 1.82 (tt, J = 7.2 and 6.6 Hz, 4H, $OCH_2\underline{CH_2}$), 1.74 (tt, J = 7.2 and 6.6 Hz, 2H, $OCH_2\underline{CH_2}$), 1.49–1.44 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.37–1.25 (m, 72H, $OC_3H_6\underline{C_{12}H_{24}}CH_3$), 0.88–0.86 (m, 9H, $OC_{15}H_{30}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 994.9 (100), 995.7 (66). Calcd for $C_{61}H_{106}BrNO_4$ ($[M]^+$): 995.73.

1-*tert*-Butoxycarbonyl-2-(4-(3,4,5-trimethoxybenzoylamino)phenyl)pyrrole and 2-(4-(3,4,5-trimethoxybenzoylamino)phenyl)pyrrole, s3b. To a 1,2-dimethoxyethane solution (20 mL) of **s2b** (357.7 mg, 0.98 mmol), 1-*tert*-butoxycarbonylpyrrole-2-boronic acid (243.0 mg, 1.15 mmol), and tetrakis(triphenylphosphine)palladium(0) (62.2 mg, 0.054 mmol) at room temperature under nitrogen was added an aqueous solution (1.5 mL) of Na_2CO_3 (365.7 mg, 0.05 mmol). The mixture was heated at reflux for 4 h, cooled then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated to give a solid. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 30% EtOAc/hexane) to give **s3b**´ (362.1 mg, 80%) as a white solid. R_f = 0.25 (30% EtOAc/hexane). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.71 (br, 1H, NH), 7.63 (d, J = 8.4 Hz, 2H, Ar-H), 7.37 (d, J = 8.4 Hz, 2H, Ar-H), 7.34–7.33 (m, 1H, pyrrole-H), 7.08 (s, 2H, Ar-H), 6.23–6.22 (m, 1H, pyrrole-H), 6.20–6.19 (m, 1H, pyrrole-H), 3.94 (s, 6H, OCH_3), 3.91 (s, 3H, OCH_3), 1.41 (s, 9H, Boc). MALDI-TOF-MS: *m/z* (% intensity): 452.4 (100), 453.4 (30). Calcd for $C_{25}H_{28}N_2O_6$ ($[M]^+$): 452.19. The product **s3b**´ (362.1 mg, 0.80 mmol) was heated at 190 °C for 15 min. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent 30% EtOAc/CH_2Cl_2) to give **s3b** as a white solid (229.3 mg, 78%). R_f = 0.78 (30% EtOAc/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 8.44 (br, 1H, pyrrole-NH), 7.70 (br, 1H, NH), 7.65–7.64 (d, J = 8.4 Hz, 2H, Ar-H), 7.50–7.49 (d, J = 8.4 Hz, 2H, Ar-H), 7.08 (s, 2H, Ar-H), 6.88–6.87 (m, 1H, pyrrole-H), 6.52–6.51 (m, 1H, pyrrole-H), 6.31–6.30 (m, 1H, pyrrole-H), 3.94 (s, 6H, OCH_3), 3.91 (s, 3H, OCH_3). MALDI-TOF-MS: *m/z* (% intensity): 351.7 (100), 352.7 (20). Calcd for $C_{20}H_{19}N_2O_4$ ($[M - H]^-$): 351.13.

1-*tert*-Butoxycarbonyl-2-(4-(3,4,5-tridodecyloxybenzoylamino)phenyl)pyrrole and 2-(4-(3,4,5-tridodecyloxybenzoylamino)phenyl)pyrrole, s3c. To a 1,2-dimethoxyethane solution (20 mL) of **s2c** (1.02 g, 1.23 mmol), 1-*tert*-butoxycarbonylpyrrole-2-boronic acid (308.7 mg, 1.46 mmol), and tetrakis(triphenylphosphine)palladium(0) (69.5 mg, 0.060 mmol) at room temperature under nitrogen was added an aqueous solution (2.0 mL) of Na_2CO_3 (567.2 mg, 5.32 mmol). The mixture was heated at reflux for 14 h, cooled then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated to give a solid. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 4.5% EtOAc/hexane) to give **s3c**´ (926.3 mg, 82%) as a white solid. R_f = 0.23 (4.5% EtOAc/hexane). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.69 (br, 1H, NH), 7.62 (d, J = 9.0 Hz, 2H, Ar-H), 7.35 (d, J = 9.0 Hz, 2H, Ar-H), 7.34–7.33 (m, 1H, pyrrole-H), 7.04 (s, 2H, Ar-H), 6.23–6.22 (m, 1H, pyrrole-H), 6.19–6.18 (m, 1H, pyrrole-H), 4.05–4.00 (m, 6H, OCH_2), 1.82 (tt, J = 7.2 and 6.6 Hz, 4H, O $CH_2\underline{CH_2}$), 1.75 (tt, J = 7.2 and 6.6 Hz, 2H, $OCH_2\underline{CH_2}$), 1.49–1.44 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.41 (s, 9H, Boc), 1.37–1.25 (m, 48H, $OC_3H_6\underline{C_8H_{16}}CH_3$), 0.88–0.86 (m, 9H, $OC_{15}H_{30}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 913.1 (100), 914.2 (58). Calcd for $C_{58}H_{93}N_2O_6$ ($[M - H]^-$): 913.70. The product **s3c**´ (915.1 mg, 1.0 mmol) was heated at 190 °C for 25 min. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: $CHCl_3$) to give **s3c** (629.4 mg, 77%) as a white solid. R_f = 0.18 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 8.43 (br, 1H, pyrrole-NH), 7.68 (br, 1H, NH), 7.63 (d, J = 9.0 Hz, 2H, Ar-H), 7.48 (d, J = 9.0 Hz, 2H, Ar-H), 7.04 (s, 2H, Ar-H), 6.87–6.86 (m, 1H, pyrrole-H), 6.51–6.50 (m, 1H, pyrrole-H), 6.31–6.29 (m, 1H, pyrrole-H), 4.04 (t, J = 6.6 Hz, 4H, OCH_2), 4.01

(t, J = 6.6 Hz, 2H, OCH_2), 1.81 (tt, J = 7.8 and 6.6 Hz, 4H, $OCH_2\underline{CH_2}$), 1.74 (tt, J = 7.8 and 6.6 Hz, 2H, $OCH_2\underline{CH_2}$), 1.50–1.45 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.33–1.25 (m, 48H, $OC_3H_6\underline{C_8H_{16}}CH_3$), 0.88–0.86 (m, 9H, $OC_{19}H_{38}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 812.9 (100), 813.9 (56). Calcd for $C_{53}H_{85}N_2O_4$ ([M – H]$^-$): 813.65.

1-*tert*-Butoxycarbonyl-2-(4-(3,4,5-trihexadecyloxybenzoylamino)phenyl)pyrrole and 2-(4-(3,4,5-trihexadecyloxybenzoylamino)phenyl)pyrrole, s3d. To a 1,2-dimethoxyethane solution (20 mL) of **s2d** (523.4 mg, 0.52 mmol), 1-*tert*-butoxycarbonylpyrrole-2-boronic acid (137.6 mg, 0.65 mmol), and tetrakis(triphenylphosphine)palladium(0) (36.3 mg, 0.031 mmol) at room temperature under nitrogen was added an aqueous solution (1.0 mL) of Na_2CO_3 (207.3 mg, 1.95 mmol). The mixture was heated at reflux for 6 h, cooled then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated to give a solid. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 9.5% EtOAc/hexane) to give **s3d′** (413.6 mg, 73%) as a white solid. R_f = 0.23 (9.5% EtOAc/hexane). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.69 (br, 1H, NH), 7.62 (d, J = 9.0 Hz, 2H, Ar-H), 7.35 (d, J = 9.0 Hz, 2H, Ar-H), 7.34–7.33 (m, 1H, pyrrole-H), 7.04 (s, 2H, Ar-H), 6.22 (m, 1H, pyrrole-H), 6.19–6.18 (m, 1H, pyrrole-H), 4.04 (t, J = 6.0 Hz, 4H, OCH_2), 4.01 (t, J = 6.0 Hz, 2H, OCH_2), 1.82 (tt, J = 7.2 and 6.6 Hz, 4H, O $CH_2\underline{CH_2}$), 1.75 (tt, J = 7.2 and 6.6 Hz, 2H, $OCH_2\underline{CH_2}$), 1.49–1.44 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.41 (s, 9H, Boc), 1.37–1.25 (m, 72H, $OC_3H_6\underline{C_{12}H_{24}}CH_3$), 0.88–0.86 (m, 9H, $OC_{15}H_{30}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 1082.2 (100), 1083.1 (68). Calcd for $C_{70}H_{118}N_2O_6$ ([M]$^+$): 1082.89. The product **s3d′** (413.0 mg, 0.38 mmol) was heated at 190 °C for 25 min. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: $CHCl_3$) to give **s3d** as a white solid (165.4 mg, 44%). R_f = 0.28 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 8.43 (br, 1H, pyrrole-NH), 7.68 (br, 1H, NH), 7.63 (d, J = 9.0 Hz, 2H, Ar-H), 7.48 (d, J = 9.0 Hz, 2H, Ar-H), 7.04 (s, 2H, Ar-H), 6.87–6.86 (m, 1H, pyrrole-H), 6.51–6.50 (m, 1H, pyrrole-H), 6.31–6.29 (m, 1H, pyrrole-H), 4.04 (t, J = 6.6 Hz, 4H, OCH_2), 4.01 (t, J = 6.6 Hz, 2H, OCH_2), 1.81 (tt, J = 7.8 and 6.6 Hz, 4H, $OCH_2\underline{CH_2}$), 1.74 (tt, J = 7.8 and 6.6 Hz, 2H, $OCH_2\underline{CH_2}$), 1.50–1.45 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.33–1.25 (m, 72H, $OC_3H_6\underline{C_{12}H_{24}}CH_3$), 0.88–0.86 (m, 9H, $OC_{19}H_{38}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 983.6 (100), 984.6 (71). Calcd for $C_{65}H_{110}N_2O_4$ ([M]$^+$): 982.85.

1,3-Bis(5-(4-(3,4,5-trimethoxybenzoylamino)phenyl)pyrrol-2-yl)-1,3-propanedione, 2b′. A THF solution (10 mL) of **s3b** (68.7 mg, 0.19 mmol) was treated with malonyl chloride (9.6 mg, 0.14 mmol) at room temperature and stirred for 3 h at the same temperature. After confirming the consumption of the starting pyrrole by TLC analysis, the mixture was washed with saturated 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 (Wakogel C-300, eluent: 4.5% MeOH/$CHCl_3$) and recrystallized from $CHCl_3$/hexane to afford **2b′** (26.6 mg, 35%) as a pale yellow solid. R_f = 0.22 (4.5% MeOH/$CHCl_3$). ^{1}H NMR (600 MHz, DMSO-d_6, 20 °C; diketone **2b′** was obtained as a mixture of keto and enol tautomers in the ratio of 1:0.42): δ (ppm) keto from 12.05 (br, 2H, pyrrole-NH), 10.21 (br, 2H, NH), 7.91–7.88 (m, 4H, Ar-H), 7.81–7.76 (m, 4H, Ar-H), 7.28 (s, 4H, Ar-H), 7.21–7.20 (m, 2H, pyrrole-H), 6.70–6.69 (m, 2H, pyrrole-H), 4.31 (s, 2H, CH), 3.87 (s, 12H, OCH_3), 3.73 (s, 6H, OCH_3); enol from 16.91 (br, 1H, OH), 11.88 (br, 2H, pyrrole-NH), 10.20 (br, 2H, NH), 8.03–8.02 (m, 4H, Ar-H), 7.96–7.94 (m, 4H, Ar-H), 7.27 (s, 4H, Ar-H), 7.11–7.10 (m, 2H, pyrrole-H), 6.87 (s, 1H, CH), 6.75–6.74 (m, 2H, pyrrole-H), 3.86 (s, 12H, OCH_3), 3.72 (s, 6H, OCH_3). MALDI-TOF-MS: *m/z* (% intensity): 771.2 (100), 772.2 (48). Calcd for $C_{43}H_{39}N_4O_{10}$ ([M – H]$^-$): 771.27.

BF_2 complex of 1,3-bis(5-(4-(3,4,5-trimethoxybenzoylamino)phenyl)pyrrol-2-yl)-1,3-propanedione, 2b. To a CH_2Cl_2 solution (40 mL) of **2b′** (20.6 mg, 0.025 mmol), $BF_3{\cdot}OEt_2$ (13.5 μL, 0.11 mmol) was added and stirred for 45 min at room temperature. After removal of the solvent, flash column chromatography (eluent: 4.5% MeOH/$CHCl_3$) and crystallization from $CHCl_3$/hexane afforded **2b** (8.3 mg, 41%) as a pale red solid. R_f = 0.38 (5% MeOH/$CHCl_3$). ^{1}H NMR (600 MHz, DMSO-d_6, 20 °C): δ (ppm) 12.39 (br, 2H, pyrrole-NH), 10.27 (br, 2H, NH), 7.98 (d, J = 9.0 Hz, 4H, Ar-H), 7.85 (d, J = 9.0 Hz, 4H, Ar-H), 7.48–7.47 (m, 2H, pyrrole-H), 7.30 (s, 4H, Ar-H), 7.22 (s, 1H, CH), 6.92–6.91 (m, 1H, pyrrole-H), 3.88 (s, 12H, OCH_3), 3.74 (s, 6H, OCH_3). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 525.0 (0.94). MALDI-TOF-MS: *m/z* (% intensity): 819.3 (100), 820.3 (50). Calcd for $C_{43}H_{38}BF_2N_4O_{10}$ ([M – H]$^-$): 819.27. This compound was further characterized by X-ray diffraction analysis.

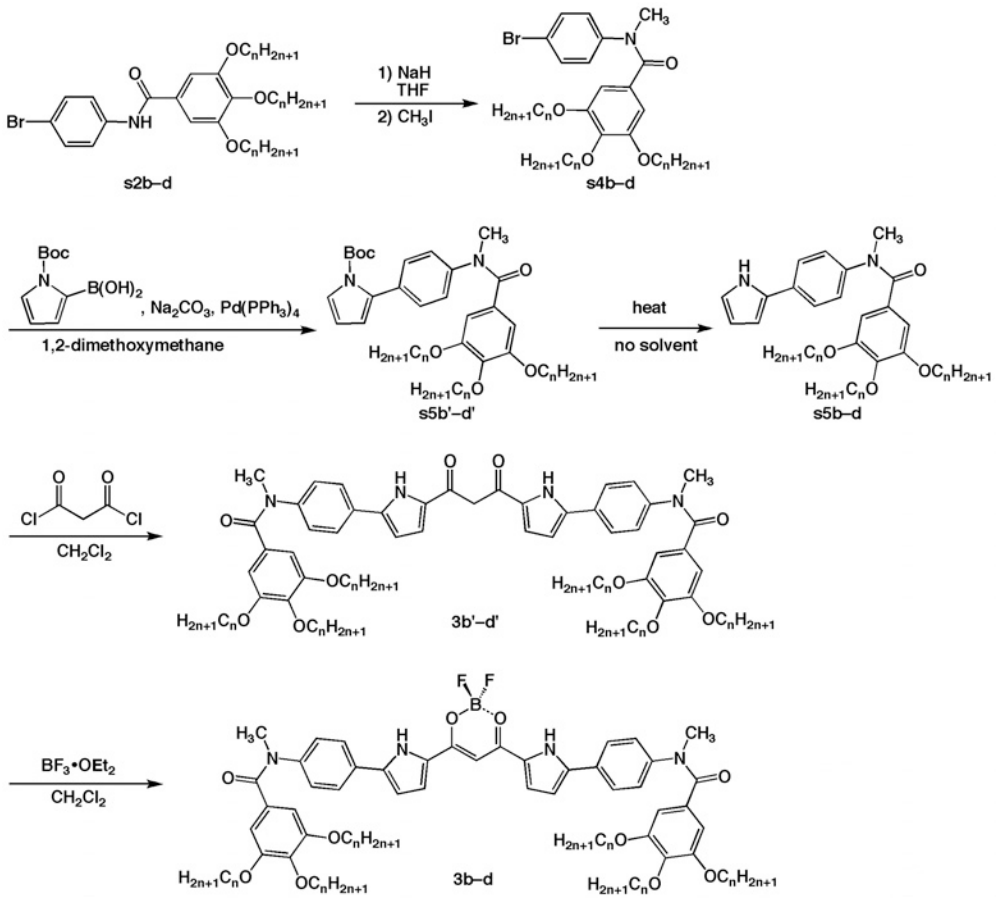
1,3-Bis(5-(4-(3,4,5-tridodecyloxybenzoylamino)phenyl)pyrrol-2-yl)-1,3-propanedione, 2c′. A CH_2Cl_2 solution (20 mL) of **s3c** (474.4 mg, 0.58 mmol) was treated with malonyl chloride (49.3 mg, 0.35 mmol) at room temperature and stirred for 2 h at the same temperature. After confirming the consumption of the starting pyrrole by TLC analysis, the mixture was washed with saturated 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 (Wakogel C-300, eluent: 2% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to afford **2c′** (212.0 mg, 43%) as a pale yellow solid. R_f = 0.23 (2% MeOH/$CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; diketone **2c′** was obtained as a mixture of keto and enol tautomers in the ratio of 1:0.41); δ (ppm) keto from 9.60 (br, 2H, pyrrole-NH), 7.77 (br, 2H, NH), 7.71–7.68 (m, 4H, Ar-H), 7.60–7.57 (m, 4H, Ar-H), 7.16–7.15 (m, 2H,

pyrrole-H), 7.04 (s, 4H, Ar-H), 6.58-6.57 (m, 2H, pyrrole-H), 4.25 (s, 2H, CH), 4.05–4.00 (m, 12H, $\underline{OCH_2}$), 1.85–1.80 (m, 8H, $OCH_2\underline{CH_2}$), 1.79–1.72 (m, 4H, $OCH_2\underline{CH_2}$), 1.48–1.44 (m, 12H, $OC_2H_4\underline{CH_2}$), 1.35–1.25 (m, 144H, $OC_3H_6\underline{C_8H_{16}}$), 0.88–0.86 (m, 18H, $OC_{11}H_{22}\underline{CH_3}$); enol from 16.69 (br, 1H, OH), 9.44 (br, 2H, pyrrole-NH), 7.76 (br, 2H, NH), 7.71–7.68 (m, 4H, Ar-H), 7.60–7.57 (m, 4H, Ar-H), 7.06 (s, 4H, Ar-H), 6.98–6.97 (m, 2H, pyrrole-H), 6.62–6.61 (m, 2H, pyrrole-H), 6.37 (s, 1H, CH), 4.05–4.00 (m, 12H, $\underline{OCH_2}$), 1.85–1.80 (m, 8H, $OCH_2\underline{CH_2}$), 1.79–1.72 (m, 4H, $OCH_2\underline{CH_2}$), 1.48–1.44 (m, 12H, $OC_2H_4\underline{CH_2}$), 1.35–1.25 (m, 144H, $OC_3H_6\underline{C_8H_{16}}$), 0.88–0.86 (m, 18H, $OC_{11}H_{22}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 1696.8 (100), 1697.6 (48). Calcd for $C_{109}H_{171}N_4O_{10}$ ($[M - H]^-$): 1697.30.

BF_2 complex of 1,3-bis(5-(4-(3,4,5-tridodecyloxybenzoylamino)phenyl)pyrrol-2-yl)-1,3-propanedione, 2c. To a CH_2Cl_2 solution (45 mL) of **2c′** (138.9 mg, 0.082 mmol), $BF_3{\cdot}OEt_2$ (100 μL, 0.81 mmol) was added and stirred for 1 h at room temperature. After removal of the solvent, silica gel column chromatography (Wakogel C-300, eluent: 2% MeOH/CH_2Cl_2) and crystallization from $CHCl_3$/MeOH afforded **2c** (83.2 mg, 59%) as a red solid. R_f = 0.32 (2% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.39 (br, 2H, pyrrole-NH), 8.01 (br, 2H, NH), 7.66 (d, J = 9.0 Hz, 2H, Ar-H), 7.49 (d, J = 9.0 Hz, 2H, Ar-H), 7.22–7.21 (m, 2H, pyrrole-H), 7.11 (s, 4H, Ar-H), 6.65–6.64 (m, 2H, pyrrole-H), 6.57 (s, 1H, CH), 4.04–4.00 (m, 12H, OCH_2), 1.80 (tt, J = 7.8 and 6.6 Hz, 8H, $OCH_2\underline{CH_2}$), 1.75 (tt, J = 7.8 and 6.6 Hz, 4H, $OCH_2\underline{CH_2}$), 1.49–1.45 (m, 12H, $OC_2H_4\underline{CH_2}$), 1.35–1.25 (m, 96H, $OC_3H_6\underline{C_8H_{16}}CH_3$), 0.88–0.86 (m, 18H, $OC_{11}H_{22}\underline{CH_3}$). UV/vis ($CH_2Cl_2$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 523.0 (0.77). MALDI-TOF-MS: *m/z* (% intensity): 1744.6 (100), 1745.6 (90). Calcd for $C_{109}H_{170}BF_2N_4O_{10}$ ($[M - H]^-$): 1744.30.

1,3-Bis(5-(4-(3,4,5-trihexadecyloxybenzoylamino)phenyl)pyrrol-2yl)-1,3-propanedione, 2d′. A THF solution (3 mL) of **s3c** (201.73 mg, 0.21 mmol) was treated with malonyl chloride (16.01 mg, 0.11 mmol) at room temperature and stirred for 2 h at the same temperature. After confirming the consumption of the starting pyrrole by TLC analysis, the mixture was washed with saturated Na_2CO_3 aq. and water, dried over anhydrous Na_2SO_4, filtered, and evaporated to dryness. The residue was then chromatographed over flash silica gel column (eluent: 1.5% MeOH/CH_2Cl_2) and recrystallized from $CHCl_3$/MeOH to afford **2d′** (43.01 mg, 21%) as a pale yellow solid. R_f = 0.26 (1.5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; diketone **2d′** was obtained as a mixture of keto and enol tautomers in the ratio of 1:0.18); δ (ppm) keto from 9.57 (br, 2H, pyrrole-NH), 7.76 (br, 2H, NH), 7.71–7.68 (m, 4H, Ar-H), 7.60–7.57 (m, 4H, Ar-H), 7.16–7.15 (m, 2H, pyrrole-H), 7.05 (s, 4H, Ar-H), 6.58-6.57 (m, 2H, pyrrole-H), 4.25 (s, 2H, CH), 4.05–4.00 (m, 12H, $\underline{OCH_2}$), 1.85–1.80 (m, 8H, $OCH_2\underline{CH_2}$), 1.79–1.72 (m, 4H, $OCH_2\underline{CH_2}$), 1.48–1.44 (m, 12H, $OC_2H_4\underline{CH_2}$), 1.35–1.25 (m, 144H, $OC_3H_6\underline{C_{12}H_{24}}$), 0.88–0.86 (m, 18H, $OC_{15}H_{30}\underline{CH_3}$); enol from 16.69 (br, 1H, OH), 9.41 (br, 2H, pyrrole-NH), 7.75 (br, 2H, NH), 7.71–7.68 (m, 4H, Ar-H), 7.60–7.57 (m, 4H, Ar-H), 7.08 (s, 4H, Ar-H), 6.98–6.97 (m, 2H, pyrrole-H), 6.62–6.61 (m, 2H, pyrrole-H), 6.36 (s, 1H, CH), 4.05–4.00 (m, 12H, $\underline{OCH_2}$), 1.85–1.80 (m, 8H, $OCH_2\underline{CH_2}$), 1.79–1.72 (m, 4H, $OCH_2\underline{CH_2}$), 1.48–1.44 (m, 12H, $OC_2H_4\underline{CH_2}$), 1.35–1.25 (m, 144H, $OC_3H_6\underline{C_{12}H_{24}}$), 0.88–0.86 (m, 18H, $OC_{15}H_{30}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 2033.7 (100), 2034.2 (74). Calcd for $C_{133}H_{220}N_4O_{10}$ ($[M - H]^-$): 2033.68.

BF_2 complex of 1,3-bis(5-(4-(3,4,5-trihexadecyloxybenzoylamino)phenyl)pyrrol-2-yl)-1,3-propanedione, 2d. To a CH_2Cl_2 solution (4 mL) of **2d′** (15.4 mg, 0.0075 mmol), $BF_3{\cdot}OEt_2$ (6.0 μL, 0.048 mmol) was added and stirred for 1 h at room temperature. After removal of the solvent, flash silica gel column chromatography (eluent: 1% MeOH/CH_2Cl_2) and crystallization from $CHCl_3$/MeOH afforded **2d** (5.9 mg, 37%) as a pale red solid. R_f = 0.22 (1% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.45 (br, 2H, pyrrole-NH), 7.94 (br, 2H, NH), 7.69 (d, J = 9.0 Hz, 2H, Ar-H), 7.54 (d, J = 9.0 Hz, 2H, Ar-H), 7.22–7.21 (m, 2H, pyrrole-H), 7.09 (s, 4H, Ar-H), 6.67–6.66 (m, 2H, pyrrole-H), 6.56 (s, 1H, CH), 4.04–4.00 (m, 12H, OCH_2), 1.81 (tt, J = 7.8 and 6.6 Hz, 8H, $OCH_2\underline{CH_2}$), 1.75 (tt, J = 7.8 and 6.6 Hz, 4H, $OCH_2\underline{CH_2}$), 1.49–1.45 (m, 12H, $OC_2H_4\underline{CH_2}$), 1.35–1.25 (m, 96H, $OC_3H_6\underline{C_{12}H_{25}}CH_3$), 0.88–0.86 (m, 18H, $OC_{15}H_{30}\underline{CH_3}$). UV/vis ($CH_2Cl_2$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 524.0 (0.71). MALDI-TOF-MS: *m/z* (% intensity): 2081.6 (100), 2082.6 (94). Calcd for $C_{133}H_{218}BF_2N_4O_{10}$ ($[M - H]^-$): 2081.68.



Supporting Figure 2 Synthesis of dipyrrolyldiketone BF_2 complexes **3b–d**.

Methyl *N*-(4-bromophenyl)-3,4,5-trimethoxybenzamide, s4b. The apparatus was charged with anhydrous THF (17.5 mL) of NaH as a suspension in 60% mineral oil (41.2 mg, 1.71 mmol). Benzamide **s2b** (398.4 mg, 1.09 mmol) in anhydrous THF (17.5 mL) was added dropwise. After 4 h, CH_3I (186.9 mg, 1.32 mmol) was added to the mixture and stirred for 5 h at the room temperature. After confirming the consumption of the starting benzamide by TLC analysis, the reaction mixture was added dropwise into H_2O (50 mL) and stirred for 30 min, and the mixture was washed with dilute HCl aq., extracted with ether, then organic layer was washed three times with dilute HCl aq., saturated NaCl aq., dried over anhydrous Na_2SO_4, filtered, and evaporated to dryness. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 50% EtOAc/hexane) to give **s4b** (238.5 mg, 58%) as a white solid. R_f = 0.45 (50% EtOAc/hexane). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.39 (d, J = 9.0 Hz, 2H, Ar-H), 6.94 (d, J = 9.0 Hz, 2H, Ar-H), 6.52 (s, 2H, Ar-H), 3.80 (s, 3H, OCH_3), 3.65 (s, 6H, OCH_3), 3.47 (s, 3H, NCH_3). FAB-MS: *m/z* (% intensity): 379.5 (100), 380.5 (79). Calcd for $C_{17}H_{19}BrNO_4$ ($[M]^+$): 379.04.

Methyl *N*-(4-bromophenyl)-3,4,5-tridodecyloxybenzamide, s4c. The apparatus was charged with anhydrous THF (15.0 mL) of NaH as a suspension in 60% mineral oil (45.6 mg, 1.90 mmol). Benzamide **s2c** (829.3 mg, 1.0 mmol) in anhydrous THF (17.0 mL) was added dropwise. After 4 h, CH_3I (170.9 mg, 1.20 mmol) was added to the mixture and stirred for 6 h at the room temperature. After confirming the consumption of the starting benzamide by TLC analysis, the reaction mixture was added dropwise into H_2O (50 mL) and stirred for 30 min, and the mixture was washed with dilute HCl aq., extracted with ether, washed three times with dilute HCl aq., saturated NaCl aq., dried over anhydrous Na_2SO_4, filtered, and evaporated to dryness. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: $CHCl_3$/hexane = 3/4) to give **s4c** (591.0 mg, 70%) as a white solid. R_f = 0.45 ($CHCl_3$/hexane = 3/4). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.35 (d, J = 9.0 Hz, 2H, Ar-H), 6.91 (d, J = 9.0 Hz, 2H, Ar-H), 6.47 (s, 2H, Ar-H), 3.89 (t, J = 6.6 Hz, 2H, OCH_2), 3.71 (t, J = 6.6 Hz, 4H, OCH_2), 3.45 (s, 3H, NCH_3), 1.69–1.64 (m, 6H, $OCH_2\underline{CH_2}$), 1.46–1.37 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.37–1.25 (m, 48H, $OC_3H_6\underline{C_8H_{16}}CH_3$), 0.89–0.86 (m, 9H, $OC_{15}H_{30}\underline{CH_3}$). FAB-MS: *m/z* (% intensity): 841.4 (100), 842.2 (79). Calcd for $C_{17}H_{19}BrNO_4$ ($[M]^+$): 841.56.

Methyl *N*-(4-bromophenyl)-3,4,5-trihexadecyloxybenzamide, s4d. The apparatus was charged with anhydrous THF (22.0 mL) of NaH as a suspension in 60% mineral oil (74.9 mg, 3.12 mmol). Benzamide

s2d (1.57 g, 1.58 mmol) in anhydrous THF (24.0 mL) was added dropwise. After 4 h, CH_3I (260.0 mg, 1.83 mmol) was added to the mixture and stirred for 12 h at the room temperature. After confirming the consumption of the starting benzamide by TLC analysis, the reaction mixture was added dropwise into H_2O (100 mL) and stirred for 30 min, and the mixture was washed with dilute HCl aq., extracted with ether, washed three times with dilute HCl aq., saturated NaCl aq., dried over anhydrous Na_2SO_4, filtered, and evaporated to dryness. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: $CHCl_3$/hexane = 3/4) to give **s4d** (1.03 g, 68%) as a white solid. R_f = 0.40 ($CHCl_3$/hexane = 3/4). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.35 (d, J = 9.0 Hz, 2H, Ar-H), 6.91 (d, J = 9.0 Hz, 2H, Ar-H), 6.47 (s, 2H, Ar-H), 3.89 (t, J = 6.6 Hz, 2H, OCH_2), 3.71 (t, J = 6.6 Hz, 4H, OCH_2), 3.45 (s, 3H, NCH_3), 1.69–1.64 (m, 6H, $OCH_2\underline{CH_2}$), 1.46–1.37 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.37–1.25 (m, 72H, $OC_3H_6\underline{C_{12}H_{24}}CH_3$), 0.89–0.86 (m, 9H, $OC_{15}H_{30}\underline{CH_3}$). FAB-MS: *m/z* (% intensity): 1009.5 (100), 1010.5 (79). Calcd for $C_{17}H_{19}BrNO_4$ ([M]$^+$): 1009.75.

1-*tert*-Butoxycarbonyl-2-(4-(3,4,5-trimethoxybenzoyl-*N*-methylamino)phenyl)pyrrole and 2-(4-(3,4,5-trimethoxybenzoyl-*N*-methylamino)phenyl)pyrrole, s5b. To a 1,2-dimethoxyethane solution (15 mL) of **s4b** (229.0 mg, 0.60 mmol), 1-*tert*-butoxycarbonylpyrrole-2-boronic acid (169.5 mg, 0.80 mmol), and tetrakis(triphenylphosphine)palladium(0) (44.1 mg, 0.038 mmol) at room temperature under nitrogen was added an aqueous solution (1.5 mL) of Na_2CO_3 (283.5 mg, 2.47 mmol). The mixture was heated at reflux for 6 h, cooled then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated to give a solid. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 45% EtOAc/hexane) to give **s5b´** (207.4 mg, 74%) as a white solid. R_f = 0.55 (45% EtOAc/hexane). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.31–7.30 (m, 1H, pyrrole-H), 7.27 (d, J = 8.4 Hz, 2H, Ar-H), 7.04 (d, J = 8.4 Hz, 2H, Ar-H), 6.60 (s, 2H, Ar-H), 6.20 (t, J = 3.0 Hz, 1H, pyrrole-H), 6.13–6.12 (m, 1H, pyrrole-H), 3.78 (s, 3H, OCH_3), 3.65 (s, 6H, OCH_3), 3.52 (s, 3H, NCH_3), 1.39 (s, 9H, Boc). MALDI-TOF-MS: *m/z* (% intensity): 465.3 (100), 466.3 (18). Calcd for $C_{26}H_{29}N_2O_6$ ([M – H]$^-$): 465.20. The product **s5b´** (204.8 mg, 0.44 mmol) was heated at 190 °C for 15 min. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent 50% EtOAc/hexane) to give **s5b** (118.0 mg, 74%) as a white solid. R_f = 0.44 (50% EtOAc/hexane). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 8.38 (br, 1H, pyrrole-NH), 7.36 (d, J = 8.4 Hz, 2H, Ar-H), 7.05 (d, J = 8.4 Hz, 2H, Ar-H), 6.87–6.86 (m, 1H, pyrrole-H), 6.58 (s, 2H, Ar-H), 6.48–6.47 (m, 1H, pyrrole-H), 6.29–6.28 (m, 1H, pyrrole-H), 6.31–6.30 (m, 1H, pyrrole-H), 3.78 (s, 3H, OCH_3), 3.62 (s, 6H, OCH_3), 3.50 (s, 3H, NCH_3). MALDI-TOF-MS: *m/z* (% intensity): 365.3 (100), 366.3 (18). Calcd for $C_{21}H_{21}N_2O_4$ ([M – H]$^-$): 365.15.

1-*tert*-Butoxycarbonyl-2-(4-(3,4,5-tridodecyloxybenzoyl-*N*-methylamino)phenyl)pyrrole and 2-(4-(3,4,5-tridodecyloxybenzoyl-*N*-methylamino)phenyl)pyrrole, s5c. To a 1,2-dimethoxyethane solution (15 mL) of **s4c** (423.3 mg, 0.50 mmol), 1-*tert*-butoxycarbonylpyrrole-2-boronic acid (131.8 mg, 0.62 mmol), and tetrakis(triphenylphosphine)palladium(0) (35.6 mg, 0.030 mmol) at room temperature under nitrogen was added an aqueous solution (2.0 mL) of Na_2CO_3 (175.9 mg, 1.65 mmol). The mixture was heated at reflux for 6 h, cooled then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated to give a solid. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 10% EtOAc/hexane) to give **s5c´** (418.2 mg, 90%) as a white solid. R_f = 0.23 (10% EtOAc/hexane). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.31–7.30 (m, 1H, pyrrole-H), 7.22 (d, J = 8.4 Hz, 2H, Ar-H), 7.01 (d, J = 8.4 Hz, 2H, Ar-H), 6.54 (s, 2H, Ar-H), 6.23–6.22 (m, 1H, pyrrole-H), 6.09–6.08 (m, 1H, pyrrole-H), 3.88 (t, J = 6.6 Hz, 2H, OCH_2), 3.71 (t, J = 6.6 Hz, 4H, OCH_2), 3.48 (s, 3H, NCH_3), 1.69–1.63 (m, 6H, $OCH_2\underline{CH_2}$), 1.43–1.34 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.39 (s, 9H, Boc), 1.32–1.25 (m, 48H, $OC_3H_6\underline{C_8H_{16}}CH_3$), 0.88–0.86 (m, 9H, $OC_{11}H_{22}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 827.5 (100), 828.5 (37). Calcd for $C_{25}H_{27}N_2O_6$ ([M – Boc]$^-$): 827.16. The product **s5c´** (410.2 mg, 0.44 mmol) was heated at 190 °C for 20 min. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: $CHCl_3$) to give **s5c** (332.4 mg, 90%) as a white solid. R_f = 0.18 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 8.34 (br, 1H, pyrrole-NH), 7.31 (d, J = 8.4 Hz, 2H, Ar-H), 7.01 (d, J = 8.4 Hz, 2H, Ar-H), 6.85–6.84 (m, 1H, pyrrole-H), 6.52 (s, 2H, Ar-H), 6.46–6.44 (m, 1H, pyrrole-H), 6.28–6.26 (m, 1H, pyrrole-H), 3.87 (t, J = 6.6 Hz, 2H, OCH_2), 3.70 (t, J = 6.6 Hz, 4H, OCH_2), 3.48 (s, 3H, NCH_3), 1.67–1.61 (m, 6H, $OCH_2\underline{CH_2}$), 1.40–1.37 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.33–1.24 (m, 48H, $OC_3H_6\underline{C_8H_{16}}CH_3$), 0.88–0.86 (m, 9H, $OC_{11}H_{22}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 827.6 (100), 828.8 (29). Calcd for $C_{54}H_{87}N_2O_4$ ([M – H]$^-$): 827.67.

1- *tert*-Butoxycarbonyl-2-(4-(3,4,5-trihexadecyloxybenzoyl-*N*-methylamino)phenyl)pyrrole and 2-(4-(3,4,5-trihexadecyloxybenzoyl-*N*-methylamino)phenyl)pyrrole, s5d. To a 1,2-dimethoxyethane solution (15 mL) of **s4d** (506.0 mg, 0.50 mmol), 1-*tert*-butoxycarbonyl-pyrrole-2-boronic acid (131.8 mg, 0.62 mmol), and tetrakis(triphenylphosphine)palladium(0) (33.0 mg, 0.028 mmol) at room temperature under nitrogen was added an aqueous solution (2.0 mL) of Na_2CO_3 (239.7 mg, 2.25 mmol). The mixture was heated at reflux for 7 h, cooled then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated to give a solid. The residue was then chromatographed over silica gel column

(Wakogel C-300, eluent: 12.5% EtOAc/hexane) to give **s5d′** (504.0 mg, 92%) as a white solid. R_f = 0.23 (12.5% EtOAc/hexane). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.32–7.31 (m, 1H, pyrrole-H), 7.22 (d, J = 8.4 Hz, 2H, Ar-H), 7.01 (d, J = 8.4 Hz, 2H, Ar-H), 6.54 (s, 2H, Ar-H), 6.19 (t, J = 3.0 Hz, 1H, pyrrole-H), 6.09–6.08 (m, 1H, pyrrole-H), 3.88 (t, J = 6.6 Hz, 2H, OCH_2), 3.71 (t, J = 6.6 Hz, 4H, OCH_2), 3.48 (s, 3H, NCH_3), 1.69–1.63 (m, 6H, $OCH_2\underline{CH_2}$), 1.40–1.35 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.39 (s, 9H, Boc), 1.30–1.29 (m, 72H, $OC_3H_6\underline{C_{12}H_{24}}CH_3$), 0.88–0.86 (m, 9H, $OC_{15}H_{30}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 995.4 (100), 996.4 (68). Calcd for $C_{66}H_{111}N_2O_4$ ([M – Boc]$^-$): 995.85. The product **s5d′** (500.0 mg, 0.45 mmol) was heated at 190 °C for 20 min. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: $CHCl_3$) to give **s5d** as a white solid (366.2 mg, 80%). R_f = 0.20 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 8.34 (br, 1H, pyrrole-NH), 7.31 (d, J = 8.4 Hz, 2H, Ar-H), 7.01 (d, J = 8.4 Hz, 2H, Ar-H), 6.85–6.84 (m, 1H, pyrrole-H), 6.52 (s, 2H, Ar-H), 6.46–6.44 (m, 1H, pyrrole-H), 6.28–6.26 (m, 1H, pyrrole-H), 3.87 (t, J = 6.6 Hz, 2H, OCH_2), 3.70 (t, J = 6.6 Hz, 4H, OCH_2), 3.48 (s, 3H, NCH_3), 1.67–1.61 (m, 6H, $OCH_2\underline{CH_2}$), 1.40–1.37 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.33–1.24 (m, 72H, $OC_3H_6\underline{C_{12}H_{24}}CH_3$), 0.88–0.86 (m, 9H, $OC_{15}H_{30}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 995.5 (100), 996.5 (66). Calcd for $C_{66}H_{111}N_2O_4$ ([M – H]$^-$): 995.85

1,3-Bis(5-(4-(3,4,5-trimethoxybenzoyl-*N*-methylamino)phenyl)pyrrol-2-yl)-1,3-propanedione, 3b′. A CH_2Cl_2 solution (8 mL) of **s5b** (58.0 mg, 0.16 mmol) was treated with malonyl chloride (12.3 mg, 0.087 mmol) at room temperature and stirred for 3 h at the same temperature. After confirming the consumption of the starting pyrrole by TLC analysis, the mixture was washed with saturated 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 (Wakogel C-300, eluent: 4% MeOH/$CHCl_3$) and recrystallized from $CHCl_3$/hexane to afford **3b′** (24.8 mg, 39%) as a pale yellow solid. R_f = 0.25 (4% MeOH/$CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; diketone **3b′** was obtained as a mixture of keto and enol tautomers in the ratio of 1:0.12): δ (ppm) keto from 9.51 (br, 2H, pyrrole-NH), 7.46, (d, J = 8.4 Hz, 4H, Ar-H), 7.12–7.11 (m, 2H, pyrrole-H), 7.11 (d, J = 8.4 Hz, 4H, Ar-H), 6.56 (s, 2H, Ar-H), 6.54–6.53 (m, 2H, pyrrole-H), 4.23 (s, 2H, CH), 3.78 (s, 6H, OCH_3), 3.62 (s, 12H, OCH_3), 3.51 (s, 6H, NCH_3); enol from 16.7 (br, 1H, OH), 9.38 (br, 2H, pyrrole-NH), 7.47 (d, J = 8.4 Hz, 4H, Ar-H), 6.95–6.94 (m, 2H, pyrrole-H), 6.58–6.57 (m, 2H, pyrrole-H), 7.10 (d, J = 8.4 Hz, 4H, Ar-H), 6.34 (s, 1H, CH), 3.79 (s, 6H, OCH_3), 3.64 (s, 12H, OCH_3), 3.52 (s, 6H, NCH_3). MALDI-TOF-MS: *m/z* (% intensity): 799.7 (100), 800.7 (51). Calcd for $C_{45}H_{43}N_4O_{10}$ ([M – H]$^-$): 799.29.

BF_2 complex of 1,3-bis(5-(4-(3,4,5-trimethoxybenzoyl-*N*-methylamino)phenyl)pyrrol-2-yl)-1,3-propanedione, 3b. To a CH_2Cl_2 solution (15 mL) of **3b′** (16.7 mg, 0.021 mmol), $BF_3{\cdot}OEt_2$ (26.0 μL, 0.21 mmol) was added and stirred for 40 min at room temperature. After removal of the solvent, silica gel column chromatography (Wakogel C-300, eluent: 5% MeOH/CH_2Cl_2) and crystallization from CH_2Cl_2/hexane afforded **3b** (12.8 mg, 72%) as a pale yellow solid. R_f = 0.38 (5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.62 (br, 2H, pyrrole-NH), 7.53 (d, J = 8.4 Hz, 4H, Ar-H), 7.21–7.20 (m, 2H, pyrrole-H), 6.68–6.67 (m, 1H, pyrrole-H), 6.58 (s, 4H, Ar-H), 6.53 (s, 1H, CH), 3.79 (s, 6H, OCH_3), 3.65 (s, 12H, OCH_3), 3.54 (s, 6H, NCH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 515.0 (0.87). MALDI-TOF-MS: *m/z* (% intensity): 847.8 (100), 848.8 (90). Calcd for $C_{45}H_{42}BF_2N_4O_{10}$ ([M – H]$^-$): 847.30.

BF_2 complex of 1,3-bis(5-(4-(3,4,5-tridodecyloxybenzoyl-*N*-methylamino)phenyl)pyrrol-2-yl)-1,3-propanedione, 3c. A CH_2Cl_2 solution (20 mL) of **s5c** (332.4 mg, 0.40 mmol) was treated with malonyl chloride (31.2 mg, 0.22 mmol) at room temperature and stirred for 5 h at the same temperature. After confirming the consumption of the starting pyrrole by TLC analysis, the mixture was washed with saturated 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 (Wakogel C-300, eluent: 2.5% MeOH/CH_2Cl_2) and recrystallized from $CHCl_3$/MeOH to afford crude 1,3-bis(5-(4-(3,4,5-tridodecyloxybenzoyl-*N*-amino)phenyl)pyrrol-2-yl)-1,3-propanedione **3c′** (153.3 mg) as a pale yellow solid. R_f = 0.25 (2.5% MeOH/CH_2Cl_2). MALDI-TOF-MS: *m/z* (% intensity): 1724.8 (100), 1725.9 (50). Calcd for $C_{111}H_{175}N_4O_{10}$ ([M – H]$^-$): 1725.33. The crude **3c′** in CH_2Cl_2 solution (40 mL) was treated with $BF_3{\cdot}OEt_2$ (84 μL, 0.68 mmol) stirred for 1 h at room temperature. After removal of the solvent, silica gel column chromatography (Wakogel C-300, eluent: 2.5% MeOH/CH_2Cl_2) and crystallization from $CHCl_3$/ice MeOH afforded **3c** (104.2 mg, 33%) as a red solid. R_f = 0.37 (2.5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.65 (br, 2H, pyrrole-NH), 7.51 (d, J = 8.4 Hz, 4H, Ar-H), 7.19–7.18 (m, 2H, pyrrole-H), 7.13 (d, J = 8.4 Hz, 4H, Ar-H), 6.66–6.65 (m, 2H, pyrrole-H), 6.53 (s, 4H, Ar-H), 6.52 (s, 1H, CH), 3.88 (m, 4H, OCH_2), 3.72 (m, 8H, OCH_2), 3.49 (s, 6H, NCH_3), 1.68–1.63 (m, 12H, $OCH_2\underline{CH_2}$), 1.49–1.38 (m, 4H, $OCH_2\underline{CH_2}$), 1.33–1.31 (m, 12H, $OC_2H_4\underline{CH_2}$), 1.28–1.24 (m, 96H, $OC_3H_6\underline{C_8H_{16}}CH_3$), 0.88–0.86 (m, 18H, $OC_{11}H_{22}\underline{CH_3}$). UV/vis ($CH_2Cl_2$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 513.0 (0.97). MALDI-TOF-MS: *m/z* (% intensity): 1772.7 (100), 1773.7 (73). Calcd for $C_{111}H_{174}BF_2N_4O_{10}$ ([M – H]$^-$): 1773.33.

BF_2 complex of 1,3-bis(5-(4-(3,4,5-trihexadecyloxybenzoyl-*N*-methylamino)phenyl)pyrrol-2-yl)-1,3-propanedione, 3d. A CH_2Cl_2 solution (14

mL) of **s5d** (358.0 mg, 0.36 mmol) was treated with malonyl chloride (30.5 mg, 0.21 mmol) at room temperature and stirred for 3 h at the same temperature. After confirming the consumption of the starting pyrrole by TLC analysis, the mixture was washed with saturated 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 (eluent: 1.5% MeOH/CH_2Cl_2) and recrystallized from $CHCl_3$/MeOH to afford crude 1,3-bis(5-(4-(3,4,5-trihexadecyloxybenzoyl-*N*-amino)phenyl)pyrrol-2-yl)-1, 3-propanedione **3d′** (111.2 mg) as a pale yellow solid. R_f = 0.18 (1.5% MeOH/CH_2Cl_2). MALDI-TOF-MS: *m/z* (% intensity): 2060.6 (100), 2061.6 (72). Calcd for $C_{135}H_{222}N_4O_{10}$ ([M – H]$^-$): 2060.70. The crude **3d′** in CH_2Cl_2 solution (35 mL) was treated with $BF_3{\cdot}OEt_2$ (66 μL, 0.54 mmol) stirred for 1 h at room temperature. After removal of the solvent, silica gel column chromatography (Wakogel C-300, eluent: 2% MeOH/CH_2Cl_2) and crystallization from CH_2Cl_2/MeOH afforded **3d** (72.0 mg, 20%) as a red solid. R_f = 0.44 (2% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.63 (br, 2H, pyrrole-NH), 7.51 (d, J = 8.4 Hz, 4H, Ar-H), 7.19–7.18 (m, 2H, pyrrole-H), 7.13 (d, J = 8.4 Hz, 4H, Ar-H), 6.66–6.65 (m, 2H, pyrrole-H), 6.53 (s, 4H, Ar-H), 6.52 (s, 1H, CH), 3.88 (m, 4H, OCH_2), 3.72 (m, 8H, OCH_2), 3.49 (s, 6H, NCH_3), 1.68–1.63 (m, 12H, $OCH_2\underline{CH_2}$), 1.49–1.38 (m, 4H, $OCH_2\underline{CH_2}$), 1.33–1.31 (m, 12H, $OC_2H_4\underline{CH_2}$), 1.28–1.24 (m, 96H, $OC_3H_6\underline{C_{12}H_{24}}CH_3$), 0.88–0.86 (m, 18H, $OC_{15}H_{30}\underline{CH_3}$). UV/vis ($CH_2Cl_2$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 513.0 (0.95). MALDI-TOF-MS: *m/z* (% intensity): 2109.5 (100), 2110.5 (94). Calcd for $C_{113}H_{174}BF_2N_4O_{10}$ ([M – H]$^-$): 2109.71.

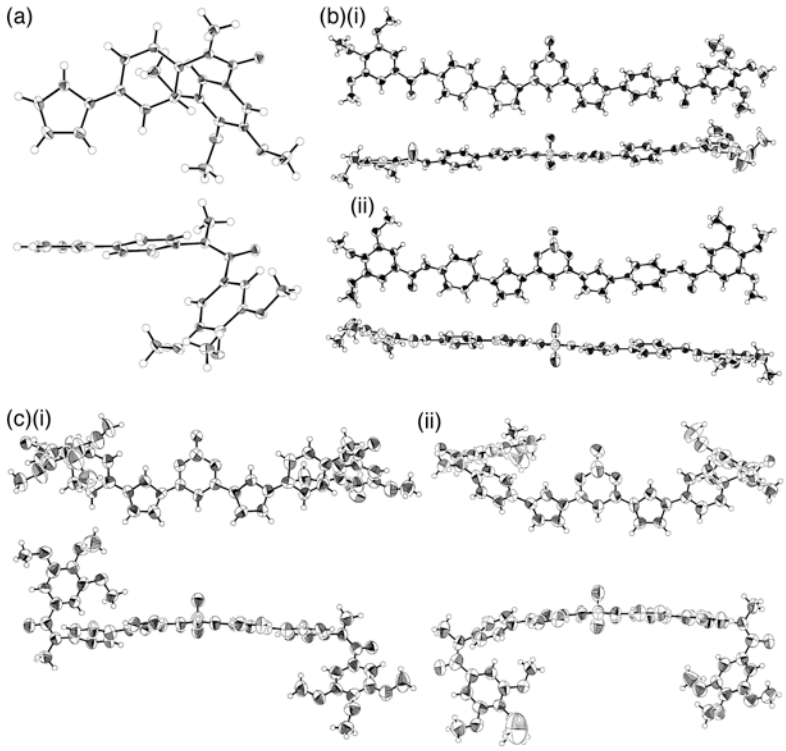
[S1] G. Johansson, V. Percec, G. Ungar and D. Abramic, *J. Chem. Soc., Perkin Trans 1*, 1994, 447.
[S2] H. Maeda, Y. Haketa and T. Nakanishi, *J. Am. Chem. Soc.*, 2007, **129**, 13661.

2. X-ray crystallographic data

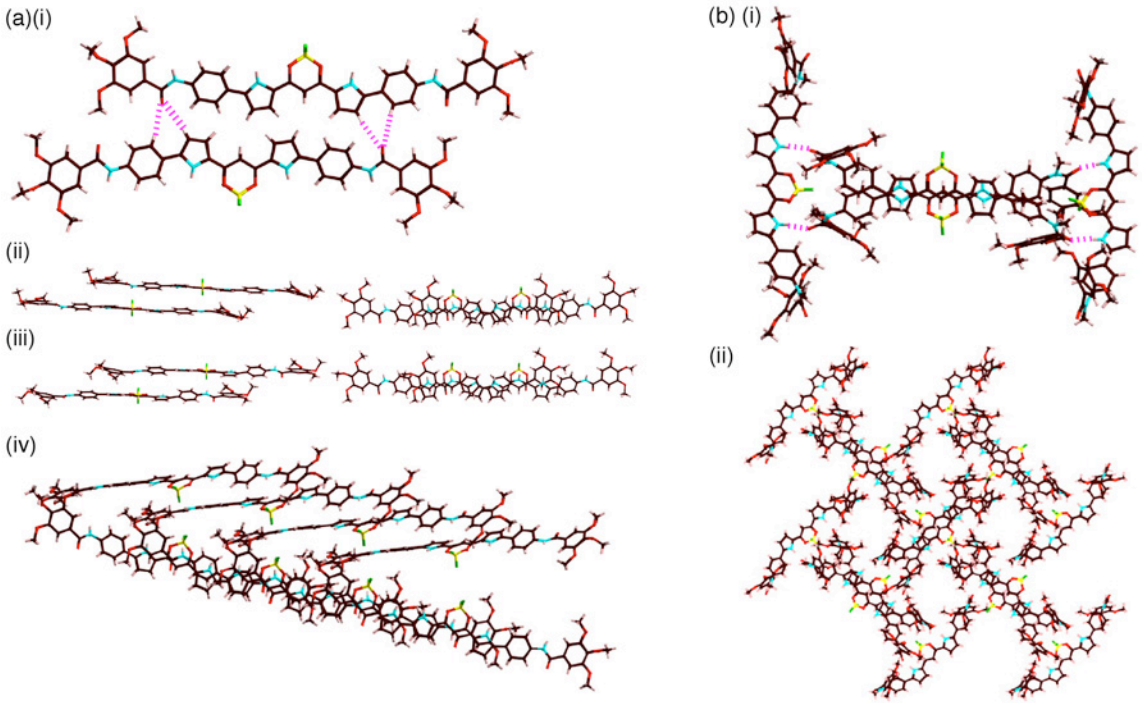
Single-crystal X-ray analysis. Crystallographic data for a pyrrole derivative **s5b** and BF_2 complexes **2b** and **3b** are summarized in Supporting Table 1. A single crystal of **s5b** was obtained by vapor diffusion of hexane into CH_2Cl_2 solution of **s5b**. The data crystal was a colorless prism of approximate dimensions 0.50 mm × 0.30 mm × 0.05 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 **2b** was obtained by vapor diffusion of hexane into an acetone solution of **2b**. The data crystal was a red-colored prism of approximate dimensions 0.45 mm × 0.10 mm × 0.07 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. In each case, the non-hydrogen atoms were refined anisotropically. A single crystal of **3b** was obtained by vapor diffusion of heptane into $CHCl_3$ solution of **3b**. The data crystal was a red-colored prism of approximate dimensions 0.30 mm × 0.20 mm × 0.10 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.[S3] The scattering arising from the presence of disordered solvents in the crystals was removed by use of the utility SQUEEZE in the PLATON software package.[S4] CIF files (CCDC-824850–824852) 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 **s5b**, **2b**, and **3b**.

	S5b	**2b**	**3b**
formula	$C_{21}H_{22}N_2O_4$	$C_{43}H_{39}N_4O_{11}BF_2 \cdot 0.5C_3H_6O$ ·water	$C_{45}H_{43}N_4O_{10}BF_2$
fw	366.41	865.63	848.64
crystal size, mm	0.50 × 0.30 × 0.05	0.45 × 0.10 × 0.07	0.30 × 0.20 × 0.10
crystal system	orthorhombic	triclinic	monoclinic
space group	*Pbca* (no. 61)	*P*-1 (no. 2)	$P2_1/c$ (no. 14)
a, Å	9.166(2)	10.755(3)	22.3431(4)
b, Å	17.124(4)	16.694(6)	21.4597(4)
c, Å	23.657(5)	23.830(9)	24.7703(5)
α, °	90	91.432(14)	90
β, °	90	99.301(12)	105.6660(8)
γ, °	90	103.498(11)	90
V, Å^3	3713.3(15)	4097(2)	11435.6(4)
ρ_{calcd}, gcm^{-3}	1.311	1.412	0.986
Z	8	2	8
T, K	123(2)	123(2)	93(2)
μ, mm^{-1}	0.091 (Mo-Kα)	0.107 (Mo-Kα)	0.619 (Cu-Kα)
no. of reflns	32797	29879	157385
no. of unique reflns	4241	14024	16887
variables	248	1094	1142
λ, Å	0.71075 (Mo-Kα)	0.71075 (Mo-Kα)	1.54187 (Cu-Kα)
R_1 ($I > 2\sigma(I)$)	0.0391	0.0897	0.1076
wR_2 ($I > 2\sigma(I)$)	0.0935	0.1657	0.2759
GOF	1.050	0.801	0.914



Supporting Figure 3 ORTEP drawings (top and side view) of single-crystal X-ray structures of (a) **s5b**, (b) **2b** (two independent structures (i) and (ii)), and (c) **3b** (two independent structures (i) and (ii)). Thermal ellipsoids are scaled to the 50% probability level.



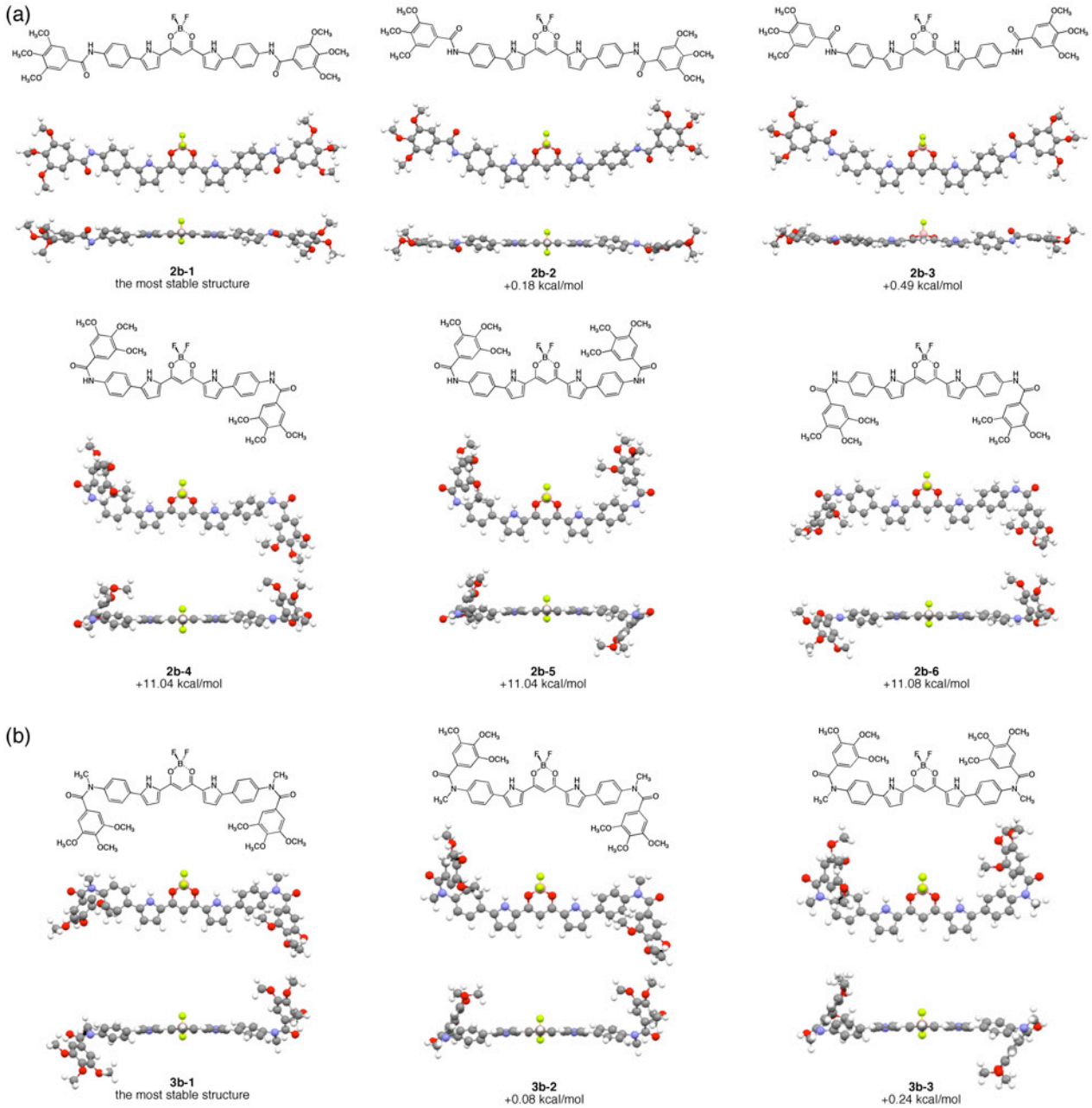
Supporting Figure 4 Assembled structures of (a) **2b** ((i) dimeric structure and (ii, iii) two kinds of stacking structures (top and side view), and (iv) assembled structures) and (b) **3b** ((i) assembled structure and (ii) packing diagram) in the solid state: Atom color code: brown, pink, yellow, green, blue, and red represent carbon, hydrogen, boron, fluorine, nitrogen, and oxygen, respectively.

[S3] *CrystalStructure (Ver. 3.8), Single Crystal Structure Analysis Software,* Rigaku/MSC and Rigaku Corporation, 2006.

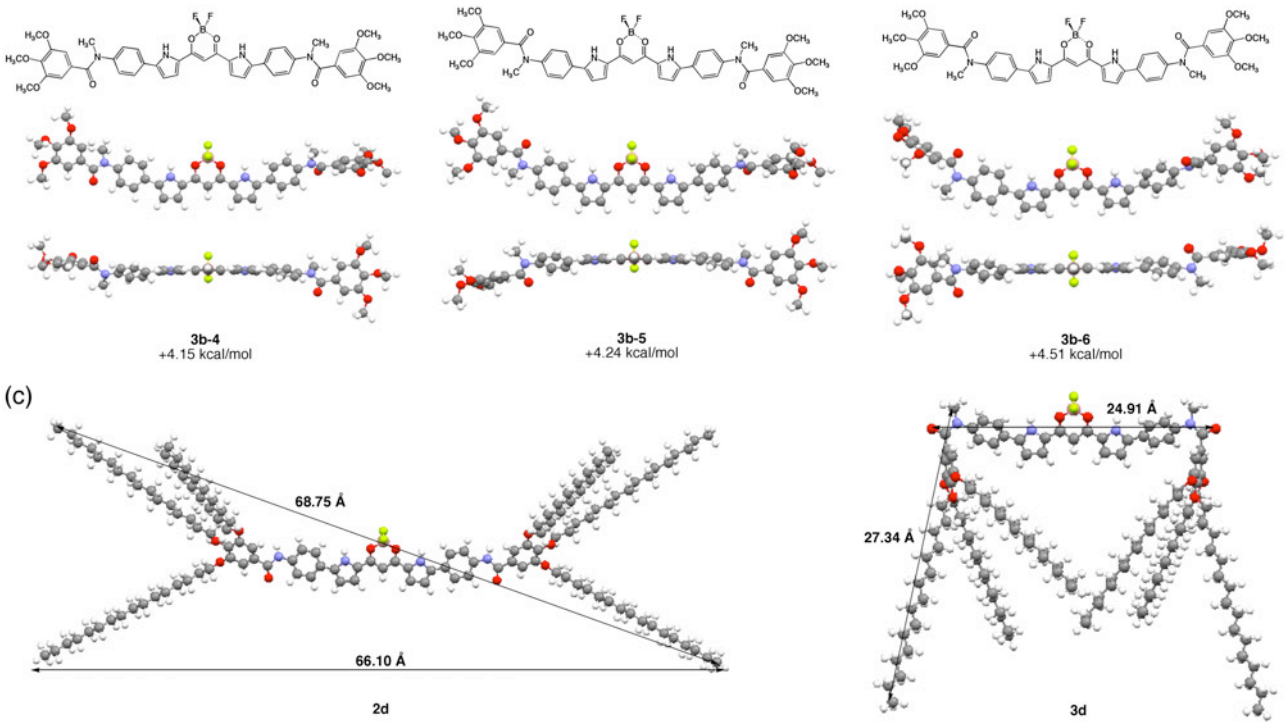
[S4] (a) A. L. Spek, *PLATON, A Multipurpose Crystallographic Tool*, Utrecht University, Utrecht, 2005. (b) P. van der Sluis, A. L. Spek, *Acta Crystallogr. Sect. A*, 1990, **46**, 194.

3. Optimization of anion receptors

DFT and AM1 calculation. Ab initio calculations of anion receptors were carried out by using Gaussian 03 program[S5] 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 **2b** and **3b** and at AM1 level for **2d** and **3d**.



Supporting Figure 5 Optimized structures of (a) **2b**, (b) **3b** (six conformations according to the orientation of amide moieties for each compound) at B3LYP/6-31G(d,p) level, and (c) **2d** and **3d** at AM1 level. As observed in (a) and (b), the relative stabilities according to the orientations of amide moieties suggest that amide-NH **2b** and amide-N-methyl **3b** prefer *trans*- and *cis*-conformations, respectively.



Supporting Figure 5 (Continued).

Cartesian Coordination of 2b-1

–2858.0781581 hartree

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C,2.5612145278,0.1991171854,4.5269686294
C,1.5647398733,0.5267637728,1.0771552307
C,2.1075299109,0.9198617312,-0.1478951969
C,1.3250785452,0.8023228885,-1.2981183179
C,-2.2374125818,2.9683188715,-16.3705308099
C,-4.3441252226,-0.4216383341,-16.1361647175
C,1.8133747398,1.0767137996,-2.6212514709
C,3.0612864662,1.4571556641,-3.1240238329
C,2.9419894001,1.5571697164,-4.5178327415
C,1.619947437,1.2391170541,-4.8647065304
C,-5.3646245488,-0.6783989296,-11.8424764703
C,2.1820736028,-0.1433871227,5.8948021147
C,0.9674962069,1.2011799393,-6.1705106789
C,1.0749005456,-0.9651689966,6.1725792967
C,0.7262715146,-1.275404669,7.4787724739
C,1.4761765396,-0.7844516248,8.5607907537
C,2.5908065899,0.0308555575,8.2999413596
C,2.9230638726,0.3407293865,6.9867985658
C,1.7224771776,1.0401363192,-7.3452412982
C,1.1322403206,1.0004769608,-8.6025889499
C,-0.2635268493,1.1161642801,-8.7187462186
C,-1.0305218195,1.2786557762,-7.552886941
C,-0.4270879444,1.3252692277,-6.304752459
C,-2.8435134166,-3.7028135149,13.639864691
C,-1.2442155294,-1.6873449642,16.7581733278
C,-2.0063422127,1.3667232191,-14.6286695692
C,-3.2938685711,0.8429807243,-14.4394596289
F,-1.4327453375,-0.8666670338,0.0022184572
F,-1.4046718132,1.4153266101,0.263888407
C, 3. 7940466425, 0. 6191689073, 4. 0043006037

Cartesian Coordination of 2b-2

–2858.0778879 hartree
H,3.5975363483,-0.4955193928,-0.0160027959
H,9.3110203046,-2.5275130417,-1.0014845542
H,7.8521090418,0.9770293101,1.0168593579
H,5.5804647842,0.0802806833,0.9730225962
H,-15.2489023183,-1.5660881162,1.8169964657
H,-16.4942030158,-2.1798877126,0.6961509567
H,-16.593139711,-0.5011296273,1.3028516956
H,-16.7769332504,1.5755327835,-1.6709198069
H,-16.5184242712,3.2124477473,-0.985443787
H,-17.943253423,2.2530998794,-0.5005542138
H,-10.7289411394,-0.9867310315,0.3686833678
H,10.060303175,0.7537125403,0.5644847691
H,-3.6005115279,-0.5044498162,0.0386073134
H,13.7570592567,-1.4005530677,0.0219746541
H,11.3270767522,2.1332347382,-0.3462290423
H,-12.6246129723,-1.0374502833,-0.3625350427
H,-11.896864083,3.1757334145,0.1325093529
H,-14.3951184119,5.7589427887,0.6822989851
H,-13.1677712342,5.0665260033,-0.4139214798
H,-13.0203870895,4.840168137,1.3526527707
H,-2.2452525288,-4.4611699291,-0.3580582255
H,0.002313358,-3.4289676142,-0.2183507409
H,17.6108525695,-0.5541560281,1.5005397137
H,16.0699718819,-0.4392209921,2.391601226
H,16.8849828247,1.0486513124,1.8163294
H,17.2387317841,3.7785255426,-0.4465385587
H,15.6513306207,3.8943616722,-1.2537113892
H,16.6640990781,2.4298429246,-1.4670488659
H,2.2611731607,-4.4651267199,-0.3253368675
H,4.9527522417,-4.477434493,-0.3282584859
H,12.4009713517,5.5678885737,-0.1288958823
H,11.4665746758,4.2529544966,0.6306657395
H,11.7207767373,4.2656844955,-1.1402198953
N,-3.6326439791,-1.5035952023,-0.1034258406
N,10.0197713492,-0.1273851086,0.0737570358
N,-10.0778805763,-0.2990650386,0.0202467012
N,3.6360790362,-1.5036522063,-0.0523984832
O,1.2376787431,-0.340330252,0.0402557816
O,-9.9101191652,1.9252582933,-0.5271470395
O,-15.1634696534,-0.9209197301,-0.1698158736
O,16.0146416721,-0.1372841148,0.3242699725
O,15.7933382584,2.6489338109,0.4212574754
O,-1.2312170739,-0.3376129399,0.0201573833
O,-14.5642736888,3.7656069266,0.4422611678
O,11.3705116548,-1.7825085473,-0.775220802
O,-16.2081846915,1.6229924804,0.3401196254
O,13.4153101872,3.8334654777,0.0065974808
H,-4.9361315029,-4.4830233658,-0.3827229738
H,-5.58676383,0.2293636933,-0.8293724911
H,-7.8729278065,1.121769375,-0.7188403755
H,-9.2892831276,-2.711998199,0.6151146462
H,-7.0005595209,-3.5899793056,0.5657687483
H,7.0104404621,-3.4085202346,-1.1047251749
B,0.0030775513,0.5263402614,0.1558259016
C,-8.7418395597,-0.7283060389,-0.0468343189
C,-7.6762806407,0.0957347961,-0.444866838
C,-8.4741754842,-2.0636784199,0.3018253673
C,14.6825694455,1.8726457512,0.2136753695
C,14.7927146083,0.4742027902,0.2153317483
C,-16.8893620733,2.2042032272,-0.7801270109
C,-15.9176390242,-1.3001592854,0.9882837364
C,6.3783695562,-0.4923714719,0.5092350761
C,7.6697331072,0.0127485385,0.5480800068
C,8.7436738059,-0.7114262559,0.0038792244
C,8.4904189166,-1.9622673533,-0.5845781641
C,7.190679775,-2.4520562316,-0.6242464563
C,-7.1817273912,-2.5631334667,0.2651217018
C,-10.5991013844,0.9549835844,-0.2293726383
C,13.659276281,-0.3218888018,0.0380828224
C,11.237235074,-0.6521270507,-0.3220595202
C,13.4171287316,2.4701367762,0.025992726
C,12.2852818571,1.6698446119,-0.1451542329
C,-12.961258533,-0.0276744299,-0.1517862082
C,-14.3395808458,0.1662053404,-0.021278712
C,-14.858067293,1.4535982585,0.177480879
C,-13.9733596711,2.554302169,0.2453242213
C,-12.6012207441,2.3551184015,0.1042958318
C,-12.0907801876,1.0636979073,-0.0879438343
C,12.40839277,0.2693557566,-0.1340152192
C,-13.7265136521,4.9134400304,0.517100523
C,-2.8978385691,-3.6039556095,-0.2751896688
C,-2.489412922,-2.2719612209,-0.1606424365
C,-4.7465938291,-2.2905613691,-0.1665787513
C,-1.1989417054,-1.6431067322,-0.0872190635
C,0.0026130675,-2.3524768233,-0.1289464159
C,1.2046955364,-1.6459709263,-0.0685982045

C,16.6748461415,0.0004960837,1.5886406115
C,16.3597870484,3.2165014776,-0.767367054
C,2.4958749356,-2.2750759799,-0.1248913298
C,2.9099703126,-3.6036964875,-0.2575189921
C,4.3125154089,-3.609382096,-0.2700501695
C,4.7533767484,-2.2836022132,-0.1410554518
C,12.1750316377,4.5018357082,-0.1695719509
C,-6.1033645329,-1.7516616285,-0.1306165415
C,6.1067777174,-1.7381818901,-0.0843692181
C,-6.3860534219,-0.42132489,-0.4858485922
F,0.0131232475,1.4291679649,-0.8725124768
F,-0.0057001278,1.1026561713,1.3986399769
C,-4.3001453898,-3.6163175401,-0.2768487492

Cartesian Coordination of 2b-3

–2858.0773828 hartree
H,-4.925601846,-4.4751639497,-0.4615351626
H,-15.2696634342,-1.6159383778,1.7070645467
H,15.6984351802,-2.7398226036,0.1239361885
H,14.1399852189,-2.3974566433,-0.6718396919
H,14.2809926471,-2.2880119285,1.1081600594
H,17.9776951529,1.9189013433,0.664487198
H,16.8649989989,0.7834815783,1.4753535857
H,16.5971662394,2.552343796,1.6050759384
H,15.3401172245,5.342947361,-1.2278937556
H,14.2712672326,4.2670035196,-2.1669468764
H,-2.2349232041,-4.4490746979,-0.3880305033
H,-3.607156723,-0.511049786,0.119180407
H,0.0092544559,-3.4205748895,-0.1049015249
H,2.2632890737,-4.4232414218,-0.4024903375
H,4.9534537535,-4.4183457721,-0.4955251074
H,3.5904004251,-0.460428613,0.0232512926
H,-5.5784476336,0.2444526248,-0.7759334886
H,-7.8681123848,1.1301569403,-0.680952716
H,-9.2994007928,-2.7404856961,0.5245080232
H,-7.0083069065,-3.6137955291,0.4890449252
H,6.9752496404,-3.3179761904,-1.3011909518
H,9.2590296412,-2.4272870937,-1.2425435316
H,7.8875830507,1.0093796762,0.9469151001
H,5.6098386669,0.09170708,0.9447220048
H,-10.7365122632,-1.0092516762,0.3091192677
H,10.7112460538,-0.7903654214,-0.6570793069
H,-11.9051257674,3.157581111,0.1454706248
H,-12.6258016854,-1.0459041329,-0.4353731037
H,12.5558928609,-0.9780820287,0.3102028015
H,11.9224150019,3.2741318967,0.1053820467
H,-14.4098912777,5.7294536022,0.7180403266
H,-13.1704031386,5.058129059,-0.3776291699
H,-13.0421942787,4.7984635925,1.3858975471
N,-3.6343492926,-1.50461339,-0.0588789069
N,10.0682207548,-0.2004133568,-0.1498193004
N,-10.0823650419,-0.3132515128,-0.016116245
N,3.6319226642,-1.4660777759,-0.0580784627
O,1.2230648685,-0.3205937879,0.1157587168
O,-9.9112887549,1.9225135523,-0.5132182033
O,15.2531017339,-0.7781307012,0.0368264862
O,-14.5756827113,3.7409898486,0.4385253087
O,16.1854127307,1.7189616972,-0.2675250338
O,-1.2374512963,-0.3333015779,0.1115870452
O,14.4466247642,3.9027226838,-0.1166190471
O,9.9025096521,1.8867685033,0.7993113083
O,-16.2176614911,1.599588049,0.2792379303
O,-15.1664524143,-0.9336432398,-0.2664529585
H,15.8791974074,3.6868436927,-1.6305438385
H,-17.9445772464,2.245740969,-0.565828075
H,-16.7641772512,1.5972611722,-1.7384708672
H,-16.5163613263,3.2184729851,-1.0128857285
H,-16.5050537704,-2.2082340277,0.5638692966
H,-16.6090434973,-0.5410535344,1.2009749017
B,-0.0120373962,0.4806313064,0.4686723773
C,-2.8913740688,-3.5968583722,-0.2862241584
C,-2.4883851619,-2.2687420472,-0.118766203
C,-4.744925149,-2.2909901603,-0.1688249378
C,-1.2021092138,-1.6391462076,0.0011063026
C,0.0034319687,-2.34384237,-0.0174672502
C,1.2011158515,-1.6265014221,0.0027079839
C,15.0197821109,4.3086339071,-1.3657999231
C,16.9395108153,1.7421870784,0.9515037187
C,2.4942344548,-2.2420222711,-0.1209515778
C,2.9101482775,-3.5616207662,-0.3203077029
C,4.3113057849,-3.5572040547,-0.3811792227
C,4.7493546994,-2.2342304849,-0.2167322848
C,14.8026568622,-2.1187396294,0.1575195303
C,-6.1032571019,-1.7555183643,-0.1406867241
C,6.1023287676,-1.6853474778,-0.1869374246
C,-6.3823338784,-0.4162886799,-0.4638255705
C,-7.6740871694,0.0975455992,-0.430897392
C,-8.7445349252,-0.7385299518,-0.0731007782
C,-8.480276554,-2.0826577557,0.2431127378
C,-7.1865173419,-2.5792627826,0.2140424586
C,7.1661456267,-2.3800155855,-0.7898773444
C,8.4555883902,-1.8718319105,-0.7639462179
C,8.7345532065,-0.6430528233,-0.140713194
C,7.6832054327,0.0646980649,0.4646946003
C,6.3961999598,-0.4611525895,0.4385520979
C,-15.9309499573,-1.3343234066,0.8775461394
C,-16.8875833064,2.2052085008,-0.8348386565
C,13.964238245,2.6198645809,-0.0714167429
C,14.8388495104,1.5240229358,-0.0976144481
C,12.5893022321,2.4213646272,0.0674212284
C,-10.6023657975,0.9452936514,-0.2444752481
C,10.5884947128,0.9933944637,0.318187118
C,-13.7391507852,4.8873814813,0.5442081549
C,12.07739014,1.1284588479,0.1718936799
C,-12.095574528,1.0500387894,-0.1160826972
C,-12.6087519356,2.3374330221,0.0948424712
C,-13.9823440827,2.533629937,0.2252455754
C,-14.865803577,1.4341755099,0.1273902676
C,-14.3445272901,0.150863092,-0.0898321423
C,-12.9648450266,-0.0401973523,-0.2094766964
C,12.9442059226,0.0216066068,0.15795441
C,14.3214427551,0.2169297869,0.0292366726
F,-0.0166443607,1.6173710592,-0.2859630242
F,-0.015607061,0.7034632227,1.8223738375
C,-4.2934095369,-3.611667522,-0.314411204

Cartesian Coordination of 2b-4

–2858.0605646 hartree
H,-2.7417388293,-0.8157467146,-0.9139692547
H,-8.8000460207,-0.2083749298,-1.671383811

H,-6.4331175074,-3.5430222422,-0.3432722159
H,-4.4682231371,-2.0904752741,-0.1700496434
H,7.0110225266,-1.4724247479,1.8353170162
H,7.0798869227,-2.0759931504,3.512461488
H,7.6576174905,-3.1084422039,2.1730757888
H,11.1105716466,-3.8959783347,3.1966444507
H,11.7686375996,-4.6570913369,1.7117976102
H,10.4213113129,-5.4285385295,2.5925031676
H,11.0080977031,3.2773487123,-0.5087385721
H,-8.6276427271,-3.7879160706,-1.4974633277
H,4.1804932766,1.0385864105,-0.5521204719
H,-12.4525957425,-1.3461317859,-1.7240842591
H,-9.3052313036,-1.4919131531,1.2033076161
H,9.570045749,0.7169356922,1.6753666675
H,12.1546369087,-0.9991756602,-1.3016669254
H,12.7634800732,-4.5323924873,-1.8887061257
H,12.0481324868,-3.01799035,-2.5033335531
H,1.8614933285,4.5293499435,-0.2721697918
H,-0.0547503959,2.9415248849,-0.4376267917
H,-14.8180294465,2.1214547295,-1.3692143707
H,-13.1115207272,2.0322604817,-1.8800112983
H,-13.5250555945,2.6047161456,-0.2336404211
H,-12.7327519181,0.7409517509,3.6530950714
H,-14.1915038117,0.5161110367,2.6343680451
H,-13.8075669739,2.1240915462,3.3103326739
H,-2.5180262023,3.3458632039,-0.3969017319
H,-5.1148674256,2.645410933,-0.4832453235
H,-8.9525196937,0.5704905996,4.1484276653
H,-8.3256530253,0.156209675,2.5296625935
H,-9.2161171404,-1.0644893226,3.4856148798
N,3.958246159,2.0223899836,-0.5061369962
N,-8.847572981,-2.8758978786,-1.1139369134
N,10.499906875,2.4225610786,-0.3136899962
N,-3.0493001601,0.1325334866,-0.7541769751
O,-0.4327118044,-0.3547304872,-0.7941941448
O,12.4759806963,1.4751122492,-0.8497881674
O,8.8808799978,-1.5153427119,2.7688860969
O,-13.8065720531,0.5569040492,-0.5729730051
O,-12.6347407006,1.5893882193,1.7431549815
O,1.9486660163,0.2866960154,-0.7099682548
O,11.6073651561,-3.581832387,-0.5403519292
O,-10.9463413256,-3.4767076891,-1.6829534698
O,9.8700257362,-3.7992490245,1.5175970731
O,-10.3766594809,0.5008794046,2.7253460343
H,4.4577898126,5.2295397862,-0.1618453513
H,6.2764167624,1.0123874659,-1.4667341929
H,8.7013056423,0.7133580786,-1.4317304371
H,9.1334223984,4.4031997061,0.7307686134
H,6.6916691739,4.7099618644,0.7006593068
H,-6.8368442041,1.2505062165,-1.5025227031
B,0.9872672434,-0.8759470617,-0.8235776585
C,9.0925655858,2.5274536779,-0.3284743068
C,8.2647258334,1.5768160244,-0.9446300981
C,8.5021721594,3.6635300704,0.2466937968
C,-12.0396653666,0.5521569183,1.0725661297
C,-12.6056359929,0.0739766364,-0.1183918471
C,10.8638412812,-4.4748906058,2.2992150163
C,7.5843575076,-2.0829100825,2.5444781691
C,-5.4058847489,-1.6648904491,-0.5155863481
C,-6.5186483592,-2.4917863649,-0.603219406
C,-7.7628661131,-1.9809856474,-1.0036195627
C,-7.8586119474,-0.6173980333,-1.32546142
C,-6.7447172333,0.2056515201,-1.2238482653
C,7.124629565,3.8358477938,0.2250227374
C,11.3424696595,1.3199741713,-0.409620238
C,-11.9873869072,-0.9592444102,-0.8254583462
C,-10.2246048417,-2.6667362249,-1.11543931
C,-10.8382359454,-0.0167471357,1.5510532956
C,-10.218085409,-1.0426607413,0.8366730934
C,9.9987059175,-0.1428201193,1.1754181252
C,9.6833934809,-1.4146696073,1.6600822036
C,10.2322581991,-2.5587936048,1.0627146193
C,11.1200124497,-2.416454331,-0.0279176047
C,11.4485806048,-1.1445986397,-0.4947149302
C,10.8778078112,-0.0084276133,0.0985474392
C,-10.7937973574,-1.5090327404,-0.3561320781
C,12.5112445454,-3.5021538802,-1.6350192435
C,2.7113138385,3.8636382039,-0.3183365144
C,2.6569711718,2.4753441625,-0.4737044446
C,4.834194368,3.0603042357,-0.3669726637
C,1.5743781651,1.5354075099,-0.5799370486
C,0.2282637365,1.9047671533,-0.5470072479
C,-0.7446190169,0.9105486107,-0.6594742555
C,-13.8003252802,1.9126911295,-1.0339042101
C,-13.3824724489,1.2043818322,2.9042655189
C,-2.1578477434,1.1770413784,-0.6378484386
C,-2.9125469456,2.3475669728,-0.520160625
C,-4.2662424003,1.9834780707,-0.5756966651
C,-4.3355251618,0.5901910266,-0.7249590575
C,-9.1485402928,0.002437918,3.2382902488
C,6.2829607712,2.8766904428,-0.3649265816
C,-5.4936353067,-0.2944420113,-0.8188160257
C,6.8861879961,1.7490295288,-0.9514693926
F,1.1961030333,-1.4932685623,-2.0265732217
F,1.169219194,-1.6940703699,0.2591394591
C,4.0642342506,4.2274467169,-0.2500794513
H,13.425193117,-2.9588014434,-1.3658040759

Cartesian Coordination of 2b-5

–2858.0605612 hartree

H,-3.5865010039,-1.5274400611,-0.3400516345
H,7.7211380568,-0.102288915,1.7031876765
H,9.2758256825,-3.799261709,0.1556623659
H,9.6452954071,4.4228046061,-3.2206210866
H,9.8820249217,5.4819834046,-1.7929823545
H,8.5375522987,5.7920508595,-2.9253930655
H,6.0331916259,1.2671007043,-2.0024276188
H,6.2102921461,1.6503162054,-3.7355011563
H,6.3570311556,2.9512124968,-2.5186823682
H,-5.4053856686,-0.7973698234,-1.4832561391
H,10.6570448489,-2.1150917729,1.403750126
H,-10.633365275,-1.8509527697,-1.7579931664
H,3.5485272838,-1.6276190729,0.4603213808
H,-0.0800533445,-4.5193470154,0.2197192544
H,5.4476810534,-0.9792824688,1.5283341149
H,-7.4108624663,0.7689364827,4.0468620566
H,-7.3427384267,-0.0061846904,2.4412649341
H,-8.9035247686,0.1359334215,3.3024074626
H,-4.9635963299,-5.5009951619,-0.6814919677
H,-2.3067804501,-5.5269931405,-0.2612120516

H,-9.126932874,4.0645677144,3.4030313265
H,-10.0488555276,5.1731577954,2.336274867
H,-8.5073570215,5.7040551953,3.0653824305
H,-7.7330075452,5.657657932,-0.4361759047
H,-8.7224113695,6.4944752192,-1.6674338551
H,-7.886505834,4.9752530545,-2.0852040812
H,10.6744002677,2.3716019536,1.7126841516
H,10.3805917875,5.988791676,1.8615732223
H,9.9509906903,4.4237470767,2.6024247328
H,11.4466270363,4.574519509,1.6358816494
H,2.1672640382,-5.5932204906,0.3740289822
H,4.8457958213,-5.6385752197,0.6209732229
H,-9.3701354618,-3.5907679506,-0.5036103576
N,3.5709613187,-2.6356987118,0.5114498509
N,-9.9872775357,-1.1876400632,-1.3459933628
N,9.9978354476,-1.4372889068,1.0390777566
N,-3.6301248922,-2.533449866,-0.4140215773
O,-1.2371735863,-1.4025701029,-0.0676390962
O,11.613574111,0.0168113766,1.6428228335
O,-8.120982921,1.9283453184,2.560870425
O,9.6639743667,4.6434161833,0.5445024955
O,-8.2825282029,4.4096998089,1.5200749229
O,1.2018364214,-1.4389450168,0.2514060601
O,-9.6040104875,4.8385255949,-0.901854581
O,-11.5378318021,0.2940433993,-2.0455455183
O,8.2265663499,4.2051543416,-1.7012376871
O,7.9644428249,1.6224558699,-2.7197724596
H,-7.642483844,0.1289465693,-1.7938062781
H,-7.1195974964,-4.5293852935,-0.1867859154
H,6.9886983872,-4.6883550976,-0.0252178995
H,-10.4706224714,2.6805750153,-2.068289783
H,-9.1825941486,-0.0403552861,1.0042461762
H,8.9821351641,-0.2380553806,-1.2563949327
B,-0.0376844436,-0.57526819,0.3421739397
C,-7.5334561733,-0.8819500637,-1.420469768
C,-6.2636180824,-1.4141239749,-1.2324603531
C,6.5580658107,1.8980409526,-2.7308881446
C,9.1410566503,5.0169109286,-2.4497709657
C,-9.4377803269,3.5702098539,-0.4074320594
C,-8.8202042294,3.3526085687,0.8334655966
C,8.4323719914,-3.1854345474,0.4585793681
C,7.5639550296,-1.096848273,1.3037283909
C,9.5302402199,3.3455118372,0.1495301273
C,8.7933601675,3.1473666065,-1.0403088486
C,8.6057342433,1.8454111825,-1.5273213438
C,-8.6719307818,-1.6570280313,-1.1506327439
C,-0.0596328449,-3.4397277109,0.1870157867
C,1.1498471709,-2.7485120475,0.2850700653
C,-1.2319370125,-2.7130809991,-0.029490083
C,6.2736449379,-1.5994574312,1.1920597126
C,-6.0766551095,-2.7359921602,-0.7881102682
C,6.0298348228,-2.900693999,0.7155701223
C,-7.9426038836,0.6279360928,3.105236275
C,-4.7454215058,-3.3019724097,-0.5888852757
C,-4.3261677984,-4.6402433728,-0.5415150228
C,-2.939628651,-4.6540843739,-0.3315957333
C,-2.5143244823,-3.3252282189,-0.2475376432
C,-9.0481849364,4.8527254656,2.6482229032
C,-8.4052341353,5.521610797,-1.2871576033
C,10.07240407,2.2511231047,0.8216191861
C,9.8623148606,0.9521482494,0.3346436155
C,-9.856310322,1.1987074852,-0.6271764553
C,10.4054652093,4.9066064174,1.7288192539
C,2.8242355004,-4.7370224698,0.4270035767
C,2.4269188177,-3.3968097409,0.4036796913
C,4.6757835022,-3.4335236405,0.5928249909
C,-9.2399726543,0.9662939726,0.6130431191
C,-8.7244324079,2.0380956831,1.3429455391
C,9.1317758198,0.7496716467,-0.8381826087
C,4.2214888266,-4.7604492323,0.5440553604
C,-8.4966067013,-2.9817782324,-0.7188565227
C,-7.2250049654,-3.5103882458,-0.5448450622
C,7.1410368485,-3.6858499641,0.361299353
C,10.5448009217,-0.158762763,1.0686975789
C,-9.9618835862,2.4961071949,-1.1297719844
C,-10.5105464586,0.1024562675,-1.4075536378
F,-0.2030353695,-0.1837820159,1.6464870542
F,0.0942128835,0.457530687,-0.5399480531
C,8.6632568421,-1.8806627401,0.921551339

Cartesian Coordination of 2b-6

–2858.0605011 hartree

H,3.5217930959,-1.9789453665,0.5052897419
H,13.761267904,2.3781883392,-2.8656431592
H,14.5634339661,2.9998132688,-1.3871938632
H,-12.9519761073,0.1973634965,-2.2385642592
H,15.0941492528,2.9757139767,2.2924034845
H,14.9740037408,1.214975568,2.0231775214
H,13.7053111473,2.0680294949,2.9484957985
H,12.9356058586,0.0707122197,1.980528756
H,10.0792449208,-0.7034307815,-1.1382118856
H,-10.1985637749,-0.752760848,0.9256537274
H,-10.019501095,-3.2367337854,-1.6770563174
H,9.9587287557,-3.2665230775,1.4631973156
H,-3.5996497223,-1.973518249,-0.469516037
H,2.1961750838,2.0006190201,0.2849261344
H,-0.0610702165,0.9592775218,0.2013848687
H,-14.2226421568,4.2100260984,-2.1148734158
H,-12.5733865979,3.6295149488,-2.4670887888
H,-12.9489783741,4.3435990918,-0.8678162626
H,-12.9240609927,2.4829247959,3.0948683134
H,-14.3439415025,2.6179701106,2.0078862462
H,-4.9542024924,2.0217435482,-0.5405736402
H,-9.4613550492,1.2157950386,3.8588695832
H,-8.8747163101,0.5780830386,2.2986940397
H,5.5850764828,-2.6678405908,-0.1690968735
H,7.8616888756,-3.5412926353,0.0787139833
H,9.1113243108,0.1744913051,1.8422482577
H,6.8350665753,1.0545314831,1.6001471648
H,-6.8755681659,1.0796348173,-1.6589786401
H,-9.1439616694,0.2089257794,-1.9891248305
N,-3.6483897907,-0.9670105642,-0.4066251402
N,9.9367808757,-2.31364994,1.1187448767
N,-9.9990319658,-2.2864112149,-1.3254430494
N,3.5655342805,-0.9720481756,0.4449682213
O,1.177701431,-2.1387685841,0.1724895877
O,-12.5150238491,3.1789884324,1.1644854663
O,13.7324950553,2.4665175066,0.8975658926
O,10.6197479584,1.3906174609,-2.5414031713
O,12.0831147919,-2.317282604,1.8183279258

O,-1.2667295984,-2.1358282127,-0.1154928703
O,-10.7406757844,1.5167538171,2.3321664376
O,12.4749921147,3.1318617559,-1.40046762
O,-12.1351559902,-2.2790440566,-2.0547137772
O,-13.767870173,2.4486993086,-1.2234622302
H,4.8746695768,2.0165851008,0.5425859185
H,8.9057517963,2.3896104739,-1.8835961934
H,9.3704199991,2.5893607491,-3.5942289336
H,10.2855069834,3.4459878653,-2.3199547224
H,13.816367286,4.1341164858,-2.5454400059
B,-0.0724918381,-2.9878984985,0.2581369868
C,11.192964131,-1.7258895694,1.2181645354
C,-12.4587635274,0.4627308187,-1.3111653845
C,-11.2531352335,-1.6920287449,-1.441333386
C,-11.253726413,1.1148660056,1.133847242
C,-10.912862599,-0.0716635892,0.4834943065
C,10.825929623,-0.0711395349,-0.6740406459
C,11.1902885429,1.1101924587,-1.324774001
C,12.1680104863,1.9518481327,-0.7745360892
C,12.7939536111,1.5896080931,0.4399327058
C,12.4455419355,0.3974080453,1.0728601387
C,11.4521541455,-0.4262743823,0.5223985097
C,-11.5142554069,-0.3932087231,-0.7438240971
C,14.4063448311,2.1494719089,2.1089416623
C,2.841042682,1.1377514574,0.3691405351
C,2.4303615402,-0.1980870319,0.3341254264
C,4.6757262543,-0.1856821855,0.5610942796
C,1.1441470049,-0.829369765,0.2218129695
C,-0.0566376292,-0.1198122586,0.1511670255
C,-1.2428405296,-0.8265580328,-0.0534535472
C,-13.3384615941,3.7336441173,-1.6870303178
C,-13.3880620367,3.0698497724,2.2965671381
C,-2.5212349066,-0.1933740802,-0.2321414489
C,-2.9306763307,1.1422723723,-0.2776589154
C,-4.3174114141,1.1509089511,-0.4869291672
C,-4.7529464394,-0.1804496385,-0.5684505818
C,-9.7530640148,0.6981476983,2.944340604
C,6.0247011075,-0.7288166184,0.6936429878
C,-6.0952509437,-0.7221863634,-0.7617210423
C,6.3417529489,-2.0375706792,0.2890751474
C,7.6324568171,-2.5355937593,0.4188164434
C,8.6540788829,-1.7441641021,0.9638305534
C,8.3454684981,-0.4414276443,1.3863194259
C,7.0567004208,0.0540981355,1.2426442692
C,-7.1086421976,0.0724919338,-1.3287933395
C,-8.3933213629,-0.4171084146,-1.5218555251
C,-8.717895318,-1.7267361699,-1.133166613
C,-7.7133934871,-2.5314200282,-0.574678692
C,-6.4264765142,-2.0389262162,-0.395322759
C,9.7492862545,2.5272917857,-2.5722327946
C,13.734488676,3.1476252757,-2.0855147654
C,-12.796412592,1.655428179,-0.667954505
C,-12.2013631268,1.9902801313,0.5577658908
F,0.033157498,-4.0007861198,-0.6500422302
F,-0.2256799801,-3.4089746095,1.5545549178
C,4.235974694,1.1459642206,0.5122944478
H,-13.5592098541,4.0895422139,2.646423203
H,-2.2909990649,2.0051881786,-0.1611682705
H,-10.1500177606,-0.2921876752,3.2005545448
H,-7.9537943264,-3.5437571506,-0.2628260434
H,-5.6850871176,-2.6806259124,0.0719331707

Cartesian Coordination of 3b–1

–2936.6756521 hartree

H,-11.9375551897,4.2050864874,-1.4772895393
H,6.8159081595,1.1965214127,2.1378346653
H,-6.676836402,1.3408145046,-2.0015074935
H,-8.9135382384,0.4461134215,-2.5032234807
H,-7.8997895192,-3.2186014947,-0.5052324389
H,-5.6727329951,-2.3319740702,0.0119190016
H,7.8621547261,-3.2953096175,0.3327539691
H,8.2564862191,1.5996548676,-3.945746412
H,9.1864089286,2.7776659595,-2.9753891099
H,12.5922680728,3.6997603063,-3.8812982733
H,4.8979817733,2.2400327128,1.0202813023
H,8.0217168877,1.6737104372,-2.1784402109
H,9.087054853,0.2771289816,2.3778001744
H,-12.1917596865,4.5516246621,0.2615365203
H,-12.3422692986,1.8054830675,3.6696411132
H,-13.7252522876,2.3386682708,2.6604986653
H,-12.8161690999,3.5258765278,3.6372818974
H,-2.2318088438,2.2948575793,-0.0929880105
H,-4.8632457057,2.3227364586,-0.6604791236
H,-8.9197658561,0.143072727,4.0162967588
H,-8.414184602,-0.1556830354,2.3310676262
H,-9.7424988309,-1.1112492389,3.0512914576
H,5.5992043757,-2.3848864818,0.0773075938
N,9.9402297938,-2.1294929258,1.5248366269
N,-9.8475508537,-1.9956440068,-1.8479235958
N,3.5728997322,-0.7330751569,0.7736842761
N,-3.5836610457,-0.6712947361,-0.4260782059
O,1.1896041686,-1.8758080874,0.4113427073
O,13.1213995735,2.801185392,-0.1846618486
O,9.7689064563,0.7686351043,-2.8821520181
O,12.1467114617,-1.7560131868,1.9143056382
O,-1.2343929556,-1.8530594546,0.0037491026
O,-10.1948156797,0.8905180167,2.6480771102
O,11.5294391245,2.8666695413,-2.3672005665
O,-11.9974056721,-1.6025260833,-2.4682272997
O,-13.192017343,2.8658665763,-0.4766301302
O,-11.838460289,2.9132603458,1.9680352842
C,-10.7562342673,0.8249988709,1.4059615484
C,-6.3639439787,-1.719289939,-0.5597794717
C,8.7544222236,1.7731005165,-2.9896502367
C,12.6661874317,2.8205299554,-3.2385177846
C,-12.2776130188,1.8918622154,-0.160779452
C,-11.6353386527,1.8824738103,1.0857306177
C,4.2544652363,1.3762436938,0.9390074575
F,-0.2936580419,-3.1039405598,1.7485709662
F,0.066649367,-3.7429402867,-0.4292415133
H,-3.5353405405,-1.6777806167,-0.4913858246
H,-12.5811161947,0.8623827863,-2.0214232844
H,-9.8630990714,-1.0143740929,0.7310292042
H,-9.8533270678,-2.8872851297,-3.7807202852
H,-10.802891532,-3.7293035258,-2.5476781227
H,-9.0195738561,-3.8087160236,-2.5062371291
H,10.9516799738,-3.8887628602,2.0643694398
H,9.1744529236,-3.952411918,2.2253936813
H,2.2275540787,2.253390526,0.6820558433
H,-0.0308493586,1.2298623259,0.4275667966

H,-13.5138303155,4.8182468603,-0.9114727127
C,8.6368373219,-1.5722241504,1.3689218912
C,8.3229572352,-0.3003259804,1.8687570059
C,7.0424203954,0.2190703036,1.7241506138
C,-6.9439922134,0.3478494053,-1.6545465547
C,-8.2047025737,-0.1577524643,-1.9472401101
C,-8.5682343733,-1.4489396901,-1.5379386982
H,10.1586835286,-3.0735261232,3.4203548028
C,-7.6277108366,-2.2236924153,-0.8436950104
C,-10.5254960573,-0.1967663255,0.4835986464
C,10.3533360984,-0.2491660109,-0.8083125504
C,10.5044827128,0.7966304283,-1.722034772
C,11.4341908975,1.8189952097,-1.4873598314
C,12.235459296,1.7733751351,-0.3248967525
C,12.0948445518,0.7177406484,0.5745189737
C,11.1438772559,-0.2877712913,0.3419348336
C,-11.1698463571,-0.1730151425,-0.7633937181
C,13.9724078778,2.7954965723,0.9539370393
C,2.8643647195,1.3833431786,0.7524118756
C,2.4468554362,0.0525641421,0.6566284258
C,4.6837045004,0.0407452147,0.9506967993
C,1.1616281752,-0.5671952237,0.4811139033
C,-0.0305035547,0.151351086,0.3651740324
C,-1.2068687211,-0.5447886114,0.0812691389
C,-12.6631976321,4.1841512615,-0.6538615781
C,-12.7358817248,2.6128451705,3.044267854
C,-2.4678544858,0.0971908889,-0.1754948905
C,-2.8662522472,1.4348833661,-0.2524333454
C,-4.2348855011,1.449798737,-0.5603533882
C,-4.6692186429,0.1205307912,-0.6690955265
C,-9.2690386313,-0.1217251577,3.0175242876
C,6.0256620462,-0.5190856874,1.0927374801
C,-5.9944478538,-0.4216301444,-0.959134733
C,6.3459340225,-1.7996603698,0.6060938011
C,7.6286124186,-2.3171965472,0.7414035983
C,-11.0424011634,-1.2825047992,-1.7679864448
C,-12.0496209934,0.8640131611,-1.0774732345
C,11.1206535489,-1.4195288698,1.329141344
C,10.061792363,-3.3336587122,2.3597878303
C,-9.8806078053,-3.1765605325,-2.7236844544
B,-0.0716559523,-2.7120218169,0.4529841416
H,3.5216084508,-1.7412653726,0.7970919218
H,12.6455017996,1.9148963138,-3.8556213718
H,13.5995693575,2.8624876811,-2.6688047691
H,9.634016277,-1.0254443163,-1.0361902787
H,12.7205777119,0.6328526817,1.453079737
H,14.6171292181,1.9083979216,0.9726275103
H,14.5898014453,3.6906313684,0.869264307
H,13.3966325473,2.839542049,1.8865217914

Cartesian Coordination of 3b–2

–2936.6756398 hartree

H,-1.1926223867,-7.1867039975,5.5822784436
H,1.8444844339,-8.8146104545,9.0137160396
H,3.5651892131,-8.9574760824,8.5368461981
H,5.3059482776,-10.1068763363,4.6780608416
H,4.8734821485,-11.1969652862,6.0348144939
H,6.1481400543,-9.9636869659,6.2449448109
H,0.6549809698,1.438963184,2.3775513455
H,0.7790772543,-2.8096472677,5.1416075511
H,4.3610733609,-7.4272197677,2.107272331
H,2.6763402835,-7.0091859635,2.5211308624
H,3.0527380758,-8.5985705159,1.7943402973
H,-2.0255472195,5.7673635837,-1.9743025784
H,1.0897095815,6.4200208647,1.5766462396
H,0.9469537197,-0.3232806726,4.1229286649
H,2.8606841544,-10.1013016367,9.715835861
H,-0.6246445894,-4.7947480047,5.46906451
H,1.3364684502,7.9134075963,-0.3495801048
H,-0.0697992068,-10.5052005653,6.7203608912
H,1.0801919951,-8.6131338672,3.0351821833
H,0.8573952568,8.4486865156,-4.7738418682
H,-2.8182172051,8.8655972296,-6.9628439389
H,-3.8552528999,6.9587181111,-9.8728480228
H,-4.1271705014,7.3111096581,-8.1452207398
H,-3.383554269,8.5448080588,-9.2024845587
H,1.1130437884,3.8840209416,2.4783584564
N,-1.631365424,-8.8311172042,3.4950034909
N,-1.1661614396,9.985813666,-3.589766
N,-0.5704346151,-2.4877699435,2.1865851599
N,-0.3874112712,4.2890353948,-0.4065667023
O,-1.0332601485,-0.6078536376,0.3544503822
O,1.8947046184,6.6563955299,-6.3008219557
O,2.299137064,-10.455020505,7.8013899331
O,4.2642884629,-9.2095370516,6.2547916343
O,-0.9669941055,1.6862900541,-0.5280262914
O,-2.1752821025,6.8949882648,-8.7632257254
O,-1.6903281982,-10.7455247009,4.7186916266
O,0.2393048018,5.7483434557,-8.3567137751
O,3.6892626541,-8.3437998553,3.7700485078
O,-2.2593635444,10.7657147164,-5.4219027538
C,2.9865005342,-9.3415456704,5.7727585991
C,-0.2817845669,-3.2806886046,3.2601890075
C,3.4137309987,-7.8200946818,2.4785468046
C,-0.2965032309,6.6858268358,-1.0486791216
C,-0.6255478986,-4.6995801611,3.3129053767
C,-1.3721843455,6.6347755936,-1.9530645934
C,0.6827898907,5.5541187759,1.0751977073
F,-0.2230317479,-0.141089213,-1.79470664
F,-2.4653221584,0.0954585334,-1.350546754
H,-0.8434442413,3.9438999914,-1.2388049895
H,-1.1032810026,-2.7397604448,1.3666846343
H,-2.5090133667,7.6549368662,-3.462273753
H,0.8353448141,9.8073710232,-1.8406292315
H,0.9905572965,5.2745978619,-10.1798979786
H,1.4701157023,5.1072502464,-4.9629377563
H,-0.9742894165,11.3296957658,-1.9902294151
H,-2.6131809881,11.2561826486,-2.6818368915
H,-1.3245979569,12.0797705278,-3.5720063214
H,-2.9213184722,-10.2649434539,2.6670712656
H,-3.1635730333,-8.596183498,2.0797436155
H,-0.7155831429,-4.989586059,1.1676535488
H,-1.2947488058,-7.3697208795,1.2922483294
C,0.09086891,1.1226143712,1.5122131003
C,-0.350585989,-0.1965375953,1.395134301
C,2.6666741234,-9.514512826,8.8157942297
C,5.1932196715,-10.1841658515,5.7640420321
C,-0.1249398946,-1.2013280594,2.3990527115
C,0.4816165214,-1.1805847679,3.6582399913
H,-3.7364358635,-9.0772452367,3.6948701135

C,0.3829998024,-2.4730583607,4.1946218843
C,1.9921260815,-9.919286339,6.5750648999
C,0.6605561315,6.1749555842,-9.6583703863
C,1.9711730769,5.2762565228,-5.9245922644
C,-0.838658185,-5.4516729217,2.1429711288
C,-1.1598008155,-6.8026487803,2.2080511703
C,-1.2796229969,-7.4505814632,3.446007645
C,-1.0818178003,-6.7047144879,4.617101331
C,-0.7521198173,-5.3568216416,4.5495565732
C,0.4837893307,7.855809946,-1.0184637211
C,-1.5602592132,9.8888322613,-4.9214100343
C,0.6812282824,-10.0230090314,6.1062517774
C,-1.0627942743,-9.7486161324,4.3769520568
C,2.6521705504,-8.8677469305,4.4853824473
C,1.338578746,-8.9651824916,4.024084458
C,0.190715558,8.1496718215,-5.5728762502
C,0.6279912159,7.1620337039,-6.4595346245
C,-0.1861057936,6.7518808244,-7.5250639475
C,-1.4524772797,7.3536467195,-7.7011636635
C,-1.8742363619,8.3545986887,-6.8277710621
C,-1.0585313543,8.7458691114,-5.755160475
C,0.350317471,-9.5374296922,4.8403242841
C,-3.4542559306,7.4697356306,-8.9967153905
C,0.6853632665,4.2345677476,1.5501093329
C,0.0158680696,3.4479883991,0.6080097518
C,0.0058656362,5.5717684903,-0.1533996446
C,-0.2837566728,2.0441830779,0.5316491146
C,0.2041449974,8.9244486576,-1.8602951642
C,-1.6600592765,7.7071416043,-2.7895087397
C,-0.8690170046,8.8637543766,-2.7619571739
C,-2.9428727703,-9.2132736914,2.9508619137
C,-1.5423528867,11.2374348391,-2.9159051458
B,-1.1874186354,0.2341112218,-0.8942834338
H,-0.1663321214,6.6335609153,-10.2086714449
H,1.4963264265,6.8804083387,-9.5843446368
H,1.5302513355,4.6300728224,-6.6879431489
H,3.034214618,5.0510202483,-5.8189140996

Cartesian Coordination of 3b–3

–2936.6752753 hartree

H,-0.0947021838,-4.1542408559,0.1871255618
H,10.1297995739,2.8421406703,1.2596552106
H,9.4431322169,6.3284183284,0.5055304324
H,9.0695877182,4.9236052149,1.5398339888
H,10.6709809229,5.0573705674,0.7584902219
H,2.1526779003,-5.2271466527,0.3384958465
H,-7.8242491491,6.4970902555,0.0505229006
H,9.1442448684,-0.5677086977,-1.1648255123
H,4.8225751659,-5.2746844775,0.6798998054
H,-9.3676440024,-3.1537536156,-0.6619897217
H,-7.1301494296,-4.0923450747,-0.2434815649
H,6.9782766624,-4.2665748999,0.0508369339
H,-9.9248478936,3.1677042933,-1.4404464082
H,-9.298454047,-0.3635717954,0.9321604287
H,-7.1206514266,5.022412321,-0.664809234
H,5.3727225978,-0.6822774805,1.8178291183
H,-7.8180533117,-0.5638990474,4.2177234839
H,-7.6643640306,-0.9373213475,2.4796265136
H,-9.2827916525,-0.7788658258,3.2222796545
H,-4.9667166447,-5.136223847,-0.779863726
H,-2.3196952752,-5.1626589018,-0.2903216703
H,-9.0679287413,3.0020672634,4.2889126161
H,-9.7193649623,4.4553310426,3.4644831796
H,-8.2224654344,4.5671793605,4.4323103448
H,-7.078183414,5.2647345848,1.1089606947
N,-9.9391965431,-0.7783965391,-1.7213652528
N,9.9430263757,-1.0672924836,1.4765525403
N,-3.6255771604,-2.1687033244,-0.5503050439
N,3.5442677494,-2.2721344998,0.6008289899
O,-1.243383607,-1.0383395478,-0.1362820688
O,-8.2113771903,1.0055466623,3.0191405033
O,9.0770074727,4.6398292649,-0.52991143
O,-7.9724583835,3.6633531229,2.633756445
O,1.1859467595,-1.0741662344,0.2534637404
O,-8.9647487325,4.8411839264,0.3024599145
O,-11.2324935445,1.0447278763,-2.1277881638
O,8.0269875735,3.5230028022,-2.7550467897
O,8.1684516304,0.7641406061,-3.1411054232
O,11.2930439501,0.7146397868,1.8809135552
C,8.9572075463,4.2448169689,-3.571857681
C,-7.2215887727,-3.1077357565,-0.6909871882
C,7.1180599262,-3.297913691,0.5198291256
C,10.3478165145,0.2456793096,1.2525040803
C,-9.5484093476,2.6931241178,-0.5422800426
C,-10.3176555393,0.5424247899,-1.4834244133
C,8.6144403264,-1.5404129672,1.266344473
F,0.1022669735,0.8174466883,-0.5828678765
F,-0.2569677277,0.1907844585,1.5987493693
H,3.523390633,-1.2629135105,0.571778477
H,-3.5834639285,-1.1613892051,-0.4906040072
H,-7.5816486375,0.4235505913,-2.2310528055
H,-5.348624702,-0.5068290077,-1.8292334404
H,6.2047261729,0.3227096316,-2.5769130121
H,6.5770797966,0.3356698079,-4.3216868158
H,6.4201902482,1.8796543463,-3.4354265771
H,9.6116064626,3.5550674354,-4.1174288323
H,9.5590920814,4.9315534023,-2.9691933617
H,10.5726481756,-2.8983294178,2.2852847455
H,10.6084877026,-1.5453615005,3.441490571
H,11.837768066,-1.6435242728,2.1718898683
H,-10.5612552747,-1.1869394405,-3.7154423982
H,-11.8253357243,-1.298725871,-2.482464259
H,8.3569891614,4.8151706228,-4.2832000248
H,9.257676274,-3.3933788301,0.3741128917
H,7.6475351342,0.1819961455,2.1262085128
C,2.4068784495,-3.0320454681,0.433493684
C,4.6466235247,-3.071168959,0.7016268841
C,-9.2033948792,0.7059080872,0.8055529413
C,-8.6578999317,1.4890847878,1.8235587985
C,9.1374769782,0.4993745009,-0.9819026625
C,4.1982950093,-4.3965970081,0.6020002444
H,-10.5802623899,-2.5734791209,-2.5993048192
C,-8.4848170989,-2.5788218323,-0.9242733462
C,-8.9953216855,3.4796674169,0.4701427988
C,-8.5474544819,2.8876158886,1.6601491685
C,8.4045733105,-2.8061255137,0.6990558638
C,7.5007611194,-0.7866013101,1.6609593127
C,9.1297080139,3.2794659352,-0.6126814296
C,8.5948573949,2.7239364936,-1.7965654911
C,8.6101022087,1.3329765174,-1.9715781625

C,-8.6349837266,-1.2935795586,-1.4675354036
C,-0.0735077163,-3.0747060335,0.1530422517
C,1.1328591895,-2.3829592798,0.2823230583
C,-1.2399796162,-2.3478882446,-0.0921999043
C,6.2134780831,-1.2761678907,1.4710819769
C,-6.0609301605,-2.3708695617,-0.9894442004
C,5.9940795292,-2.5413747495,0.8976592802
C,-8.2534427279,-0.3979816043,3.2315125564
C,-4.7388863723,-2.9379402871,-0.7341614811
C,-4.328191177,-4.2757776425,-0.6425136951
C,-2.9467970901,-4.2894971517,-0.3984498649
C,-2.5185344434,-2.9604973762,-0.3355562151
C,-8.8073166376,3.9283884339,3.7678869684
C,-7.662143044,5.4277928825,0.1995014202
C,9.6740849229,2.445230013,0.3622264435
C,9.6676078662,1.0531334531,0.1850746136
C,-9.6438496898,1.3099789,-0.3827557787
C,9.5990991896,5.2572502133,0.6391026945
C,2.8055441021,-4.3719392062,0.4375106344
C,6.7567107122,0.8416292939,-3.3710287472
C,-6.220399951,-1.0876473765,-1.5422858415
C,-7.4835439822,-0.5603903695,-1.785849786
C,-10.7753629802,-1.504683288,-2.6883185913
C,10.7900177001,-1.836267262,2.400099545
B,-0.0553404527,-0.2080706791,0.3025997008

Cartesian Coordination of 3b–4

–2936.6690282 hartree
H,14.4583131519,1.4713166455,3.8405109446
H,-6.9833995178,-3.3726046674,-0.8348078324
H,7.0992468663,-2.4322048152,-1.3916938577
H,9.3202385728,-1.4826621988,-1.0831824099
H,7.6249194192,1.6266813619,1.3734462481
H,5.4316610459,0.6580244155,1.0968402963
H,-7.9081362122,1.4759528422,-0.8330658159
H,-14.0423830017,4.9355704145,2.103964104
H,-15.248452575,4.0217076617,1.1518194601
H,-17.6528925863,1.7847611236,2.5067378225
H,-4.8046562733,-3.976099556,-1.6610808467
H,-13.6463498146,4.4022038794,0.4485336577
H,-9.3027936499,-2.5947640596,-0.7820031328
H,16.0977156943,1.2803878514,3.1460006293
H,18.3411057406,0.3520413705,0.5247953583
H,17.3092289312,0.2555307612,-0.9283005339
H,17.0665549926,-0.8950672174,0.4256566814
H,2.3719841396,-3.7622297726,-1.0588987961
H,5.0591966413,-3.6506397688,-0.9918187036
H,16.0365120482,2.8201758659,-3.3458596336
H,14.4080426731,3.2375252878,-2.7487658982
H,14.7129499247,1.6279985518,-3.4635250218
H,-5.6194623512,0.7075807068,-0.9502504535
N,-10.1305543116,0.0171004737,-0.7735639728
N,9.964581822,0.6866072601,0.3982528574
N,-3.6533689225,-1.112024879,-0.6012428232
N,3.591407038,-0.852321772,-0.1751108011
O,-1.3196434023,0.0766594122,-0.0818633987
O,-16.1237008711,-0.5276803926,-0.1293912176
O,-13.635063593,2.9564494719,1.9585209116
O,-11.1651556958,-1.9121027479,-0.0437122092
O,1.1339640744,0.1644485723,0.0606855688
O,15.5767484895,1.9529881047,-1.5866246197
O,-16.0792057859,1.8050451277,1.2266112307
O,10.7507159686,0.2001624421,-1.7115760661
O,14.7046918784,-0.1788391851,2.5809757283
O,16.4645074567,1.0707252827,0.8037490839
C,14.6425888822,1.4146902466,-0.7529842752
C,6.2686007023,0.1881223047,0.5882808
C,-14.1841615908,4.14078032,1.3691137927
C,-16.7557695302,1.1885176516,2.3302775064
C,14.2521415311,0.3655261218,1.4051227025
C,15.1376516401,0.9413576778,0.4834241855
C,-4.215823999,-3.1416664515,-1.3095501266
F,-0.2258989789,0.8344000841,1.8486980459
F,-0.1608296455,2.1035830571,-0.0648224349
H,3.5007311561,0.1245290963,0.0626717525
H,-3.6714860551,-0.1727100297,-0.2319477425
H,12.2382976324,-0.2075248747,1.8343653461
H,12.8872205832,1.608262654,-2.0079931152
H,9.7402689437,1.270272309,2.4185727786
H,9.5265307283,2.5848177457,1.2382283268
H,11.1415471226,1.961182349,1.5778194611
H,-11.3921779506,1.4510266995,-1.6494000107
H,-9.7595042044,1.368265345,-2.3314423758
H,-2.1265932073,-3.8942541919,-1.415399024
H,0.0588128155,-2.8829732484,-0.7720116786
H,15.5184212608,0.1531195709,4.4067106243
C,-8.8007190286,-0.4997863864,-0.8062112885
C,-8.5005385225,-1.8754686394,-0.816734262
C,-7.1799384524,-2.3052060439,-0.8498457658
C,7.2099998264,-1.5458832914,-0.7752284274
C,8.4756467504,-1.0098787992,-0.6034956351
C,8.6650111713,0.1576133084,0.1630647127
H,-10.0364091969,2.163947095,-0.7671378379
C,7.5351574273,0.7398294249,0.7600305926
C,13.2858615895,1.2954529595,-1.0519715318
C,-12.4714703467,1.2468560762,0.7841230477
C,-13.6806475668,1.8224145219,1.1869176512
C,-14.8986494902,1.2082445499,0.864707681
C,-14.8936567265,-0.0037715506,0.1376073302
C,-13.6839661905,-0.5872123755,-0.237478128
C,-12.471161725,0.0452561146,0.0735412304
C,12.4053593848,0.7353868583,-0.1151864017
C,-16.1858683305,-1.7576079738,-0.8399641949
C,-2.8194928691,-3.0966825746,-1.1888668577
C,-2.4775794832,-1.8182811543,-0.7377935631
C,-4.7255426592,-1.8889054618,-0.9349873148
C,-1.2257411594,-1.1860656393,-0.4247440184
C,0.0058383864,-1.8398892908,-0.4958737803
C,1.1715122415,-1.1024095748,-0.2778373228
C,15.2276540463,0.748618665,3.5391842635
C,17.3364380901,0.1331157334,0.1585408263
C,2.4928508884,-1.6462775258,-0.4260049236
C,2.9755299327,-2.9028403863,-0.8044830206
C,4.3760361498,-2.8414521786,-0.779426524
C,4.74807581,-1.5467398147,-0.384763585
C,15.1441490382,2.4313898402,-2.8540534026
C,-6.1025236435,-1.4045247988,-0.890312541
C,6.0712851585,-0.9619637606,-0.1885854542
C,-6.4105056916,-0.0345860069,-0.8916702944
C,-7.7265076236,0.4082909667,-0.8451317929

C,10.9818416569,0.5334800243,-0.5564667356
C,12.8888113276,0.2698220291,1.1100400842
C,-11.2076590751,-0.7055612736,-0.2583162045
C,-10.3397554999,1.3275354791,-1.4061046782
C,10.0992556295,1.6787068501,1.4692306837
B,-0.1473617023,0.8509391917,0.4785714561
H,-17.0418894793,0.1603025107,2.0901569257
H,-16.1268008458,1.2010174171,3.2278402953
H,-11.5505607295,1.7378555656,1.0768144807
H,-13.6520794692,-1.539003294,-0.7510813849
H,-17.2468350717,-1.9856370039,-0.9484870365
H,-15.7306869515,-1.6703521143,-1.8340630664
H,-15.6936206873,-2.5683314269,-0.2891639236

Cartesian Coordination of 3b–5

-2936.6688954 hartree
H,15.5965765292,3.3858009731,-3.5972366419
H,-10.3902755244,-1.7618785496,2.1562527011
H,-11.3795891965,-2.2766833482,0.7738481179
H,-11.8541388102,-0.8623738494,1.722499321
H,16.273995729,1.0511328125,2.6095926265
H,18.2980425437,0.5434853181,-0.278133762
H,17.1438581431,0.5743096471,-1.6389335375
H,17.0577653002,-0.7343142267,-0.4156612098
H,0.0354626278,-3.1204935714,-0.45626479
H,5.0231970532,-3.7401192818,-1.1216290142
H,14.0153522445,3.6571518593,-2.8165897678
H,14.3023199359,2.1672661579,-3.7611552616
H,-5.6872024898,0.3591150511,-0.0681818529
H,-4.8629989111,-4.2524393538,-1.0507019716
H,2.3405388336,-3.9131156628,-1.0026845165
H,15.8271845354,-0.2321134078,3.7715748994
H,7.0030740789,-2.4210457085,-1.5643093608
H,-6.982509304,-3.7435672386,0.0474625229
H,12.3484694545,-0.4069985738,1.4514657354
H,12.6139462833,1.881499801,-2.1784441259
H,-12.7222268883,-1.0974451039,-0.8220547277
H,-11.9819030666,2.8914702393,0.6050250238
H,-14.436741202,5.5080767274,1.1365889556
H,-13.0267938253,4.9362231141,0.2029353877
H,-13.2767969139,4.375901253,1.8816406244
H,-2.1749604588,-4.1393432846,-0.9778753044
H,11.1782970863,1.7373079344,1.550435204
H,-3.6889341326,-0.5286095565,0.5441006454
H,9.8628682116,0.9133652271,2.4100014565
H,-16.9596224983,-0.5503889623,-0.027367421
H,5.4696321624,0.3463795389,1.3530210142
H,7.657657732,1.345918592,1.5632160008
H,9.5303635544,2.3518107854,1.4164627201
H,14.6970746018,1.1114205779,3.4556124506
H,9.2221949864,-1.4427323879,-1.3259294556
N,-3.6807930875,-1.4432750033,0.116669898
N,9.9333431162,0.5778029769,0.323388062
N,-10.1890175664,-0.5102446887,0.489103577
N,3.5695565217,-1.0692309751,0.0637128117
O,-16.279401935,1.6797066235,-0.4165304111
O,15.3175158811,2.2810417683,-1.9358461506
O,-9.9911727923,1.5898074113,-0.4344465734
O,1.1227567882,-0.1356876865,0.565551474
O,-15.2446045048,-0.8003163079,-1.2037562514
O,16.4330821372,1.1484336454,0.2434723569
O,14.8665710592,-0.3727073112,1.9931255184
O,-1.3326846765,-0.2607409659,0.5851908942
O,-14.6235970778,3.6135372159,0.4776655563
O,10.5535349896,0.3512497847,-1.8829942054
H,3.4786277764,-0.1205854506,0.3968248503
H,-7.9926906984,1.1001563996,0.2369884429
H,-9.2887927761,-3.0006692422,0.2949857835
H,-16.3693050186,2.0214392516,-2.4769545622
H,-16.2028684738,3.4902886928,-1.462108651
H,-17.7433500002,2.5891147332,-1.4870492888
H,-15.8125663197,-1.8020357414,0.5410933928
H,-16.7858568757,-2.0857230654,-0.9266915368
B,-0.1353120406,0.4836703987,1.1333110825
C,15.0874186403,1.0073213319,0.0202521248
C,4.7196426106,-1.7113044205,-0.2949273331
C,14.7621955438,2.9015271342,-3.0887002735
C,-6.1389070219,-1.7571371244,-0.0280330032
C,6.042288259,-1.1130704697,-0.1391564537
C,-6.4654587662,-0.3919146427,0.0345831193
C,-4.2626857346,-3.4329606427,-0.6834478196
C,-0.01282024,-2.1073597588,-0.0842936851
C,1.1544582652,-1.3662321642,0.1124454045
C,15.4516516796,0.4517270617,3.0079618251
C,17.2716339823,0.3279643732,-0.5806253298
C,2.4699312573,-1.8635440518,-0.1811645882
C,2.9457473339,-3.0665227146,-0.7118190698
C,4.3429795832,-2.9721543265,-0.7836158001
C,14.3009342455,0.290790534,0.9331472962
C,-16.6565965731,2.4972960223,-1.5322840991
C,-16.2598276241,-1.3282063337,-0.3424177251
C,6.2746906227,-0.0436911502,0.7369524078
C,7.538769895,0.5239808498,0.8696843106
C,8.6304173672,0.0388852416,0.1319729705
C,8.4070959478,-1.0477827692,-0.7371460281
C,7.1435632022,-1.6003245237,-0.868217619
C,-7.1929340045,-2.6792027774,0.0756874758
C,-10.7029128637,0.6862989098,-0.0089400995
C,12.9205760657,0.1783268729,0.7402390077
C,10.8712065742,0.5648478091,-0.7201269563
C,14.4746913436,1.6077335533,-1.1030686023
C,13.1014794079,1.4717076022,-1.3037163725
C,-13.0723115324,-0.1184810104,-0.5161691414
C,-14.4345878776,0.1644642208,-0.6579986681
C,-14.935078243,1.4274240624,-0.313621191
C,-14.0487634203,2.416356022,0.1700411779
C,-12.1989740668,0.8635816094,-0.0453329055
C,12.3209962615,0.768554601,-0.3748921886
C,-13.7806758154,4.6573305454,0.9490065838
C,-2.8618704569,-3.3704264687,-0.6546508109
C,-2.5077176931,-2.1179421014,-0.1443582444
C,-4.7621751921,-2.2159854049,-0.1954316804
C,-1.2454651908,-1.4877753923,0.1306901454
C,-8.5057909688,-2.2541196698,0.2311825675
C,-7.7747326584,0.0445514247,0.2021583711
C,-8.8241480245,-0.8858995353,0.2989384911
C,10.135987049,1.4407128344,1.491196519
C,-11.0017905311,-1.407073126,1.3228705288
F,-0.1168097481,0.3381952115,2.4980996984
F,-0.2047255198,1.7799549857,0.7115175353

C,-12.6877340125,2.1364575496,0.2850854053

Cartesian Coordination of 3b–6
–2936.6684577 hartree
H,-2.5214051382,-4.5499505928,-15.3251625316
H,-0.9058589963,0.7321846554,16.6688269604
H,2.3069791898,-0.4686360867,17.6105147738
H,2.6754488023,0.6895408542,16.3017511921
H,3.0273962917,-1.0556165169,16.0866677645
H,2.3466053618,-1.2425245715,-11.3515585019
H,-2.1138643064,1.2682524188,15.4609470812
H,3.0807514929,-3.1340679482,12.8219749634
H,1.4935653677,-3.9470765393,12.9421260985
H,1.402840224,-1.9485126648,11.7202913105
H,-0.4684690108,1.8452475816,12.4964003864
H,-1.6151872134,-2.4361268596,-12.5185979989
H,-2.1384075568,4.4700761065,4.6062940245
H,2.7502703226,-4.2575175162,14.1695009617
H,-1.3411530139,2.4612959362,16.5388952298
H,-2.5691852625,-2.9174939004,-14.6070188716
H,-2.4510051474,-4.3552597218,-13.5518894009
H,0.385137302,0.4938693791,5.4389550882
H,0.5901883329,-0.3073767936,7.7367233167
H,-2.412813654,2.5120044314,8.973395857
H,-2.6592236302,3.2745885064,6.6719797789
H,-0.4879958426,3.6299088606,-7.2745354232
H,-0.08337645,2.7723306608,-9.5100221922
H,-0.3161545222,-1.2590882095,-8.006465357
H,-0.7606617385,-0.396496298,-5.7799943852
N,0.1543798519,0.1803559877,-10.2416345348
N,-0.8358958904,0.5862648004,9.89314276
N,-0.6836147039,1.51592778,-3.8614387354
N,-0.9506289399,1.6791887306,3.4010273657
O,-0.332341703,0.4869335808,-1.4230219288
O,-0.7316181802,-3.9108434616,-14.6564940543
O,1.8483999447,-2.4678011336,14.374785203
O,1.948214532,-3.9268600131,-14.9832690737
O,-0.4155245214,0.5453933447,1.0441520703
O,3.5924235479,-2.5919004396,-13.1576617465
O,-1.2884356066,-1.6076316514,-10.0952279199
O,1.0006958745,-0.5378196318,16.0595437143
O,-0.1379028119,1.8094363262,15.0447885968
O,1.3200781387,-0.2136725913,9.782688912
C,-0.9109716052,1.7555705501,0.9656495175
C,0.8318960875,-0.3799825984,14.7074613855
C,0.2095198373,0.7740396748,14.2127622833
C,-0.0096464827,0.9253825195,12.83986542
C,-0.5500716813,-2.448573416,-12.7085704424
C,-0.0055203751,-3.1843584773,-13.7603698371
C,-1.8020496447,3.6430658385,3.9982269622
F,-0.8407767637,-1.4143103081,-0.1587580546
F,1.2903561129,-0.5647295356,-0.108163471
H,-0.6130113191,0.7276246473,3.399608308
H,-0.2628087829,0.6009177175,-3.7897357392
H,-2.0187964243,4.3984480343,1.9180263252
H,-1.5464193509,3.3836528375,-0.2966328333
H,5.255312579,-2.1396647749,-14.2230659277
H,3.9503724397,-0.93347849,-14.3789258197
H,3.8276627793,-2.5001388887,-15.2371852682
H,2.4548145444,-5.7553473817,-15.701634146
H,0.9585298824,-5.7526270065,-14.7285124296
H,-2.3575112532,1.5817533564,11.0388402207
H,-2.0408672238,-0.1024487921,11.472424142
H,-2.9047277477,0.2723731575,9.9710831472
H,0.9779305228,0.6105729659,-12.1226733885
H,1.6040948759,1.6124658851,-10.7987531343
H,2.5555028949,-5.6236232674,-13.9234086504
H,-1.8449153777,4.3008397461,-2.5840414402
H,-1.74299518,4.261172514,-5.2734375916
C,0.3387946704,0.0873111129,10.4537200173
C,-0.3631632606,-1.0511164954,-10.6719004064
C,2.3148201059,-3.5007785517,13.5159672119
C,0.2875499404,-1.7227742958,-11.8495650881
C,0.4073106761,-0.0672822581,11.9512743816
C,1.0501090624,-1.2165935319,12.4348920457
H,-0.0197014161,1.9079358038,-11.4641744461
C,1.2483522521,-1.3845758983,13.8049131926
C,-1.1378158594,2.3843950185,-0.2594437592
C,-0.8264371518,1.7001732437,-1.4359529741
C,4.1767939866,-2.0063890238,-14.3269090973
C,1.9724391724,-5.35012708,-14.8102640028
C,-1.0149451635,2.2572937061,-2.7475214118
C,-1.4874238905,3.4913734871,-3.2041160293
C,-1.4240885223,3.4748993589,-4.6048959096
C,-0.9155400535,2.2288609484,-5.0024618202
C,-2.1464618134,-3.9252081642,-14.5136991837
C,-1.1623998707,1.9465546961,5.8604291571
C,-0.6600468538,1.6953556221,-6.3375535136
C,-0.2542458338,0.9299439854,6.2013578537
C,-0.1232600711,0.4679630511,7.5062486465
C,-0.8995091779,1.0274929434,8.5359112259
C,-1.803914018,2.0517969071,8.203940245
C,-1.9352397173,2.497504533,6.895374835
C,-0.4685561737,2.5555839161,-7.4275232058
C,-0.2273885197,2.0621842643,-8.706010029
C,-0.1637302633,0.6802306354,-8.947636313
C,-0.3461609612,-0.1895246282,-7.855415014
C,-0.5935298057,0.3112870301,-6.5868826231
C,-1.1853165023,1.535125728,15.9822516816
C,2.3393180334,-0.3287958321,16.5284138473
C,2.2253993003,-2.5129022451,-13.0658107476
C,1.395584639,-3.2263715696,-13.942159066
C,1.6726782849,-1.7568232791,-12.0275891029
C,-1.3116186044,2.4231526737,4.4875259547
C,-1.1980380727,2.3693469269,2.2340862678
C,-1.7293727958,3.6100456785,2.5978634804
C,0.7111777296,1.131246695,-11.2083254832
C,-2.1020942231,0.5941078366,10.6392822527
B,-0.050763718,-0.2962655573,-0.1593025457

Cartesian Coordination of 2d (AM1)
–1.705462 hartree
H,19.6378899861,-6.6200200413,-1.26972
H,-20.1734399996,0.1830100425,5.17951
H,-20.9530500028,-1.3100299559,4.52976
H,-26.0312599973,1.2594900548,9.73309
H,-26.8106300005,-0.2334899435,9.08335
H,-15.3313899883,5.5602100323,-2.30011
H,-15.5268399875,5.9538300327,-0.54899
H,-20.9627100006,-0.3003899559,2.22162

H,-20.1825599975,1.1924500425,2.87161
H,-19.0048600014,-0.65802996,0.69686
H,-18.2211799982,0.8326400384,1.34814
H,-19.0017200035,-1.66980996,3.01194
H,-18.2213800004,-0.1763899616,3.66235
H,-17.370029978,10.4379800366,-1.76358
H,-17.1748699789,10.0441400362,-3.51442
H,-19.0176399694,14.52892004,-4.72853
H,-19.2127999686,14.9227200405,-2.97772
H,32.6191799779,-10.5056700687,-4.91996
H,31.7247199754,-11.6818500668,-5.95649
H,21.8827499901,-4.7106200461,-2.22944
H,20.9876599876,-5.8868100442,-3.26601
H,20.8880000401,19.035419956,-5.94776
H,22.5110800411,19.5194099526,-5.30468
H,21.0839100409,19.4297199556,-4.19233
H,16.1817200036,1.7214599659,0.31862
H,15.9173700028,1.3154399665,-1.44465
H,13.5801999916,-4.0069900286,-0.98295
H,19.2118200314,14.9233299595,-2.97361
H,19.0164300306,14.53004996,-4.72451
H,23.9333899812,-8.9384400504,-2.34629
H,24.8280699837,-7.7623200523,-1.30951
H,24.0299399876,-5.8698200506,-2.76788
H,23.1351499852,-7.0461000487,-3.80444
H,29.1235099788,-10.0803300613,-2.38597
H,28.2289599763,-11.2565900594,-3.42265
H,27.9929600055,2.6258799411,8.94428
H,28.7727800024,1.1335599394,8.29361
H,20.7705200273,12.9626299563,-2.70716
H,20.5750900265,12.5693599567,-4.45808
H,17.8111300123,5.8416499625,-2.63845
H,18.0067800131,6.2350899621,-0.88742
H,22.906019998,-0.9526700482,6.04691
H,22.1261200011,0.5396999534,6.69756
H,22.9149500001,0.0579899517,3.7396
H,22.1349200033,1.5503099534,4.39033
H,20.9536599972,-1.3114300441,4.5291
H,20.1736100004,0.1809799575,5.17978
H,32.4020900042,2.0078799318,13.14197
H,31.912910007,3.3386099328,12.01412
H,32.6947600039,1.8424299312,11.36176
H,31.2716399763,-11.2395200658,-2.92435
H,30.3771399739,-12.415740064,-3.96096
H,30.4729799803,-9.3470700642,-4.3825
H,29.5784399778,-10.5233700623,-5.41911
H,28.7639500003,0.1229699394,10.60084
H,27.9841400034,1.6152799411,11.2515
H,22.4162900359,17.0534199528,-5.67063
H,22.6116700367,17.4466599524,-3.9199
H,28.3252099828,-8.1880000596,-3.84433
H,27.4306399803,-9.3643200578,-4.88095
H,12.0831100002,0.0758899746,-0.9174
H,18.2906400267,12.6806999615,-2.36708
H,18.0952600259,12.2873899619,-4.11799
H,20.1331800361,17.1663199576,-3.58029
H,19.9378000353,16.773049958,-5.3311
H,26.0811499787,-10.0975300549,-2.88449
H,26.9757399812,-8.9213100568,-1.84777
H,17.369400022,10.4381699634,-1.76053
H,17.1740200212,10.0448299638,-3.51146
H,16.4480600173,8.1958199654,-1.15394
H,16.2526800164,7.8024199658,-2.90491
H,15.3309000117,5.5604699677,-2.29819
H,15.5265500125,5.9535999673,-0.54699
H,-18.0962899741,12.2864900381,-4.12148
H,-18.2914399733,12.6803000385,-2.37065
H,-21.0852399591,19.4286700444,-4.19751
H,-22.5125799589,19.5179700474,-5.30969
H,-20.8895699599,19.033850044,-5.95286
H,-16.1817099964,1.7218900341,0.31787
H,-15.9175699972,1.3154000335,-1.44533
H,-25.2824900173,-8.2068299468,-4.34036
H,-26.1771900148,-7.0307899449,-3.30351
H,-24.8271900163,-7.7639699477,-1.3072
H,-23.9324500188,-8.9398399496,-2.34422
H,-18.9285699822,8.4772500399,-1.49628
H,-18.733299983,8.0834100394,-3.24715
H,21.4962400312,14.8120599547,-5.0646
H,21.691660032,15.2053299543,-3.31372
H,20.9627999994,-0.3004500441,2.22155
H,20.1822000025,1.1917499575,2.87245
H,18.732560017,8.0840899606,-3.24498
H,18.9280600179,8.4774299601,-1.49402
H,22.6805999861,-6.6033800478,-0.7711
H,21.7856899836,-7.7792900459,-1.80804
H,-4.7136000111,-5.2618899901,-2.11367
H,-21.692699968,15.2045200457,-3.31755
H,-21.4975099688,14.8107400453,-5.06835
H,5.9182599966,-1.5927300125,0.66894
H,8.3057499977,-1.0913900175,0.8695
H,9.1284699922,-3.7019100192,-2.5316
H,6.7192399912,-4.1744100141,-2.71699
H,-6.7192800088,-4.1742999859,-2.71699
H,-9.1285000078,-3.7017399808,-2.53161
H,-8.3057100023,-1.0909699825,0.86927
H,-5.9182300034,-1.5923599875,0.66873
H,-27.4301200197,-9.3663699422,-4.8782
H,-28.3247600172,-8.1903199404,-3.84133
H,-18.0071199869,6.2351200379,-0.88918
H,-17.8116899877,5.8411900375,-2.64012
H,-16.2533499836,7.8019500342,-2.90734
H,-16.4485199827,8.1958400346,-1.15646
H,-13.5801500084,-4.0068599714,-0.98219
H,-20.5328300115,-5.4455399568,-0.23066
H,-19.6372700139,-6.6205199587,-1.26839
H,-20.7713899727,12.9620300437,-2.71047
H,-20.5761899735,12.5682500433,-4.4613
H,-19.8500099774,10.7195900418,-2.10339
H,-19.6547899783,10.3257900414,-3.85423
H,-22.4177399641,17.0518700472,-5.67492
H,-22.6128899633,17.4456300476,-3.92427
H,-16.8894699924,3.5992900356,-2.03396
H,-17.0862599916,3.993530036,-0.28243
H,-14.402509993,3.3157000303,-1.6875
H,-14.6034099922,3.7025900307,0.06387
H,-29.5777600222,-10.5258799377,-5.41599
H,-30.4723600197,-9.3498599358,-4.37911
H,-31.2702800237,-11.2425899342,-2.92092
H,-30.3757200261,-12.418529936,-3.95779

H,-29.1223100212,-10.0829299387,-2.38292
H,-28.2277100237,-11.2589199406,-3.41985
H,-23.1349300148,-7.0472399513,-3.80244
H,-24.0297800124,-5.8712199494,-2.76564
H,-22.6798700139,-6.6045699522,-0.76917
H,-21.7849200164,-7.7802299541,-1.80634
H,-26.9747100188,-8.9234299432,-1.84509
H,-26.0800600213,-10.0993899451,-2.88205
H,-19.9391899647,16.771710042,-5.33566
H,-20.1343399639,17.1654800424,-3.58493
H,4.7135199889,-5.2620500099,-2.11363
H,-20.9875900124,-5.8875299558,-3.26439
H,-21.8827300099,-4.7115699539,-2.22759
H,-0.0000200085,-4.04291,-1.55297
H,-31.7238800246,-11.6848199332,-5.953
H,-32.6184100221,-10.5089099313,-4.9162
H,-24.8673599991,0.4170300524,5.25755
H,-24.087909996,1.9100000507,5.90731
H,-2.0083500105,-4.9911899958,-1.97952
H,-18.377700009,-4.2856099613,0.31193
H,-17.4810800115,-5.4566499632,-0.72873
H,-19.7369500075,-3.5514999584,-1.68858
H,-18.84111001,-4.7274899603,-2.72623
H,-17.567570005,-2.365089963,-1.11634
H,-16.6630000075,-3.5546699649,-2.18149
H,-32.5511300286,-13.5822099315,-4.51901
H,-33.9171900266,-12.6177599286,-5.21609
H,-33.4480700261,-12.4031599296,-3.47941
N,3.711829995,-2.3895600078,-0.78751
N,-3.711820005,-2.3894099922,-0.78759
N,10.2645999957,-2.0288900216,-0.65931
N,-10.2645900043,-2.0285499784,-0.65945
O,1.2342299974,-1.2110500026,-0.21484
O,11.2392599928,-3.4381100237,-2.22192
O,-11.2393300072,-3.4382799763,-2.22156
O,-15.9935200072,-3.4028999663,-0.20107
O,-16.4987000013,-0.5979699653,0.04028
O,15.9936199928,-3.4032100337,-0.20183
O,-14.2386299975,1.17316003,-0.17418
O,16.4987199987,-0.5983300347,0.04039
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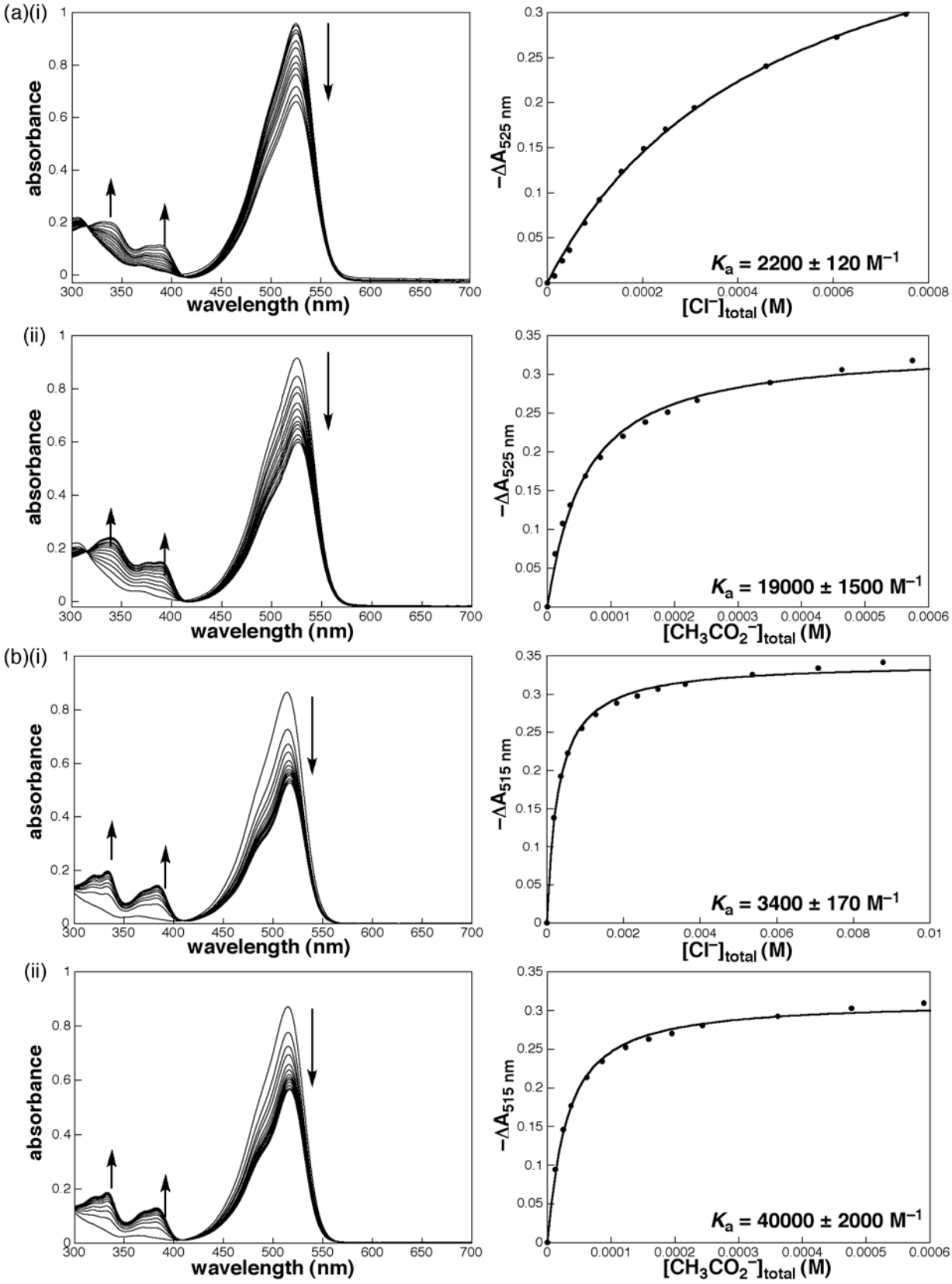
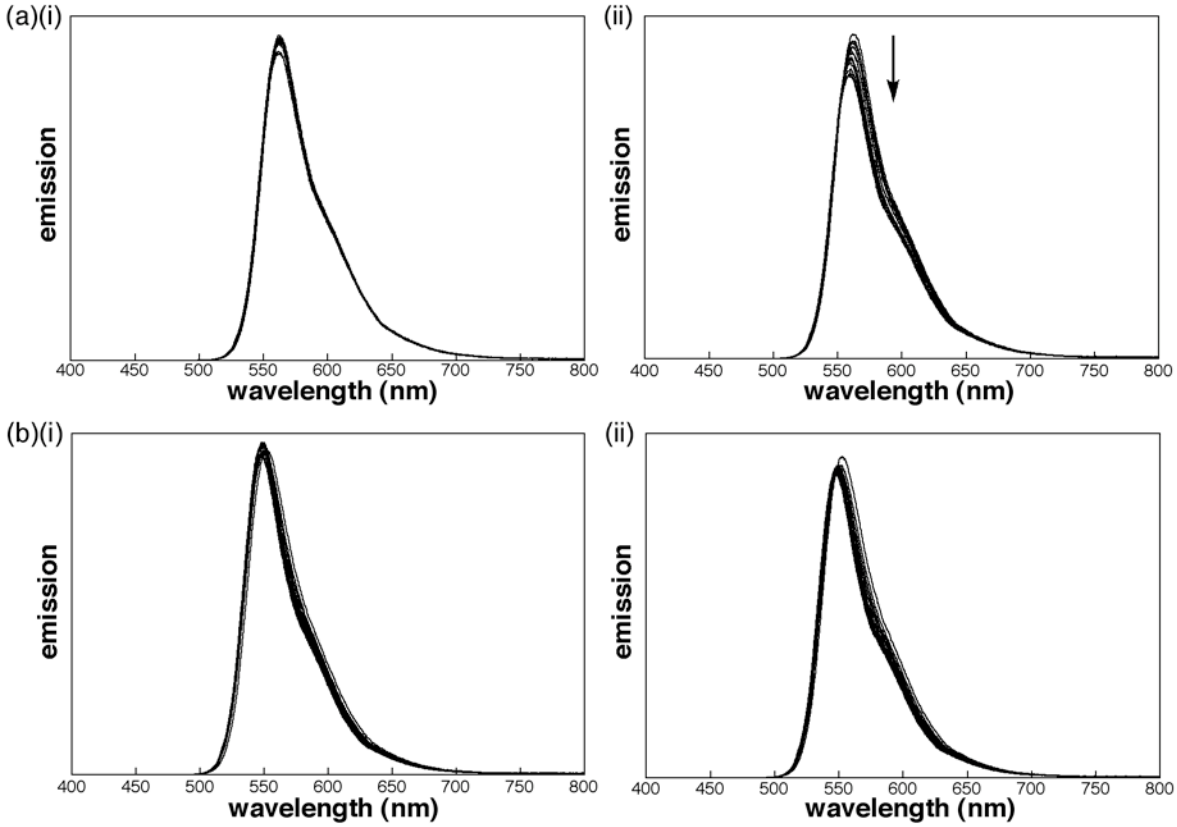
[S5 (as a complete ref. 9)] *Gaussian 03* (Revision C.01), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, 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, J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

4. Anion-binding properties



Supporting Figure 6 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of (a) **2b** (1.0×10^{-5} M) upon the addition of (i) Cl^- and (ii) $CH_3CO_2^-$ and (b) **3b** (1.0×10^{-5} M) upon the addition of (i) Cl^- and (ii) $CH_3CO_2^-$ in $CHCl_3$. Anions were added as tetrabutylammonium (TBA) salts.

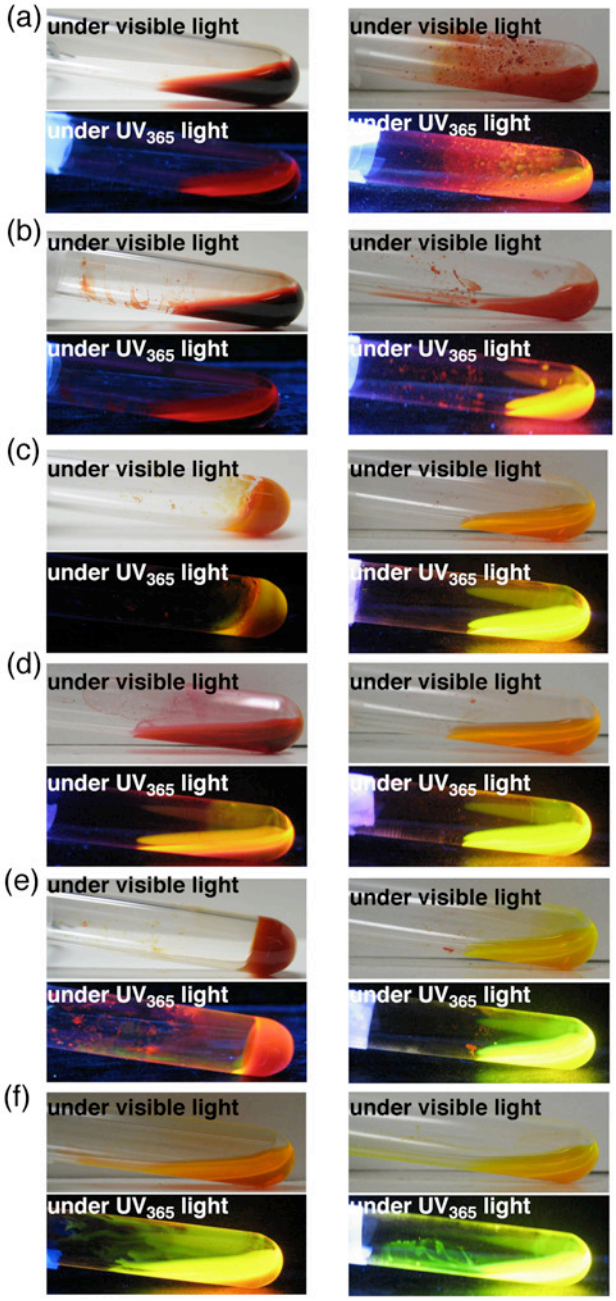


Supporting Figure 7 Fluorescence emission spectral changes of (a) **2b** (1.0×10^{-5} M, excited at 525 nm) upon the addition of (i) Cl^- and (ii) $CH_3CO_2^-$ and (b) **3b** (1.0×10^{-5} M, excited at 515 nm) upon the addition of (i) Cl^- and (ii) $CH_3CO_2^-$ in $CHCl_3$. Anions were added as TBA salts. Under the conditions excited at each absorption maximum, there are negligibly small changes in spectra by the addition of anions in (a)(i) and (b)(i,ii).

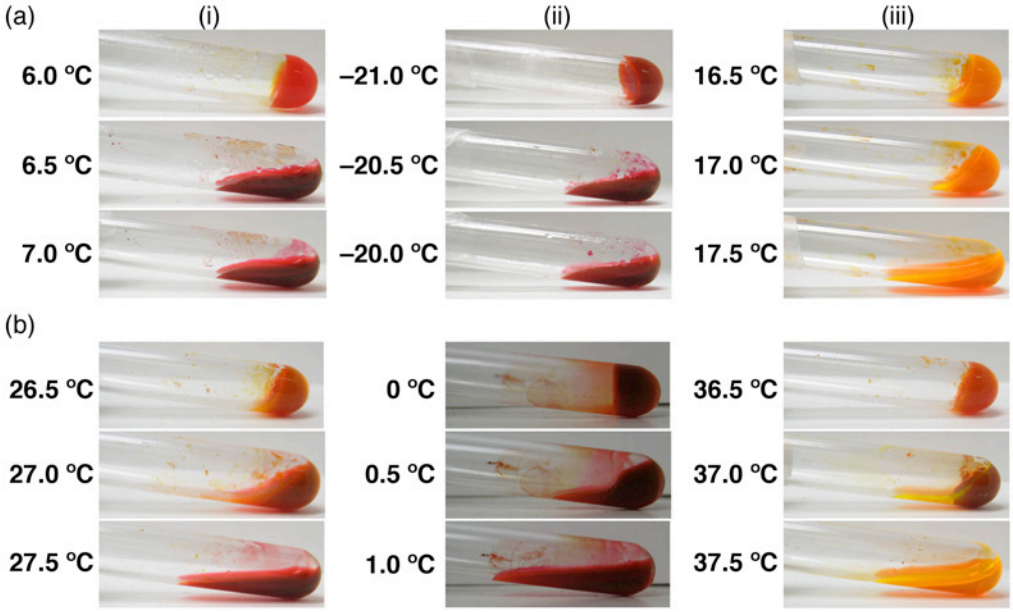
5. Formation of supramolecular gels

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.

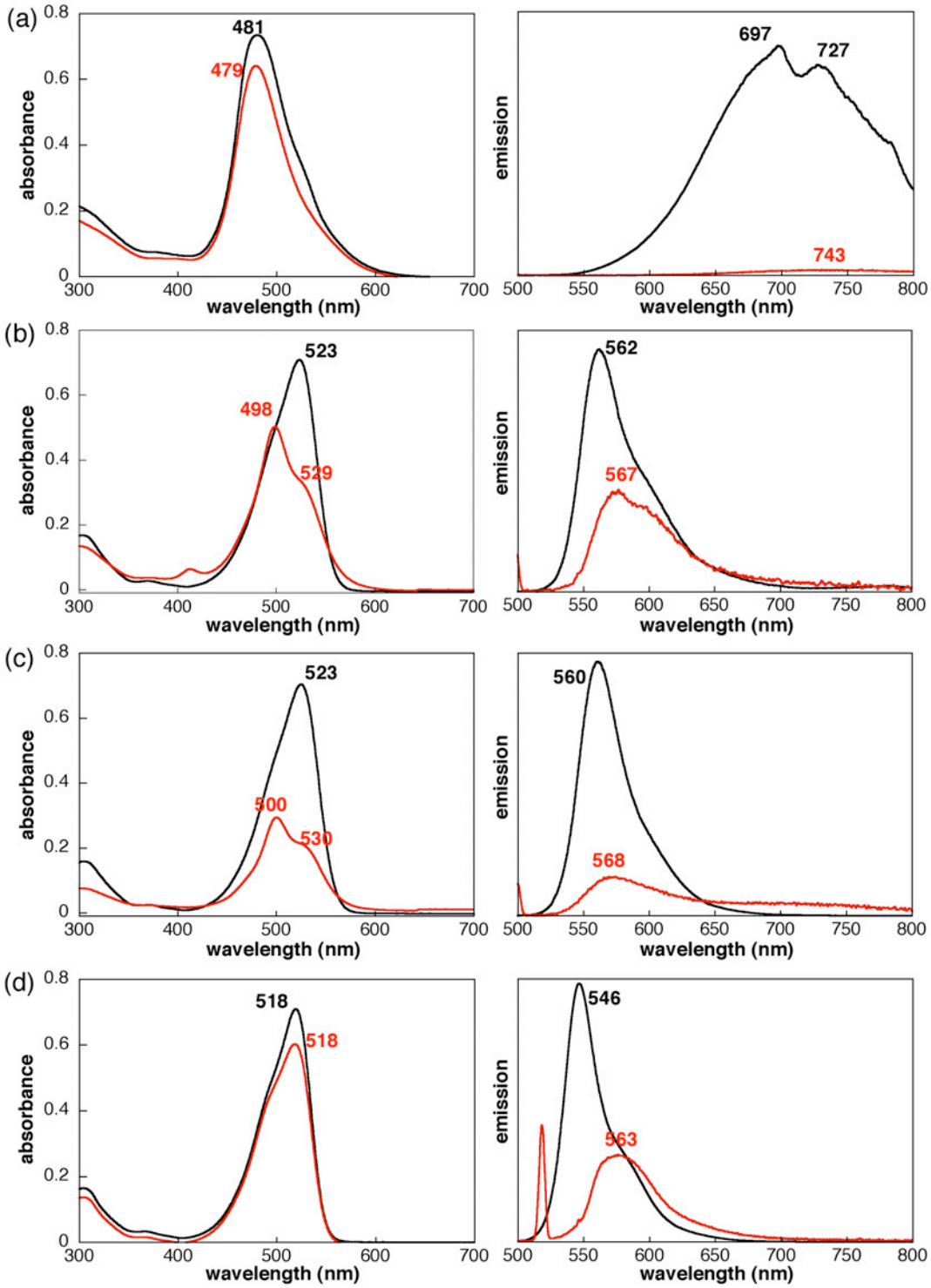
Synchrotron X-ray diffraction analysis (XRD). High-resolution XRD analyses were carried out using a synchrotron radiation X-ray beam with a wavelength of 1.00 Å on BL40B2 at SPring-8 (Hyogo, Japan). A large Debye-Scherrer camera with a camera lengths of 531.527 (xerogel of **2d** prepared from CH_2Cl_2), 535.504 (xerogel of **2d** prepared from 1,4-dioxane), and 530.981 (solid state of **3d**) mm was 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 30 (xerogel of **2d** prepared from CH_2Cl_2 and solid state of **3d**) and 10 (xerogels of **2d** prepared from 1,4-dioxane) sec.



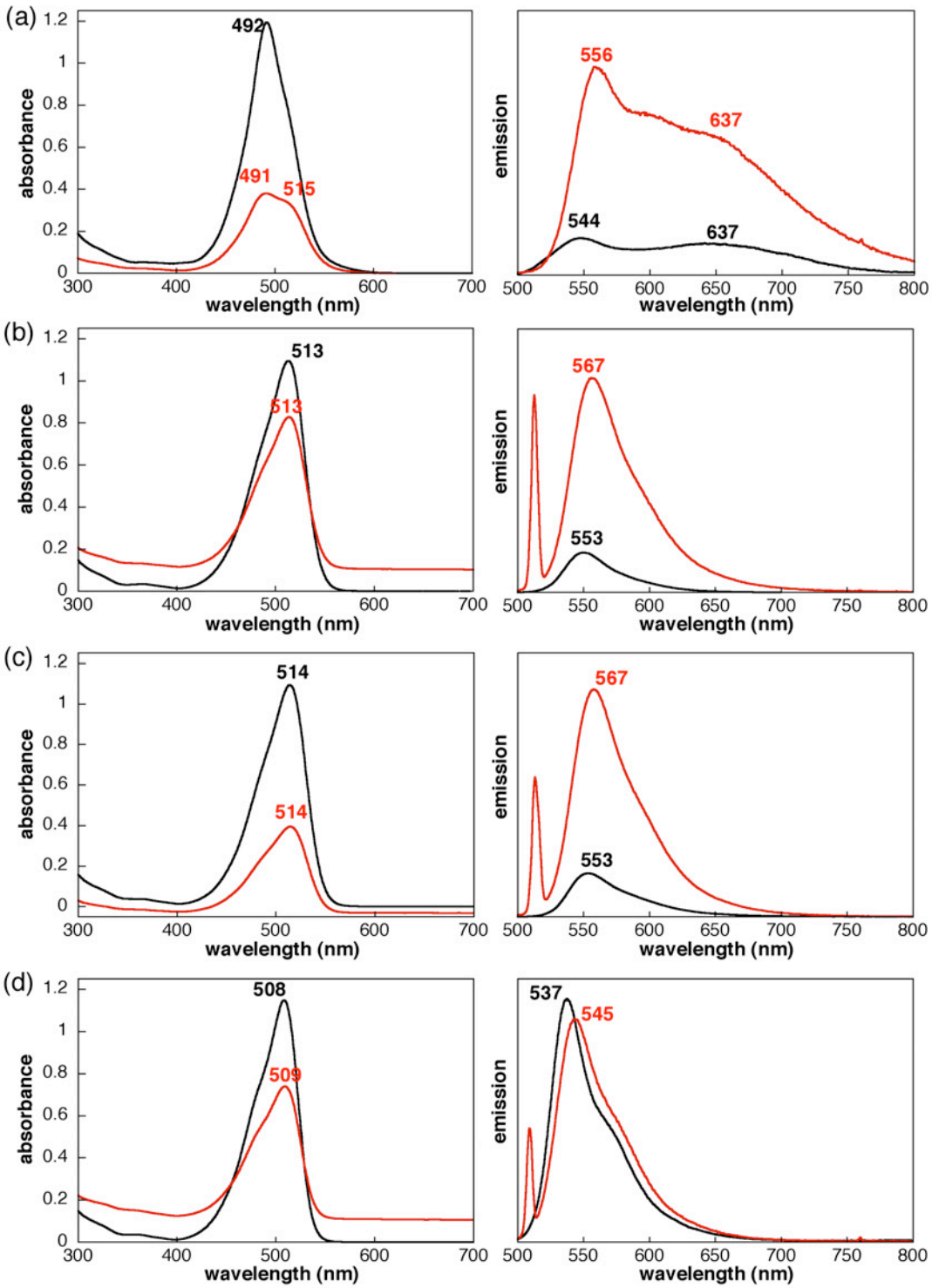
Supporting Figure 8 Photographs of gels, precipitates, or solutions of **2d** (left) and **3d** (right) (10 mg/mL) obtained from (a) octane, (b) cyclohexane, (c) CH_2Cl_2, (d) $CHCl_3$, (e) 1,4-dioxane, and (f) THF.



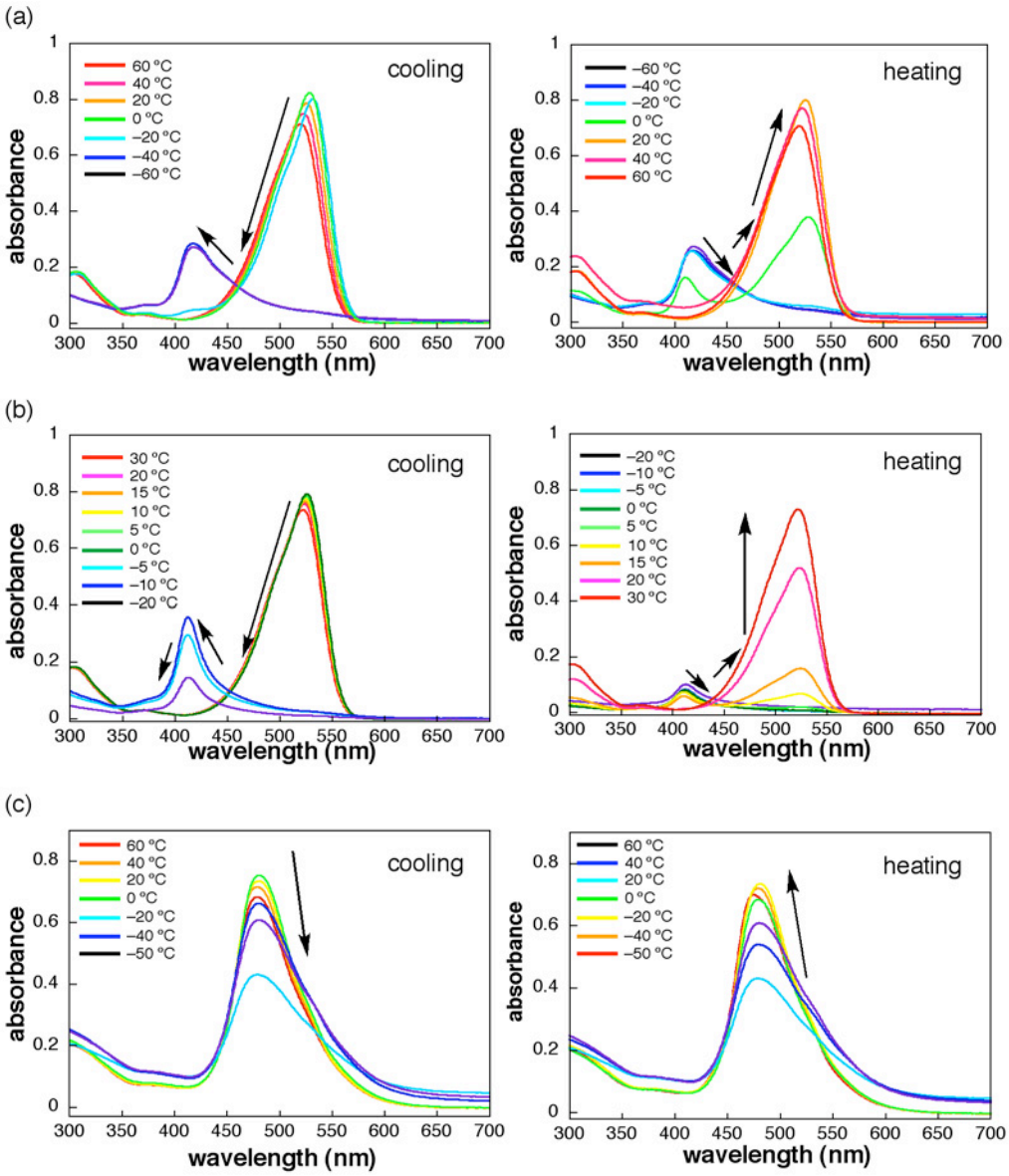
Supporting Figure 9 Phase transitions of (a) **2c** and (b) **2d** in (i) CH_2Cl_2, (ii) $CHCl_3$, and (iii) 1,4-dioxane (10 mg/mL).



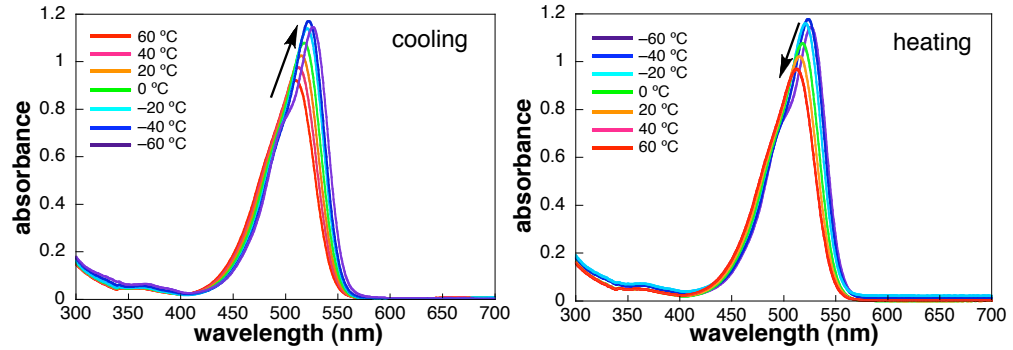
Supporting Figure 10 UV/vis absorption (left) and fluorescence emission (right, $\lambda_{ex} = \lambda_{max}$) spectra of **2d** at 1×10^{-5} M (black) and 10 mg/mL (red): (a) octane, (b) CH_2Cl_2, (c) $CHCl_3$, and (d) 1,4-dioxane. The concentration of 10 mg/mL in CH_2Cl_2, $CHCl_3$, and 1,4-dioxane provides supramolecular gels.



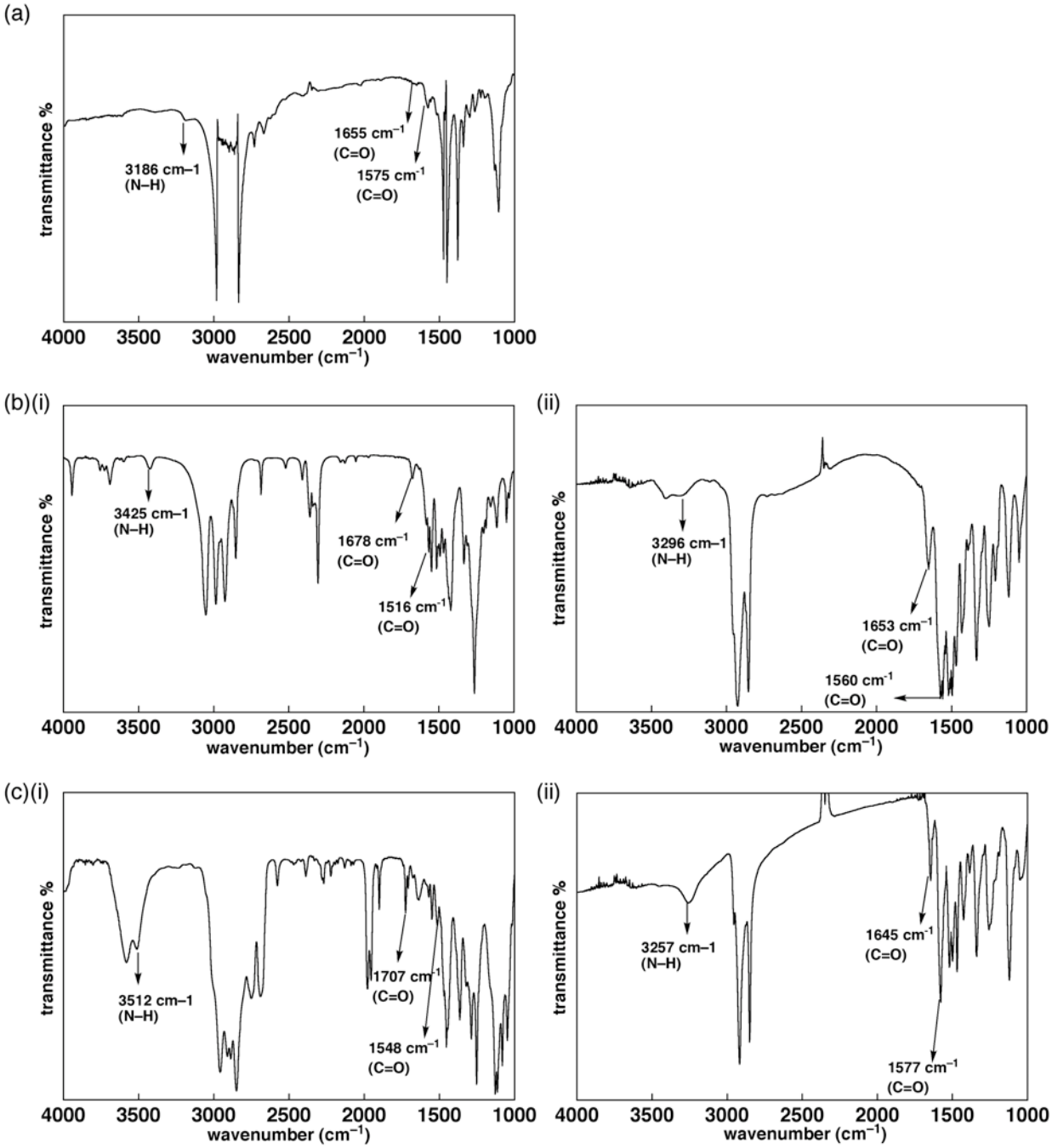
Supporting Figure 11 UV/vis absorption (left) and fluorescence emission (right, $\lambda_{ex} = \lambda_{max}$) spectra of **3d** at 1×10^{-5} M (black) and 10 mg/mL (red): (a) cyclohexane, (b) CH_2Cl_2, (c) $CHCl_3$, and (d) 1,4-dioxane. The concentration of 10 mg/mL in cyclohexane, CH_2Cl_2, $CHCl_3$, and 1,4-dioxane provides solutions. Cyclohexane was used due to poor solubility of **3d** in octane.



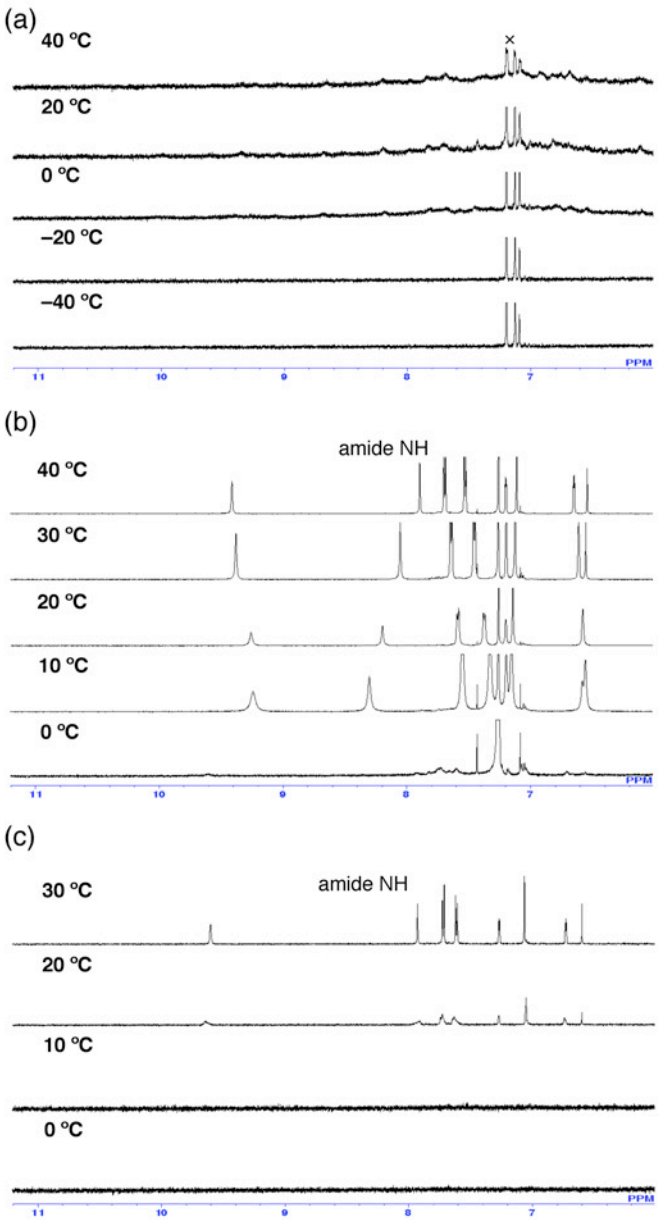
Supporting Figure 12 Variable-temperature UV/vis absorption spectra of **2d** (1.0×10^{-5} M) (a) in octane from 60 to –50 °C (left) and from –50 to 60 °C (right), (b) in $CHCl_3$ from 60 to –60 °C (left) and from –60 to 60 °C (right), and (c) in CH_2Cl_2 from 30 to –20 °C (left) and –20 to 30 °C (right). UV/vis absorption spectra in CH_2Cl_2 and $CHCl_3$ showed the dramatic changes such as blue-shifted bands at low temperatures (< –5 °C), suggesting the formation of H-aggregates even in diluted solutions.



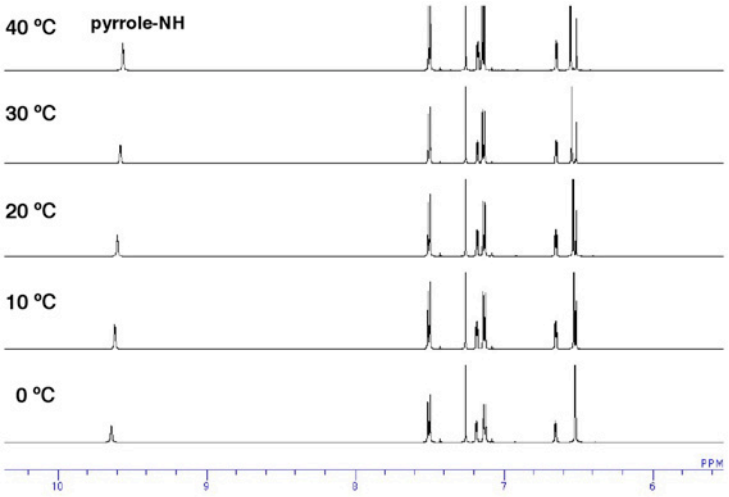
Supporting Figure 13 Variable-temperature UV/vis absorption spectra of **3d** (1.0×10^{-5} M) in $CHCl_3$ from 60 to –60 °C (left) and from –60 to 60 °C (right).



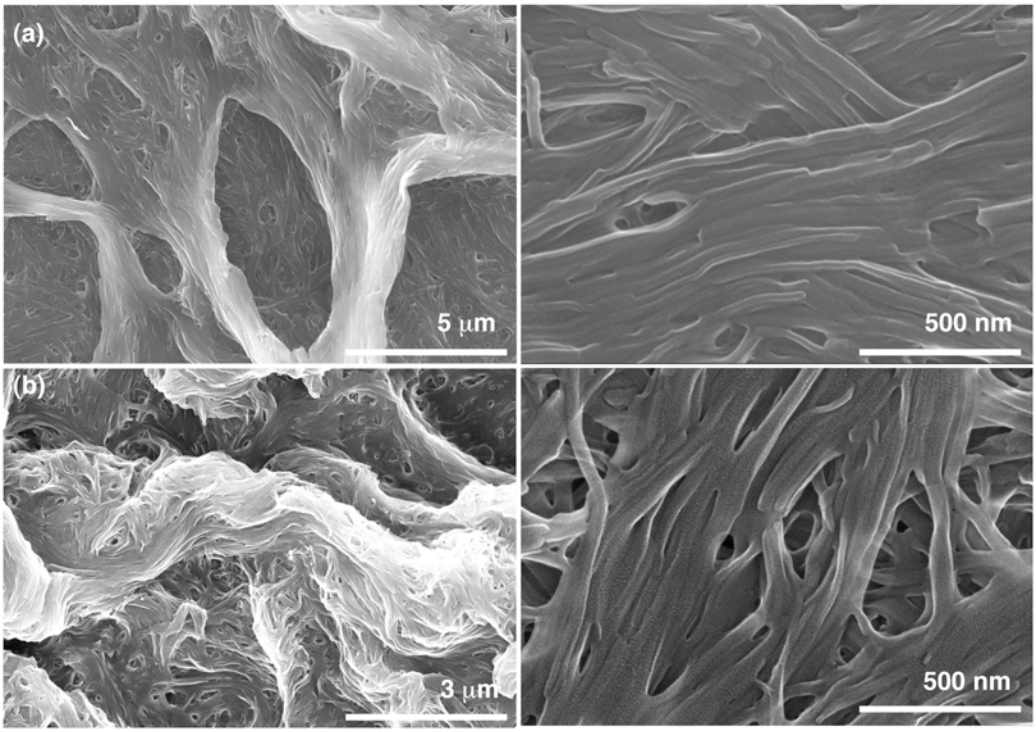
Supporting Figure 14 FT-IR spectra of **2d** (a) in octane (2.5×10^{-3} M), (b)(i) in CH_2Cl_2 (2.5×10^{-3} M) and (ii) as xerogel from CH_2Cl_2, and (c)(i) in 1,4-dioxane (2.5×10^{-3} M) and (ii) as xerogel from 1,4-dioxane at room temperature. Arrows indicate amide N–H and C=O vibration modes.



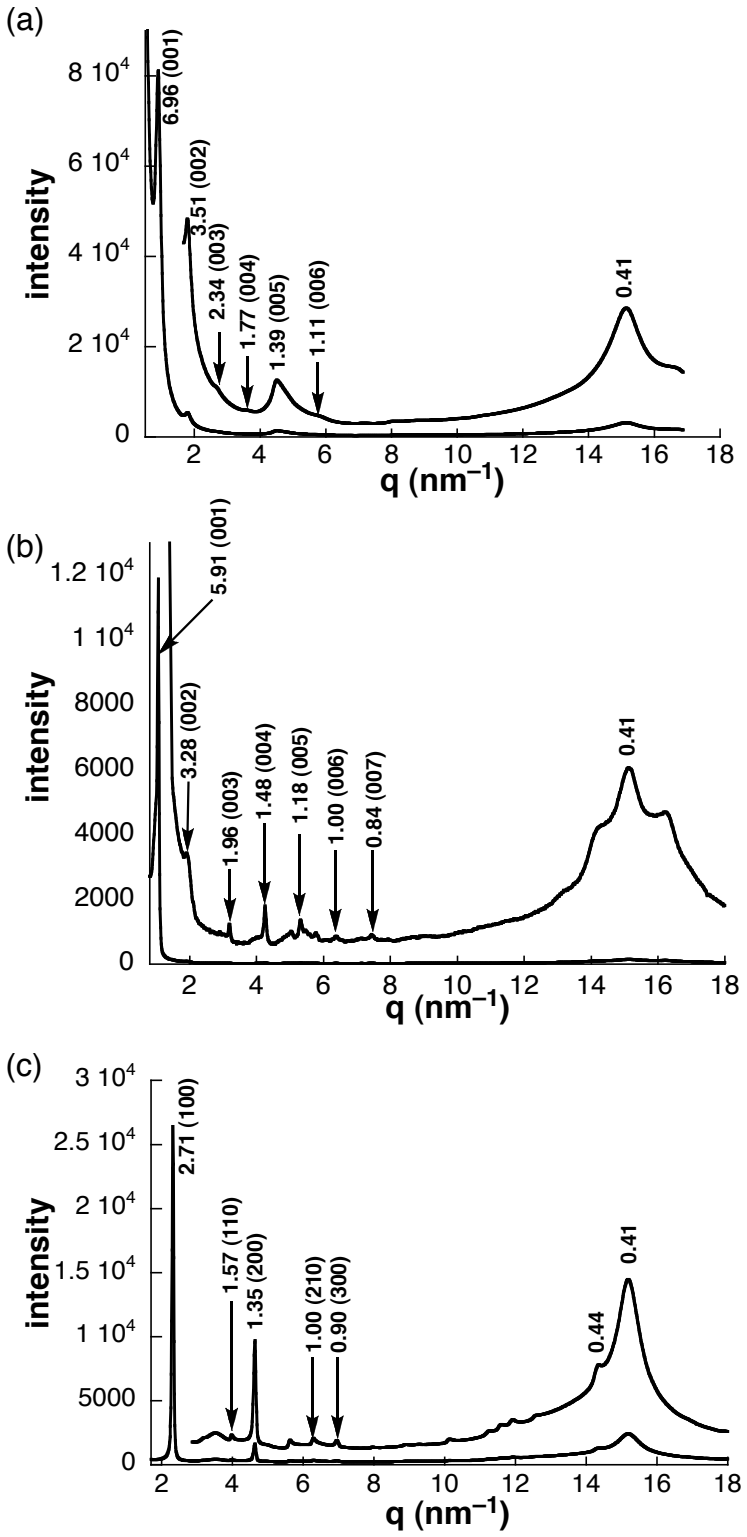
Supporting Figure 15 Variable-temperature ^{1}H NMR spectral changes of **2d** (a) in octane-d_{18} (1×10^{-3} M) from 40 to –40 °C, (b) in $CDCl_3$ (5×10^{-3} M) from 60 to 0 °C, and (c) in CD_2Cl_2 (5×10^{-3} M) from 30 to 0 °C. Impurity included in octane-d_{18} is indicated as X.



Supporting Figure 16 Variable-temperature ^{1}H NMR spectral changes of **3d** in $CDCl_3$ (5×10^{-3} M) from 40 to 0 °C.



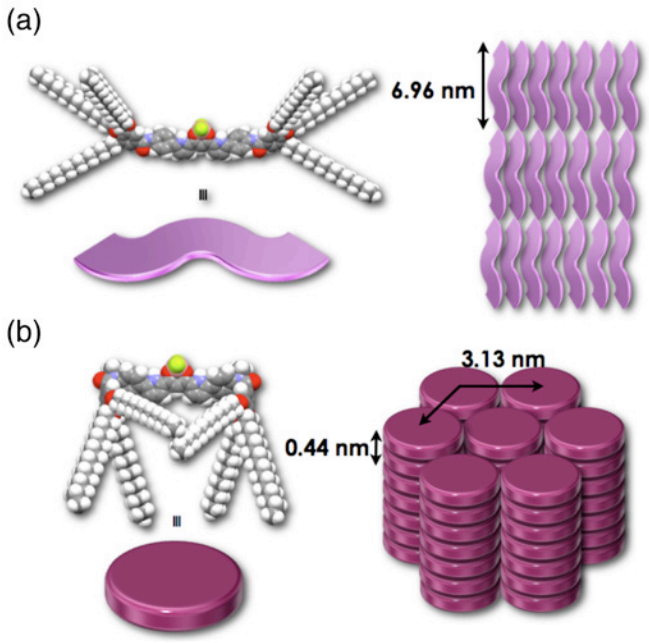
Supporting Figure 17 SEM images of xerogels prepared from (a) CH_2Cl_2 and (b) 1,4-dioxane of **2d** (10 mg/mL).



Supporting Figure 18 XRD patterns of (a) xerogels of **2d** prepared from (i) CH_2Cl_2 and (ii) 1,4-dioxane and (b) solid state of **3d**. Only assignable peaks are indicated. The measurements were conducted to the xerogels (for **2d**) in sample tubes frozen and pumped at 0 °C or –40 °C.

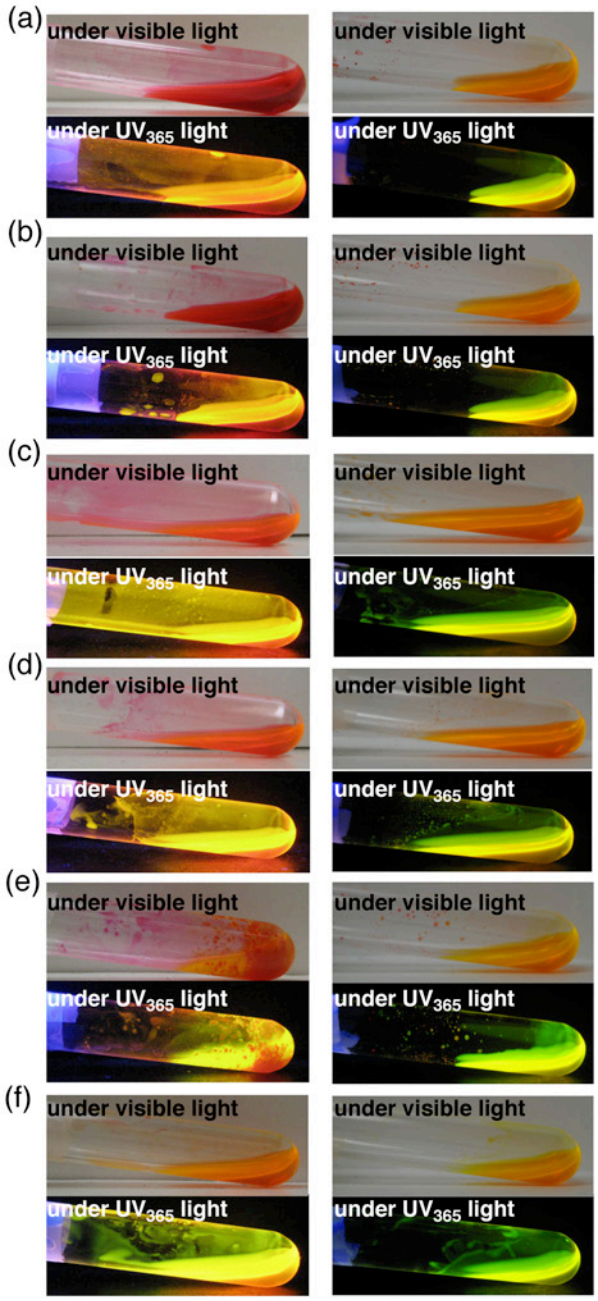
Supporting Table 2 Summary of XRD data of (a) xerogels of **2d** prepared from (i) CH_2Cl_2 and (ii) 1,4-dioxane and (b) solid state of **3d**. Lattice paramater of hexagonal columnar structure of **3d**: a = 3.13 nm, c = 0.44 nm, Z = 1.

	q (nm^{-1})	d_{obs} (nm)	d_{cal} (nm)	hkl
(a) (i)	0.90	6.96	6.96	001
	1.78	3.51	3.48	002
	2.68	2.34	2.32	003
	3.54	1.78	1.74	004
	4.51	1.39	1.39	005
	5.66	1.11	1.16	006
(a) (ii)	1.06	5.91	5.91	001
	1.92	3.28	2.96	002
	3.20	1.96	1.97	003
	4.26	1.48	1.48	004
	5.31	1.18	1.18	005
	6.29	1.00	0.99	006
	7.44	0.84	0.84	007
(b)	2.31	2.71	2.71	100
	3.98	1.57	1.56	110
	4.64	1.35	1.36	200
	6.30	1.00	1.02	210
	6.95	0.90	0.90	300

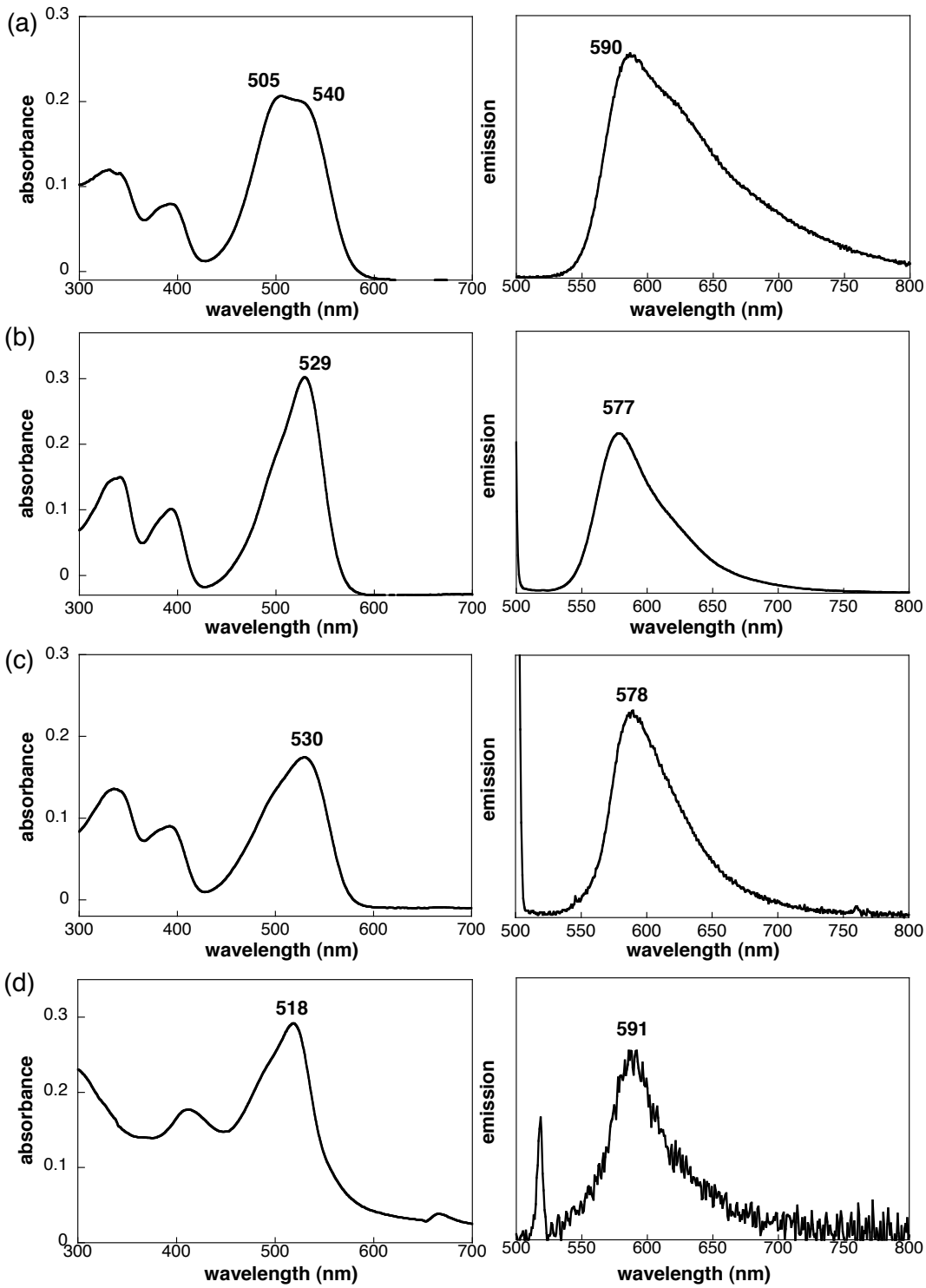


Supporting Figure 19 Possible packing model structures of (a) **2d** (the value is derived from the xerogel from CH_2Cl_2) and (b) **3d**.

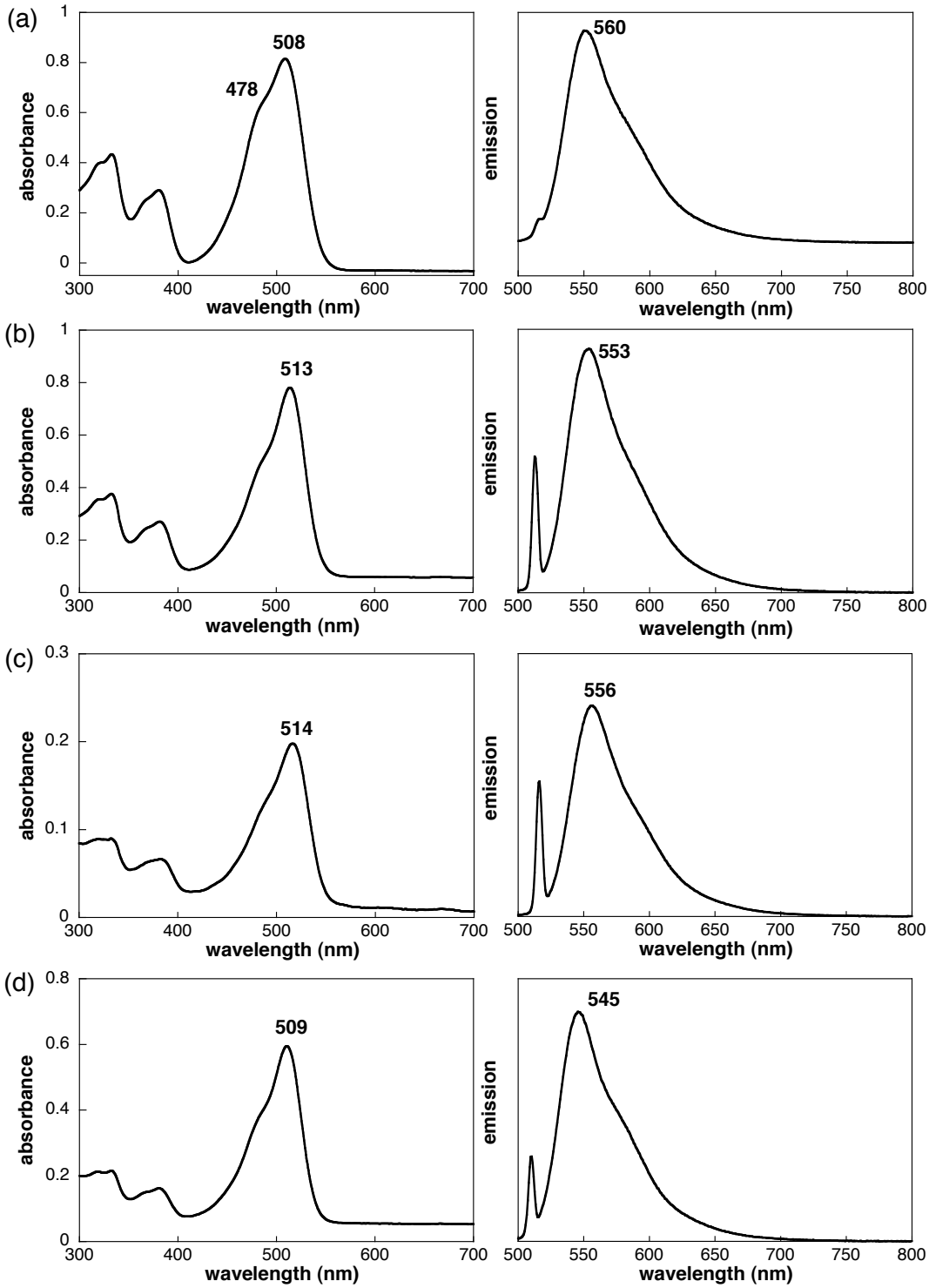
6. Anion-responsive behaviors of supramolecular gels



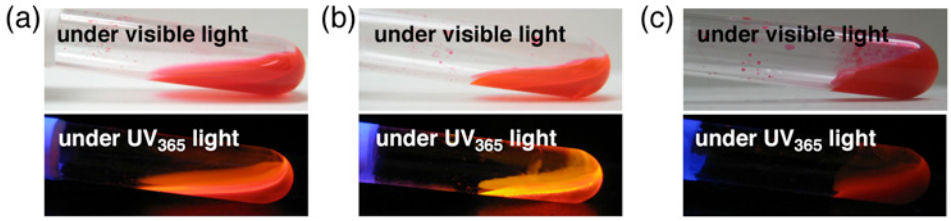
Supporting Figure 20 Photographs of precipitates or solutions of (i) **2d** and (ii) **3d** (10 mg/mL) with 1 equiv of TBACl obtained from (a) octane, (b) cyclohexane, (c) CH_2Cl_2, (d) $CHCl_3$, (e) 1,4-dioxane, and (f) THF.



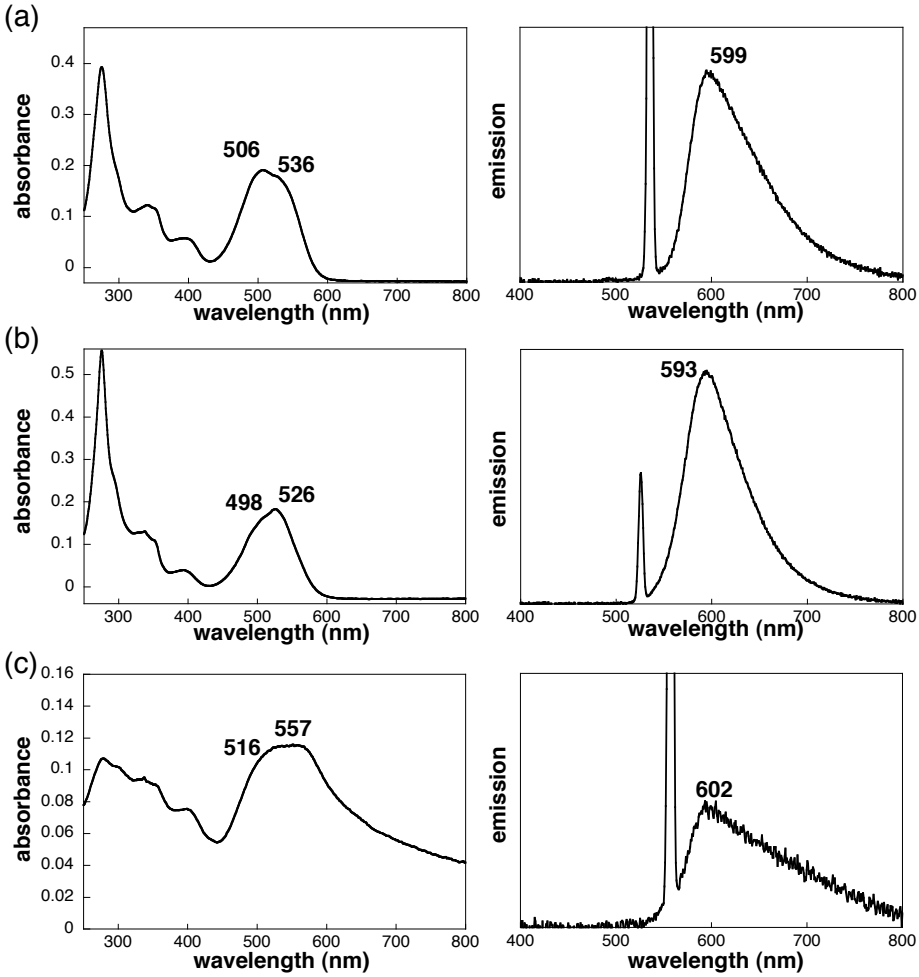
Supporting Figure 21 UV/vis absorption (left) and fluorescence emission (right, $\lambda_{ex} = \lambda_{max}$) spectra of **2d** (10 mg/mL) with 1 equiv of TBACl in (a) octane, (b) CH_2Cl_2, (c) $CHCl_3$, and (c) 1,4-dioxane.



Supporting Figure 22 UV/vis absorption (left) and fluorescence emission (right, $\lambda_{ex} = \lambda_{max}$) spectra of **3d** (10 mg/mL) with 1 equiv of TBACl in (a) cyclohexane, (b) CH_2Cl_2, (c) $CHCl_3$, and (c) 1,4-dioxane. Cyclohexane was used in the examination of anion-responsive behavior due to the poor solubility of **3d** in the absence of anions in octane.



Supporting Figure 23 Photographs of solutions of **2d** (10 mg/mL) with 1 equiv of TATA^{C3}Cl obtained from (a) octane, (b) CH_2Cl_2, and (c) 1,4-dioxane.



Supporting Figure 24 UV/vis absorption (left) and fluorescence emission (right, $\lambda_{ex} = \lambda_{max}$) spectra of **2d** (10 mg/mL) with 1 equiv of TATA^{C3}Cl in (a) octane, (b) CH_2Cl_2, and (c) 1,4-dioxane as solutions. These spectra suggest that TATA^{C3} cation interacts with the receptor–Cl^- complex (**2d**·Cl^-) to form small aggregates.