Electronic Supplementary Material (ESI) for ChemComm.
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High yielding self-assembly favored by preorganization

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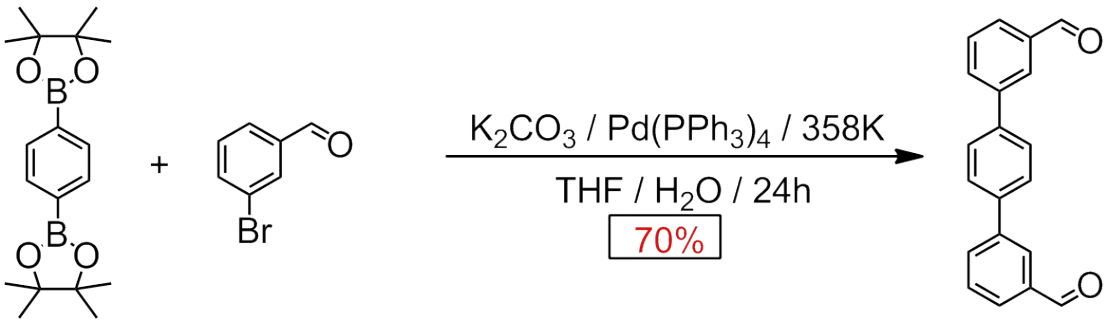
Supporting Information

Table of content

1. Materials and general methods.

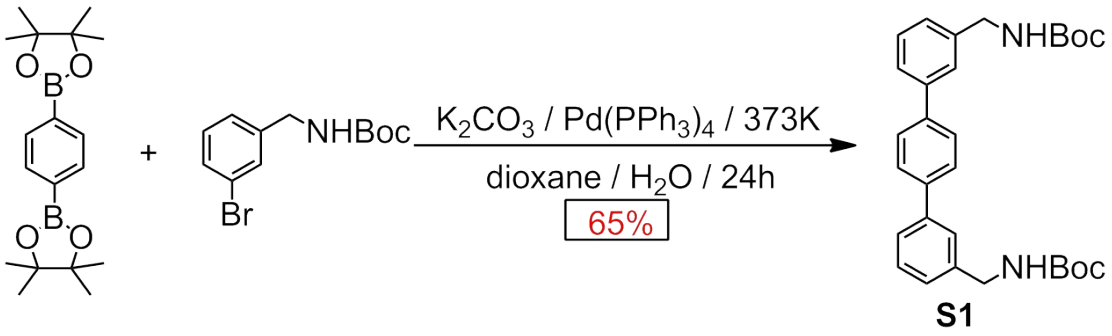
All reagents and solvents were purchased from commercial sources and used without further purification. Solvents were deoxygenated by passing N_2 through the solvent for 30 min. Manipulations were performed under a normal laboratory atmosphere unless otherwise noted. Nuclear magnetic resonance (NMR) spectra were recorded at ambient temperature using Bruker AVANCE III 400 or 500 spectrometers, with working frequencies of 400/500 and 100/125 MHz for ^{1}H and ^{13}C, respectively. Chemical shifts are reported in ppm relative to the residual internal non-deuterated solvent signals ($CDCl_3$: δ = 7.26 ppm). High-resolution mass spectra (HRMS) were measured using a SHIMADZU liquid chromatograph mass spectrometry ion trap time of flight (LCMS-IT-TOF) instrument. X-ray crystallographic data were collected on a Bruker D8 Venture diffractometer.

2. Synthesis and characterization of new compounds.



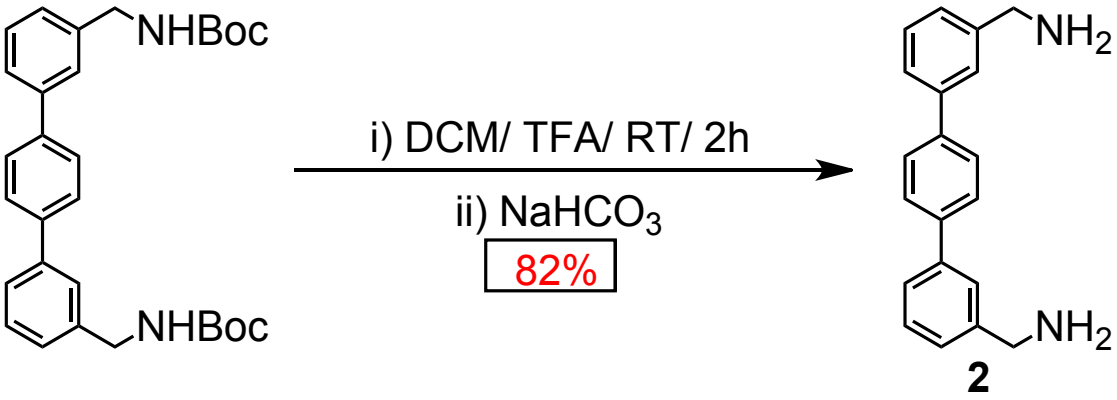
Scheme S1. Synthesis of 1.

Synthesis of compound 1: 1,4-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzene (1 g, 3.0 mmol), 3-bromobenzaldehyde (1.2 g, 6.6 mmol) and $Pd(PPh_3)_4$ (80 mg) were added to a mixture containing THF (50 mL) and aqueous solution of potassium carbonate (2 M; 15 mL). The mixture was vigorously stirred at 358K for 24 h. After the mixture was cooled to room temperature, it was poured into deionized water (150 mL). The aqueous layer was extracted with dichloromethane three times. The combined organic layers were washed with water and dried over magnesium sulfate. After vacuum evaporation of the solvent, the crude sample was purified by flash column chromatography (DCM / PE (1:1); silica gel, 200-300 mesh), yielding pure **1** (600mg, 70%) as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 10.1 (s, 2H), 8.15 (s, 2H), 7.91 (d, J = 8.0 Hz, 2H), 7.88 (d, J = 8.0 Hz, 2H), 7.74 (s, 4H), 7.64 (t, J = 8.0 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.3, 141.3, 139.3, 137.0, 132.9, 129.6, 129.0, 127.9, 127.7. HRMS-ESI for **1**, Calcd for $C_{20}H_{14}O_2$: *m/z* = 287.0994 $[M + H]^+$; Found: 287.0928 $[M + H]^+$



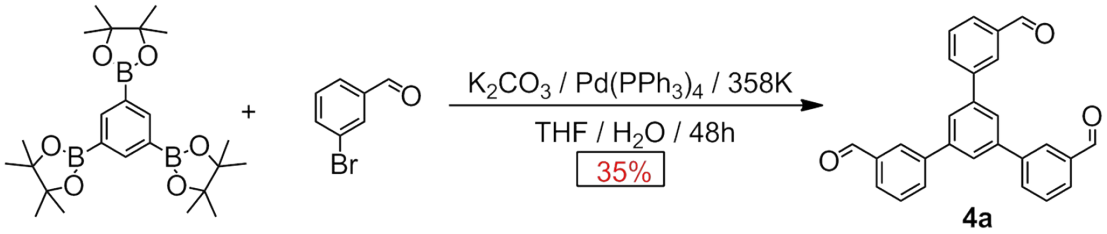
Scheme S2. Synthesis of S1.

Synthesis of compound S1: 1,4-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzene (1 g, 3.0 mmol), tert-butyl 3-bromobenzylcarbamate (1.9 g, 6.6 mmol) and $Pd(PPh_3)_4$ (80 mg) were added to a mixture containing dioxane (50 mL) and an aqueous solution of potassium carbonate (2 M; 15 mL). The mixture was vigorously stirred at 373K for 24 h. After the mixture was cooled to room temperature, it was poured into deionized water (150 mL). The aqueous layer was extracted with dichloromethane three times. The combined organic layers were washed with water and dried over magnesium sulfate. After vacuum evaporation of the solvent, the crude sample was purified by flash column chromatography (EA / PE (1:3); silica gel, 200-300 mesh), yielding pure **S1** (950mg, 65%) as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.66 (s, 4H), 7.55 (s, 2H), 7.54 (d, J = 6.0 Hz, 2H), 7.42 (t, J = 6.0 Hz, 2H), 7.28 (d, J = 6.0 Hz, 2H), 4.90 (s, 2H), 4.40 (s, 4H), 1.48 (s, 18H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 155.9, 141.0, 139.9, 129.1, 127.5, 126.2, 126.0, 125.8, 44.7, 28.4. HRMS-ESI for **S1**, Calcd for $C_{30}H_{36}N_2O_4$: *m/z* = 489.2675 $[M + H]^+$; Found: 489.2650 $[M + H]^{2+}$



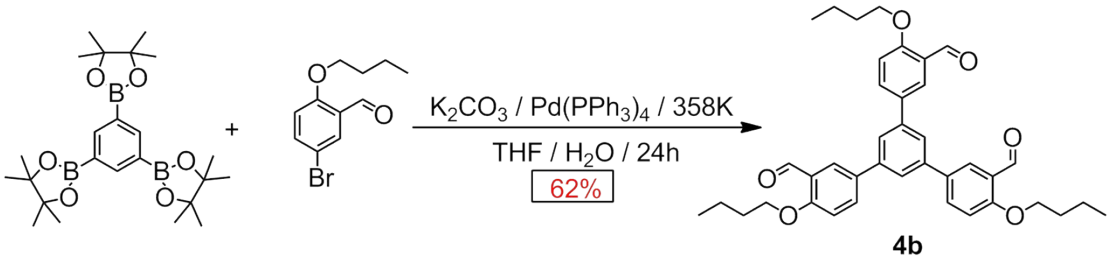
Scheme S3. Synthesis of 2.

Synthesis of compound 2: Trifluoroacetic acid (10 mL, 131 mmol) was added to a solution of **S2** (0.5 g, 1.02 mmol) in DCM (10 mL). The resultant mixture was stirred at room temperature for 2 h. Remaining solvent was removed under vacuum to give the corresponding ammonium salt as a white solid. Saturated sodium bicarbonate solution was added and the aqueous solution was extracted with dichloromethane three times. The combined organic layers were washed with water and dried over magnesium sulfate. After vacuum evaporation of the solvent, pure **2** (240mg, 82%) was prepared as a white solid without further purification. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.68 (s, 4H), 7.60 (s, 2H), 7.54 (d, J = 6.4 Hz, 2H), 7.44 (t, J = 6.4 Hz, 2H), 7.32 (d, J = 6.4 Hz, 2H), 4.90 (s, 2H), 3.96 (s, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 162.2, 135.5, 132.2, 127.6, 125.5, 123.1, 120.6, 118.7, 39.6. HRMS-ESI for **2**, Calcd for $C_{30}H_{36}N_2O_4$: *m/z* = 289.1626 $[M + H]^+$; Found: 489.1657 $[M + H]^{2+}$



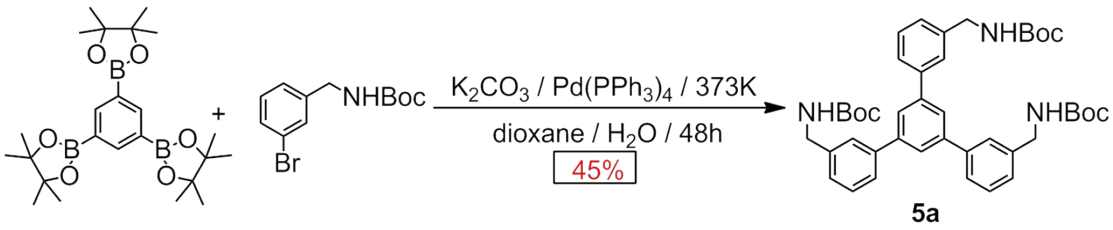
Scheme S4. Synthesis of 4a.

Synthesis of compound 4a: 1,3,5-tris(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzene (1 g, 2.2 mmol), 3-bromobenzaldehyde (1.8 g, 10.0 mmol) and $Pd(PPh_3)_4$ (80 mg) were added to a mixture of THF (50 mL) and aqueous 2 M potassium carbonate (15 mL). The mixture was vigorously stirred at 358K for 24 h. After the mixture was cooled to room temperature, solid suspension was filtered out and collected. yielding pure **4a** (300mg, 35%) as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 10.1 (s, 3H), 8.15 (s, 3H), 7.92 (d, J = 8 Hz, 3H), 7.89 (d, J = 8 Hz , 3H), 7.74 (s, 3H), 7.63 (t, J = 8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.3, 141.3, 139.3, 137.0, 132.9, 129.6, 129.0, 127.9, 127.7. HRMS-ESI for **4a**, Calcd for $C_{39}H_{42}O_6$: *m/z* = 391.1256 [*M* + H]$^+$; Found: 391.1274 [*M* + H]$^+$



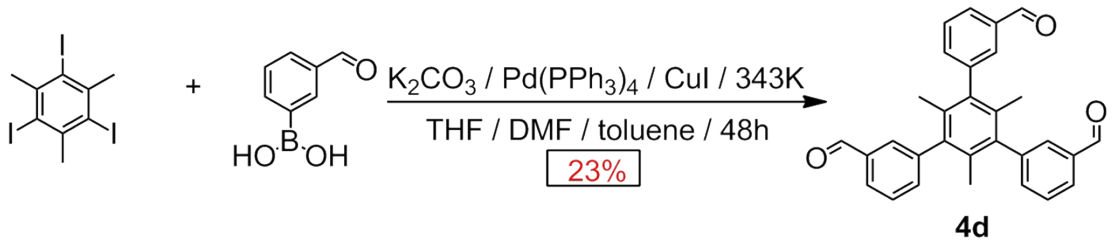
Scheme S5. Synthesis of 4b.

Synthesis of compound 4b: 1,3,5-tris(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzene (1 g, 2.2 mmol), 5-bromo-2-butoxybenzaldehyde (2.6 g, 10.0 mmol) and $Pd(PPh_3)_4$ (80 mg) were added to a mixture of THF (50 mL) and aqueous 2 M potassium carbonate (15 mL). The mixture was vigorously stirred at 358K for 24 h. After the mixture was cooled to room temperature, it was poured into 150 mL deionized water. The aqueous layer was extracted with dichloromethane three times. The combined organic layers were washed with water and dried over magnesium sulfate. After vacuum evaporation of the solvent, the crude sample was purified by flash column chromatography (EA / PE (1:3); silica gel, 200-300 mesh), yielding pure **4b** (820mg, 62%) as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 10.55 (s, 3H), 8.10 (s, 3H), 7.84 (d, J = 8.4 Hz, 3H), 7.65 (s, 3H), 7.07 (d, J = 8.4 Hz, 3H), 4.14 (t, J = 6.4 Hz, 6H), 1.86 (quint, J = 6.4 Hz, 6H), 1.55 (quint, J = 6.4 Hz, 6H), 1.01 (t, J = 6.4 Hz, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 189.7, 161.2, 140.8, 134.6, 133.0, 126.5, 124.9, 123.9, 113.1, 68.5, 31.1, 19.3, 13.8. HRMS-ESI for **4b**, Calcd for $C_{39}H_{42}O_6$: *m/z* = 607.2981 $[M + H]^+$; Found: 607.2954 $[M + H]^+$



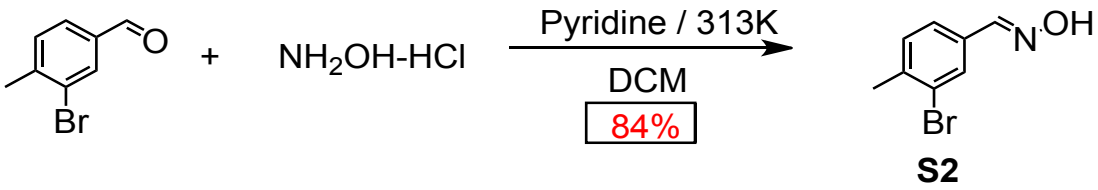
Scheme S6. Synthesis of 5a.

Synthesis of compound 5a: 1,3,5-tris(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzene (1 g, 2.2 mmol), tert-butyl 3-bromobenzylcarbamate (2.85 g, 10.0 mmol) and $Pd(PPh_3)_4$ (80 mg) were added to a mixture containing dioxane (50 mL) and an aqueous solution of potassium carbonate (2 M; 15 mL). The mixture was vigorously stirred at 373K for 48 h. After the mixture was cooled to room temperature, it was poured into 150 mL deionized water. The aqueous layer was extracted with dichloromethane three times. The combined organic layers were washed with water and dried over magnesium sulfate. After vacuum evaporation of the solvent, the crude sample was purified by flash column chromatography (EA / PE (1:3); silica gel, 200-300 mesh), yielding pure **5a** (710mg, 45%) as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.74 (s, 3H), 7.60 (s, 3H), 7.58 (d, J = 7.6 Hz, 3H), 7.44 (t, J = 7.6 Hz, 3H), 7.32 (d, J = 7.6 Hz, 3H), 4.92 (s, 3H), 4.41 (s, 6H), 1.46 (s, 27H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 155.9, 142.1, 141.4, 139.6, 129.1, 126.7, 126.4, 125.2 44.7, 28.4. HRMS-ESI for **5a**, Calcd for $C_{42}H_{51}N_3O_6$: *m/z* = 694.3778 $[M + H]^+$; Found: 694.3792 $[M + H]^+$



Scheme S7. Synthesis of 4d.

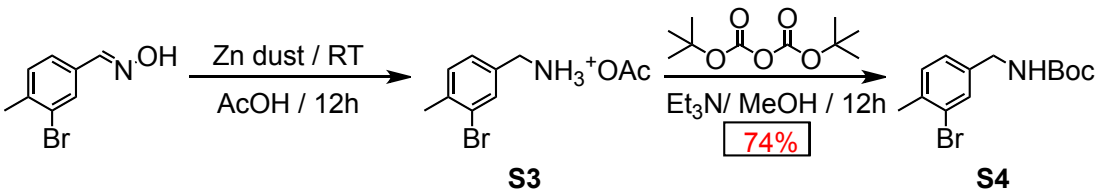
Synthesis of compound 4d: 1,3,5-triiodo-2,4,6-trimethylbenzene (1 g, 2.0 mmol) and (3-formylphenyl)boronic acid (1.8 g, 12.0 mmol) were dissolved in a solution mixture consisting of DMF (40 mL), toluene (20 mL) and THF (20 mL). The reaction mixture was degassed for 30 min, before $Pd(PPh_3)_4$ (110 mg, 0.051 mmol) and K_2CO_3 (2.8 g, 20.0 mmol) were added. The reaction mixture was stirred at 353K under an N_2 atmosphere for 48 h. After cooling to room temperature, the solvent was removed under vacuum and the residue was poured into water and then extracted with CH_2Cl_2. The resulting organic extract was washed with water (1 x 100 mL) and brine (3 x 80 mL), dried over magnesium sulfate, and then concentrated to give the crude product. The crude sample was purified by flash column chromatography (PE / EA / DCM (7:1:1); silica gel, 200-300 mesh), yielding pure **4d** (200mg, 23%) as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 10.06 (s, 3H), 7.87 (d, J = 7.6 Hz, 3H), 7.75 (s, 3H), 7.63 (t, J = 7.6 Hz, 3H), 7.51 (d, J = 7.6 Hz, 3H), 1.68 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.3, 142.6, 138.7, 136.8, 135.5, 133.4, 130.5, 129.4, 128.3, 19.5. HRMS-ESI for **4d**, Calcd for $C_{30}H_{24}O_3$: *m/z* = 433.1725 $[M + H]^+$; Found: 433.1786 $[M + H]^+$



S2

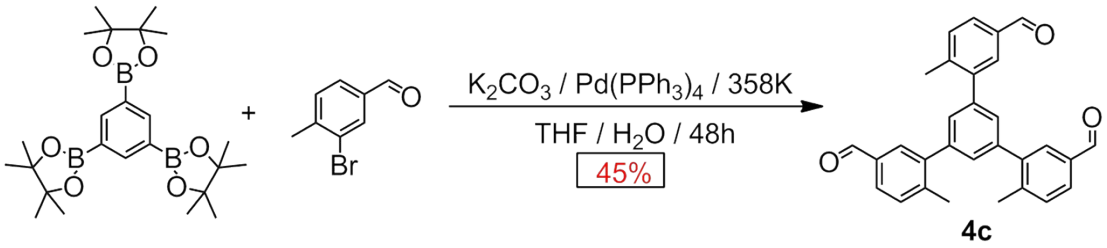
Scheme S8. Synthesis of S2.

Synthesis of compound S2: 3-bromo-4-methylbenzaldehyde (10 g, 50 mmol), hydroxylamine hydrochloride (4.1 g, 60 mmol), and pyridine (10 mL) were dissolved in DCM (120 ml). The mixture was refluxed for 6 h, before the solvent was evaporated. The reaction mixture was dissolved in water and the aqueous layer was extracted with EA (40 ml) four times. The organic layer was combined and dried with magnesium sulfate, filtered and the filtrate was collected. After evaporating the solvent, the crude sample was purified by recrystallization, yielding pure **S2** (8.9 g, 84%) as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.07 (s, 1H), 7.75 (s, 1H), 7.41 (d, J = 7.6 Hz, 1H), 7.24 (d, J = 7.6 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 149.0, 139.9, 131.3, 131.0, 130.7, 125.8, 125.3, 22.9. HRMS-ESI for **S2**, Calcd for C_8H_8BrNO: *m/z* = 213.9789 $[M + H]^+$; Found: 213.9722 $[M + H]^+$



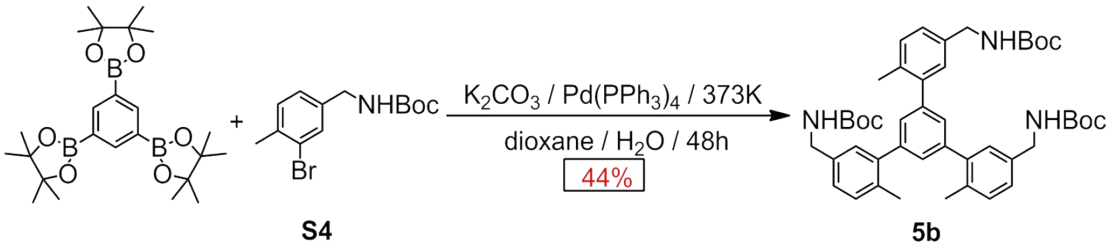
Scheme S9. Synthesis of S4.

Synthesis of compound S4: To a solution of **6** (5.00 g, 23.5 mmol) in 100 mL of acetic acid was added zinc (10 g, 156 mmol). The solution was stirred at room temperature for 12 h. The insoluble was then moved by filtration and washed with ethyl acetate. The filtrate was collected and the solvent was evaporated. An aqueous solution of sodium hydroxide was added. The aqueous layer was extracted three times with ethyl acetate. The organic layer was washed with brine, dried over magnesium sulfate. The solvent was evaporated under reduced pressure to yield **S3** as a colourless oil. Compound **S3** (4.0 g, 20 mmol) was then dissolved in MeOH (100 mL), to which Et_3N (4 ml) and Boc2O (4.8 g, 22 mmol) was then added. The reaction mixture was stirred overnight at rt. After that, the reaction mixture was cool to 0 ^oC, after which an aqueous solution of HCl (1 M; 20 mL) was slowly added. The organic layer was collected, and the aqueous phase was re-extracted with DCM (10 mL). The combined organic solution was washed with an aqueous $NaHCO_3$ (10 mL, saturated), then dried with magnesium sulfate. Removal of solvent yielded compound **S4** (5.2 g, 74%). Product was used for next step without further purification. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.43 (s, 1H), 7.16 (d, J = 7.6 Hz, 1H), 7.10 (d, J = 7.6 Hz, 1H), 4.89 (s, 1H), 4.23 (s, 2H), 2.35 (s, 3H), 1.45 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 155.8, 138.4, 136.7, 131.1, 130.8, 126.3, 124.9, 43.7, 28.4, 27.4. HRMS-ESI for **S4**, Calcd for $C_{13}H_{18}BrNO_2$: *m/z* = 300.0521 $[M + H]^+$; Found: 300.0577 $[M + H]^+$



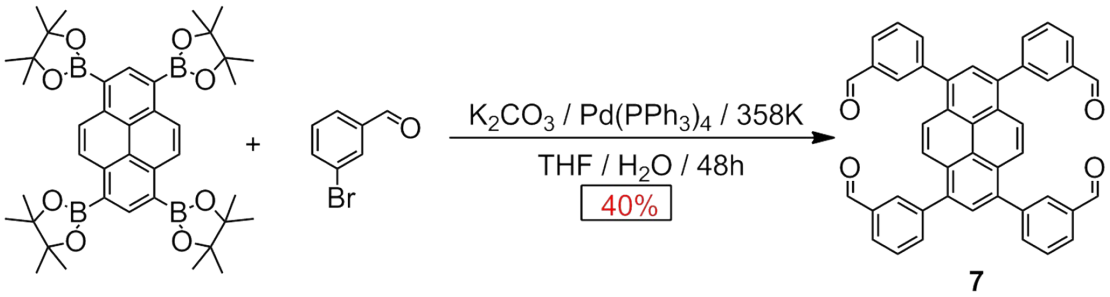
Scheme S10. Synthesis of 4c.

Synthesis of compound 4c: 1,3,5-tris(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzene (1 g, 2.2 mmol), 3-bromo-4-methylbenzaldehyde (2 g, 10.0 mmol) and $Pd(PPh_3)_4$ (80 mg) were added to a mixture containing THF (50 mL) and an aqueous solution of potassium carbonate (2 M; 15 mL). The mixture was vigorously stirred at 358K for 48 h. After the mixture was cooled to room temperature, it was poured into deionized water (150 mL). The aqueous layer was extracted with dichloromethane three times. The combined organic solution was washed with water and dried over magnesium sulfate. After removing the solvent by evaporation, the crude sample was purified by flash column chromatography (EA / PE (1:1); silica gel, 200-300 mesh), yielding pure **4c** (427 mg, 45%) as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 10.02 (s, 3H), 7.83 (s, 3H), 7.80 (d, J = 7.6 Hz, 3H), 7.47 (d, J = 7.6 Hz, 3H), 7.33 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 191.9, 142.9, 141.9, 140.8, 134.6, 131.2, 131.0, 128.9, 128.7, 21.1. HRMS-ESI for **4c**, Calcd for $C_{30}H_{24}O_3$: *m/z* = 433.1725 $[M + H]^+$; Found: 433.1759 $[M + H]^+$



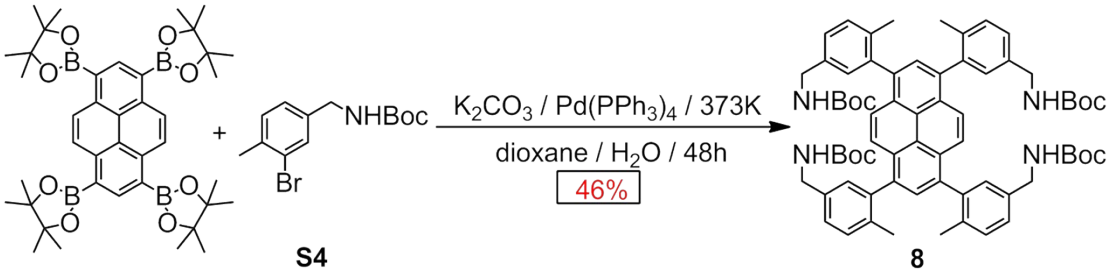
Scheme S11. Synthesis of 5b.

Synthesis of compound 5b: 1,3,5-tris(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzene (1 g, 2.2 mmol), **S4** (3.0 g, 10.0 mmol) and $Pd(PPh_3)_4$ (80 mg) were added to a mixture containing dioxane (50 mL) and an aqueous solution of potassium carbonate (2 M; 15 mL). The mixture was vigorously stirred at 373K for 48 h. After the mixture was cooled to room temperature, it was poured into deionized water (150 mL). The aqueous layer was extracted with dichloromethane three times. The combined organic solution was washed with water and dried over magnesium sulfate. After removing the solvent by evaporation, the crude sample was purified by flash column chromatography (EA / PE (1:3); silica gel, 200-300 mesh), yielding pure **5b** (710mg, 44%) as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.25 (s, 3H), 7.23 (s, 3H), 7.22 (d, J = 7.6 Hz, 3H), 7.21 (d, J = 7.6 Hz, 3H), 4.83 (s, 3H), 4.32 (s, 6H), 2.34 (s, 3H), 1.44 (s, 9H). **^{13}C NMR** (100 MHz, CDCl3): δ = 155.8, 141.7, 141.3, 136.3, 134.4, 130.7, 129.0, 128.4, 126.5, 44.4, 28.4, 20.3 HRMS-ESI for **5b**, Calcd for $C_{45}H_{57}N_3O_6$: *m/z* = 736.4247 $[M + H]^+$; Found: 736.4284 $[M + H]^+$



Scheme S12. Synthesis of 7.

Synthesis of compound 7: 1,3,6,8-tetrakis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyrene (1 g, 1.4 mmol), 3-bromobenzaldehyde (1.5 g, 8.5 mmol) and $Pd(PPh_3)_4$ (80 mg) were added to a mixture containing THF (50 mL) and an aqueous solution of potassium carbonate (2 M; 15 mL). The mixture was vigorously stirred at 358K for 48 h. After the mixture was cooled to room temperature, it was poured into deionized water (150 mL). The aqueous layer was extracted with dichloromethane three times. The combined organic solution was washed with water and dried over magnesium sulfate. After vacuum evaporation of the solvent, the crude sample was purified by flash column chromatography (DCM / PE (3:1); silica gel, 200-300 mesh), yielding pure **7** (340 mg, 40%) as a light yellow solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 10.16 (s, 4H), 8.20 (s, 4H), 8.14 (s, 4H), 8.05 (s, 2H), 8.02 (d, J = 7.6 Hz, 4H), 7.96 (d, J = 7.6 Hz, 4H), 7.75 (t, J = 7.6 Hz, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.1, 141.5, 136.7, 136.5, 136.2, 131.5, 129.5, 129.2, 129.0, 128.4, 125.8, 125.5. HRMS-ESI for **7**, Calcd for $C_{44}H_{26}O_4$: *m/z* = 619.1831 $[M + H]^+$; Found: 619.1878 $[M + H]^+$



Scheme S13. Synthesis of 8.

Synthesis of compound 8: 1,3,6,8-tetrakis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyrene (1 g, 1.4 mmol), **S4** (2.5 g, 8.5 mmol) and $Pd(PPh_3)_4$ (80 mg) were added to a mixture containing dioxane (50 mL) and an aqueous solution of potassium carbonate (2 M; 15 mL). The mixture was vigorously stirred at 373K for 48 h. After the mixture was cooled to room temperature, it was poured into deionized water (150 mL). The aqueous layer was extracted with dichloromethane three times. The combined organic solution was washed with water and dried over magnesium sulfate. After vacuum evaporation of the solvent, the crude sample was purified by flash column chromatography (EA / PE (1:1); silica gel, 200-300 mesh), yielding pure **8** (690mg, 46%) as a orange solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.74 (m, 2H), 7.67 (m, 4H), 7.33 (m, 4H), 3.32 (m, 4H), 7.29 (m, 4H), 4.91 (s, 4H), 4.36 (s, 8H), 2.07 (m, 12H), 1.42 (m, 36H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 155.9, 140.6, 136.8, 136.6, 136.1, 130.2, 129.6, 128.8, 128.3, 126.8, 125.3, 44.4, 28.4, 24.8, 20.0. HRMS-ESI for **8**, Calcd for $C_{68}H_{78}F_6N_4O_8$: *m/z* = 1079.5820 $[M + H]^+$; Found: 1079.5987 $[M + H]^+$

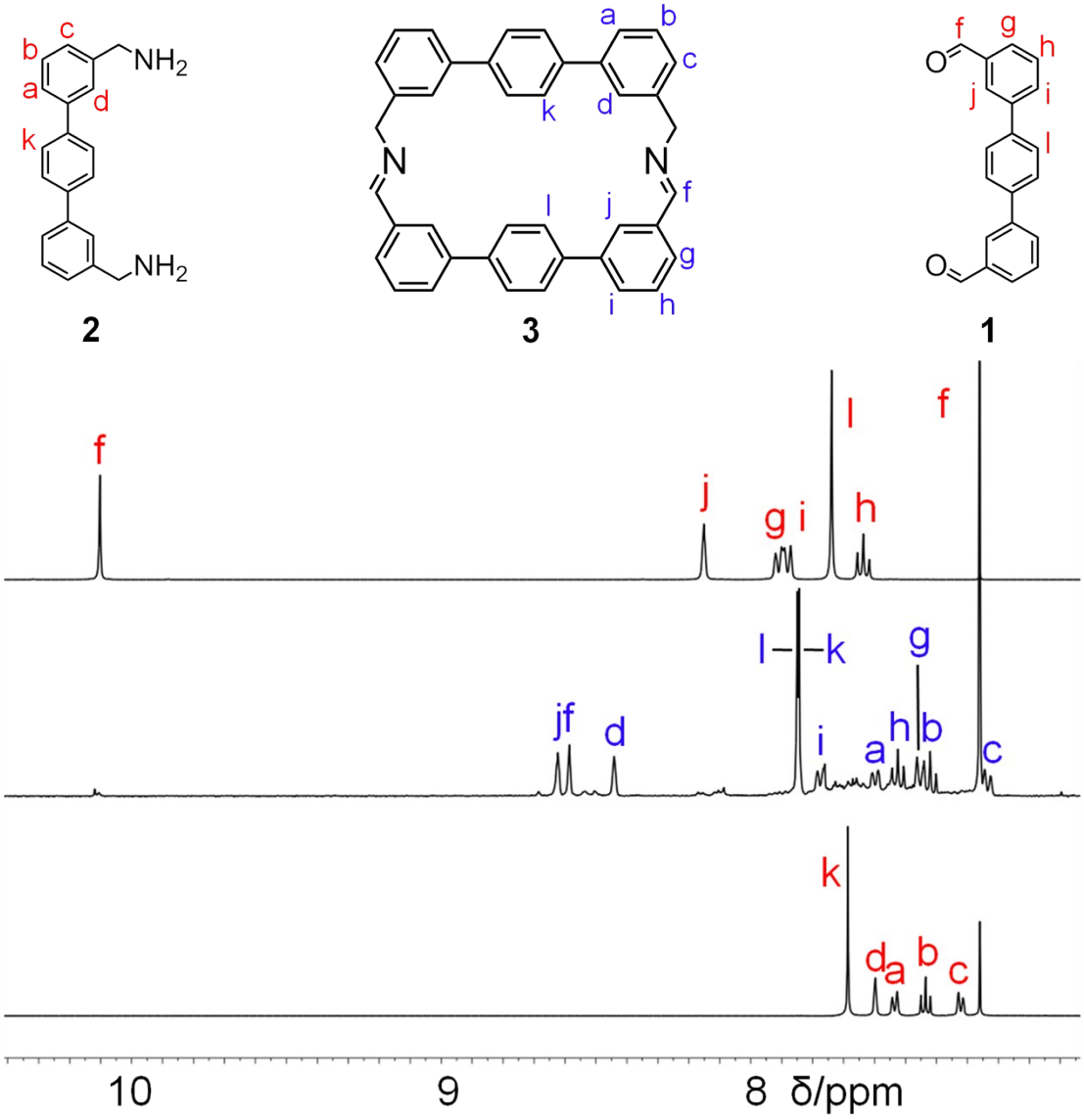


Figure S1. Partial ^{1}HNMR spectra of **1** (top), **3** (middle, crude sample by mixing **1** and **2** in $CDCl_3$) and **2** (bottom). For the full spectrum of the ring **3**, see Figure S5.

Synthesis of compound 3: The cycle **3** was obtained by condensing **1** (10 mg, 0.035 mmol), **2** (10.9 mg, 0.038 mmol) in $CDCl_3$ (7.9 mL). The mixture was vigorously stirred at 313K for 8 h. The peak assignment was made based on two-dimensional NMR spectra, including COSY (Figure S6) and NOESY (Figure S7). ^{1}H NMR diffusion-ordered spectroscopy (DOSY) experiments (Figure S8) demonstrate that **3** was produced as a relatively pure compound.

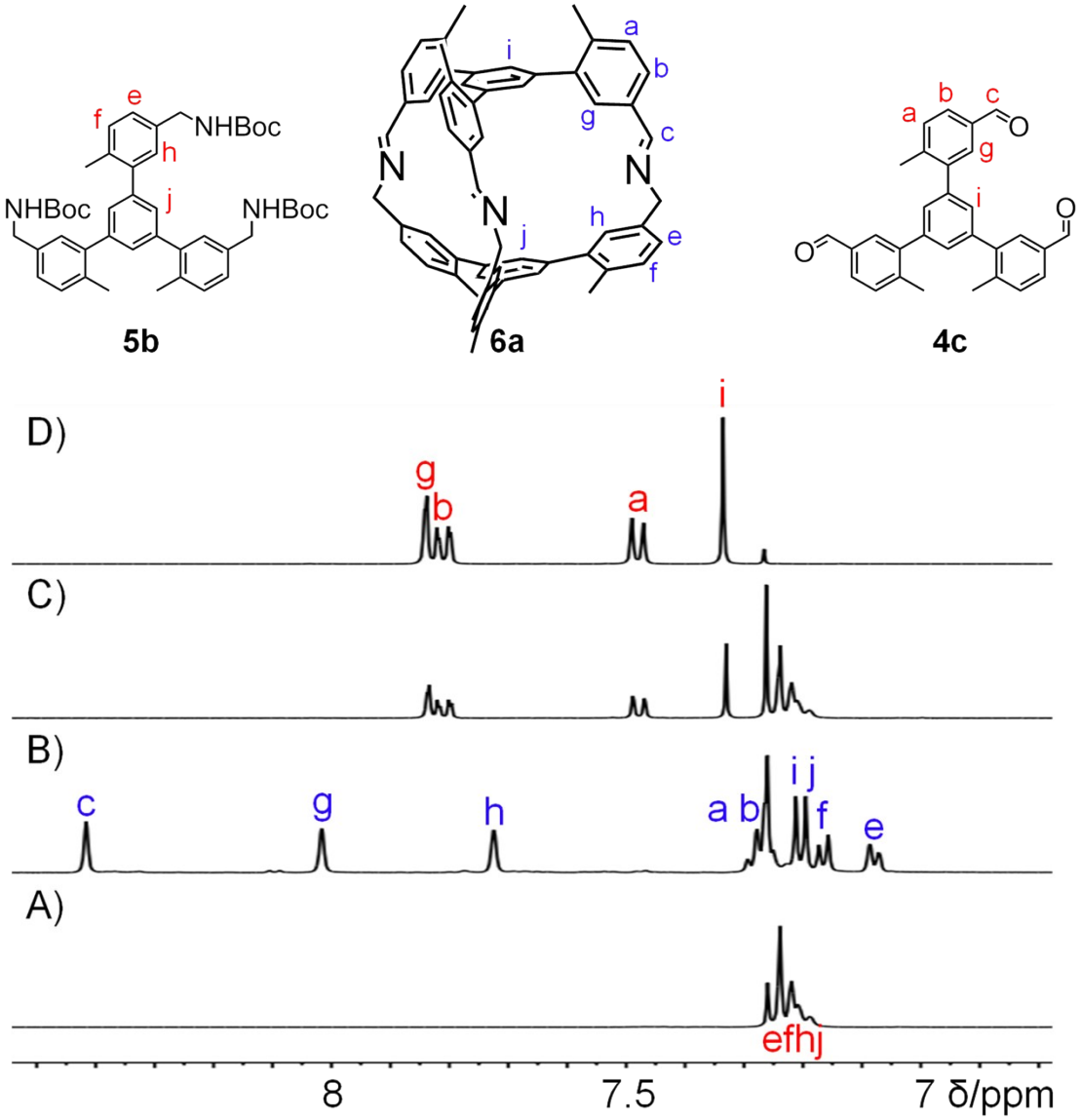


Figure S2. Partial ^{1}HNMR spectra of A) **5b**, B) **6a**, C) a 1:1 mixture of **5b** and **4c**, D) **4c**. For the full spectrum of the ring **6a**, see Figure S10.

Synthesis of compound 6a: The **6a** was obtained by mixing **4c** (10 mg, 0.023 mmol), **5b** (18.7 mg, 0.025 mmol) and 115 µl TFA in $CDCl_3$ (5.2 mL). The mixture was vigorously stirred at 313K for 24 h. After cooling to room temperature, triethylene diamine (TEDA; 460 mg) was added and the mixture was stirred at 313K for 6 h. Then the organic layer was washed with water (10ml, 6 times)

and dried over magnesium sulfate. The peak assignment was made based on two-dimensional NMR spectra, including COSY (Figure S11) and NOESY (Figure S12). ^{1}H NMR diffusion-ordered spectroscopy (DOSY) experiments (Figure S13) demonstrate that **6a** was produced as a relatively pure compound.

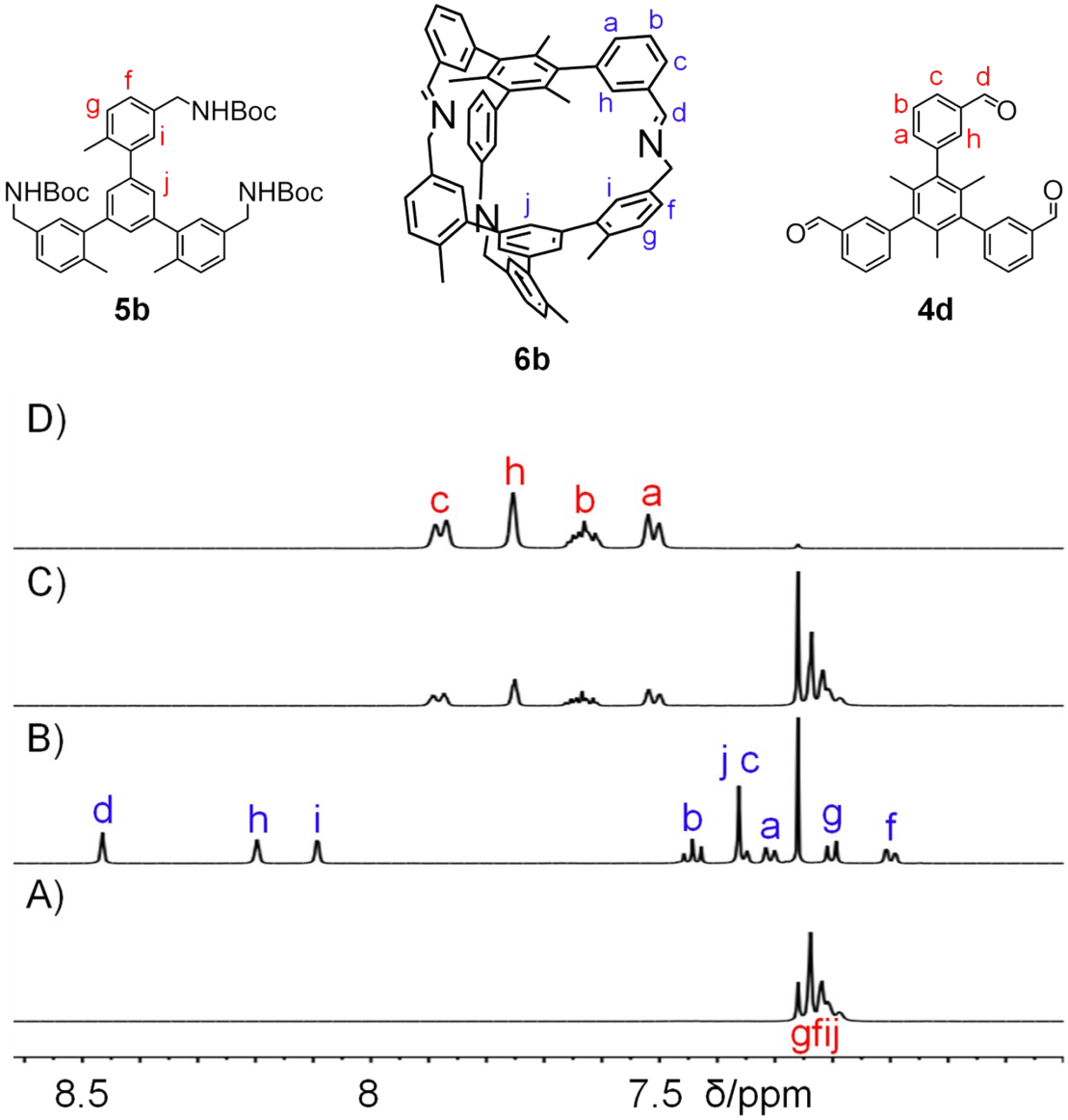


Figure S3. Partial ^{1}HNMR spectra of A) **5b**, B) **6b**, C) a 1:1 mixture of **5b** and **4d**, D) **4d**. For the full spectrum of the ring **6b**, see Figure S15.

Synthesis of compound 6b: **4d** (15 mg, 0.035 mmol), **5b** (28 mg, 0.038 mmol) and 172 µl TFA was combined in $CDCl_3$ (7.8 mL). The mixture was vigorously stirred at 313K for 24 h. After

cooling to room temperature, triethylene diamine (TEDA; 690mg) was added and the mixture was stirred at 313K for 6 h. The organic layer was washed with water (10ml, 6 times) and dried over magnesium sulfate. The peak assignment was made based on two-dimensional NMR spectra, including COSY (Figure S16) and NOESY (Figure S17). ^{1}H NMR diffusion-ordered spectroscopy (DOSY) experiments (Figure S18) demonstrate that **6b** was produced as a relatively pure compound.

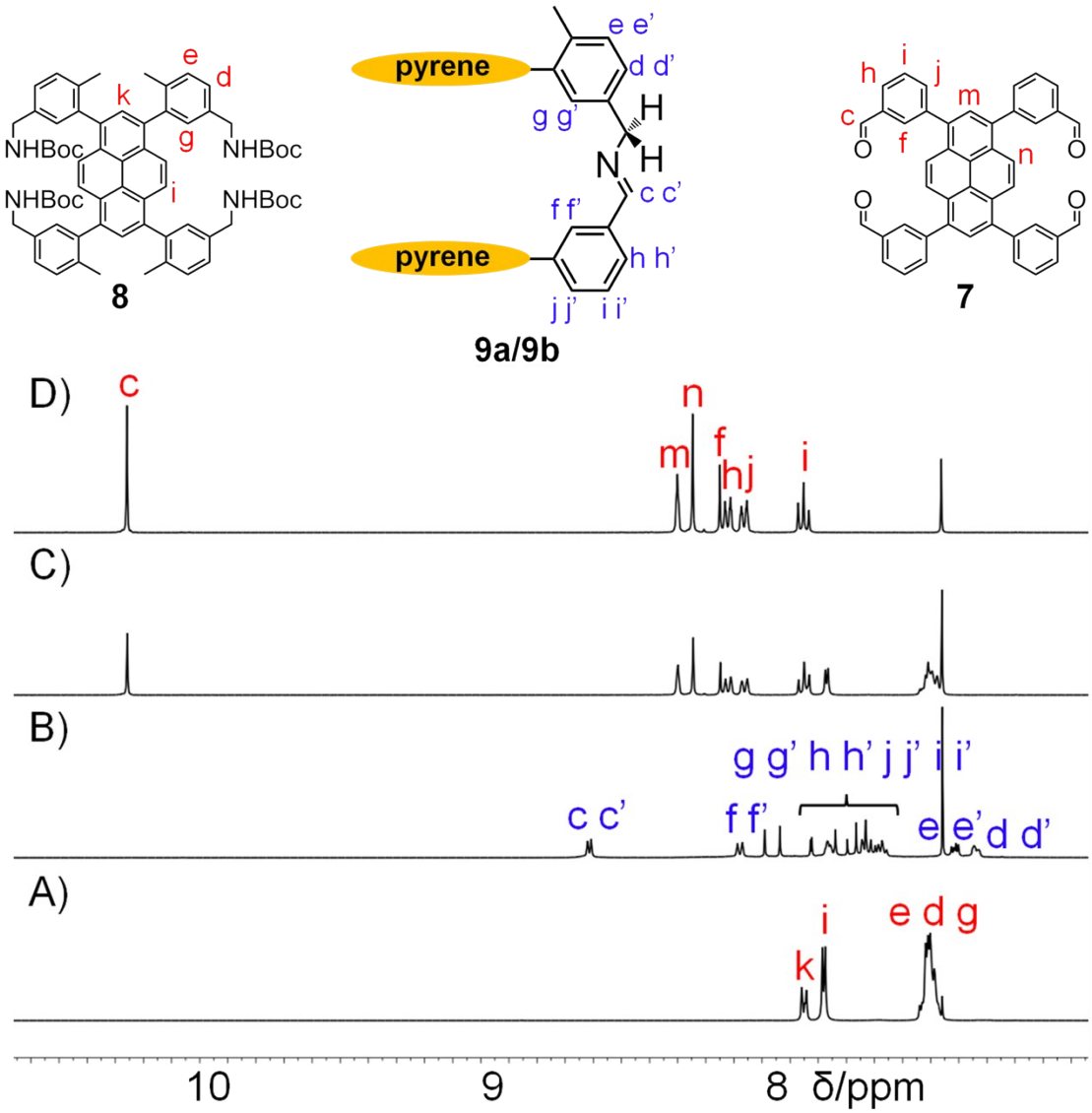


Figure S4. Partial ^{1}HNMR spectra of A) **8**, B) **9a** and **9b**, C) a 1:1 mixture of **7** and **8**, D) **7**.

Synthesis of compound 9a and 9b: **7** (10 mg, 0.016 mmol), **8** (19.2 mg, 0.018 mmol) and 80 µl TFA were combined in $CDCl_3$ (3.6 mL). The mixture was vigorously stirred at 313K for 24 h. After cooling to room temperature, triethylene diamine (TEDA; 320mg) was added and the mixture was stirred at 313K for 6 h. The organic layer was washed with water (10ml, 6 times) and dried over magnesium sulfate. The peak assignment was made based on two-dimensional NMR spectra, including COSY (Figure S21) and NOESY (Figure S22). ^{1}H NMR diffusion-ordered spectroscopy (DOSY) experiments (Figure S23) demonstrate that **9a** and **9b** were produced as relatively pure compounds.

3. Characterization of the self-assembled products.

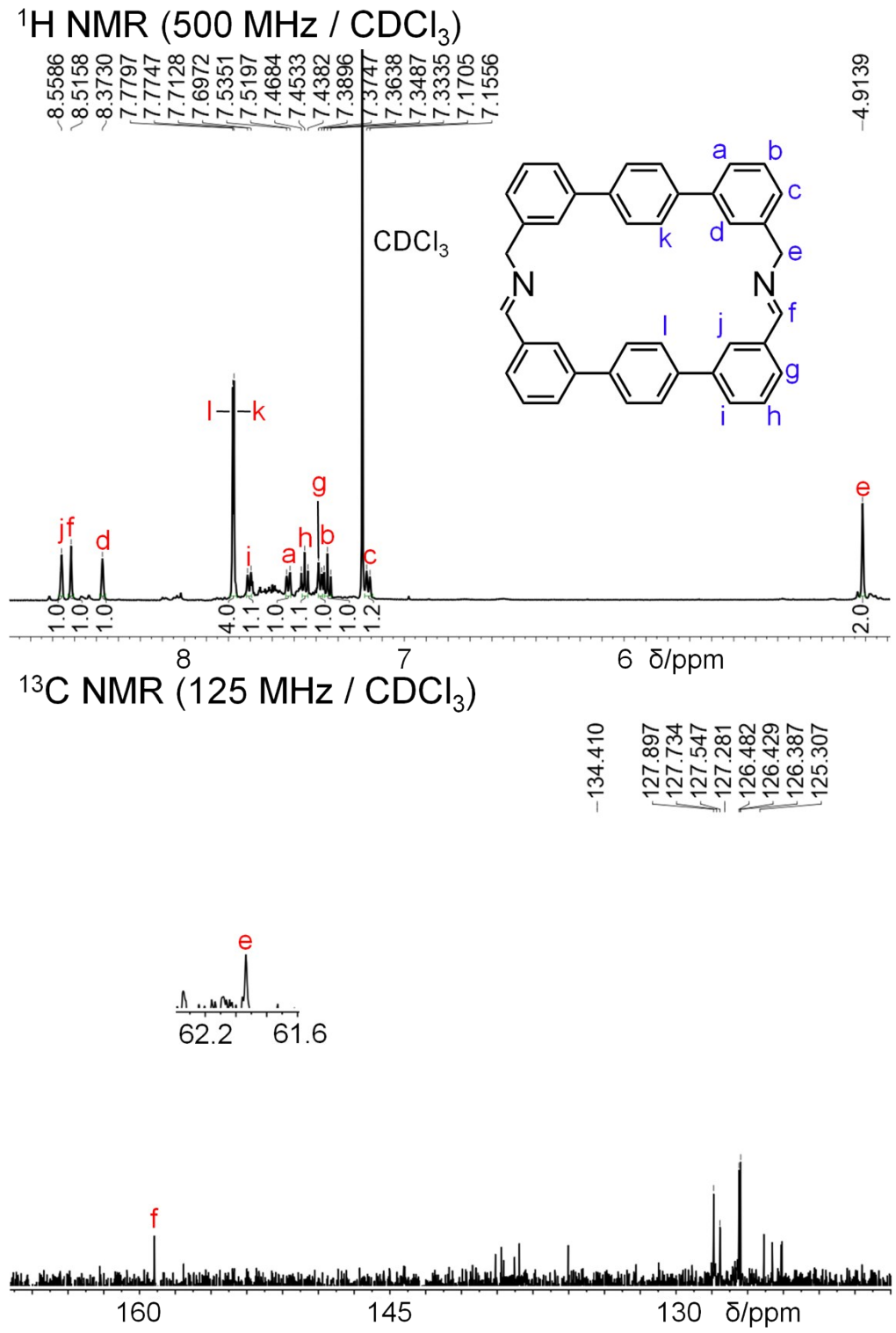


Figure S5. ^{1}H (top) and ^{13}C (bottom) spectrum of 3.

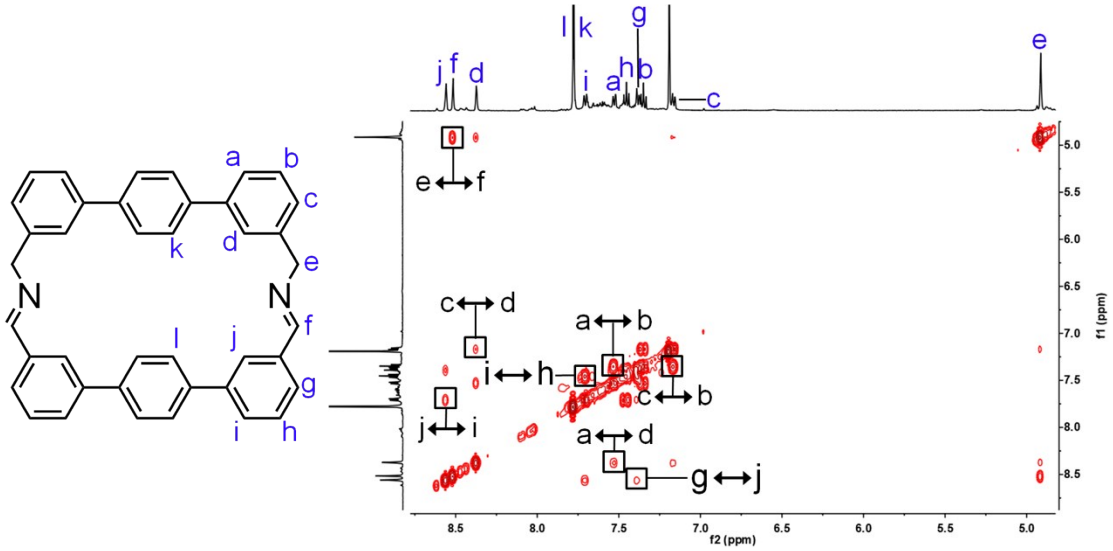


Figure S6. ^{1}H-^{1}H COSY spectrum (500 MHz, $CDCl_3$, 298 K) of 3. Key correlation peaks are labeled. The peak assignment was made in Figure S5.

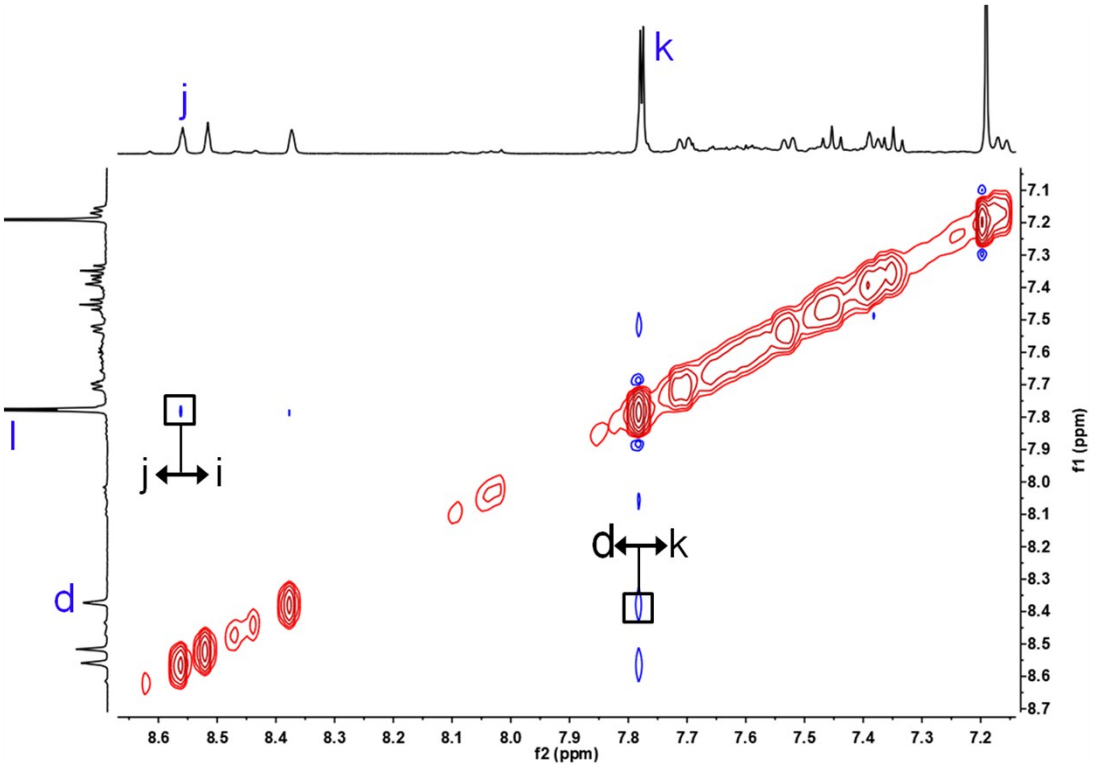


Figure S7. **Partial 1H-1H NOESY spectrum (500 MHz, CDCl3, 298K) of 3.** A key correlation peak between protons i and j, d and k are labeled.

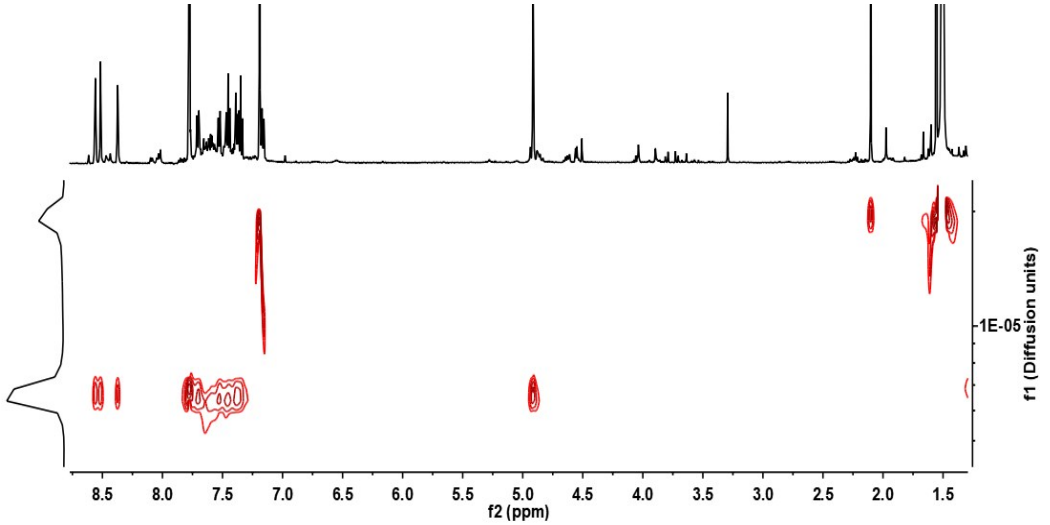


Figure S8. The DOSY spectrum of 3 (500 MHz, $CDCl_3$, 298 K).

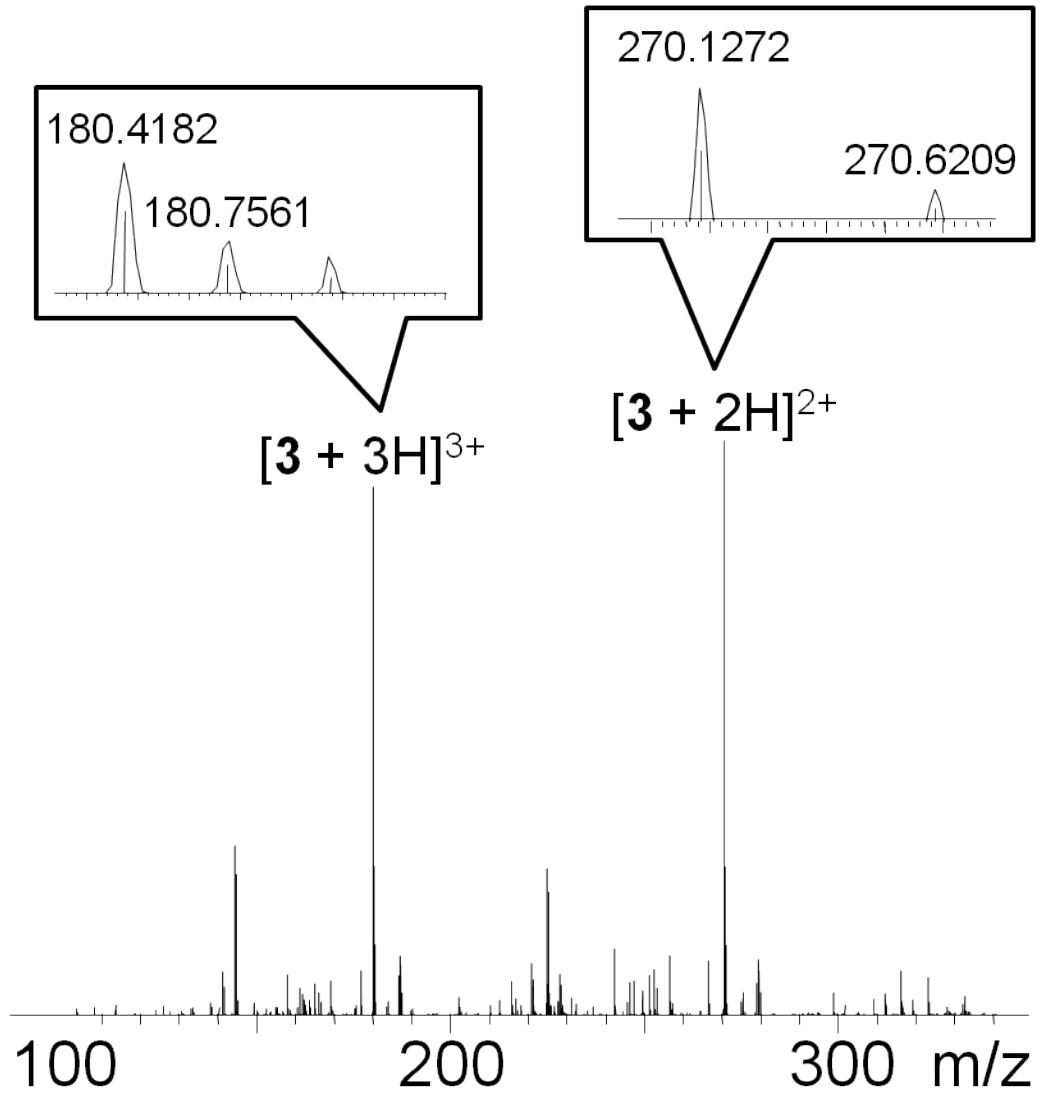


Figure S9. **ESI-HRMS of 3.** The signals labeled in the spectrum correspond to molecular cations

that contain three and two charges, respectively.

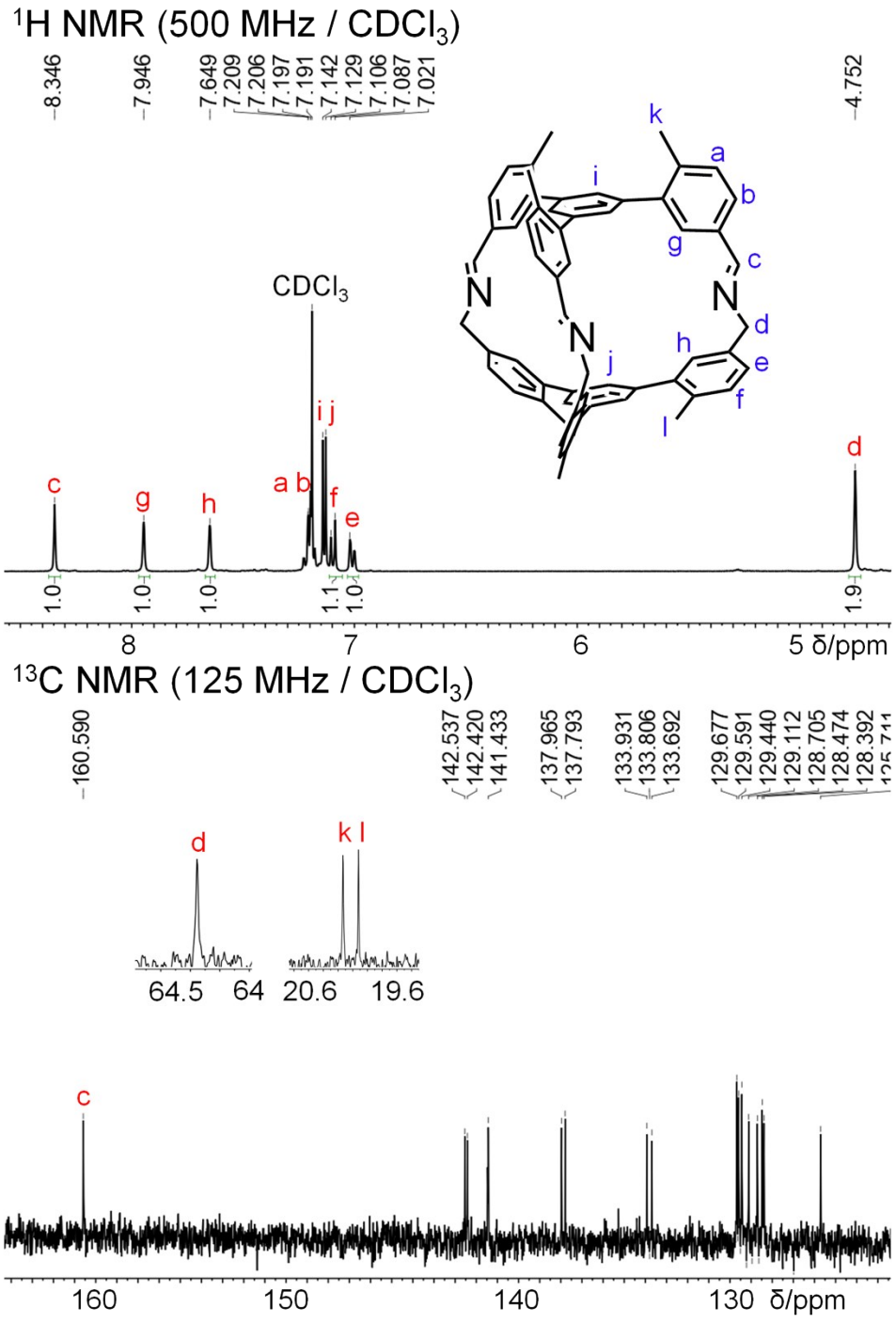


Figure S10. ^{1}H (top) and ^{13}C (bottom) spectrum of 6a.

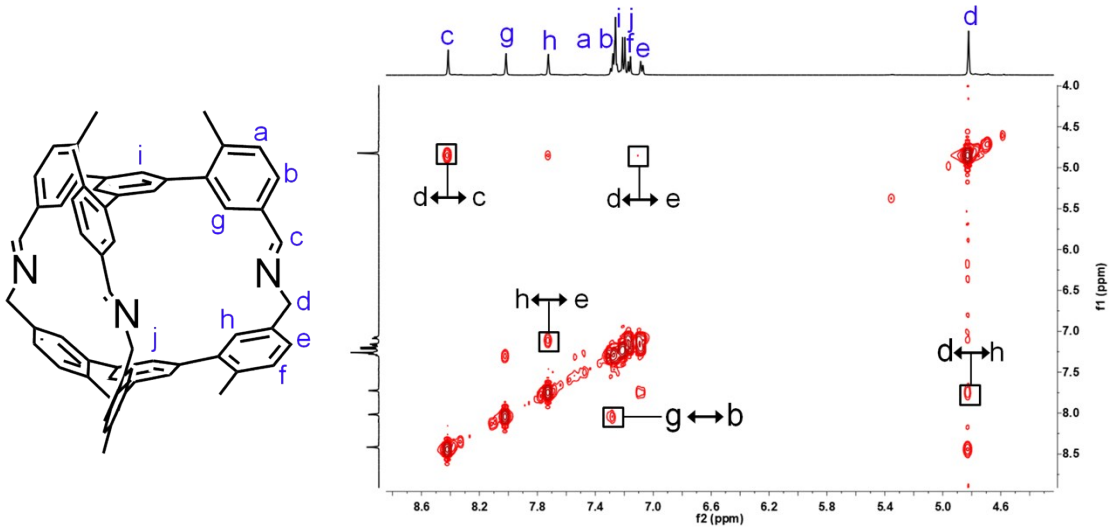


Figure S11. ^{1}H-^{1}H COSY spectrum (500 MHz, $CDCl_3$, 298 K) of 6a. Key correlation peaks are labeled. The peak assignment was made in Figure S10.

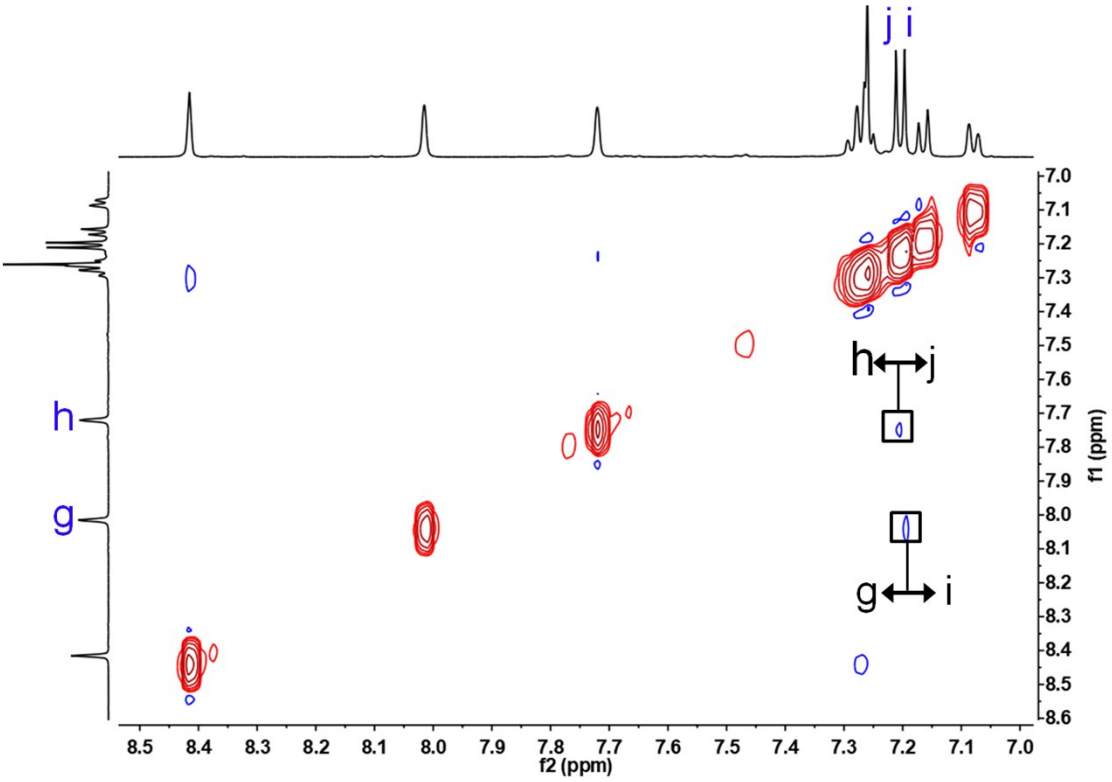


Figure S12. Partial ^{1}H-^{1}H NOESY spectrum (500 MHz, $CDCl_3$, 298K) of 6a. A key correlation peak between protons h and j, as well as g and i are labeled.

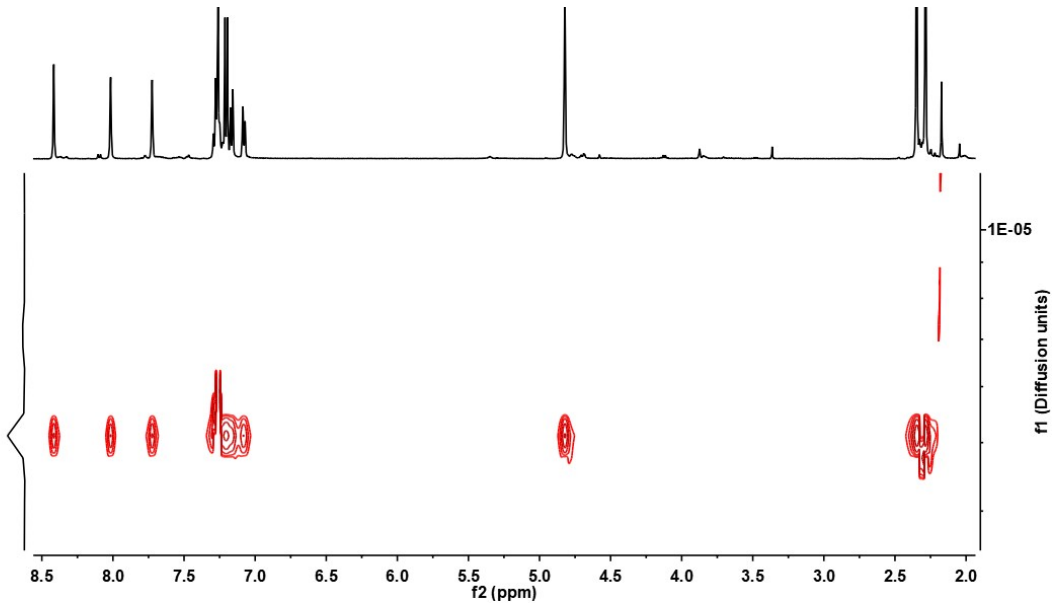


Figure S13. The DOSY spectrum of 6a (500 MHz, $CDCl_3$, 298 K).

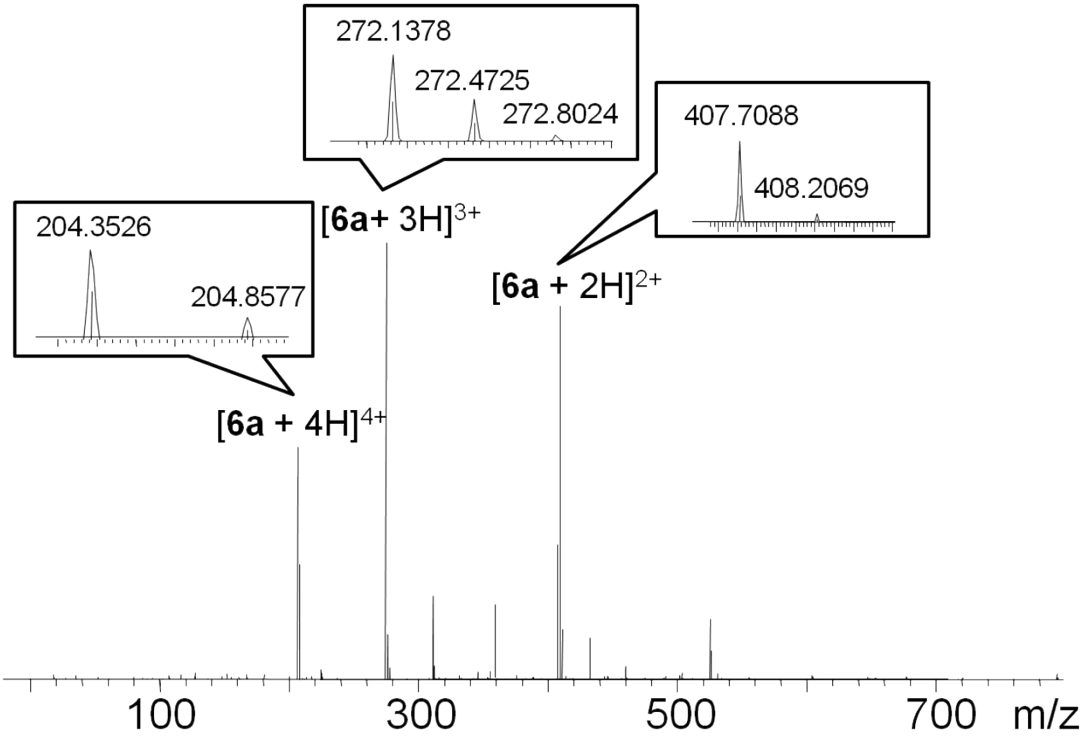


Figure S14. ESI-HRMS of 6a. The signals labeled in the spectrum correspond to molecular cations that contain four, three and two charges, respectively.

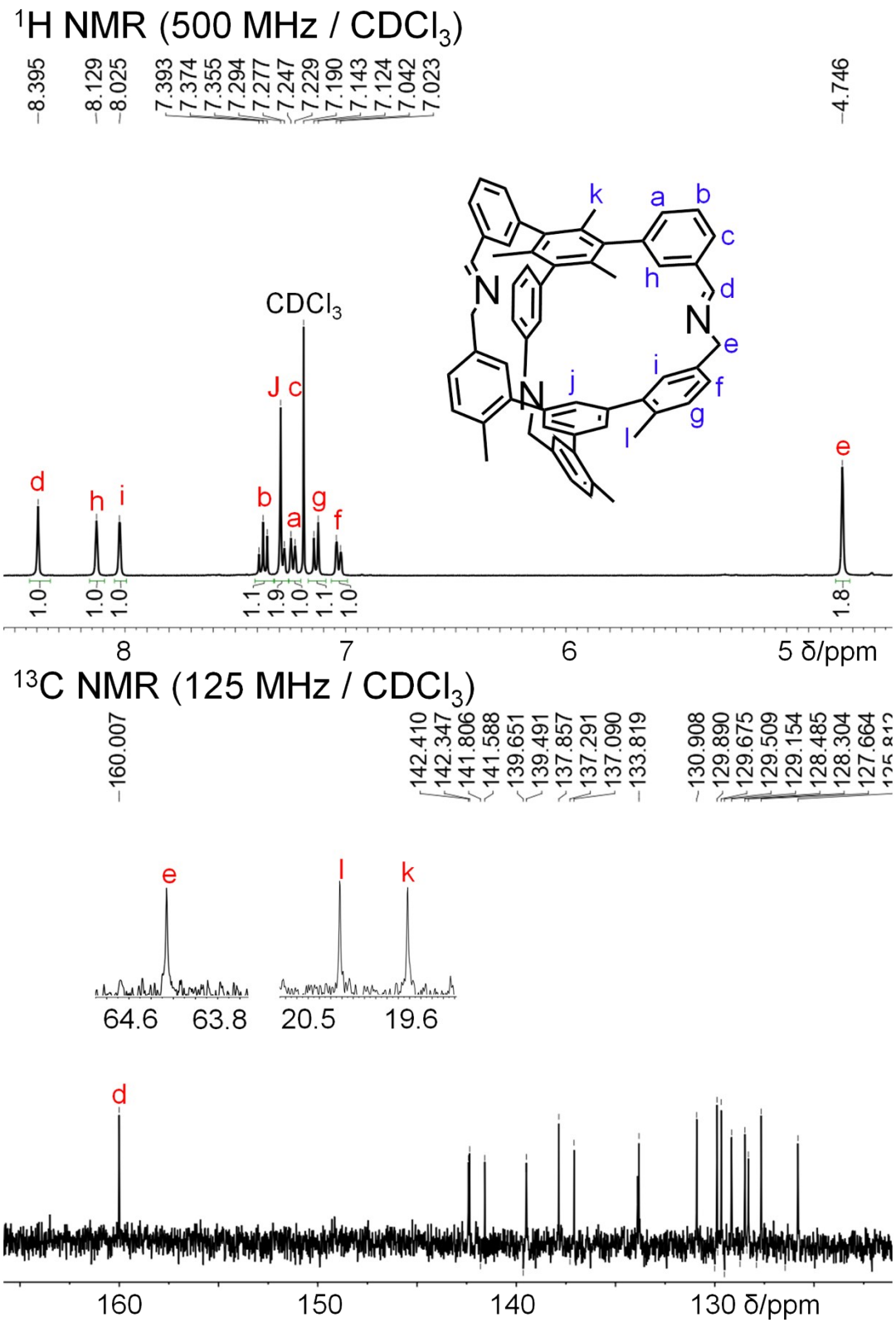


Figure S15. ^{1}H (top) and ^{13}C (bottom) spectrum of 6b.

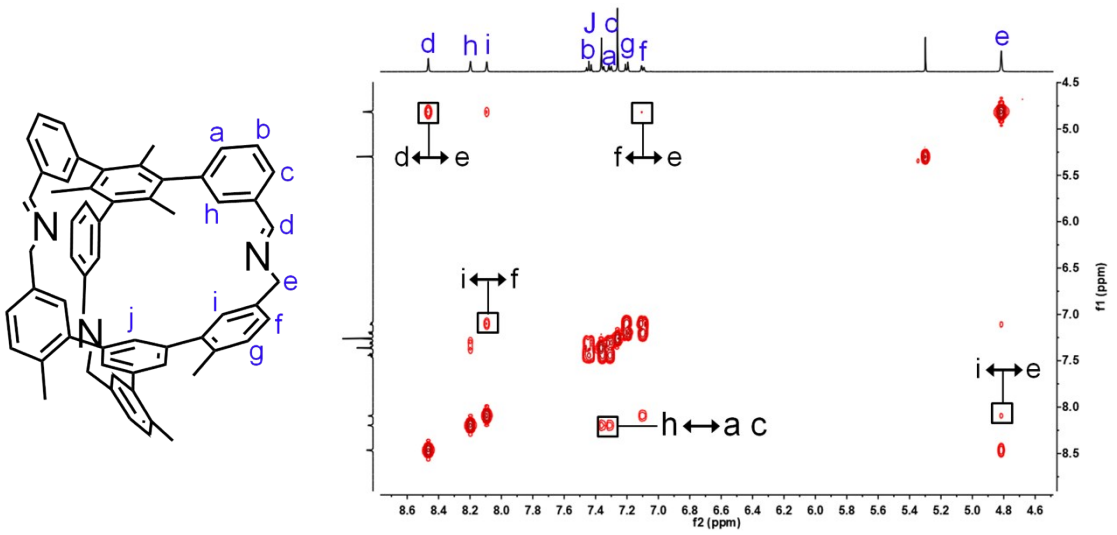


Figure S16. ^{1}H-^{1}H COSY spectrum (500 MHz, $CDCl_3$, 298 K) of 6b. Key correlation peaks are labeled. The peak assignment was made in Figure S15.

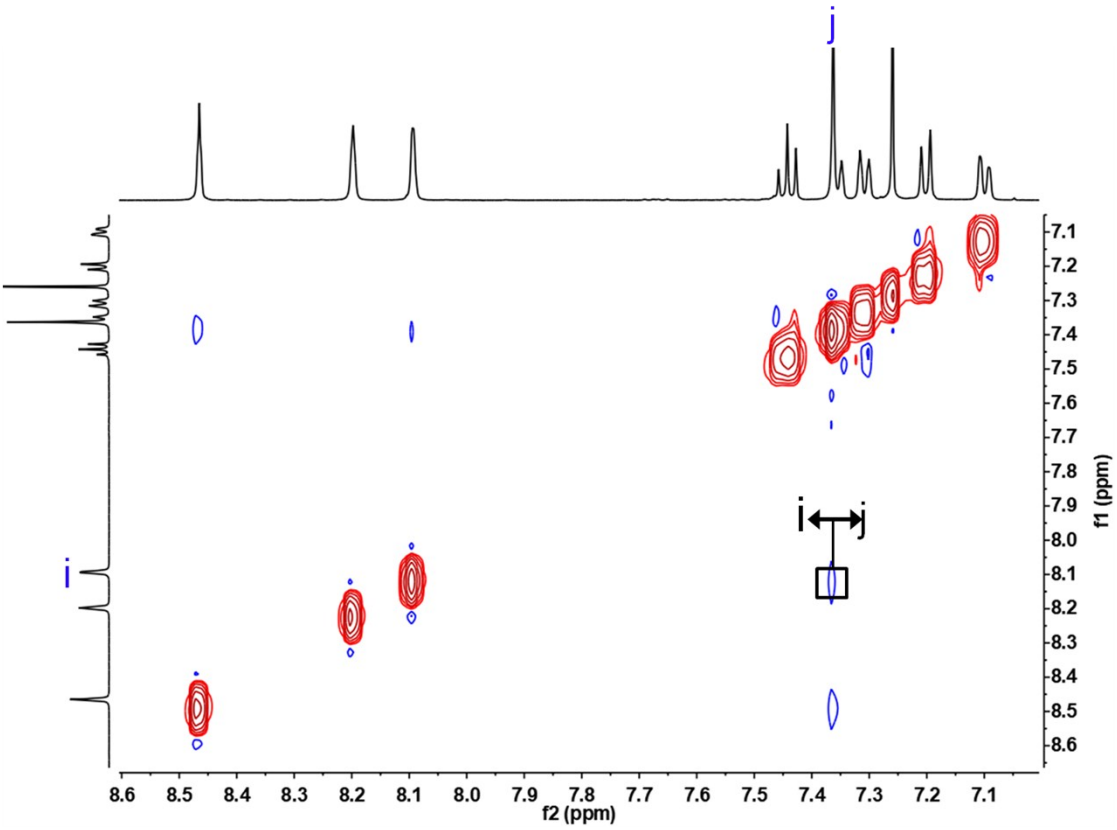


Figure S17. Partial ^{1}H-^{1}H NOESY spectrum (500 MHz, $CDCl_3$, 298K) of 6b. A key correlation peak between protons i and j are labeled.

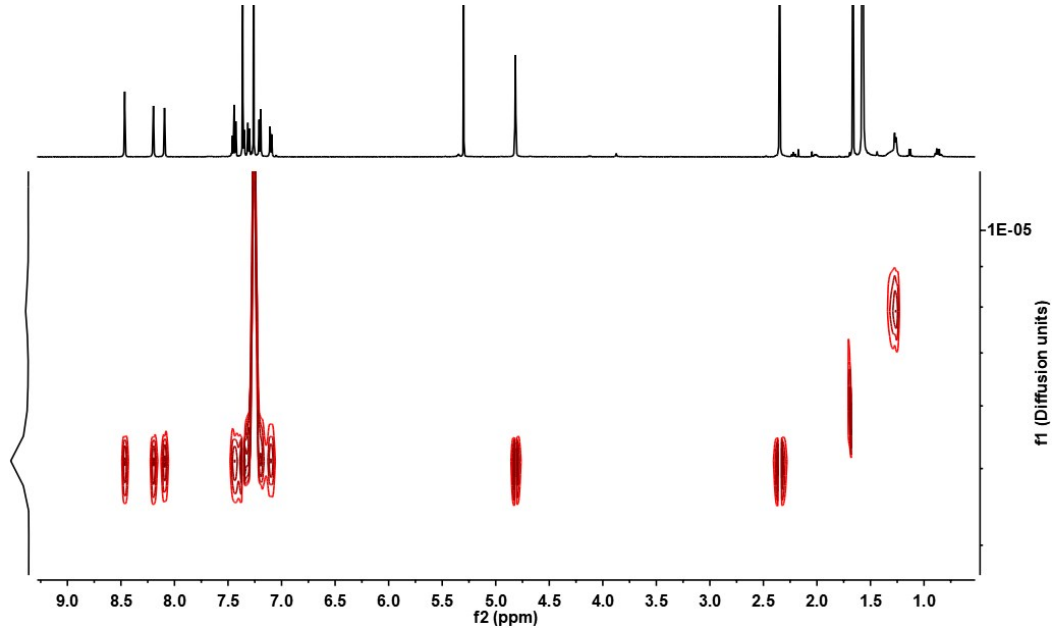


Figure S18. The DOSY spectrum of 6b (500 MHz, $CDCl_3$, 298 K).

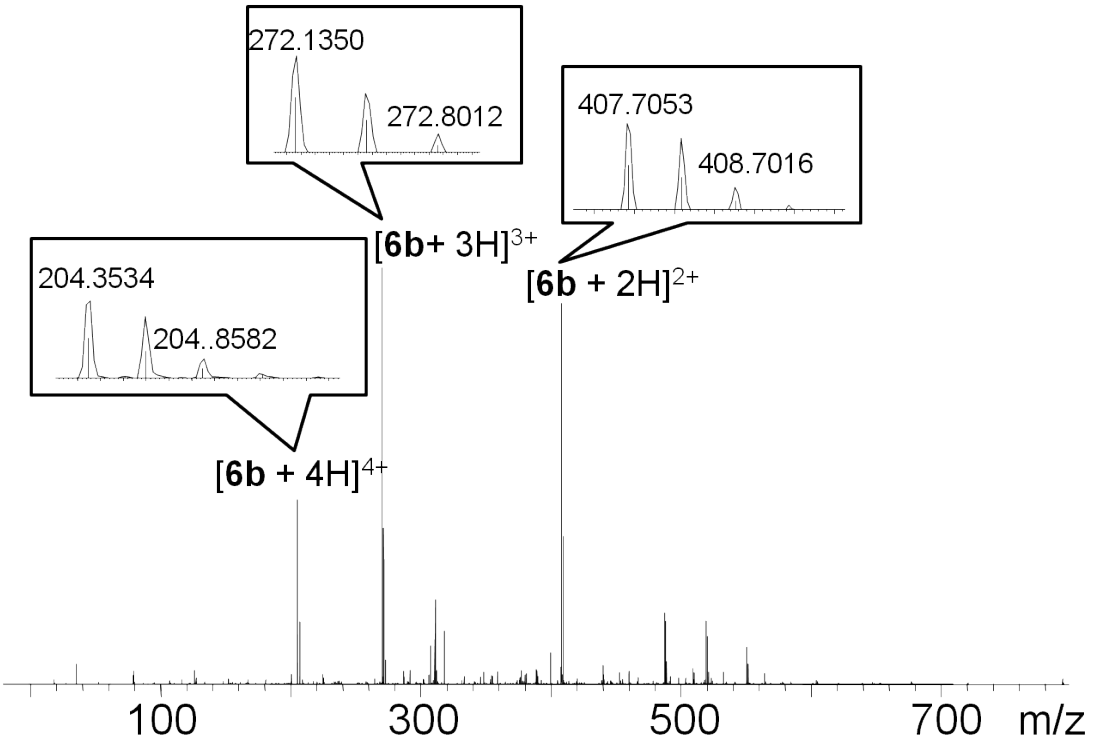


Figure S19. ESI-HRMS of 6b. The signals labeled in the spectrum correspond to molecular cations that contain four, three and two charges, respectively.

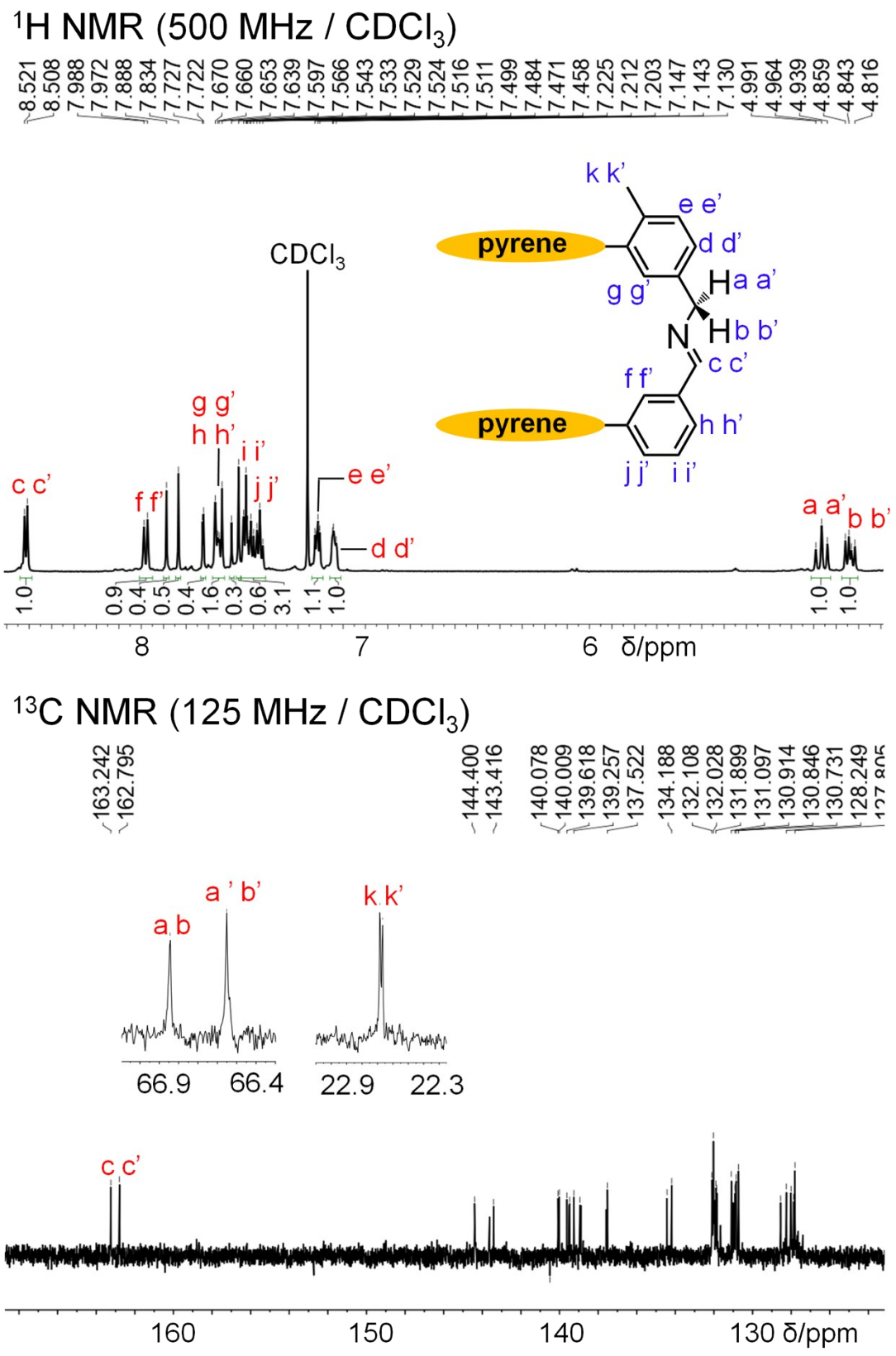


Figure S20. ^{1}H (top) and ^{13}C (bottom) spectrum of 9a and 9b.

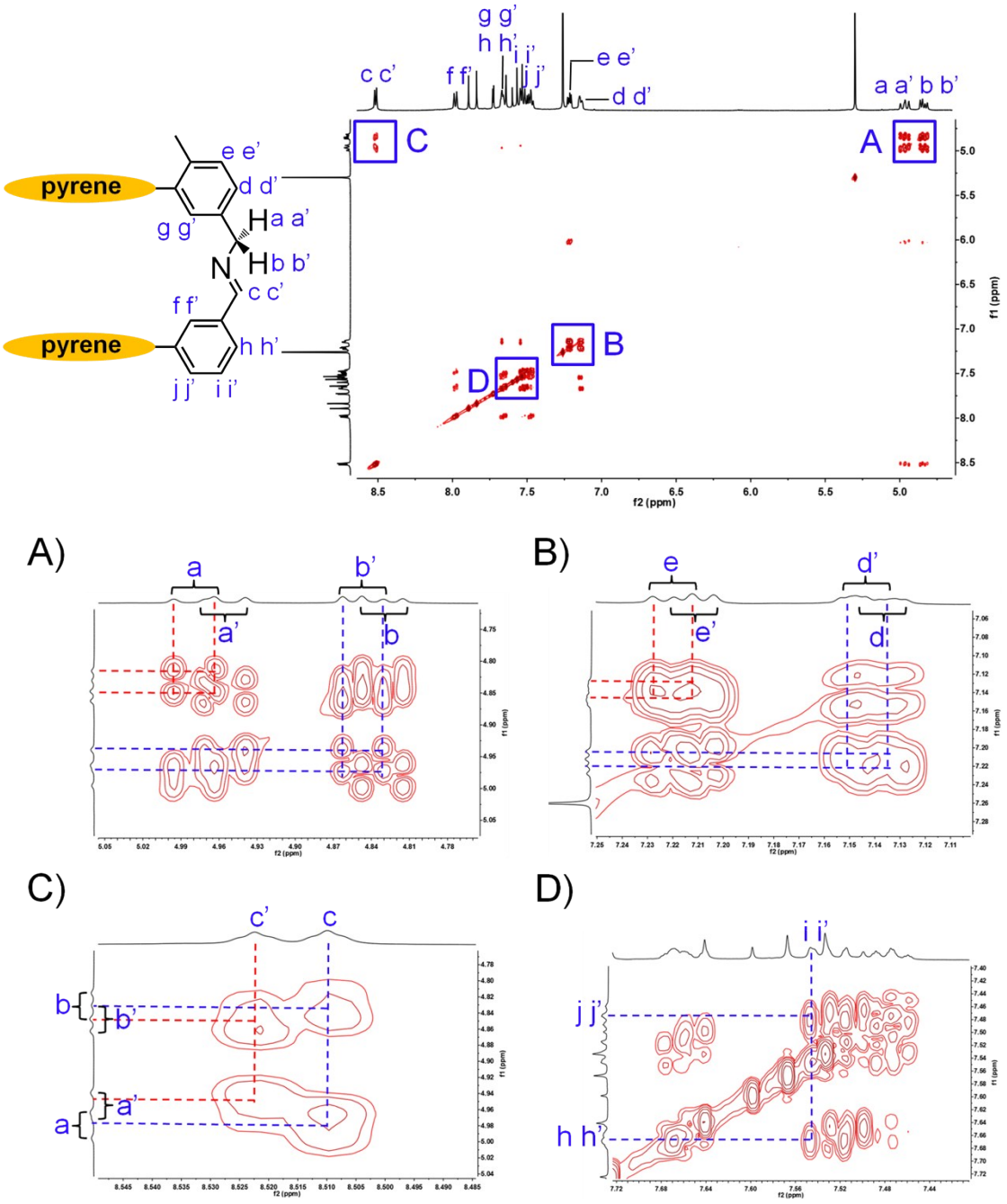


Figure S21. ^{1}H-^{1}H COSY spectrum (500 MHz, $CDCl_3$, 298 K) of 9a and 9b. Key correlation peaks are labeled. The peak assignment was made in Figure S20.

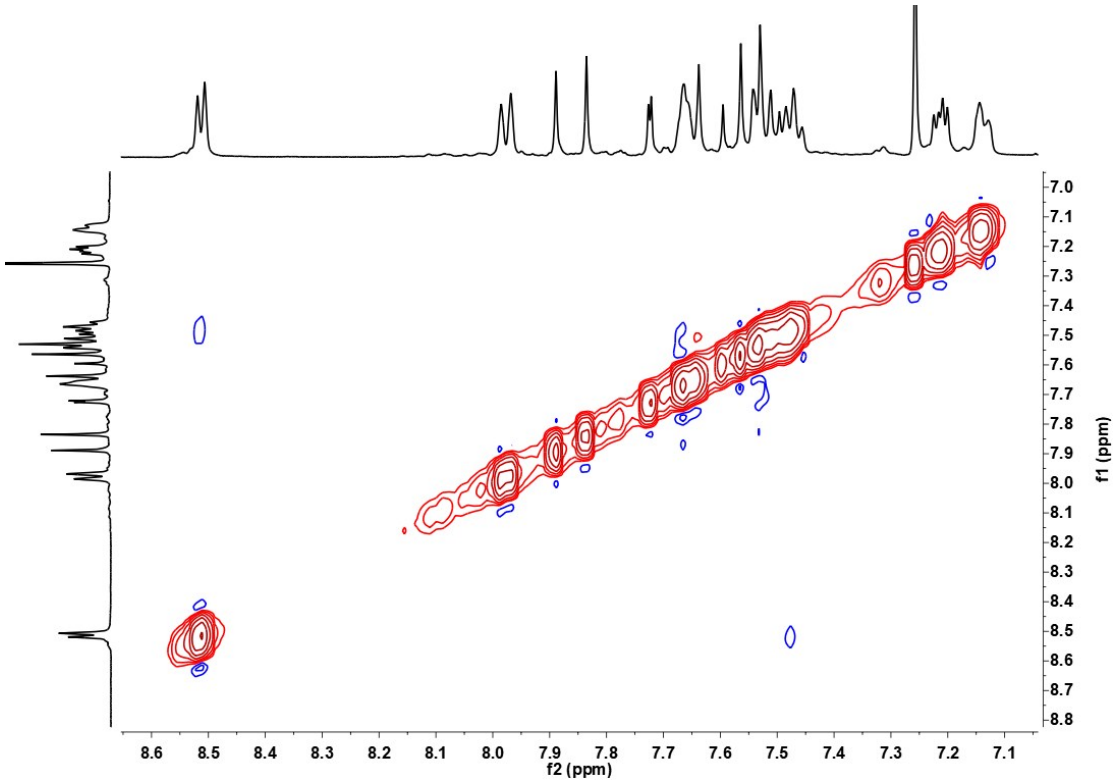


Figure S22. Partial ^{1}H-^{1}H NOESY spectrum (500 MHz, $CDCl_3$, 298K) of 9a and 9b.

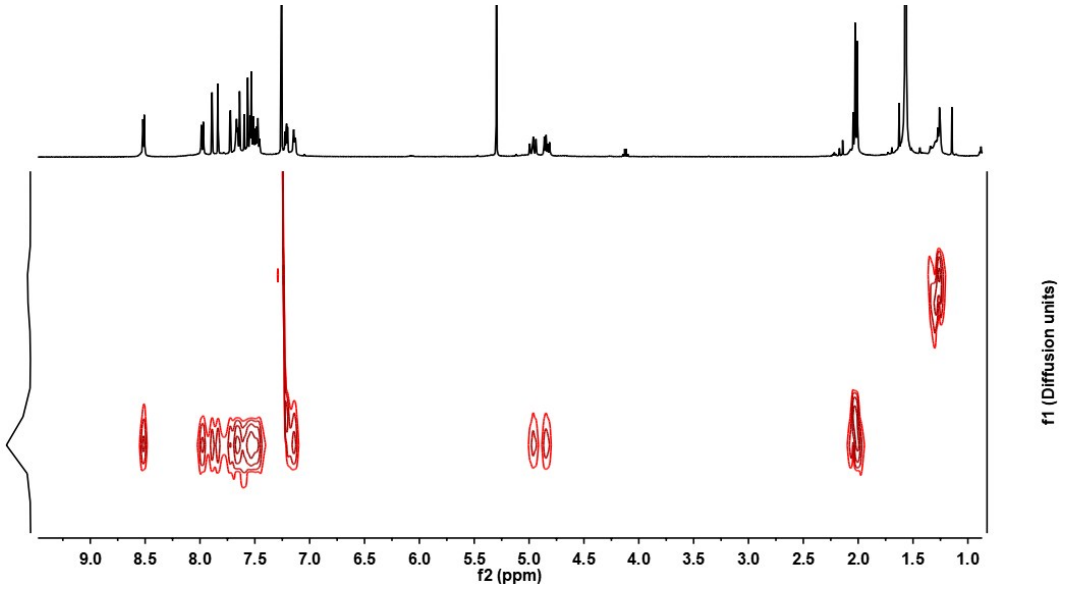


Figure S23. The DOSY spectrum of 9a and 9b (500 MHz, $CDCl_3$, 298 K).

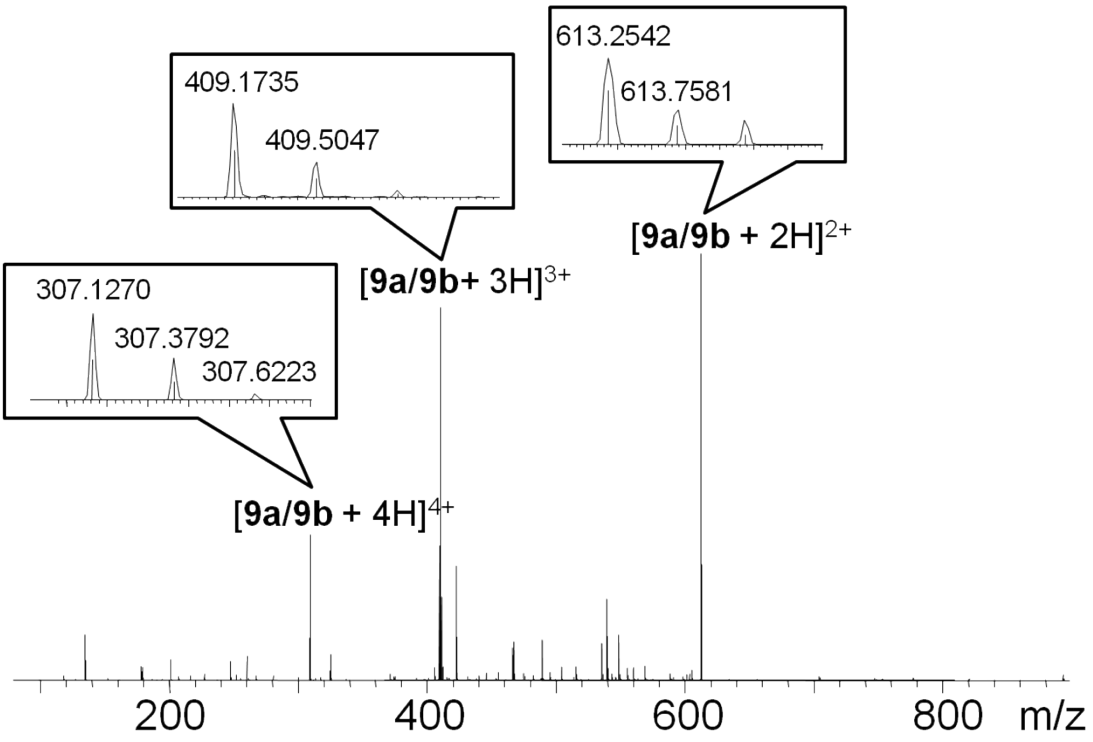


Figure S24. ESI-HRMS of 9a and 9b. The signals labeled in the spectrum correspond to molecular cations that contain four, three and two charges, respectively.

4. Control experiment.

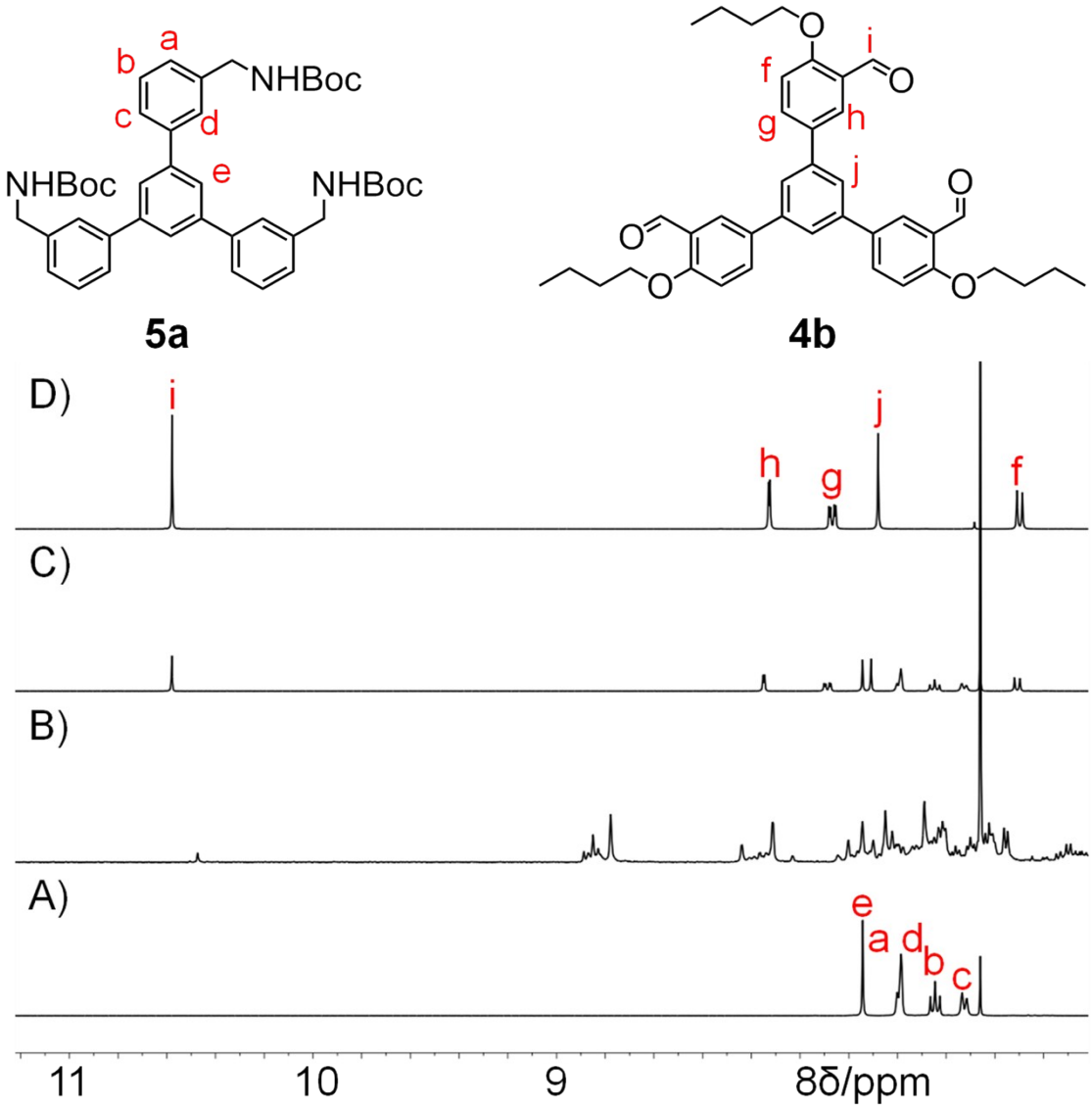


Figure S25. Partial ^{1}H NMR spectra of **4b** (D), **5a** (A), a mixture of **4b** and **5a** before (C) and after (B) the so-call deprotection-condensation was performed.

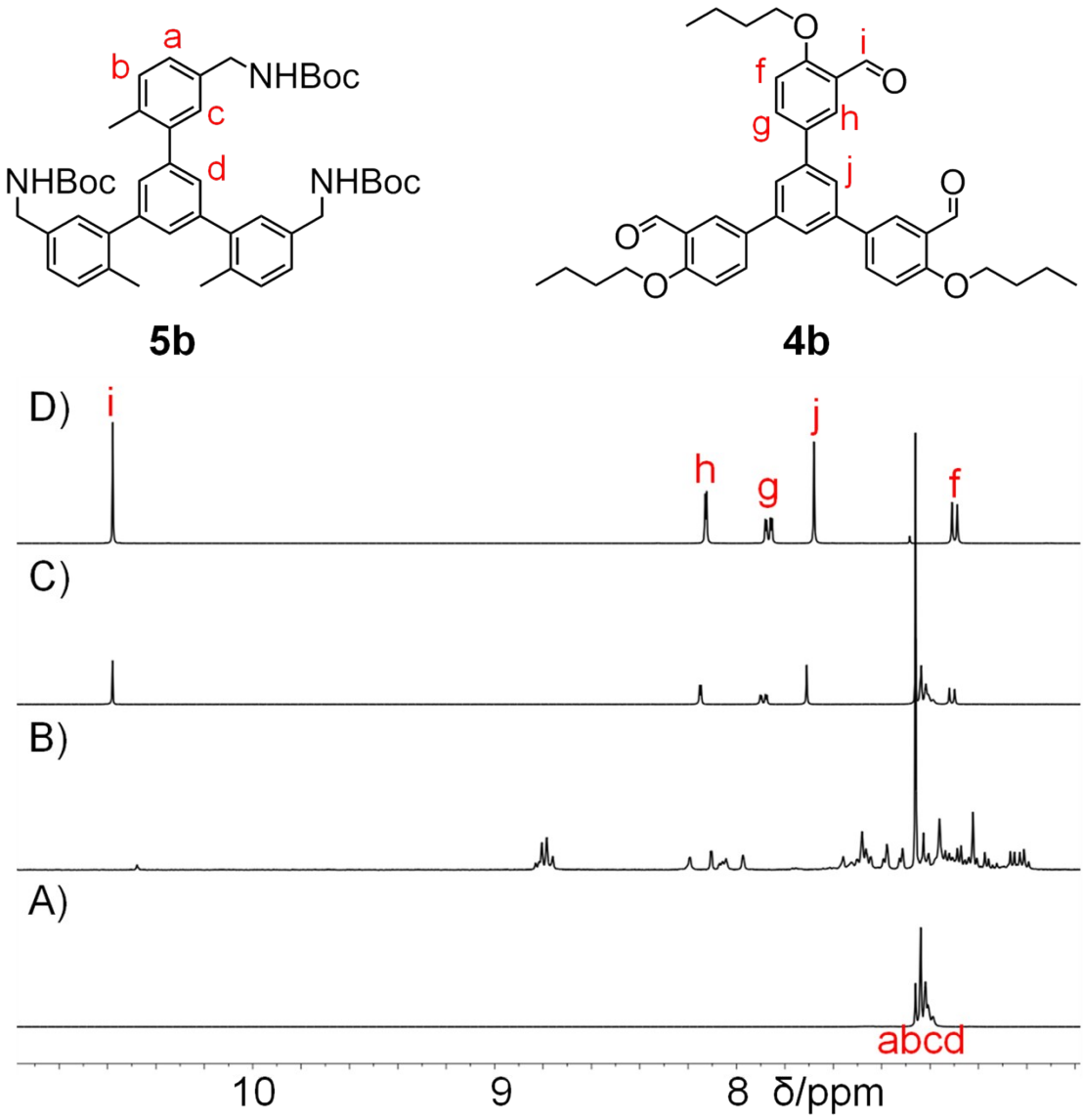


Figure S26. Partial ^{1}H NMR spectra of **4b** (D), **5b** (A), a mixture of **4b** and **5b** before (C) and after (B) the so-call deprotection-condensation was performed.

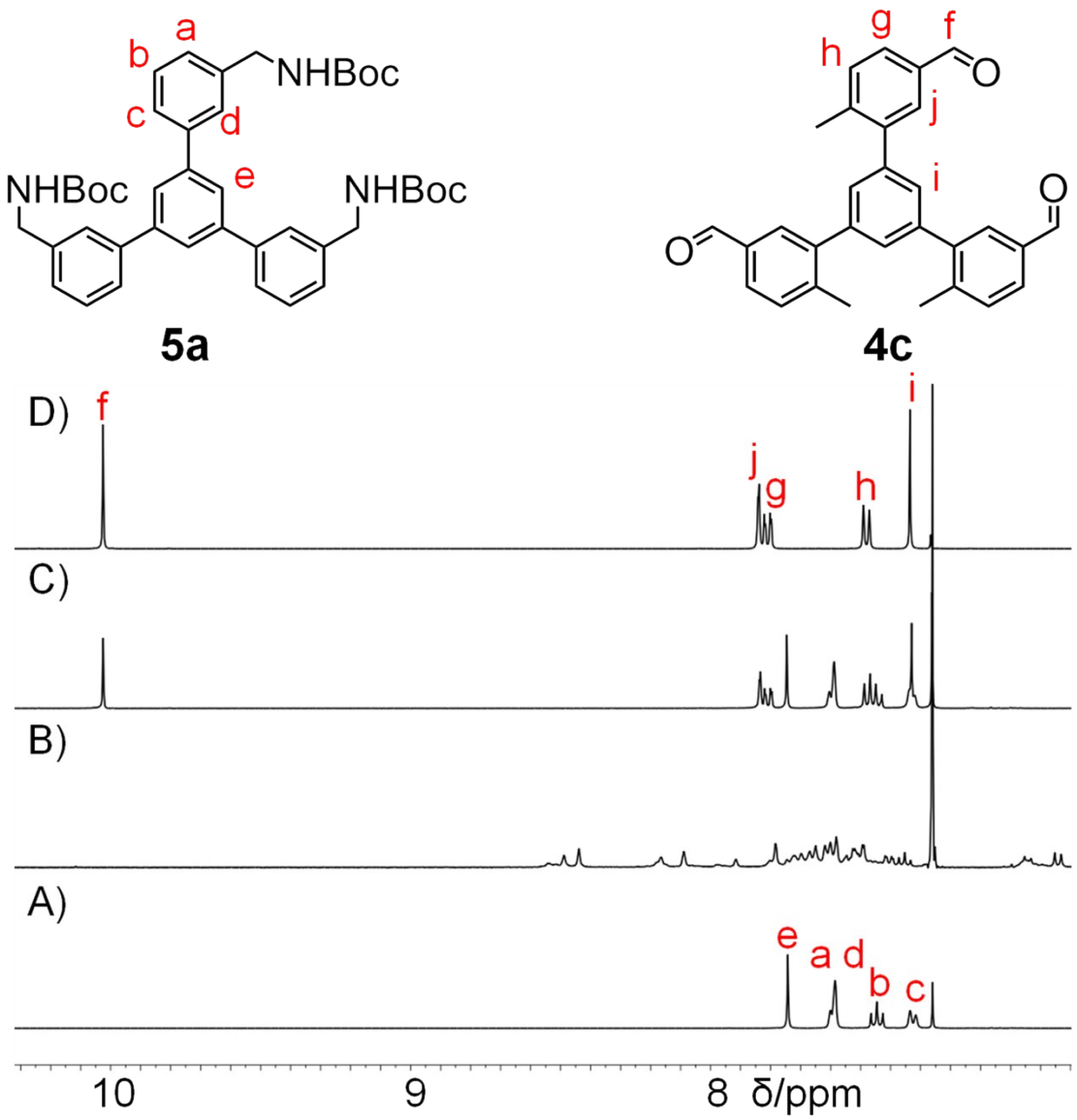


Figure S27. Partial ^{1}H NMR spectra of **4c** (D), **5a** (A), a mixture of **4c** and **5a** before (C) and after (B) the so-call deprotection-condensation was performed.

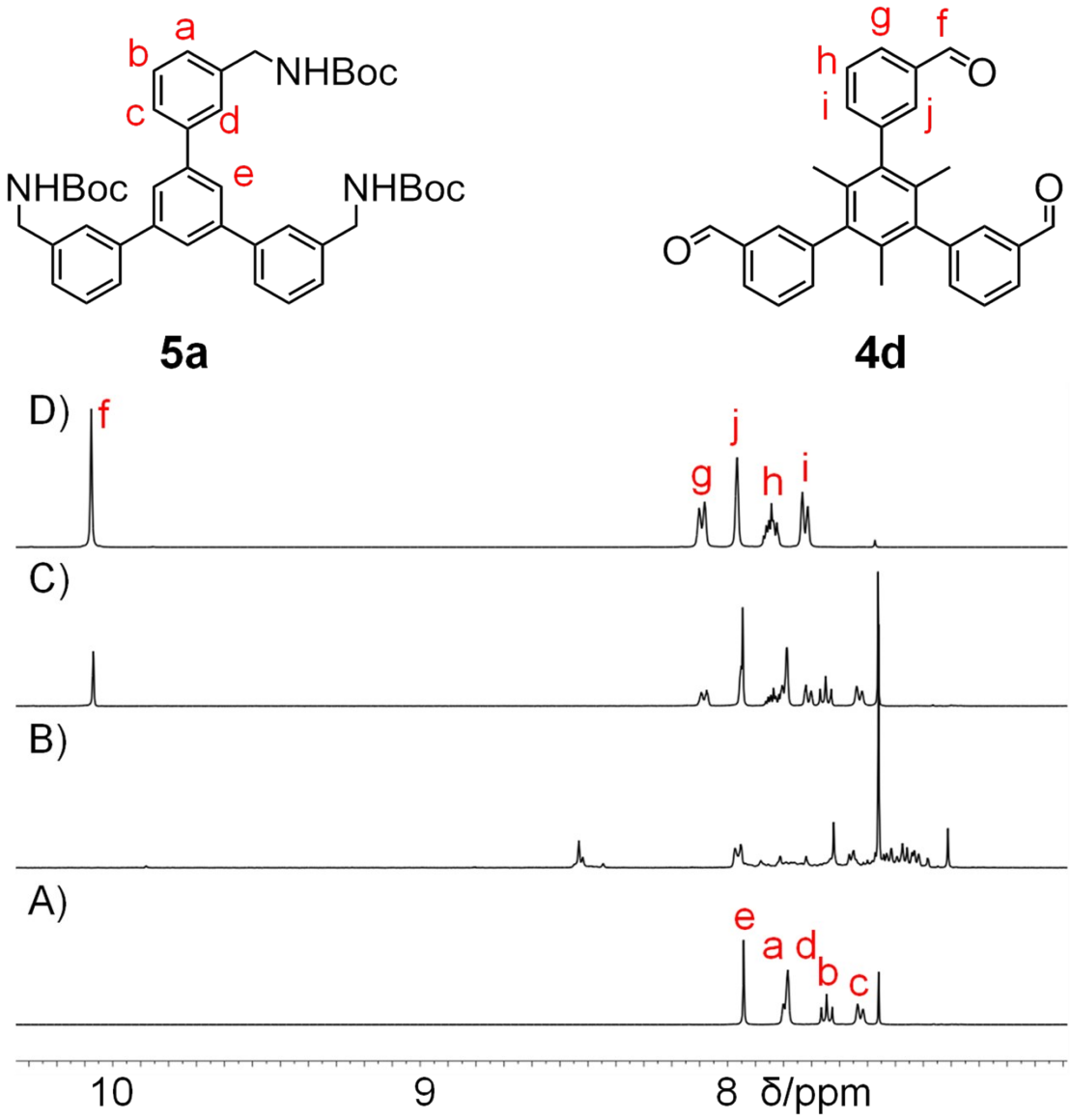


Figure S28. Partial ^{1}H NMR spectra of **4d** (D), **5a** (A), a mixture of **4d** and **5a** before (C) and after (B) the so-call deprotection-condensation was performed.

5. X-ray Crystallography.

a) Methods

Single crystals of **3**, suitable for X-ray crystallography, were grown by slow vapor diffusion of isopropyl ether into solution of **3** (in $CDCl_3$) over the course of days. Data were collected at 170 K on a Bruker D8 Venture Diffractometer equipped with a MoKα IμS source and MX optic.

b) Crystal parameters

$[C_{40}H_{30}N_2]$, Yellow block (0.19×0.24×0.28mm), Monoclinic, space group P21/n, a = 13.1968(3) Å, b = 17.0333(4) Å, c = 19.6066(5) Å, α = 90°, β = 101.946(1)°, γ = 90°, V = 4311.82(18) Å^3, Z = 6, T = 170 K, ρ_{calc} = 1.245 g/cm^3, μ(GaKα) = 0.072 mm^{-1}. A total of 13711 reflections were collected, of which 8358 were unique. Final $R_1(I > 2\sigma(I))$ = 0.0778 and wR_2 = 0.2185 (all data). The structure was solved by direct method and different Fourier syntheses. Using Olex2,[S1] the structure was solved with the ShelXT[S2] structure solution program using Intrinsic Phasing and refined with the ShelXL[S3] refinement package using Least Squares minimization. CCDC number: 1981448.

c) Solid-state structure

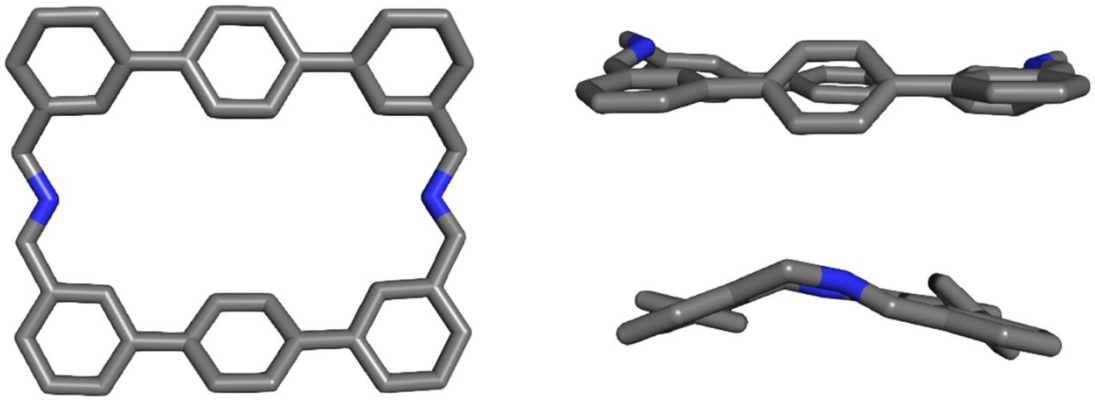


Figure S29. Different views of the solid-state structure of 3. Carbon, grey; nitrogen blue, Hydrogen atoms and disordered solvent molecules are omitted for clarity.

a) Methods

Single crystals of **6a**, suitable for X-ray crystallography, were grown by slow vapor diffusion of isopropyl ether into solution of **6a** (in $CDCl_3$) over the course of days. Data were collected at 170 K on a Bruker D8 Venture Diffractometer equipped with a MoKα IμS source and MX optic.

b) Crystal parameters

$[C_{60}H_{51}N_3\cdot]\cdot(CDCl_3)_2$, Yellow block (0.16×0.18×0.18mm), Triclinic, space group P-1, a = 13.119(3) Å, b = 15.227(2) Å, c = 15.449(4) Å, α = 106.247(6)°, β = 109.671(8)°, γ = 101.252(7)°, V = 2643.3(9) Å^3, Z = 2, T = 170 K, ρ_{calc} = 1.323 g/cm^3, μ(GaKα) = 2.188 mm^{-1}. A total of 9977 reflections were collected, of which 4719 were unique. Final $R_1(I > 2\sigma(I))$ = 0.0743 and wR_2 = 0.2282 (all data). The structure was solved by direct method and different Fourier syntheses. Using Olex2,[S1] the structure was solved with the ShelXT[S2] structure solution program using Intrinsic Phasing and refined with the ShelXL[S3] refinement package using Least Squares minimization. CCDC number: 1981450.

c) Solid-state structure

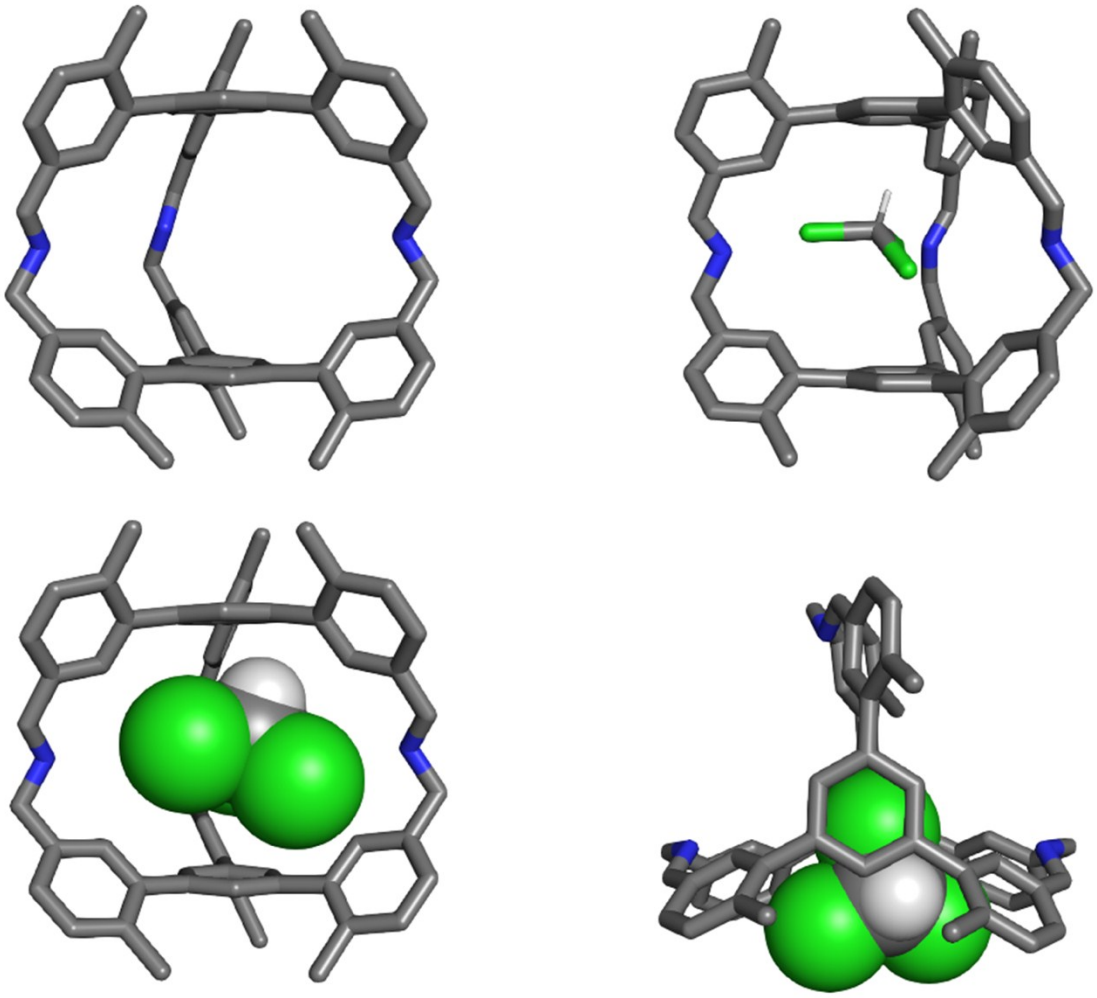


Figure S30. Different views of the solid-state structure of 6a. Carbon, grey; nitrogen blue; chlorine, green; hydrogen, white. Hydrogen atoms and disordered solvent molecules are omitted for clarity.

a) Methods

Single crystals of **6b**, suitable for X-ray crystallography, were grown by slow vapor diffusion of isopropyl ether into solution of **6b** (in $CDCl_3$) over the course of days. Data were collected at 170 K on a Bruker D8 Venture Diffractometer equipped with a MoKα IμS source and MX optic.

b) Crystal parameters

$[C_{60}H_{51}N_3\cdot]\cdot(CDCl_3)_3$, Yellow block (0.13×0.24×0.32mm), Triclinic, space group P-1, a = 11.337(6) Å, b = 20.266(11) Å, c = 26.705(16) Å, α = 71.662(16)°, β = 84.799(18)°, γ = 86.827(16)°, V = 5794(6) Å^3, Z = 4, T = 170 K, ρ_{calc} = 1.343 g/cm^3, μ(GaKα) = 2.814 mm^{-1}. A total of 21752 reflections were collected, of which 9737 were unique. Final $R_1(I > 2\sigma(I))$ = 0.1250 and wR_2 = 0.3581 (all data). The structure was solved by direct method and different Fourier syntheses. Using Olex2,[S1] the structure was solved with the ShelXT[S2] structure solution program using Intrinsic Phasing and refined with the ShelXL[S3] refinement package using Least Squares minimization. CCDC number: 1981449.

c) Solid-state structure

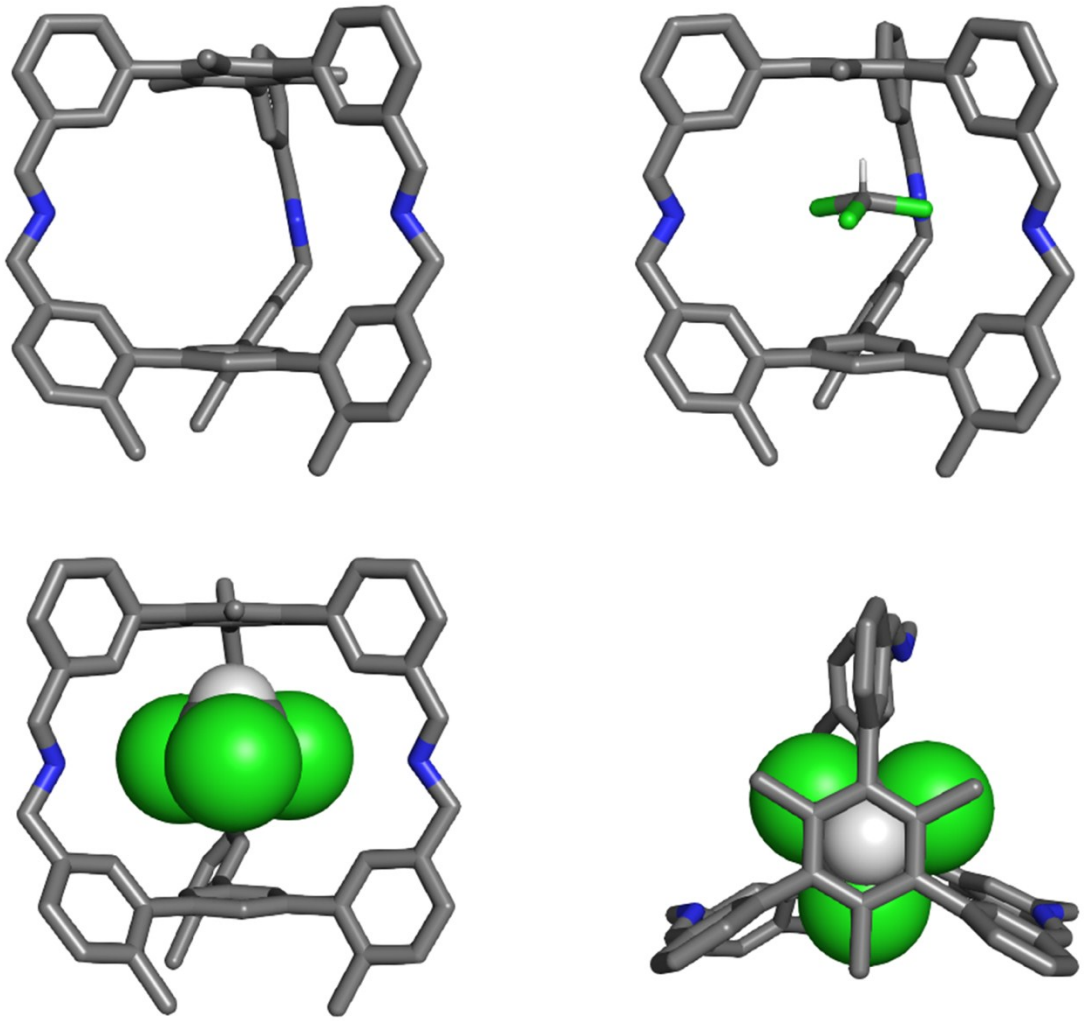


Figure S31. Different views of the solid-state structure of 6b. Carbon, grey; nitrogen blue; chlorine, green; hydrogen, white. Hydrogen atoms and disordered solvent molecules are omitted for clarity.

6. Computational Analysis

All density functional theory (DFT) calculations were performed with Gaussian 09.[S4] Geometry optimization of all the structures was carried out at the b3lyp level of theory[S5] with 6-31g(d) basis set.[S6] The vibrational frequencies of the optimized stationary points are calculated under the same level of theory, to obtain the zero-point vibrational energy (ZPVE) and thermal corrections at 298 K as well as verifying whether each of optimized stationary points is an energy minimum. The single-point energies were computed at b3lyp level of theory with 6-311++g(d,p) basis set for all the atoms, based on the gas-phase optimized structures. The distortion energies ($\Delta E_{distortion}$) for 4c, 4d, and 4a were calculated by using the equation $\Delta E_{distortion} = E_{complex} - E_{free}$. $E_{complex}$ refers to the single-point energy of the molecular fragment containing the residue of precursor within the corresponding cage framework. E_{free} refers to the single-point energy of the molecular fragment containing the residue of precursor within the corresponding free precursor.

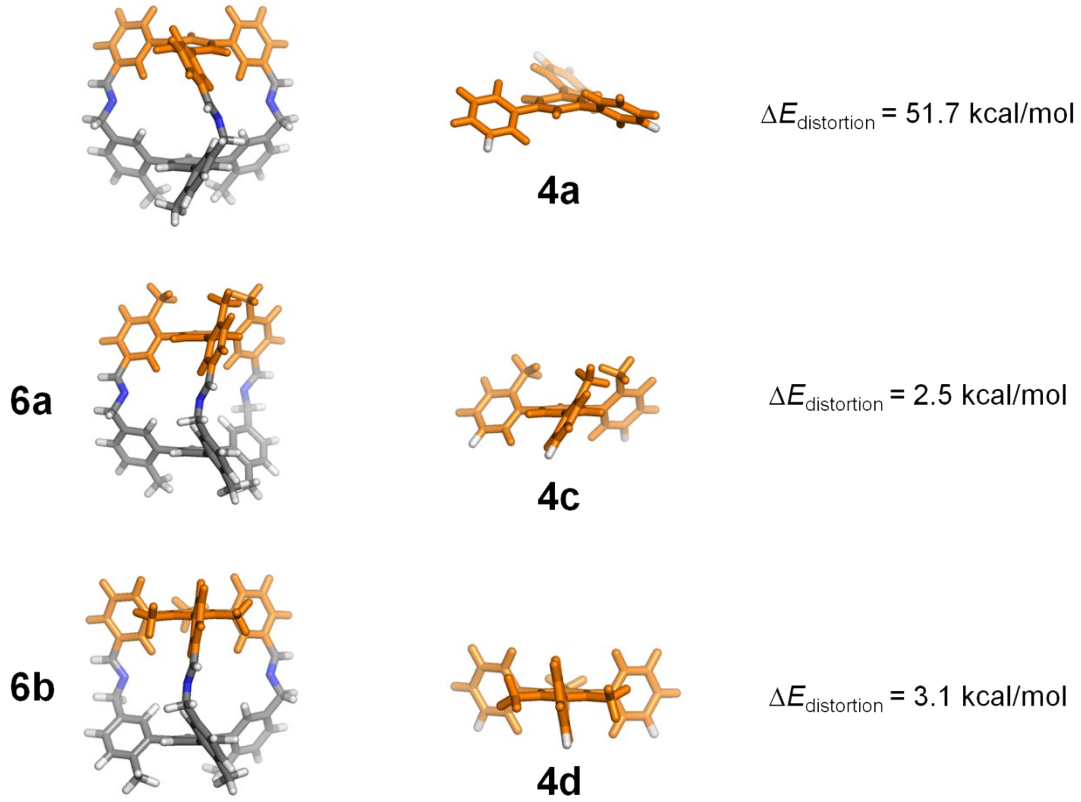


Figure S32 Optimized structures of 4a, 4c, 4d and corresponding cages. The energies of molecular fragments with orange color were calculated to obtain corresponding $\Delta E_{distortion}$.

Cartesian Coordinates for the Optimized Structures

9a

C	-2.96653200	-4.47912400	0.74937100
C	-1.55471300	-4.54867000	0.72984800
C	-0.81237300	-3.99169300	1.81969900
C	-1.49497200	-3.36817200	2.91338800

C	-2.90926100	-3.28134800	2.88858300
C	-3.60711000	-3.86889900	1.82710900
C	-0.83614500	-5.14560800	-0.35928700
C	0.52381300	-5.15076500	-0.39591700
C	1.30301900	-4.55982500	0.65431400
C	0.62110800	-3.99973000	1.78153800
C	1.36672400	-3.38898000	2.83963600
C	0.65072800	-2.84635100	3.95796100
C	-0.70939000	-2.84486500	3.99647400
C	2.71417600	-4.50108700	0.60041800
C	3.41508400	-3.90402100	1.64983900
C	2.77454300	-3.32990400	2.75078800
C	-3.68934100	-2.43322600	3.83006900
C	-3.80103600	-4.88445100	-0.42302400
C	3.48942900	-4.93800700	-0.60176800
C	3.61904600	-2.53615600	3.69763800
C	-3.32960500	-1.08922500	4.00841800
C	-4.15316700	-0.19444500	4.69763600
C	-5.34965900	-0.65591800	5.26613500
C	-5.69236500	-2.00016800	5.14517700
C	-4.87882700	-2.88073000	4.42599300
C	-4.61443300	-6.02929000	-0.40255200
C	-5.44663800	-6.32459500	-1.48357500
C	-5.48943500	-5.47507700	-2.58890400
C	-4.68860500	-4.32511000	-2.62467200
C	-3.84193900	-4.04868100	-1.54221400
C	3.54428800	-4.10061500	-1.71926200
C	4.34400800	-4.41949400	-2.82633300
C	5.08096400	-5.61182200	-2.81594700
C	5.02211300	-6.46309400	-1.71294200
C	4.23808000	-6.12673200	-0.60852400
C	4.37629400	-3.12520000	4.71724100
C	5.28233000	-2.35747800	5.45873000
C	5.47018600	-1.00910000	5.16984500
C	4.70979700	-0.39853000	4.16068000
C	3.76920600	-1.16218600	3.46074300
C	-3.74781600	1.22180300	4.73535400
C	-4.76046100	-3.40629000	-3.77523000
C	4.43919500	-3.50502000	-3.97864000
C	4.94737600	0.99226500	3.71679100
C	-2.87127000	2.53072600	-2.32090400
C	-1.45409600	2.52225900	-2.36959400
C	-0.70554100	3.04177800	-1.26493600
C	-1.39001700	3.58536600	-0.12980400

C	-2.80819900	3.62315400	-0.11831900
C	-3.50613700	3.08840500	-1.20598300
C	-0.73144400	2.04204400	-3.51331800
C	0.62815100	2.02962100	-3.54816400
C	1.41573200	2.49552300	-2.44238000
C	0.73204200	3.03039000	-1.30270800
C	1.48206600	3.56018500	-0.20500700
C	0.75936000	4.04882100	0.93393600
C	-0.60044600	4.08056800	0.96171300
C	2.83313600	2.47094300	-2.46014300
C	3.53329400	3.01457000	-1.37814600
C	2.89965100	3.57747100	-0.26651200
C	-3.56845400	4.22609700	1.02513100
C	-3.69526500	1.94638000	-3.42774800
C	3.59597400	1.87469000	-3.60190100
C	3.72750700	4.14845900	0.84121800
C	-3.52274400	3.62191600	2.28891900
C	-4.17906200	4.16184800	3.40139800
C	-4.93115000	5.32292700	3.22131400
C	-4.99380200	5.93406800	1.96965000
C	-4.31532600	5.41727700	0.86066000
C	-4.54090600	2.75196000	-4.22531700
C	-5.28828600	2.13277900	-5.23354900
C	-5.20693100	0.76239400	-5.47123000
C	-4.35734900	-0.03796900	-4.70472100
C	-3.61879400	0.56769300	-3.68297500
C	3.47331800	0.50084800	-3.86122900
C	4.16290500	-0.11895600	-4.90798600
C	5.00940400	0.66291800	-5.69660900
C	5.13567400	2.02981600	-5.45442900
C	4.43808400	2.66347100	-4.41983000
C	3.65526200	5.51499300	1.20363800
C	4.40278000	5.94418100	2.30595300
C	5.21848100	5.07320800	3.02400800
C	5.36688900	3.73960900	2.62848000
C	4.61664400	3.30386500	1.52675000
C	-4.01562600	3.53354600	4.77929000
N	-4.57429700	2.18526900	4.84421600
C	-4.19521400	-1.51333000	-5.03564300
N	-4.06076600	-2.34477000	-3.85199200
C	3.94971600	-1.58857400	-5.23506600
N	3.79096900	-2.41084300	-4.04747300
C	6.39590300	2.87102900	3.34003800
N	6.07641100	1.55378100	3.88641200

H	-4.68692100	-3.75777500	1.79139800
H	-1.40223400	-5.59419900	-1.16869000
H	1.04303600	-5.60241500	-1.23460600
H	1.22015600	-2.43770300	4.78676300
H	-1.22259700	-2.44383200	4.86355400
H	4.49610700	-3.82488400	1.57700800
H	-2.42363000	-0.71669600	3.53792500
H	-5.99067100	0.04529700	5.79076900
H	-6.60788900	-2.36774800	5.60113600
H	-5.16936000	-3.92251900	4.31914100
H	-4.59248700	-6.68497900	0.46385900
H	-6.06882800	-7.21516300	-1.45930600
H	-6.14937200	-5.69841500	-3.42440200
H	-3.23350000	-3.15098700	-1.57776700
H	2.98466600	-3.17105900	-1.73525700
H	5.70430700	-5.86686900	-3.67025600
H	5.59491800	-7.38648900	-1.70856400
H	4.20497500	-6.78323300	0.25685600
H	4.26935100	-4.18782800	4.91860300
H	5.86275000	-2.82718900	6.24861500
H	6.20829800	-0.41719300	5.70157200
H	3.18957000	-0.69808500	2.66585600
H	-2.66439700	1.39733000	4.61660500
H	-5.46873700	-3.69482800	-4.57088100
H	5.12009800	-3.82835700	-4.78479600
H	4.11405100	1.46121600	3.17741500
H	-4.59210600	3.08324300	-1.17194000
H	-1.29395500	1.69202900	-4.37125100
H	1.13976600	1.66914300	-4.43329300
H	1.32061900	4.40243900	1.79196200
H	-1.10885000	4.47899900	1.83195500
H	4.61951200	3.00288100	-1.40270600
H	-2.94449600	2.70828000	2.40160900
H	-5.45737800	5.76331300	4.06503100
H	-5.56992900	6.84934700	1.85313200
H	-5.94227200	2.74263900	-5.85312400
H	-5.79971600	0.31733100	-6.26764600
H	-2.97265500	-0.04996900	-3.06678600
H	2.83159100	-0.10304800	-3.22727100
H	5.56584300	0.20694400	-6.51290400
H	5.78717200	2.62475000	-6.09084500
H	4.35220200	6.99048100	2.59950500
H	5.77831900	5.44570400	3.87913800
H	4.71102500	2.27817000	1.18089100

H	-2.94361000	3.53521600	5.04422800
H	-4.53595900	4.15313500	5.51805500
H	-5.02259800	-1.83996300	-5.68959300
H	-3.26841000	-1.63789600	-5.61778600
H	3.01694800	-1.68253900	-5.81360200
H	4.76249600	-1.94609900	-5.89115600
H	7.24176300	2.69292000	2.65811900
H	6.82340800	3.45016800	4.16890700
C	-4.37402300	6.15532300	-0.45774400
H	-3.38837200	6.21651900	-0.93070500
H	-5.03946900	5.66194500	-1.17632300
H	-4.74786100	7.17395500	-0.31271600
C	-4.64632600	4.24923200	-4.03973400
H	-5.33294000	4.51389600	-3.22546900
H	-3.67820300	4.69862600	-3.79847100
H	-5.02720700	4.72423200	-4.94978700
C	2.83932600	6.52055600	0.42170600
H	2.89259900	6.32778500	-0.65463400
H	1.77741300	6.49886500	0.69394200
H	3.20700100	7.53517600	0.60605000
C	4.58471100	4.15712600	-4.22690200
H	3.61954600	4.63543400	-4.03029900
H	5.23816300	4.40383400	-3.38092100
H	5.01901600	4.61912900	-5.11937400

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C	-2.95445800	-2.84471900	-3.19584700
C	-2.98651500	-1.43057100	-3.23164300
C	-1.84328400	-0.71824200	-3.71918200
C	-0.68703900	-1.43439400	-4.16917200
C	-0.65734000	-2.84853200	-4.06513300
C	-1.80293100	-3.51298300	-3.61329400
C	-4.13152100	-0.68061200	-2.80319800
C	-4.13151300	0.68046700	-2.80324000
C	-2.98649800	1.43038600	-3.23173100
C	-1.84327500	0.71801500	-3.71922400
C	-0.68702100	1.43412700	-4.16925500
C	0.39250700	0.68027600	-4.73966500
C	0.39249800	-0.68059000	-4.73962600
C	-2.95442400	2.84453500	-3.19601700
C	-1.80288800	3.51276100	-3.61349800
C	-0.65730500	2.84827000	-4.06529700
C	0.57129100	-3.66086300	-4.27938300
C	-4.06502800	-3.67342000	-2.63643500

C	-4.06498900	3.67328000	-2.63665800
C	0.57133500	3.66057500	-4.27959800
C	1.78567100	-3.28769500	-3.68191700
C	2.90592100	-4.12593500	-3.70705200
C	2.82894900	-5.36051500	-4.36846100
C	1.64566400	-5.72500100	-5.00517100
C	0.52666500	-4.88980100	-4.95910200
C	-4.78068300	-4.55965600	-3.46088900
C	-5.73506500	-5.42082000	-2.92013600
C	-5.97343000	-5.42488600	-1.54640500
C	-5.27209300	-4.54857700	-0.70698300
C	-4.33207900	-3.66810000	-1.26409800
C	-4.33202900	3.66806200	-1.26431800
C	-5.27204200	4.54857600	-0.70726100
C	-5.97338500	5.42482400	-1.54674200
C	-5.73503100	5.42065700	-2.92047400
C	-4.78065200	4.55945300	-3.46117200
C	0.52672000	4.88946800	-4.95940000
C	1.64572600	5.72465600	-5.00552400
C	2.82900600	5.36020400	-4.36878700
C	2.90596700	4.12566800	-3.70729300
C	1.78571000	3.28743800	-3.68210300
C	4.12456200	-3.68570600	-3.00299700
C	-5.48839200	-4.60232600	0.75060100
C	-5.48833800	4.60242200	0.75032000
C	4.12460200	3.68548200	-3.00320200
C	-1.13269900	1.22926600	4.04217300
C	0.17212100	1.24069900	3.49487700
C	0.84037800	0.00009300	3.23988800
C	0.17210400	-1.24048900	3.49494200
C	-1.13271400	-1.22900900	4.04223900
C	-1.74742000	0.00013900	4.29696500
C	0.83479800	2.45990600	3.12901100
C	2.09407600	2.46037800	2.61299500
C	2.82617200	1.24150600	2.41304000
C	2.17107500	0.00006900	2.69900500
C	2.82616400	-1.24139000	2.41311300
C	2.09404400	-2.46023900	2.61312400
C	0.83476600	-2.45972400	3.12914000
C	4.14102900	1.22979500	1.88767500
C	4.75901700	0.00003100	1.64086200
C	4.14102800	-1.22971700	1.88775600
C	-1.92162700	-2.47038000	4.31748600
C	-1.92159700	2.47066200	4.31734200

C	4.87311400	2.47478600	1.49631600
C	4.87312400	-2.47472700	1.49647700
C	-3.08016600	-2.68642200	3.56057600
C	-3.92408900	-3.77783600	3.78870300
C	-3.57995600	-4.67878700	4.79655100
C	-2.43365800	-4.47066600	5.56577400
C	-1.59164200	-3.37296900	5.35614600
C	-1.59159500	3.37332700	5.35593100
C	-2.43359400	4.47105100	5.56547900
C	-3.57989500	4.67912800	4.79624700
C	-3.92404700	3.77810300	3.78847300
C	-3.08014000	2.68666000	3.56042600
C	5.16283200	2.64975600	0.13670400
C	5.86517400	3.75708900	-0.34795200
C	6.28642300	4.71826000	0.57275700
C	6.02664400	4.54926300	1.93333300
C	5.33239600	3.43663500	2.42546000
C	5.33246600	-3.43649700	2.42567700
C	6.02671900	-4.54914500	1.93360500
C	6.28645300	-4.71823900	0.57303200
C	5.86516100	-3.75713800	-0.34773000
C	5.16281300	-2.64978400	0.13687100
C	-5.20213100	-3.93580000	2.98261800
N	-4.95582900	-3.77379600	1.55718200
C	-5.20209000	3.93602200	2.98237900
N	-4.95578600	3.77393400	1.55695200
C	6.13873200	3.88414100	-1.83823400
N	5.00805800	4.48785600	-2.55705900
C	6.13868400	-3.88428200	-1.83801100
N	5.00799700	-4.48805400	-2.55676600
H	-1.76782600	-4.59287000	-3.50447300
H	-5.01158600	-1.22203200	-2.47291700
H	-5.01157300	1.22191600	-2.47299400
H	1.21572700	1.21670400	-5.19867600
H	1.21571100	-1.21705600	-5.19860700
H	-1.76777100	4.59265400	-3.50474200
H	1.84100200	-2.35218200	-3.13199200
H	3.69863400	-6.00969200	-4.37664700
H	1.58731200	-6.67000500	-5.53880800
H	-0.39248200	-5.19107100	-5.45428200
H	-4.57902000	-4.57155800	-4.52867200
H	-6.28336400	-6.09797000	-3.56944900
H	-6.70014600	-6.11251700	-1.11930500
H	-3.78181600	-3.01036400	-0.59907400

H	-3.78176200	3.01037400	-0.59925000
H	-6.70009900	6.11248500	-1.11968800
H	-6.28333400	6.09775900	-3.56983300
H	-4.57899900	4.57127600	-4.52895800
H	-0.39242400	5.19071200	-5.45459900
H	1.58738200	6.66962400	-5.53922500
H	3.69869700	6.00937200	-4.37701400
H	1.84103200	2.35196200	-3.13211400
H	4.20520300	-2.59398800	-2.86469800
H	-6.13373600	-5.42547800	1.10275400
H	-6.13367500	5.42560100	1.10242300
H	4.20521600	2.59377700	-2.86478800
H	-2.74863600	0.00015700	4.71802300
H	0.29579500	3.39477000	3.24497600
H	2.55685400	3.39602800	2.31653100
H	2.55680400	-3.39591200	2.31670700
H	0.29575100	-3.39457400	3.24515500
H	5.76774200	0.00001700	1.23727200
H	-3.32577600	-1.99138100	2.76319400
H	-4.21212800	-5.54209200	4.99356200
H	-2.19274400	-5.17285000	6.36091300
H	-2.19266500	5.17329400	6.36056100
H	-4.21205300	5.54245800	4.99319500
H	-3.32576400	1.99156100	2.76309700
H	4.82223500	1.88805500	-0.56061900
H	6.83138200	5.59477300	0.23043800
H	6.38816600	5.29393300	2.63899200
H	6.38829200	-5.29375100	2.63930600
H	6.83142100	-5.59476300	0.23075800
H	4.82218200	-1.88813900	-0.56049700
H	-5.68660100	-4.89767700	3.22266400
H	-5.90562800	-3.14301100	3.28067700
H	-5.90558700	3.14325000	3.28048300
H	-5.68655900	4.89791400	3.22236800
H	7.01451000	4.52148700	-2.00025300
H	6.37431700	2.88608200	-2.24095600
H	6.37424500	-2.88624400	-2.24080100
H	7.01446600	-4.52162600	-2.00001300
C	-0.39439900	3.15670800	6.25360100
H	-0.36614000	2.13145500	6.63991600
H	0.55290000	3.31936200	5.72586100
H	-0.42172600	3.84073800	7.10760300
C	5.13319700	3.26804900	3.91458700
H	4.09072100	3.43107700	4.21314200

H	5.39757500	2.25550000	4.23937600
H	5.75354900	3.97741500	4.47123900
C	-0.39444400	-3.15630000	6.25380000
H	0.55285100	-3.31905100	5.72608200
H	-0.36614500	-2.13100500	6.64000100
H	-0.42180200	-3.84023400	7.10787700
C	5.13337800	-3.26779100	3.91480600
H	5.39774000	-2.25520300	4.23948800
H	4.09093800	-3.43084100	4.21346600
H	5.75381000	-3.97708000	4.47146700

Molecular fragment of free **4a**

C	-0.20951000	1.39760500	-0.00257800
C	-1.29436700	0.50992600	-0.04267400
C	-1.10385300	-0.87928900	-0.04151400
C	0.20678500	-1.37544100	-0.00086500
C	1.31402900	-0.51633400	0.03828600
C	1.08815100	0.86761200	0.03770300
H	-2.30143700	0.90672200	-0.12769900
H	0.36777700	-2.44921300	0.00039800
H	1.93425000	1.54270500	0.12266400
C	-2.26504200	-1.80579800	-0.09979300
C	-2.21281100	-2.98490900	-0.86219900
C	-3.44570400	-1.52704200	0.60919900
C	-3.30119600	-3.85471100	-0.91257800
H	-1.32019400	-3.20723300	-1.44033500
C	-4.53491200	-2.39564900	0.55845000
H	-3.49923400	-0.63362200	1.22524500
C	-4.46746200	-3.56417900	-0.20242300
H	-5.43489200	-2.16308300	1.12184300
H	-5.31604000	-4.24182100	-0.24200700
C	-0.43055800	2.86744400	-0.00120100
C	0.42398400	3.72799400	-0.71081400
C	-1.50040200	3.43619100	0.71040500
C	0.21730500	5.10666100	-0.70849600
H	1.24246600	3.30862700	-1.28935900
C	-1.70900000	4.81455300	0.71209600
H	-2.15870300	2.79265400	1.28750400
C	-0.85062300	5.65658800	0.00288200
H	-2.53885500	5.23199900	1.27646600
H	-1.01235400	6.73113900	0.00448800
C	2.69598500	-1.06101900	0.09821300
C	3.74236600	-0.45231900	-0.61509100
C	2.99262000	-2.19880100	0.86741400

C	5.03853700	-0.96290000	-0.56210400
H	3.53101700	0.41379900	-1.23618400
C	4.28835000	-2.71067100	0.92016000
H	2.20497600	-2.66960000	1.44911600
C	5.31753900	-2.09503400	0.20559500
H	4.49555500	-3.58720100	1.52858900
H	6.32765200	-2.49355300	0.24683400

Molecular fragment of 4a within cage framework

N	0.51605700	5.01190000	-0.01698400
N	0.51018700	-4.22313600	-2.60318100
N	0.14140100	-2.57278600	4.23745700
C	4.19718000	1.41692000	-0.28957300
C	4.29862100	0.39274500	-1.23960300
H	4.40200200	0.64766600	-2.29077500
C	4.14022300	-0.95006000	-0.87086000
C	3.92967400	-1.26502300	0.47836600
H	3.80756500	-2.30384500	0.77236000
C	3.89681800	-0.26174400	1.45633200
C	4.02290800	1.07535100	1.05731700
H	3.94071900	1.86381600	1.80040700
C	4.11008400	2.83884300	-0.72369100
C	2.95223700	3.55740800	-0.41366400
H	2.15237200	3.08861700	0.14966500
C	2.76383900	4.86859400	-0.87108000
C	3.77695000	5.48092900	-1.62113600
H	3.64325100	6.49945700	-1.97917200
C	4.94432500	4.77894400	-1.92516100
H	5.72687300	5.25646500	-2.50866400
C	5.10732200	3.46267800	-1.49241200
C	1.48924600	5.56823600	-0.62144500
H	1.42029000	6.59632400	-1.01666300
C	-0.72821500	5.74790900	0.13771600
H	-0.68130300	6.75787300	-0.30553700
H	-0.89475000	5.87929100	1.21757800
C	-1.90184500	4.98376200	-0.45798500
C	-2.85106700	5.63695100	-1.24526000
H	-2.74615500	6.69969100	-1.45314200
C	-3.93995700	4.93602000	-1.76321400
H	-4.67906700	5.46701700	-2.35932200
C	-4.11186400	3.56652100	-1.53612600
C	-3.14608900	2.89342900	-0.75189100
C	-2.06799000	3.61480200	-0.21959200
H	-1.32199900	3.08890900	0.36863800

C	-5.32338000	2.86331200	-2.10766100
H	-5.07960900	2.28499000	-3.00774400
H	-6.09342000	3.58958600	-2.38756500
H	-5.76028500	2.16130000	-1.39003400
C	-3.24027700	1.42971500	-0.45723700
C	-3.31579000	0.98586900	0.87063400
H	-3.33546500	1.71987500	1.67105500
C	-3.34102400	-0.38082500	1.18247900
C	-3.28021000	-1.30652800	0.13252700
H	-3.30551000	-2.36812300	0.36137400
C	-3.20734100	-0.89787100	-1.20720800
C	-3.19390800	0.47633900	-1.48540300
H	-3.09385600	0.81148900	-2.51328000
C	-3.08363400	-1.92823200	-2.28213200
C	-2.05488900	-2.87442200	-2.16636500
H	-1.36610400	-2.80184800	-1.33029100
C	-1.86043000	-3.88420800	-3.11335300
C	-2.72972600	-3.94316900	-4.20318500
H	-2.60225200	-4.71364600	-4.96061700
C	-3.76799200	-3.01952400	-4.32367700
H	-4.44680300	-3.09200800	-5.17077800
C	-3.96837400	-2.00232600	-3.38376400
C	-5.12797100	-1.04764000	-3.56491900
H	-5.59672300	-0.79043000	-2.61014900
H	-5.89192600	-1.48924000	-4.21337700
H	-4.81561700	-0.10435600	-4.03171000
C	-0.73397600	-4.89316900	-2.94689200
H	-0.97855200	-5.57459100	-2.11833000
H	-0.64695500	-5.51029800	-3.85798100
C	1.53111600	-4.40581800	-3.34166900
H	1.50644800	-5.07995600	-4.21512000
C	2.80512500	-3.69803100	-3.11653000
C	3.88441700	-3.89821800	-3.98749000
H	3.79776900	-4.62092900	-4.79596600
C	5.05729600	-3.15903800	-3.83093800
H	5.89241600	-3.31645100	-4.50817600
C	5.15640400	-2.20830000	-2.81563300
C	4.08979800	-2.00388200	-1.92280100
C	2.92790900	-2.76387600	-2.07765000
H	2.07713800	-2.60480200	-1.42340400
C	3.67804700	-0.58914400	2.89239600
C	4.57153100	-0.13435300	3.87930200
C	4.34173500	-0.40971700	5.22618300
H	5.04596600	-0.06300500	5.97761000

C	3.20435000	-1.11969700	5.61064300
H	3.01095400	-1.31452200	6.66325800
C	2.29305700	-1.56588200	4.64435400
C	2.55030800	-1.31219500	3.28847600
H	1.82627800	-1.64785400	2.55322900
C	1.04026900	-2.21837600	5.06620100
H	0.91073800	-2.34303500	6.15509600
C	-1.11372800	-3.10003300	4.74948500
H	-1.11301300	-3.20878900	5.84805100
H	-1.24776800	-4.10590800	4.32477000
C	-2.27171300	-2.20954600	4.32252700
C	-3.28989300	-1.86628200	5.21281500
H	-3.26706200	-2.23664800	6.23555800
C	-4.34118500	-1.04889200	4.79650500
H	-5.13444400	-0.80495100	5.49998500
C	-4.40736000	-0.53032200	3.49836700
C	-3.37358000	-0.86749700	2.59432100
C	-2.33521800	-1.70688400	3.01969200
H	-1.53408100	-1.94473400	2.32713100
C	-5.57942100	0.34138500	3.10350400
H	-5.93293800	0.11228300	2.09304600
H	-5.32311600	1.40829600	3.11566500
H	-6.41421400	0.20086000	3.79794600
H	6.01339700	2.91589900	-1.74050200
H	5.45319100	0.42634400	3.58054500
H	6.06565400	-1.62354700	-2.70336500

Molecular fragment of free **4d**

C	-0.97434000	-1.01228500	0.00219100
C	0.39110000	-1.35931900	-0.03322300
C	1.36365800	-0.33874100	-0.04239000
C	0.98087400	1.01751100	-0.03398300
C	-0.38875100	1.34907200	0.00174800
C	-1.37167500	0.33976200	0.02679300
C	2.82054300	-0.70185600	-0.04682100
C	3.52172200	-0.87494600	-1.25044400
C	3.51451300	-0.87627200	1.15931300
C	4.87630800	-1.21148200	-1.24796600
H	2.99665000	-0.74278800	-2.19326000
C	4.86937700	-1.21298200	1.16446100
H	2.98480500	-0.74478500	2.09948200
C	5.55479900	-1.38133900	-0.03952000
H	5.40171600	-1.34064700	-2.19085600
H	6.60963100	-1.64300700	-0.03676800

C	-2.01675000	-2.09188100	0.01626200
C	-2.34531200	-2.76156200	1.20465000
C	-2.68855600	-2.45557600	-1.16062400
C	-3.31745100	-3.76309400	1.21754600
H	-1.83533400	-2.48890800	2.12522300
C	-3.65817100	-3.45960500	-1.15133400
H	-2.44322700	-1.94713000	-2.08969100
C	-3.97656100	-4.11621500	0.03869600
H	-4.16524100	-3.72830900	-2.07463200
H	-4.73243400	-4.89707300	0.04742200
C	-0.80184800	2.79174600	0.01557100
C	-1.22747500	3.42891400	-1.15982800
C	-0.77175700	3.53737400	1.20376900
C	-1.60975200	4.77136100	-1.14926100
H	-1.25482000	2.86427600	-2.08844800
C	-1.15742300	4.87869600	1.21796700
H	-0.44759400	3.05649600	2.12329100
C	-1.57691100	5.50056700	0.04062700
H	-1.93414000	5.24703000	-2.07137500
H	-1.87598000	6.54537100	0.05045800
C	0.80899000	-2.81687900	-0.04731700
H	1.77036600	-2.95321700	-0.54698000
H	0.92039700	-3.21040600	0.97210300
H	0.06582900	-3.44024900	-0.54982100
C	2.02806400	2.11397800	-0.05071500
H	2.26863600	2.45269300	0.96599000
H	2.96093800	1.77180900	-0.50271300
H	1.67738600	2.99039400	-0.60140900
C	-2.84283100	0.70298800	0.08373600
H	-2.99635500	1.66773200	0.57236100
H	-3.27867400	0.77968900	-0.92135300
H	-3.41864700	-0.05358100	0.62200400

Molecular fragment of 4d within cage framework

N	-0.10337700	1.99567400	4.56576900
N	-0.09567000	-4.95251900	-0.55863600
N	-0.09082800	2.96678300	-4.00186900
C	-3.87506700	0.65592800	-1.24528100
C	-3.88197300	1.41198300	-0.05272000
C	-3.88169200	0.74472400	1.18543300
C	-3.88572500	-0.66599100	1.24414600
C	-3.87873400	-1.40444300	0.04726400
C	-3.87717400	-0.74994700	-1.20391200
C	-3.84304300	-1.57397800	-2.47607600

H	-4.56000200	-2.40010500	-2.43230700
H	-2.85501800	-2.02615400	-2.62889500
H	-4.06761800	-0.97182400	-3.35714700
C	-3.85301100	2.92601800	-0.12680100
H	-2.85051900	3.29160000	-0.38379900
H	-4.13364800	3.38492900	0.82208100
H	-4.52938800	3.29816700	-0.90234600
C	-3.86105900	-1.35747900	2.59314600
H	-2.86425600	-1.30175700	3.04886700
H	-4.12558800	-2.41266100	2.51424300
H	-4.55215700	-0.88119300	3.29549800
C	-3.80459500	1.52671700	2.46487400
C	-2.57008600	1.70457100	3.09355800
H	-1.66972600	1.27841400	2.66251100
C	-2.45621100	2.44245600	4.28195700
C	-3.60475900	3.01508400	4.84416700
H	-3.52454500	3.59485200	5.76120600
C	-4.84628900	2.83485600	4.23447900
H	-5.73711300	3.27318900	4.67651200
C	-4.94704600	2.09483900	3.05594400
H	-5.91488700	1.96046700	2.57943300
C	-1.14752500	2.62231200	4.93745000
H	-1.13064000	3.33564700	5.77954200
C	1.14598000	2.23839200	5.27011800
H	1.35578300	1.33917400	5.87015600
H	1.07832100	3.08307900	5.97734900
C	2.29723200	2.46059200	4.30330500
C	3.24256800	3.46323700	4.52301300
H	3.14790400	4.12126000	5.38434600
C	4.31530300	3.62173400	3.64555100
H	5.05248200	4.39722500	3.84256800
C	4.47603100	2.80899100	2.51785000
C	3.51274200	1.80039000	2.28130000
C	2.45050500	1.64043700	3.18173800
H	1.70380200	0.87701600	2.98615600
C	5.67434000	3.01796300	1.61748900
H	5.42560700	3.61093200	0.72823100
H	6.08435000	2.06820200	1.25997100
H	6.46654800	3.55327900	2.15128500
C	3.58122900	0.88095900	1.10595600
C	3.58263500	1.37385700	-0.20656100
H	3.56187900	2.44648600	-0.37528800
C	3.58416300	0.51194300	-1.31203600
C	3.58455500	-0.87119000	-1.08230900

H	3.56512400	-1.55437800	-1.92625800
C	3.58314700	-1.39731600	0.21692200
C	3.58167600	-0.50722300	1.30018000
H	3.56085800	-0.89700300	2.31361300
C	3.51625900	-2.87511000	0.42444700
C	4.47895500	-3.58452500	1.18019200
C	4.32004400	-4.96811400	1.31640000
H	5.05693800	-5.52694700	1.88942600
C	3.24921200	-5.64876300	0.73682700
H	3.15590000	-6.72410500	0.87362500
C	2.30399100	-4.95687000	-0.02137700
C	2.45590600	-3.57497800	-0.16767000
H	1.70970500	-3.02328400	-0.73108500
C	5.67403200	-2.90838500	1.81663600
H	6.08495800	-2.12224800	1.17553100
H	6.46664900	-3.63731600	2.01523400
H	5.42075000	-2.43650900	2.77450300
C	1.15426400	-5.68311400	-0.69958500
H	1.36552000	-5.75216500	-1.77814800
H	1.08621700	-6.71831200	-0.32263800
C	-1.13955000	-5.58893300	-0.20314800
H	-1.12153500	-6.67494400	-0.00694000
C	-2.44907800	-4.93296000	-0.03196300
C	-3.59663400	-5.70771400	0.18292700
H	-3.51496800	-6.79166700	0.22644300
C	-4.83896500	-5.09126500	0.33146000
H	-5.72905400	-5.69437700	0.48981800
C	-4.94145800	-3.70066100	0.28021800
H	-5.90993500	-3.22223700	0.40257600
C	-3.80000700	-2.90325900	0.08390200
C	-2.56474500	-3.53504300	-0.07709500
H	-1.66537100	-2.94743700	-0.23183200
C	-3.79404800	1.37382600	-2.56142600
C	-4.93354900	1.59697700	-3.35447500
H	-5.90169700	1.24724700	-3.00492600
C	-4.82959900	2.24859300	-4.58390400
H	-5.71821900	2.40866600	-5.18873400
C	-3.58770800	2.69164600	-5.03882100
H	-3.50487100	3.19637400	-5.99899400
C	-2.44211800	2.49544900	-4.25633300
C	-2.55929400	1.83502200	-3.02345000
H	-1.66143500	1.67912300	-2.43384100
C	-1.13257900	2.97666800	-4.73382900
H	-1.11220300	3.35217800	-5.77152300

C	1.16001800	3.45750400	-4.55929100
H	1.37056400	4.42339900	-4.07419600
H	1.09379100	3.65446300	-5.64333100
C	2.30892900	2.50510700	-4.27228900
C	3.25337000	2.19499900	-5.25134300
H	3.16102300	2.61683900	-6.24997200
C	4.32190000	1.34908100	-4.95353600
H	5.05781100	1.13142500	-5.72469200
C	4.47924800	0.77154900	-3.68867900
C	3.51806800	1.07212800	-2.69518100
C	2.45948000	1.93749900	-3.00375700
H	1.71320000	2.14963700	-2.24433100
C	5.67063900	-0.12341200	-3.42449000
H	5.41077100	-1.18751200	-3.49080100
H	6.08743200	0.03872700	-2.42544300
H	6.46102300	0.06241100	-4.15919800

Molecular fragment of free 4c

C	0.94364800	-1.06066000	-0.16754200
C	1.27396400	0.29938400	-0.24557800
C	0.28302000	1.29148800	-0.26068800
C	-1.06090800	0.89876800	-0.18204300
C	-1.42584700	-0.45137400	-0.09200500
C	-0.41063700	-1.41854300	-0.09452100
H	2.31562600	0.58782700	-0.34620200
H	-1.83353300	1.66146800	-0.20310900
H	-0.67771700	-2.46852000	-0.01290500
C	0.62395500	2.73582300	-0.42828700
C	0.03229700	3.43766400	-1.49181200
C	1.49865800	3.42247100	0.44505000
C	0.29936000	4.78665000	-1.71423200
H	-0.63493000	2.90221800	-2.16204600
C	1.75168700	4.78013400	0.20722700
C	1.16895900	5.46242900	-0.85948000
H	2.41464600	5.31402700	0.88472800
H	1.38781700	6.51553300	-1.01542800
C	1.99073100	-2.12427400	-0.21975800
C	1.89484400	-3.09986800	-1.22578600
C	3.05585300	-2.19622500	0.70720700
C	2.83232400	-4.12381900	-1.34113200
H	1.07507400	-3.03634400	-1.93652600
C	3.98638100	-3.23591900	0.57766000
C	3.88855900	-4.19021200	-0.43374000
H	4.79998400	-3.30094700	1.29694700

H	4.62824000	-4.98327000	-0.50565100
C	-2.85756000	-0.86981300	-0.03431200
C	-3.32276700	-1.78512500	-0.99291000
C	-3.75165200	-0.39438700	0.95311400
C	-4.64574500	-2.22106000	-1.00404100
H	-2.63016700	-2.14356900	-1.74996400
C	-5.07728400	-0.84810200	0.92749700
C	-5.53105600	-1.74549100	-0.03779700
H	-5.76478400	-0.49427700	1.69278700
H	-6.56644100	-2.07586700	-0.02842600
C	-3.32380900	0.55600300	2.05109500
H	-2.30819700	0.34554900	2.39962600
H	-3.33688100	1.60224600	1.72011800
H	-4.00178700	0.48075500	2.90752100
C	2.14461200	2.75540500	1.64020100
H	1.47227800	2.03749300	2.11962500
H	3.05384400	2.20623900	1.36353100
H	2.43512900	3.50278700	2.38572500
C	3.20822200	-1.21319900	1.84764100
H	3.69786300	-0.28430300	1.52827400
H	2.24104700	-0.93245300	2.27574000
H	3.82312200	-1.64303500	2.64507100

Molecular fragment of 4c within cage framework

N	0.03525300	4.95819600	-0.16130500
N	0.06134000	-4.22590100	-2.55002000
N	-0.05656200	-2.34700200	4.31959900
C	3.79022500	1.39121300	-0.39362200
C	3.83683100	0.36150200	-1.34283700
H	3.84436900	0.61169400	-2.40038700
C	3.79022500	-0.98393100	-0.95648400
C	3.71978000	-1.29298400	0.40905600
H	3.67309900	-2.33332300	0.71928500
C	3.70161400	-0.28372100	1.38090100
C	3.73198800	1.05414200	0.96474000
H	3.67596700	1.84736300	1.70538200
C	3.69122600	2.82093000	-0.82084500
C	2.49408600	3.49576000	-0.57445700
H	1.67441800	2.98309200	-0.08139800
C	2.30166500	4.82493600	-0.97812200
C	3.35157000	5.48563600	-1.62543800
H	3.22595000	6.51759000	-1.94640300
C	4.55709600	4.82662100	-1.85787200
H	5.36952500	5.35651900	-2.34972500

C	4.75198500	3.49497200	-1.47236000
C	6.07673300	2.81879400	-1.74084700
H	6.42167900	2.24900400	-0.87150300
H	6.84522700	3.55525300	-1.99600600
H	6.01143300	2.11044900	-2.57664300
C	1.01725500	5.51039300	-0.75553100
H	0.95375800	6.53910500	-1.15075300
C	-1.20318800	5.70809800	-0.02023600
H	-1.15207600	6.70406100	-0.49385500
H	-1.36006700	5.87415100	1.05648200
C	-2.38628800	4.93425800	-0.58016900
C	-3.34099000	5.56075900	-1.38227900
H	-3.23575600	6.61479400	-1.63052400
C	-4.43573300	4.84297900	-1.86408700
H	-5.17916700	5.35296900	-2.47308800
C	-4.60879500	3.48305100	-1.58483500
C	-3.63778900	2.83811200	-0.78384800
C	-2.55369600	3.57662200	-0.28974000
H	-1.80216000	3.07164500	0.30945100
C	-5.82628700	2.76239100	-2.12090700
H	-5.59509300	2.16912700	-3.01482800
H	-6.60546100	3.47885700	-2.40101900
H	-6.24630900	2.07150100	-1.38289800
C	-3.72091400	1.38857400	-0.42890600
C	-3.73274300	0.99992500	0.91808100
H	-3.72541100	1.76674200	1.68725000
C	-3.72460800	-0.35179200	1.28818500
C	-3.69710300	-1.32130400	0.27665000
H	-3.69284500	-2.37268900	0.55021100
C	-3.69148200	-0.96736000	-1.08066500
C	-3.70932600	0.39341500	-1.41688100
H	-3.65617800	0.68489000	-2.46148600
C	-3.59439600	-2.03368200	-2.12234200
C	-2.52330300	-2.93466300	-2.04029100
H	-1.78965600	-2.80965100	-1.24976400
C	-2.34487600	-3.96490500	-2.96802200
C	-3.27404100	-4.09134800	-4.00141400
H	-3.16025500	-4.87992600	-4.74227500
C	-4.35477800	-3.21363000	-4.08564800
H	-5.07931100	-3.33897300	-4.88756800
C	-4.53995100	-2.17653700	-3.16465400
C	-5.74565600	-1.27272000	-3.29982100
H	-6.16556100	-1.00662500	-2.32493100
H	-6.52907100	-1.76206600	-3.88799000

H	-5.50065300	-0.33162300	-3.80909300
C	-1.17847100	-4.93098300	-2.83555200
H	-1.36889300	-5.60768500	-1.98853200
H	-1.10987500	-5.56096900	-3.73952600
C	1.07200200	-4.44513600	-3.29343400
H	1.03236800	-5.16150900	-4.13234500
C	2.36069200	-3.75649500	-3.10976900
C	3.44984300	-4.06835600	-3.93056000
H	3.35030400	-4.83806000	-4.69305500
C	4.66138100	-3.39807100	-3.77292000
H	5.50387800	-3.66020700	-4.40864800
C	4.82298200	-2.39148500	-2.81382700
C	3.72137100	-2.06759400	-1.98547900
C	2.51857800	-2.75899700	-2.13604500
H	1.66849000	-2.51171900	-1.50841500
C	6.15406800	-1.69037300	-2.67058100
H	6.92701300	-2.19846700	-3.25552700
H	6.48065900	-1.65877900	-1.62515200
H	6.10748400	-0.65017700	-3.01596100
C	3.57819900	-0.62779600	2.83105300
C	4.62453300	-0.37774900	3.75218200
C	4.42043500	-0.70751400	5.09699900
H	5.22103600	-0.52738100	5.81062200
C	3.22011300	-1.25978600	5.53927700
H	3.08607700	-1.49536000	6.59296300
C	2.18630600	-1.51507900	4.63204000
C	2.38736100	-1.20075300	3.27955700
H	1.57960200	-1.39085800	2.58011200
C	5.94495700	0.21225900	3.31305100
H	5.85178000	1.27273300	3.04905200
H	6.33779000	-0.29856400	2.42691600
H	6.68964000	0.13482300	4.11133200
C	0.90794700	-2.07228900	5.10454600
H	0.83160600	-2.22538500	6.19507100
C	-1.29672300	-2.84934900	4.88986000
H	-1.25949100	-2.92057900	5.99097700
H	-1.44008400	-3.87152300	4.50774900
C	-2.47818000	-1.98951800	4.46936700
C	-3.46231300	-1.61510100	5.38490300
H	-3.38623100	-1.92829500	6.42407100
C	-4.54838400	-0.84229500	4.97309600
H	-5.31436200	-0.57370600	5.69754000
C	-4.68397600	-0.40089200	3.65229300
C	-3.68394200	-0.76799200	2.72211700

C	-2.60916100	-1.56148500	3.14502400
H	-1.83452100	-1.82330800	2.43093100
C	-5.89223800	0.42274500	3.26288200
H	-6.28693900	0.12662500	2.28560700
H	-5.65970600	1.49326200	3.19973600
H	-6.69050500	0.30758300	4.00343500

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