Multi-stack porphyrin oligomer with three cleft-like cavities for efficient guest encapsulations

Rabban Rabban, [a] Dhanyashree Das, [a] Dhrubajyoti Talukdar [a] and Bappaditya Gole*[a]

[a]*Biomimetic Supramolecular Chemistry Laboratory, Department of Chemistry, School of Natural Sciences, Shiv Nadar Institution of Eminence Deemed to be University, Greater Noida, Uttar Pradesh 201314, India. Email: bappaditya.gole@snu.edu.in*

Electronic Supplementary Information

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1. Materials and Methods

1.1. General Information

All Solvents and chemicals were purchased from Finar, Rankem, Sigma-Aldrich, TCI Chemicals, Alfa-Aesar or BLD Chemicals and were used without further purification. Tetrahydrofuran (THF), dichloromethane (CH_2Cl_2), and Methanol (MeOH) were dried over MBRAUN SPS-800 solvent purification system; chloroform ($CHCl_3$), ethylacetate (EtOAc) and diisopropylethylamine (DIPEA) were distilled over P_2O_5 and calcium hydride (CaH_2) respectively prior to use. Anhydrous DMF was purchased from Sigma Aldrich and used without further purification. Reactions were monitored by thin layer chromatography (TLC) on Merck silica gel 60-F254 plates and observed under UV light. Column chromatography purifications were performed using silica gel (100-200 mess). Size exclusion preparative recycling gel permeation chromatography (GPC) was performed on the Japan Analytical Industry (JAI) LaboACE LC-5060 instrument using JAIGEL-2HR and JAIGEL-2.5HR columns at a flow rate of 7 mL/min with a mobile phase composed of 1% (vol/vol) ethanol and 0.5% (vol/vol) Et_3N in chloroform. Monitoring was carried out by UV detector at 254 nm, 300 nm, 400 nm, and 500 nm.

1.2. Nuclear Magnetic Resonance

NMR spectra were recorded on a Bruker Avance III HD 400 NMR spectrometer operating at 400 MHz for ^1H spectra and 100 MHz for ^{13}C spectra. Chemical shifts are reported in parts per million (ppm, δ) relative to the ^1H residual signal of the deuterated solvent used. ^1H NMR splitting patterns with observed first-order coupling are designated as singlet (s), doublet (d), triplet (t), or quartet (q). Coupling constants (*J*) are reported in hertz. Samples were not degassed; otherwise, it is specified. Data processing was performed with Topspin 3.6.4 software.

1.3. Mass Spectrometry

High-resolution ESI mass spectra (HR-MS) were recorded using Agilent 6540 UHD Accurate-Mass Q-TOF LC/MS system under the following operation parameters: temperature 350 °C, dry nitrogen gas flow rate 10 L/min, nebulizer pressure 30 psi, Vcap 4000 and fragmentor voltage 100 V. Mass spectra were acquired either in the positive ion mode or in negative ion mode. Accurate mass analysis calibration was carried out by ESI-low concentration tuning mix solution provided by Agilent technologies, U.S.A. The accuracy error threshold was set at 5 ppm.

MALDI-TOF mass spectra were recorded using Bruker Autoflex maX MALDI TOF/TOF instrument. The matrix used was α-Cyano-4-hydroxycinnamic acid (CHCA).

1.4 Spectroscopic studies

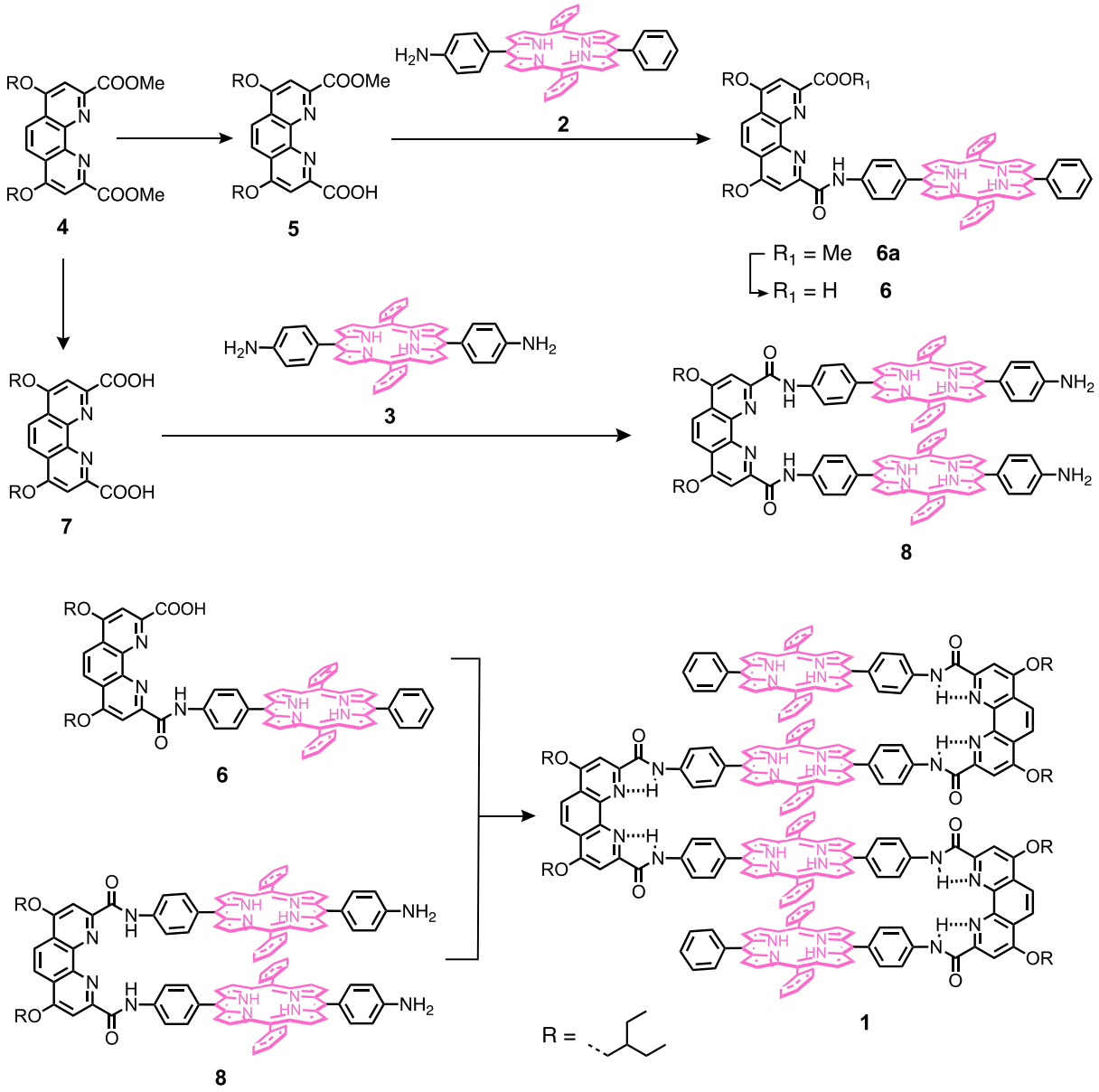
Electronic absorption spectra were measured on JASCO V-750 UV-Vis spectrophotometer. Variable temperature UV-Vis was carried out using Peltier temperature control. Steady-state emission spectra were recorded on an Edinburgh Instruments spectrophotometer equipped with standard cuvette holder SC-05 (Model: FS5) fitted with a PMT-900 detector and excited with a 150W CW Ozone-free xenon arc lamp. All solvents used were spectroscopic grade.

1.5 Computational Methods and Details

The geometry optimizations of **1** was performed by using hybrid DFT functional, B3LYP as implemented in the Gaussian 16 Rev. C02 program, with 6-31G basis set.[1] The optimized ground state structure of **1** is given below. Frequency calculations are done to estimate the ground state of these monomeric units. The absence of negative frequencies indicates minimum energy structures for these molecules.

To geometry optimize the host-guest complexes **1⊃G1**, **1⊃G1**$_2$, and **1⊃G1**$_3$, one, two, and three guest (G1) were introduced inside the cleft of the optimized structure **1**, respectively. Subsequently, the geometry optimizations were performed as before. Again, frequency calculations are performed to ascertain the minimum energy structures for these molecules.

2. Synthetic Procedures

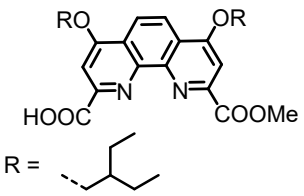


Scheme 1. Synthetic scheme of the tetraporphyrin oligomer, **1**.

5,15-di(4-aminophenyl)-10,20-diphenyl porphyrin (3): 5,15-di(4-aminophenyl)-10,20-diphenyl porphyrin was synthesized according to the modified literature.[2] In a 1 L round bottom flask, 2,2'-(phenylmethylene)bis(1H-pyrrole)[3] (2 g, 9 mmol, 1 eq) and 4-nitrobenzaldehyde (1.35 g, 9 mmol, 1 eq) was dissolved in 750 mL chloroform. The solution was then purged with N_2 for 15 min, and the flask was covered with aluminum foil to shield it from ambient light. TFA (1 mL) was then added and stirred for 3 hours at room temperature. To the mixture, *p*-chloranil (3.04

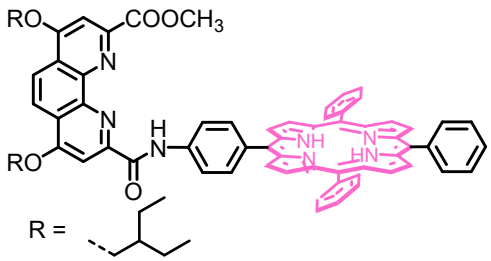
g, 12.586 mmol, 1.4 eq) was added and stirred for 10 hours at room temperature. After completion of the reaction, NEt_3 was added dropwise to neutralize the reaction mixture. The solvent was removed, and the crude product was passed through a silica gel column and DCM as an eluent. The reddish-purple solid obtained was used for the next step without characterization. In a 100 mL round-bottomed flask, it was dissolved in 50 mL conc. HCl, and then $SnCl_2 \bullet 2H_2O$ (2 g) was added portion-wise into the reaction vessel and stirred at room temperature for 45 min. Subsequently, the temperature was gradually increased to 95 °C and stirred overnight. After completion of the reaction, the residual HCl was neutralized with NH_4OH solution under ice-cold conditions. The solution was then poured into a conical flask containing 1 L of acetone. The inorganic salts precipitated and were removed through filtration. The acetone is then evaporated in rotary evaporator to obtain purple solid, which was purified by column chromatography using silica gel and 5% Ethyl acetate in Chloroform as eluent. Yield (5%, 0.260 g). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ ppm: 8.93 (d, J = 4.5 Hz, 4H), 8.82 (d, J = 4.5 Hz, 4H), 8.22 (d, J = 7.1 Hz, 4H), 8.00 (d, J = 8.0 Hz, 4H), 7.76 (m, 6H), 7.07 (d, J = 8.0 Hz, 4H), 4.03 (s, 4H), -2.74 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K) δ ppm: 146.00, 142.42, 135.67, 134.56, 132.49, 127.59, 126.61, 120.43, 119.79, 113.46. HRMS (ESI): m/z calcd for $C_{44}H_{33}N_6$ $[M+H]^+$ 645.2761 Found 645.2674.

4,7-bis(2-ethylbutoxy)-9-(methoxycarbonyl)-1,10-phenanthroline-2-carboxylic acid (5): In a dry



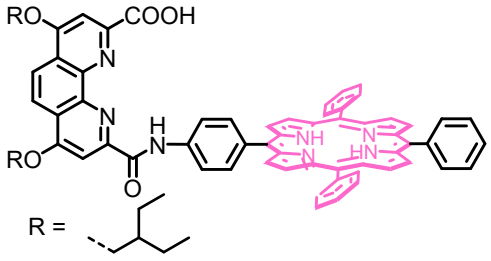
250 mL round bottom flask, dimethyl 4,7-bis(2-ethylbutoxy)-1,10-phenanthroline-2,9-dicarboxylate (**4**)[4] (1.80 g, 3.63 mmol, 1 eq) was dissolved in 80 mL of 1:1 mixture of THF:MeOH. KOH (0.223 mg, 3.99 mmol, 1.1 eq) was dissolved in 20 mL MeOH and then transferred to the solution through a syringe pump over a period of 3 hours at 0 °C. The mixture was stirred at room temperature for 12-14 hours under the nitrogen atmosphere. TLC was checked intermittently, and after completion of the reaction, the solvent was evaporated in a rotary evaporator. The crude product was purified by column chromatography with silica gel and 5% MeOH in $CHCl_3$ as eluent to obtain the sodium salt of **5**. It was acidified with a 5% citric acid solution, extracted with dichloromethane, and dried in Na_2SO_4 to get **5** as an off-white solid. Yield (63%, 1.1 g). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ ppm: δ 8.31 (s, 2H), 8.01 (s, 1H), 7.84 (s, 1H), 4.45 (dd, J = 11.8, 5.6 Hz, 4H), 4.10 (s, 3H), 1.92 (m, 2H), 1.66 (m, 8H), 1.03 (m, J = 7.4, 4.5 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K) δ ppm: 165.35, 163.42, 149.27, 149.08, 123.15, 122.95, 121.15, 121.05, 104.66, 103.71, 72.21, 71.78, 53.25, 40.85, 40.79, 23.60, 23.54, 11.23, 11.17. HRMS (ESI): m/z calcd for $C_{27}H_{35}N_2O_6$ $[M+H]^+$ 483.2490, Found 483.2427.

Methyl4,7-bis(2-ethylbutoxy)-9-((4-((1*Z*,4*Z*,10*Z*,14*Z*)-10,15,20-triphenyl-22*H*,24*H*-porphyrin-5-yl)phenyl)carbamoyl)-1,10-phenanthroline-2-carboxylate (6a): In a 10 mL round-bottomed flask,



5 (0.15 g, 0.31 mmol, 1 eq) was taken and kept under vacuum for 30 min. Anhydrous DCM (3 mL) was then added to it under N_2 atmosphere. Oxalyl chloride (0.26 mL, 3.10 mmol, 10 eq) was added dropwise in ice-cold condition to the reaction vessel. It was then stirred at room temperature for 2 hours. The acid chloride was then dried in a vacuum for 3 hours. The acid chloride was used for the next step without further purification. In the same flask, 5 mL of anhydrous THF was added to dissolve it. In another 10 mL round bottom flask, 4-(10,15,20-triphenylporphyrin-5-yl)aniline (**2**)[5] (0.195 g, 0.310 mmol, 1 eq), was taken and dissolved in anhydrous THF (5 mL). To it anhydrous DIPEA (0.43 mL, 2.480 mmol, 8 eq) was added. It was then transferred dropwise to the round bottom flask containing acid chloride under ice-cold conditions. The reaction was then stirred overnight at room temperature. After the completion of the reaction, the solvent was evaporated. The crude product was then redissolved in DCM, washed with 5 % citric acid solution and brine, and further dried over Na_2SO_4. The solvent was removed to get a purple solid. It was then purified by size exclusion Gel Permeation Chromatography (GPC) to obtain a pure product as a purple solid (eluting solvent: chloroform). Yield (44%, 0.15 g), ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ ppm: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ ppm: 11.61 (s, 1H), 8.99 (d, J = 4.8 Hz, 2H), 8.88 (d, J = 4.8 Hz, 2H), 8.85 (s, 2H), 8.44 – 8.40 (m, 8H), 8.35– 8.28 (m, 2H), 8.24 (m, 4H), 7.91 (s, 2H), 7.79 (m, 9H), 4.39 (d, J = 5.5 Hz, 2H), 4.31 (d, J = 5.5 Hz, 2H), 4.18 (s, 3H), 1.96 (m, 2H), 1.71 (m, 8H), 1.09 (m, 12H), -2.73 (s, 2H).^{13}C NMR (100 MHz, $CDCl_3$, 298 K) δ ppm: 166.06, 163.57, 163.22, 163.14, 148.88, 146.15, 145.41, 142.25, 138.09, 138.00, 135.16, 134.57, 127.68, 126.67, 123.16, 122.93, 121.50, 120.30, 120.13, 120.02, 118.67, 104.21, 102.28, 71.65, 71.54, 53.27, 53.23, 40.94, 23.66, 11.28. HRMS (ESI): m/z calcd for $C_{71}H_{65}N_7O_5$ $[M+2H]^{2+}$ 547.7518, Found 547.7567.

4,7-bis(2-ethylbutoxy)-9-((4-((1*Z*,4*Z*,10*Z*,14*Z*)-10,15,20-triphenyl-22*H*,24*H*-porphyrin-5-yl)-phenyl)-carbamoyl)-1,10-phenanthroline-2-carboxylic acid (6): In a 25 mL round-bottomed flask, **6a**



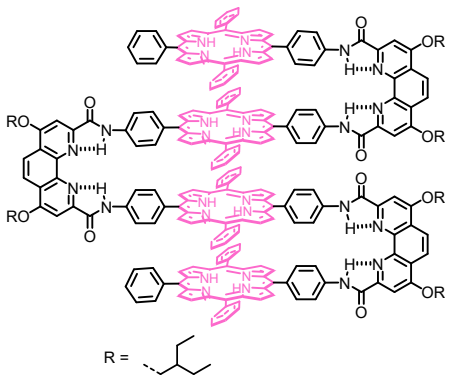
(0.160 g, 0.146 mmol, 1 eq) was taken. The compound was then dissolved in a 10 mL 2:1 mixture of THF and MeOH under an inert atmosphere. In another round bottom flask, NaOH (0.035 g, 0.878 mmol, 6 eq) was dissolved in 2 mL MeOH and then transferred to the reaction flask. The reaction was then stirred overnight at room temperature. The progress

was monitored by TLC. After completion of the reaction, the solvent was evaporated completely and then extracted with DCM, washed with 5 % citric acid solution and brine, and dried over Na_2SO_4. The solvent was evaporated to obtain the product as a purple solid. The product was used for the next step without purification. Yield (82%, 130 mg). ^{1}H NMR (400 MHz, $CDCl_3$:DMSO-d_6 (1:1), 298 K) δ ppm: 11.52 (s, 1H), 8.92 (d, *J* = 4.8 Hz, 2H), 8.83 (d, *J* = 4.8 Hz, 2H), 8.80 (s, 2H), 8.42 (d, *J* = 8.2 Hz, 4H), 8.34 – 8.26 (m, 2H), 8.18 – 8.17 (m, 4H), 8.12 (s, 2H), 8.07 (d, *J* = 6.5 Hz, 2H), 7.92 (s, 2H), 7.78 (m, 9H), 4.38 (d, *J* = 5.1 Hz, 2H), 4.34 (d, *J* = 5.4 Hz, 2H), 1.97 (m, 2H), 1.67 (m, 8H), 1.04 (m, 12H), -2.92 (s, 2H). ^{13}C could not be recorded due to the high propensity of aggregation at higher concentrations. HRMS (ESI): m/z calcd for $C_{70}H_{63}N_7O_5$ $[M+2H]^{2+}$ 540.7440, Found 540.7481.

***N*2,*N*9-bis(4-(15-(4-aminophenyl)-10,20-diphenylporphyrin-5-yl)phenyl)-4,7-bis(2-ethylbutoxy)-1,10-phenanthroline-2,9-dicarboxamide (8):** In a 25 mL round bottomed flask, dimethyl 4,7-bis(2-ethylbutoxy)-1,10-phenanthroline-2,9-dicarboxylate (**7**)[4] (0.12 g, 0.256 mmol, 1 eq) was taken and kept under vacuum for 30 min. Anhydrous DCM (4 mL) was then added to the flask under N_2 atmosphere. Oxalyl chloride (0.2 mL, 2.56 mmol, 10 eq) was added dropwise in ice-cold conditions. It was then stirred in room temperature for 2-3 hours. The acid chloride was dried under a vacuum for 3 hours. The acid chloride formed is used without further purification. In the same flask, 20 mL of anhydrous THF was added to dissolve it and transferred into a syringe. Subsequently, in another 250 mL round bottom flask, **3** (0.38 g, 0.6 mmol, 2.3 eq), was added and dissolved in anhydrous THF (300 mL) and anhydrous DIPEA (0.26 g, 2.0 mmol, 8 eq). The acid chloride solution was then added to the reaction vessel dropwise through a syringe pump over a period of 3 h at 0 ºC. The reaction was then stirred for 24 hours at room temperature. After the completion of the reaction, the solvent was evaporated. The crude product was then redissolved in DCM, washed with 5 % citric acid solution and brine, and further dried over Na_2SO_4. The solvent was removed to get a purple solid. It was then purified by GPC (eluting solvent: chloroform) and later by column chromatography using silica gel and DCM as eluent to obtain a pure product as a purple solid. Yield (8%, 0.030 g). ^{1}H NMR (400 MHz, CDCl3, 298 K) δ 11.42 (s, 2H), 8.76 (m, 8H), 8.50 (d, *J* = 7.8 Hz, 3H), 8.43 (s, 2H), 8.35 – 8.33 (m, 6H), 8.25 - 8.22 (m, 5H), 7.92 (d, *J* = 7.8 Hz, 3H), 7.36 (d, *J* = 4.1 Hz, 2H), 7.28 – 7.24 (m, 7H), 7.20 (d, *J* = 7.8 Hz, 5H), 7.05 (d, *J* = 7.8 Hz, 3H), 6.91 (t, *J* = 7.8 Hz, 6H), 4.70 (s, 4H), 4.43 (d, *J* = 5.3 Hz, 4H), 2.01 - 1.98 (m, 2H), 1.72 - 1.67 (m, 10H), 1.10 (t, *J* = 7.4 Hz, 12H), -2.98 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K) δ ppm: 163.90, 162.72, 151.20, 145.93, 144.99, 141.55, 138.64, 137.64, 135.60, 135.48, 133.82, 132.52, 128.55, 127.66, 127.01,

126.89, 125.85, 123.13, 120.84, 120.52, 119.40, 118.62, 117.96, 113.44, 101.82, 71.79, 40.95, 29.69, 23.69, 11.30. MALDI-TOF Mass: m/z calcd for $C_{114}H_{93}N_{14}O_4$ $[M+H]^+$ 1722.75, Found 1722.43.

Tetramer (1): In a 5 mL round bottom flask, **8** (0.03 g, 0.016 mmol, 1 eq), **6** (0.046 g, 0.042 mmol, 2.5 eq), HATU (0.066 g, 0.174 mmol, 10 eq) were taken under N_2 atmosphere. Anhydrous pyridine (0.5 mL) was transferred to the reaction mixture and heated at 40 °C for 36 hours. After the completion of the reaction, the reaction mixture was dissolved in DCM, washed multiple times with water, brine, and dried over Na_2SO_4. The solvent was then removed to get the crude product. Purification was carried out by GPC (eluting solvent: chloroform) and further by column chromatography using silica gel and chloroform as an eluent to obtain a pure product. Yield (12 mg, 18 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ 11.45 (s), 11.39 (s), 11.28 (s), 8.85 (d), 8.79 (d), 8.74 (d), 8.51 (s), 8.43 (s), 8.32 (s), 8.26 – 8.22 (m), 8.16 (d), 7.91 (d), 7.75 (d), 7.61 (s), 7.52 – 7.49 (m), 7.45 (t), 6.64 (s), 6.01 (s), 4.52 (d), 4.44 (d), 4.33 (d), 2.12 (m), 2.04 (m), 1.89 (m), 1.28 (t), 1.21 (t), 1.12 (t), -3.41 (s), -3.88 (s). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K) δ ppm: 164.16, 163.89, 163.04, 162.64, 162.46, 161.90, 152.48, 151.26, 150.95, 145.02, 144.55, 144.07, 142.10, 141.07, 138.88, 138.72, 138.41, 138.09, 137.62, 136.42, 135.79, 135.48, 134.28, 133.28, 132.37, 127.41, 126.45, 126.38, 125.76, 125.33, 124.50, 123.26, 122.93, 122.21, 121.02, 120.38, 119.46, 119.34, 119.27, 118.57, 118.39, 118.25, 118.12, 117.87, 101.75, 72.40, 71.96, 71.73, 41.34, 41.16, 41.13, 29.85, 23.93, 23.87, 11.63, 11.50, 11.48. MALDI-TOF Mass: m/z calcd for $C_{254}H_{211}N_{28}O_{12}$ $[M+H]^+$ 3846.68, Found 3846.89. UV-visible ($CHCl_3$, 298 K): Soret band at 417 nm, Q-bands are at 518, 555, 593, 649 nm.



3. Characterization

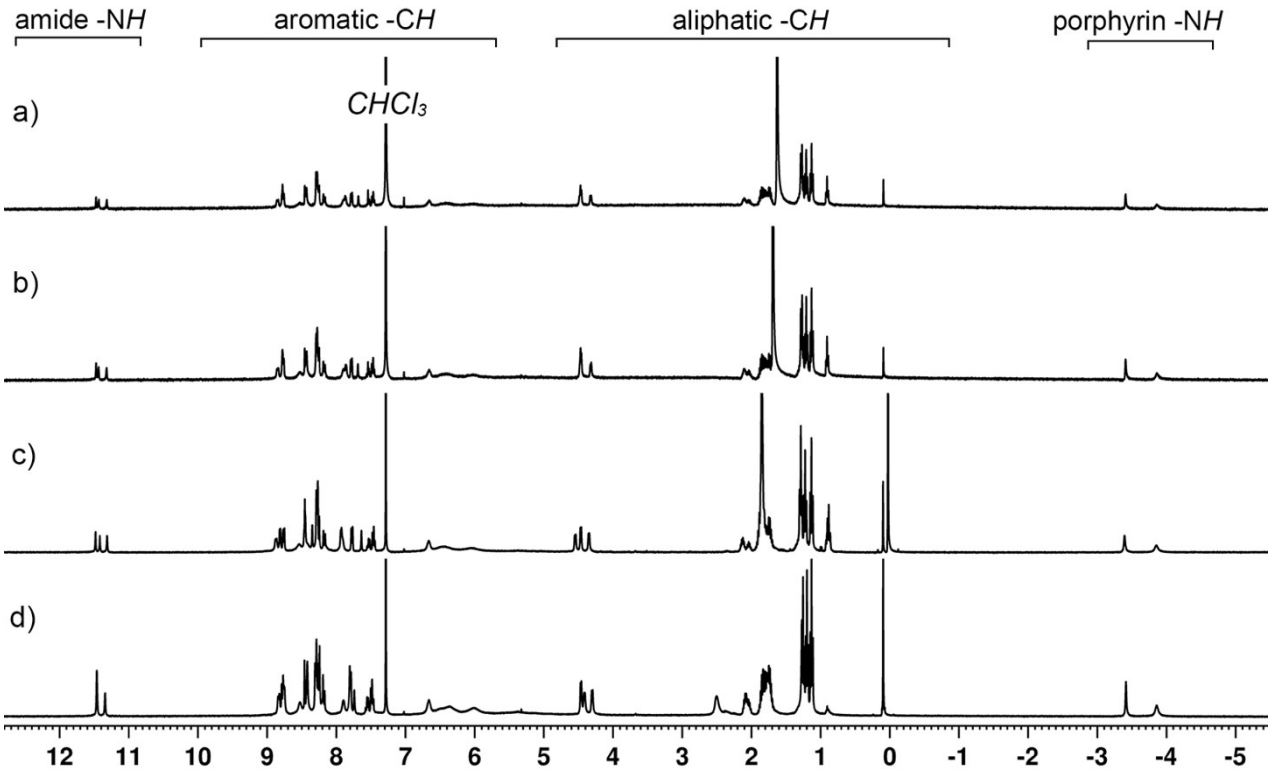


Fig. S1 Variable concentration ^{1}H-NMR spectra of **1**; (a) 0.12 mM, (b) 0.25 mM, (c) 0.5 mM, and (d) 1 mM in $CDCl_3$ at 298 K. The broadness of the peaks in the region 7 – 5 ppm did not change on dilution. Thus, confirming intramolecular behavior.

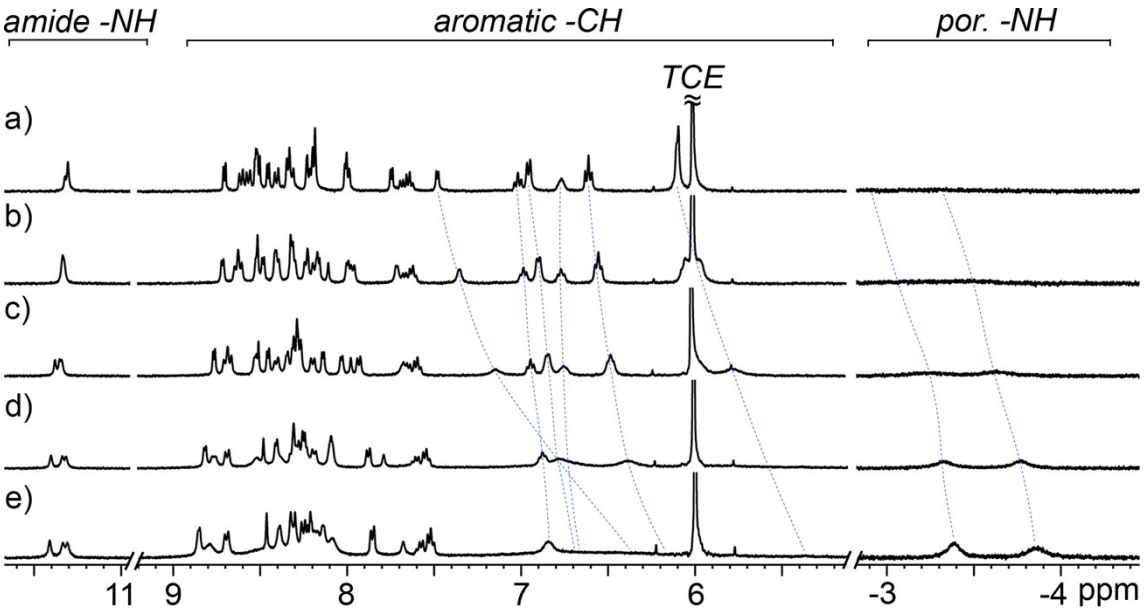


Fig. S2 Selected region VT ^{1}H NMR of 1 (0.5 mM) in $C_2D_2Cl_4$ at (a) 373 K, (b) 353 K, (c) 333 K, (d) 313 K, and (e) 298 K. At lower temperatures, along with sharp signals some broad peaks shifted upfield was seen that got resolved at the higher temperature. The dotted lines are the visual guide of the prominent shift of some signals.

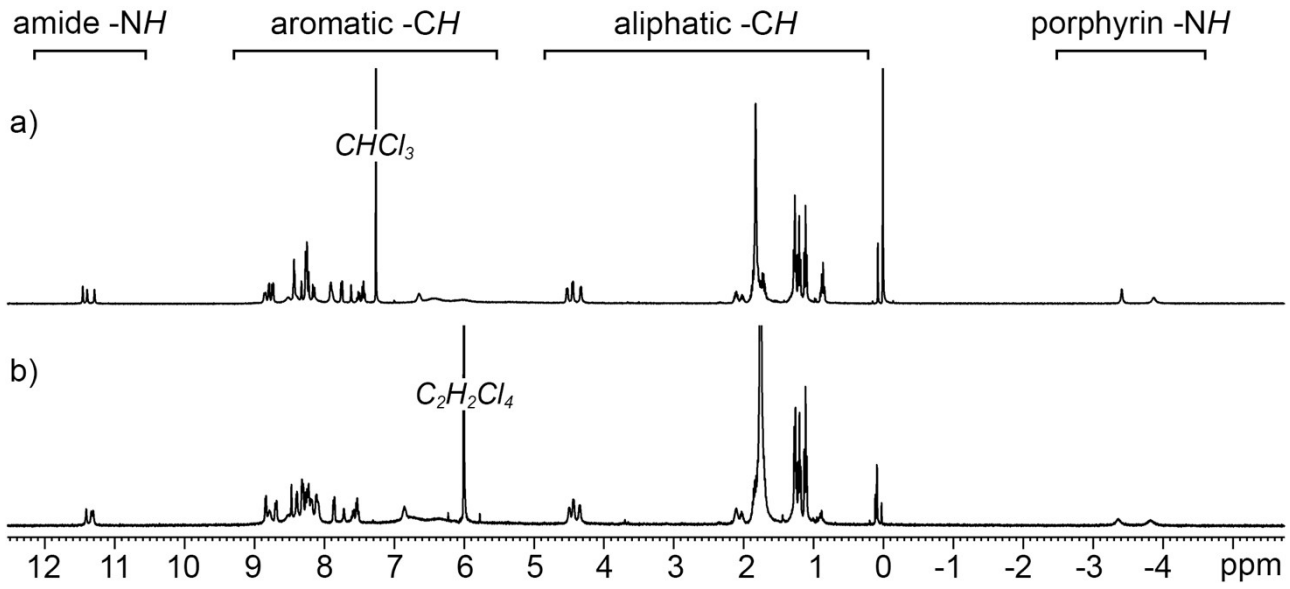


Fig. S3 ^{1}H-NMR spectra of **1** (0.5 mM) in (a) $CDCl_3$ and (b) $C_2D_2Cl_4$ at 298 K.

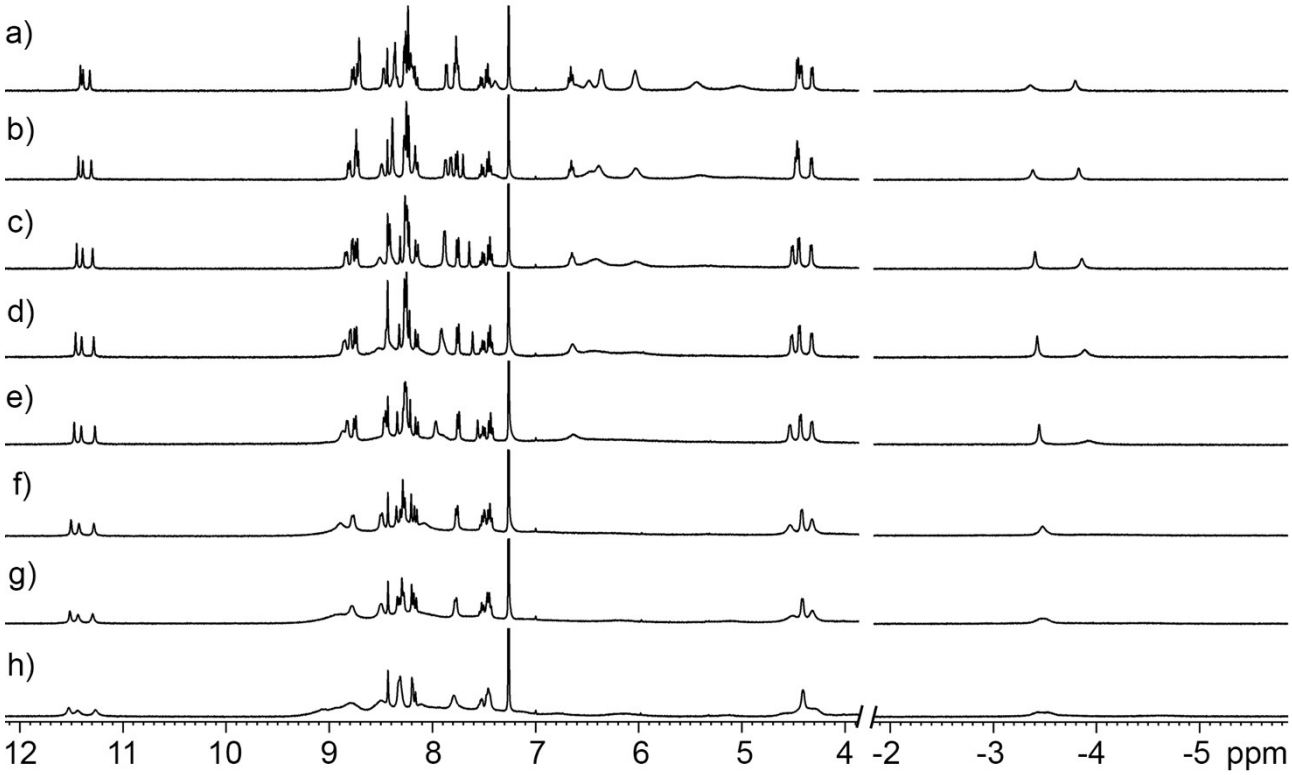


Fig. S4 The Selected region 400 MHz variable temperature ^{1}H-NMR of **1** (1 mM) in $CDCl_3$ in the range of 323 K to 243 K. (a) 323 K, (b) 313 K, (c) 303 K, (d) 293 K, (e) 283 K, (f) 263 K, (g) 253 K, (h) 243 K.

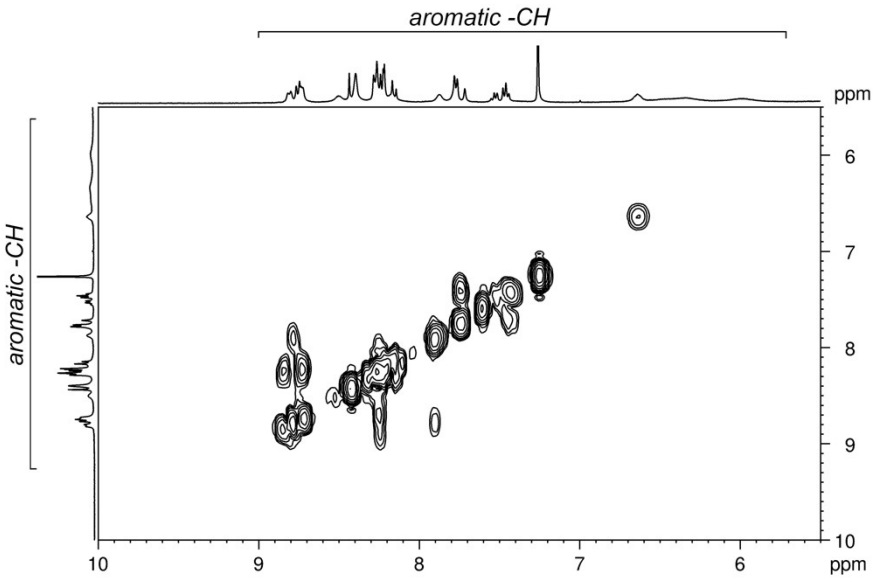


Fig. S5 400 MHz COSY NMR spectra of **1** in $CDCl_3$ at 298 K.

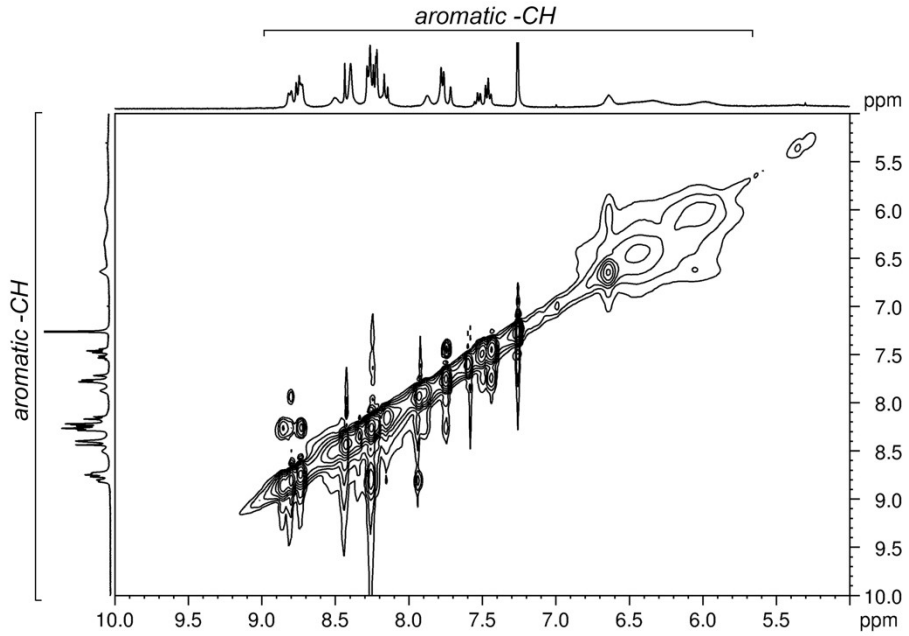


Fig. S6 400 MHz NOESY NMR spectra of **1** in $CDCl_3$ at 298 K.

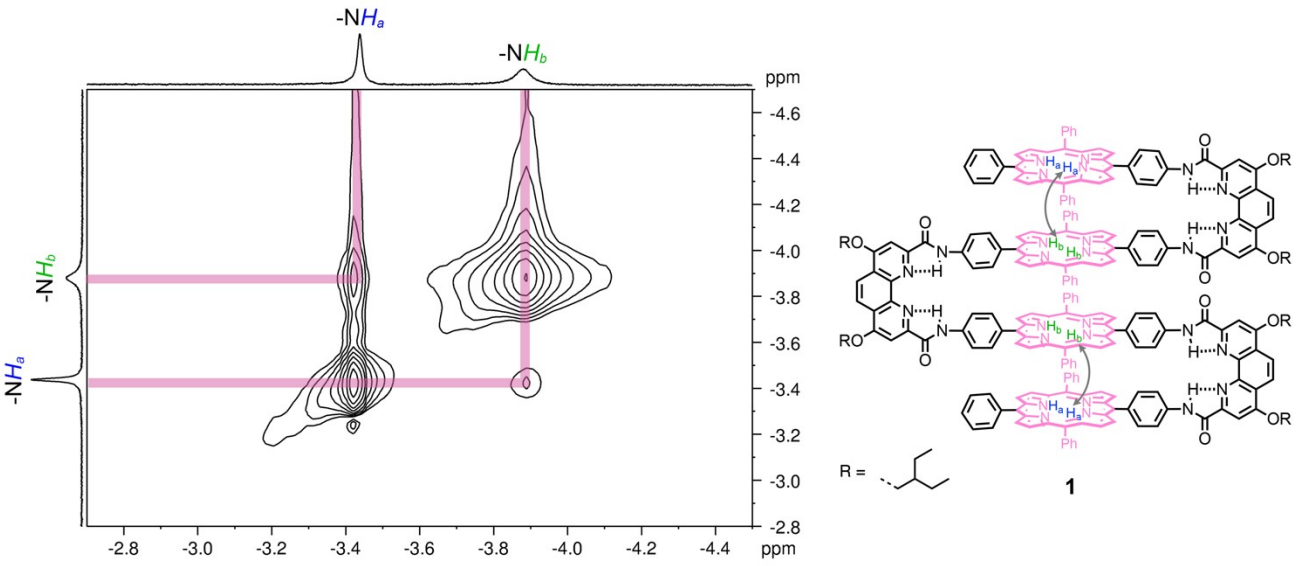


Fig. S7 400 MHz NOESY NMR spectra of **1** highlighting the correlation between two types of porphyrins -N*H* signals originated from outer and inner porphyrins. The correlation confirms the folded structure.

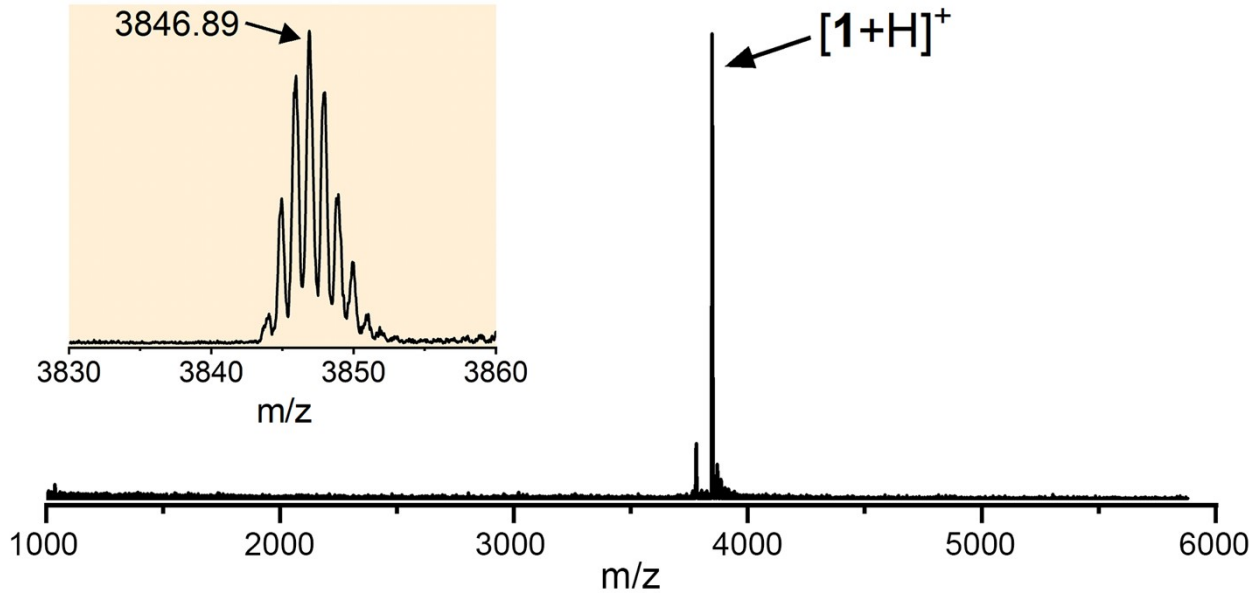


Fig. S8 MALDI-TOF mass spectra of **1**.

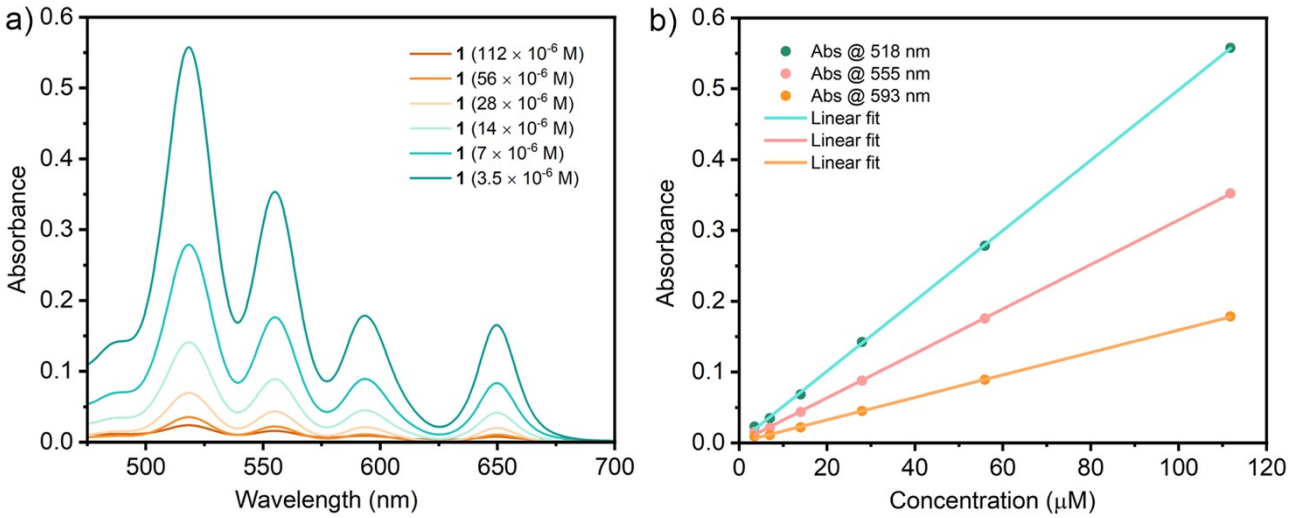


Fig. S9 (a) Concentration-dependent UV-vis spectra of **1** in $CHCl_3$ at 298 K; path length: 1 mm. (b) Concentration vs. absorbance plot shows a linear relationship between them, thus excluding the existence of any molecular association with this concentration range.

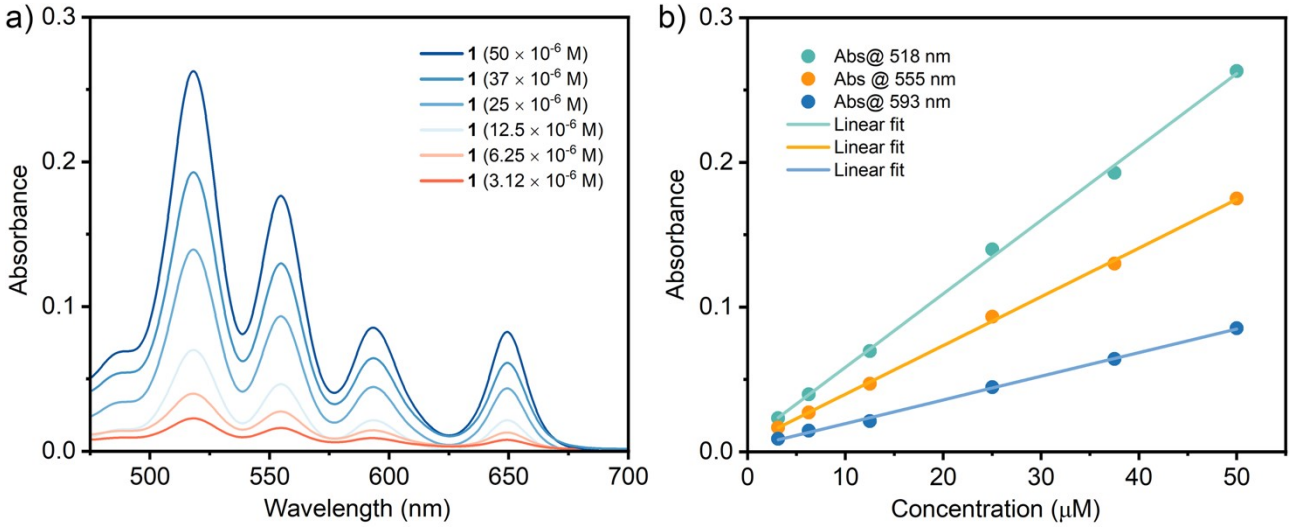


Fig. S10 (a) Concentration-dependent UV-vis spectra of **1** in 1,2-dichloroethane (DCE) at 298 K; path length: 1 mm. (b) Concentration vs. absorbance plot shows a linear relationship between them, thus excluding the existence of any molecular association with this concentration range.

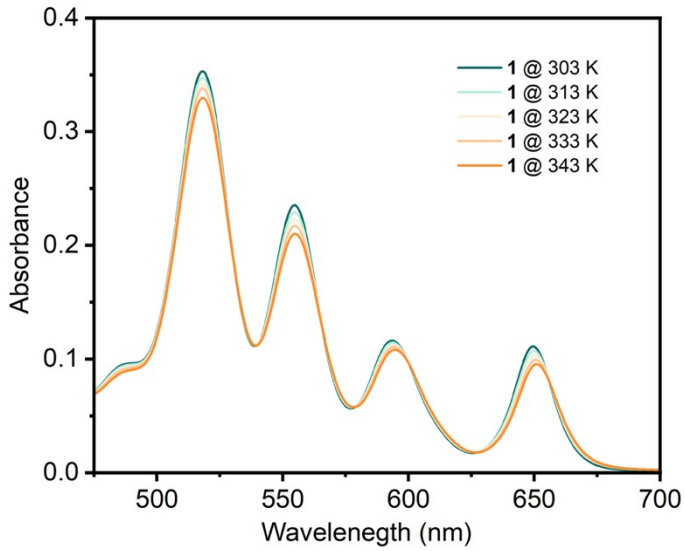


Fig. S11 Variable temperature UV-Vis absorption spectra of **1** in DCE (6.25 μM) in the temperature range 303 K to 343 K; path length: 10 mm.

4. Host-guest studies

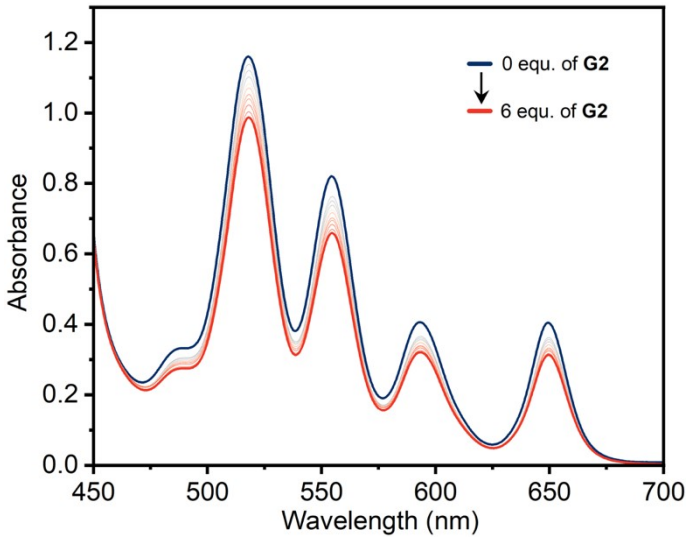


Fig. S12 UV-Vis absorption spectra of **1** (50 μM, path length: 5 mm) with the gradual addition of **G2** (0-6 equivalent) in $CHCl_3$ at 298 K. There is no significant change in the spectra except peak intensities gradually decreased, which is mostly due to the dilution effect.

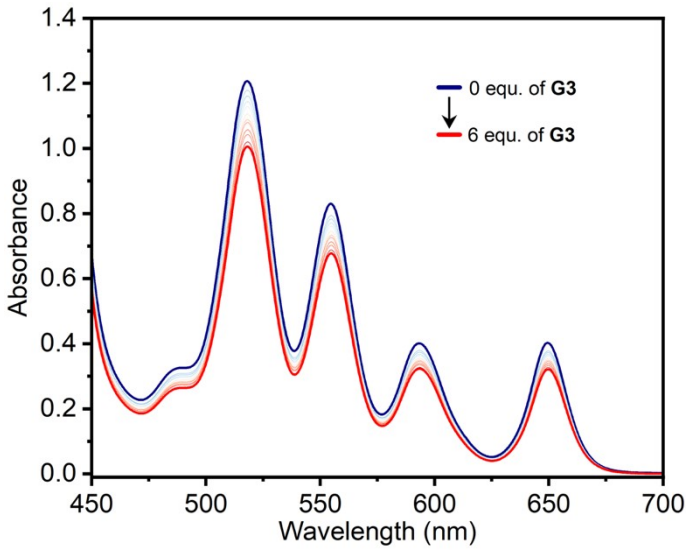


Fig. S13 UV-Vis absorption spectra of **1** (50 μM, path length: 5 mm) with the gradual addition of **G3** (0-6 equivalent) in $CHCl_3$ at 298 K. There is no significant change in the spectra except peak intensities gradually decreased, which is mostly due to the dilution effect.

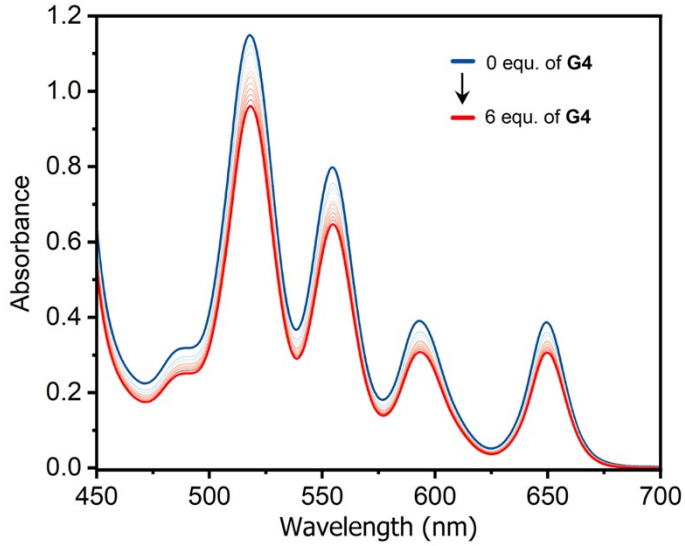


Fig. S14 UV-Vis absorption spectra of **1** (50 μM, path length: 5 mm) with the gradual addition of **G4** (0-6 equivalent) in $CHCl_3$ at 298 K. There is no significant change in the spectra except peak intensities gradually decreased, which is mostly due to the dilution effect.

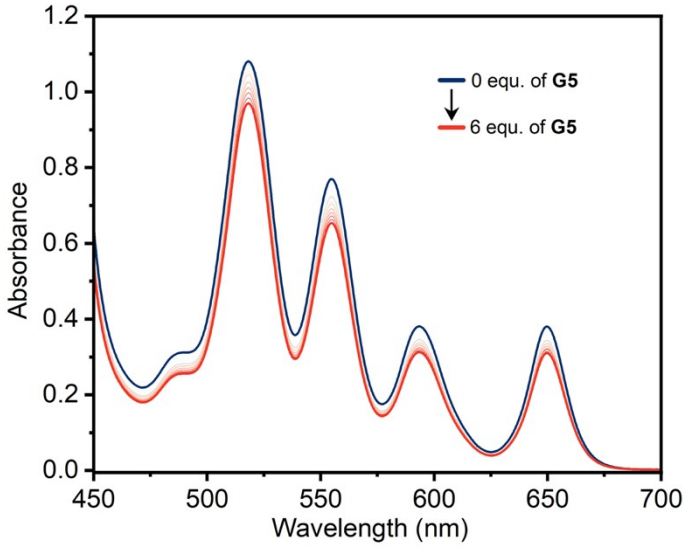


Fig. S15 UV-Vis absorption spectra of **1** (45 μM, path length: 5 mm) with the gradual addition of **G5** (0-6 equivalent) in $CHCl_3$ at 298 K. There is no significant change in the spectra except peak intensities gradually decreased, which is mostly due to the dilution effect.

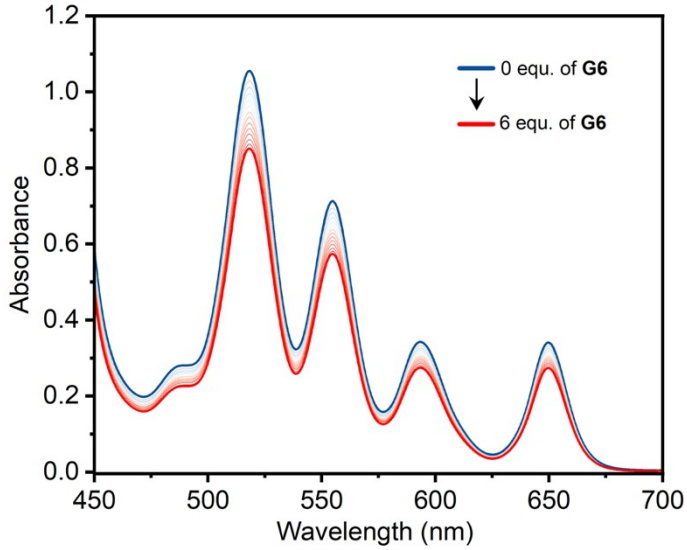


Fig. S16 UV-Vis absorption spectra of **1** (45 μM, path length: 5 mm) with the gradual addition of **G6** (0-6 equivalent) in $CHCl_3$ at 298 K. There is no significant change in the spectra except peak intensities gradually decreased, which is mostly due to the dilution effect.

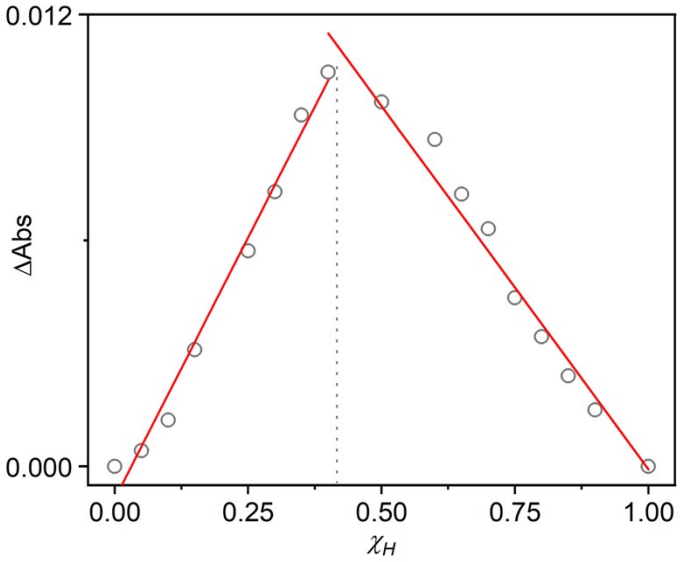


Fig. S17 Job plot for the **1** and **G1** complexation at 295 K in chloroform. The total concentration of host and guest combined was maintained at a constant value (2×10^{-5} mol/L). ΔAbs indicates $|Abs-Abs_H\cdot\chi- Abs_G.\chi|$, where Abs, Abs_H, Abs_G, and χ represent the observed absorbance, absorbance of the host, absorbance of the guest, and mole fraction, respectively.

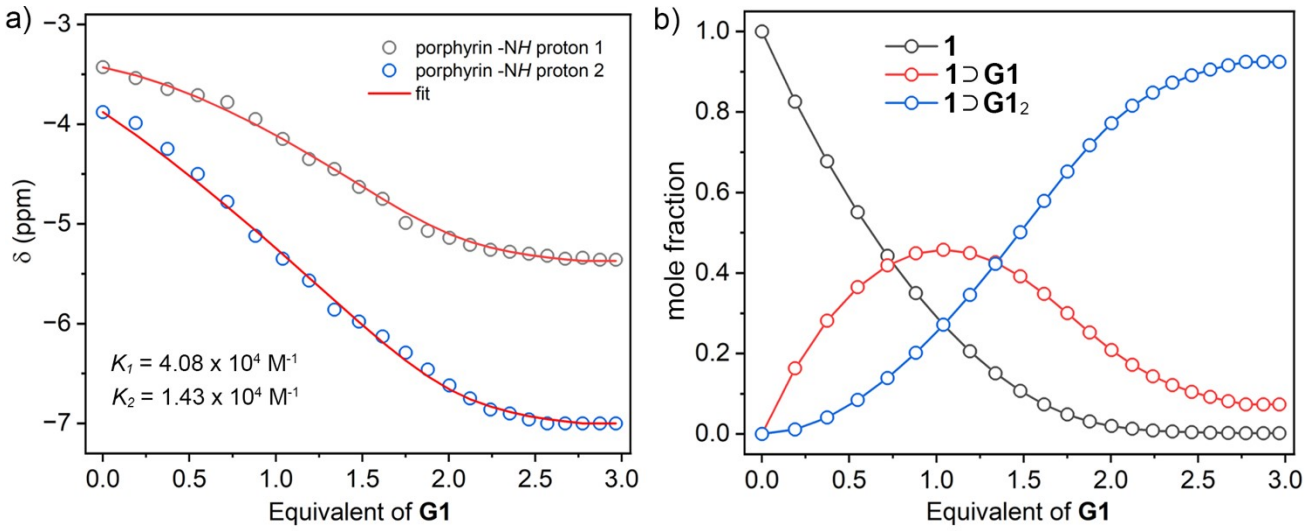


Fig. S18 (a) Variation of chemical shifts (δ) in ^{1}H-NMR (400 MHz) of two porphyrin -N*H* protons upon gradual addition of **G1** into a solution of **1** in $CDCl_3$ at 298 K. The data was fitted using a 1:2 binding model to obtain two binding constants, K_1 = 4.08×10^4 ± 54 M^{-1} and K_2 = 1.43×10^4 ± 11 M^{-1}. (b) The simulated mole fraction variation of **1**, **1⊃G1**, and **1⊃G1**$_2$ with increasing **G1** concentration. The fitting and mole fraction variation was obtained from Bindfit.[6,7]

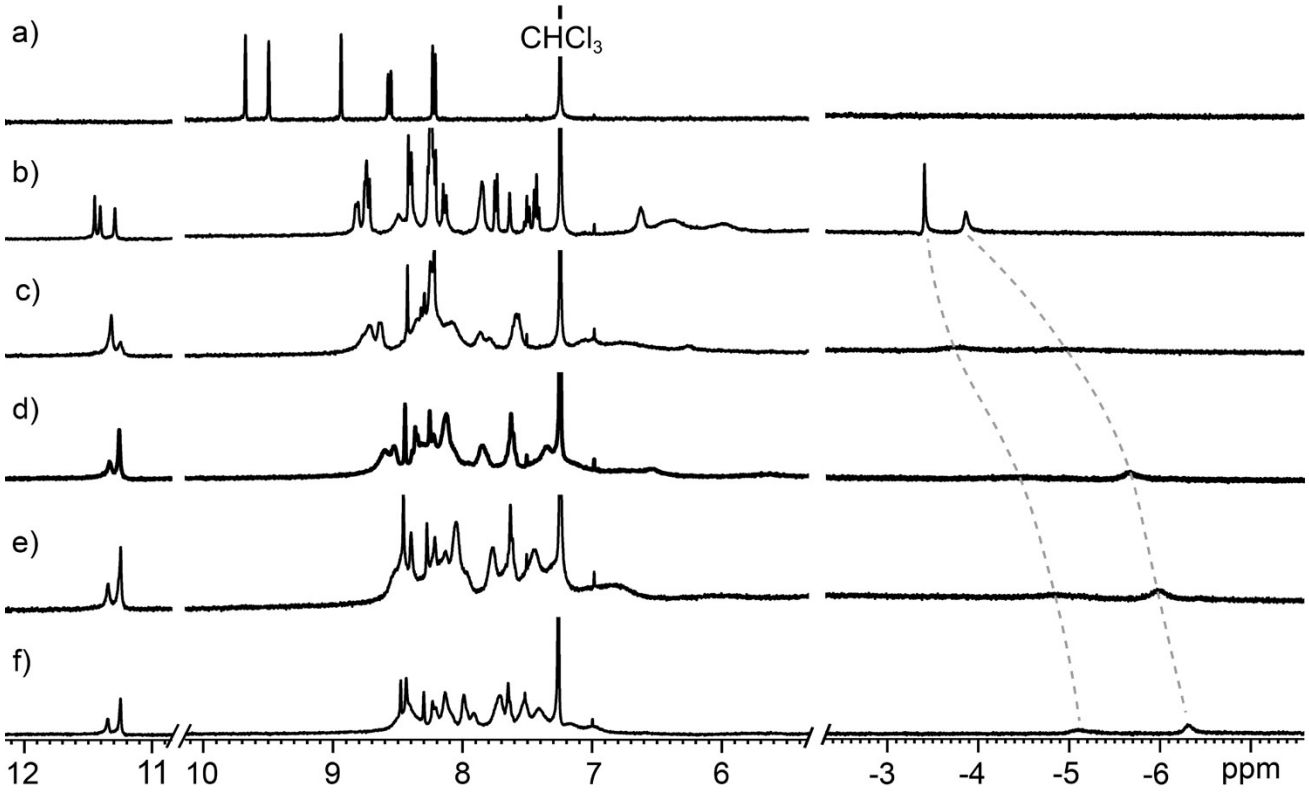


Fig. S19 The Selected region 400 MHz ^{1}H-NMR spectra of (a) **G2** (10 mM), (b) **1** (1 mM) in $CDCl_3$ and after the addition of (c) 1, (d) 2, (e) 3 and (f) 4 equivalent of guest **G2** at 298 K.

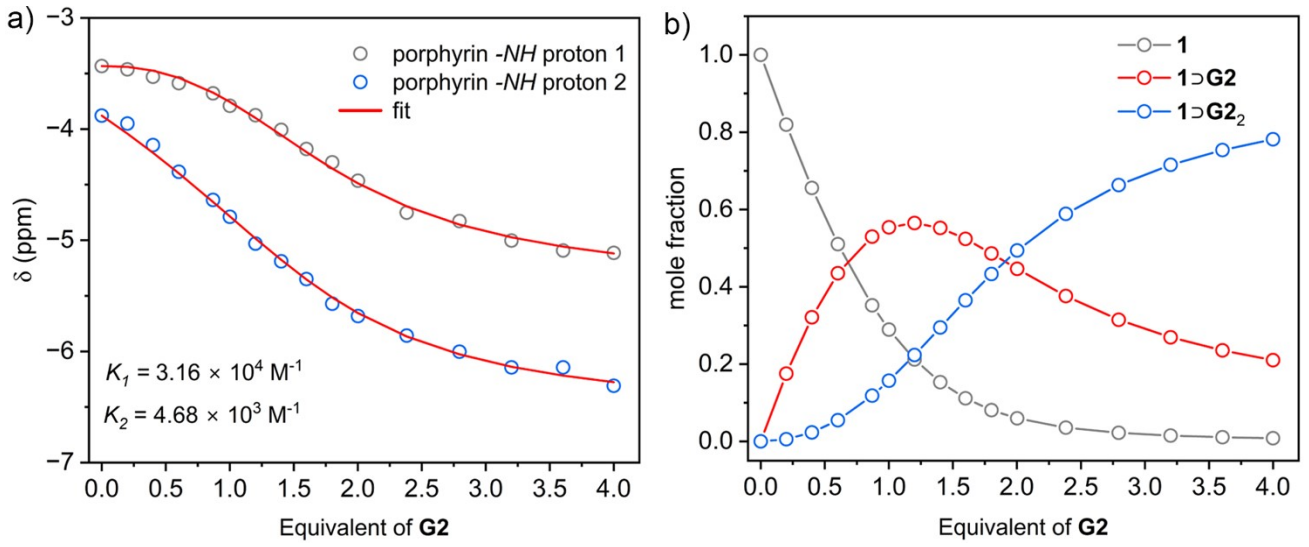


Fig. S20 (a) Variation of chemical shifts (δ) in ^{1}H-NMR (400 MHz) of two porphyrin -N*H* protons upon gradual addition of **G2** into a solution of **1** in $CDCl_3$ at 298 K. The data was fitted using a 1:2 binding model to obtain two binding constants, K_1 = 3.16×10^4 ± 33 M^{-1} and K_2 = 4.68×10^3 ± 4 M^{-1}. (b) The simulated mole fraction variation of **1**, **1⊃G2**, and **1⊃G2**$_2$ with increasing **G2** concentration. The fitting and mole fraction variation was obtained from Bindfit.

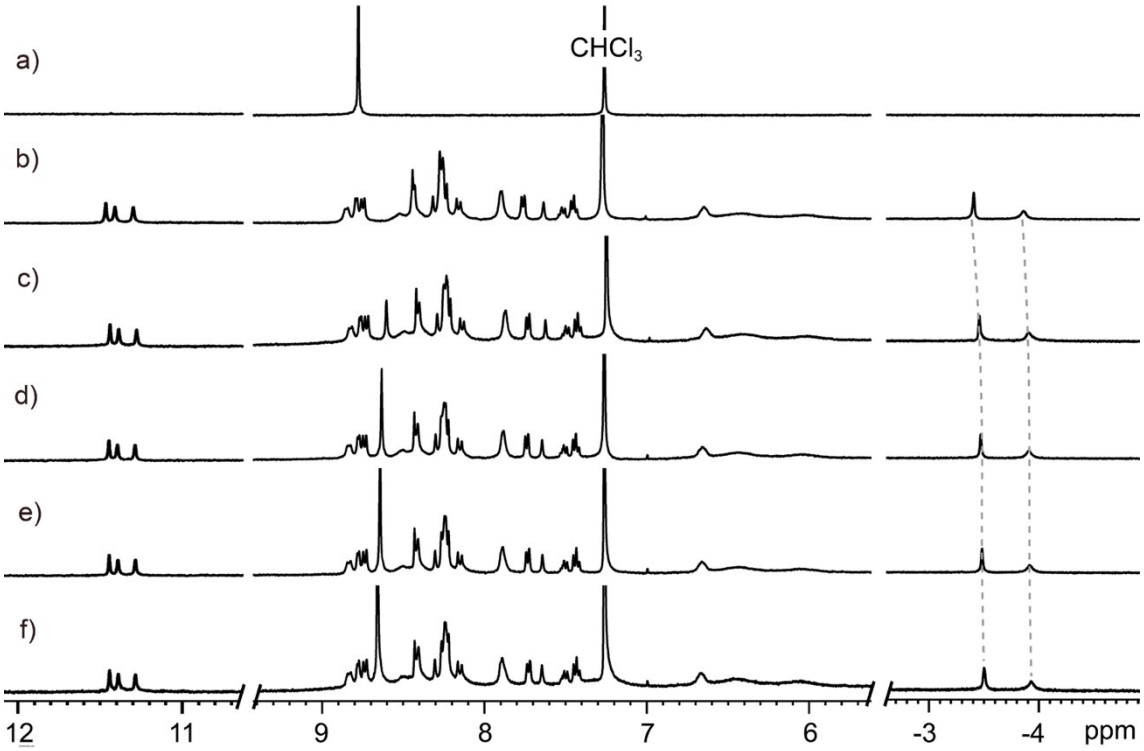


Fig. S21 The Selected region 400 MHz ^{1}H-NMR spectra of (a) **G3** (10 mM), (b) **1** (1 mM) in $CDCl_3$ and after the addition of (c) 1, (d) 2, (e) 3 and (f) 4 equivalent of guest **G3** at 298 K.

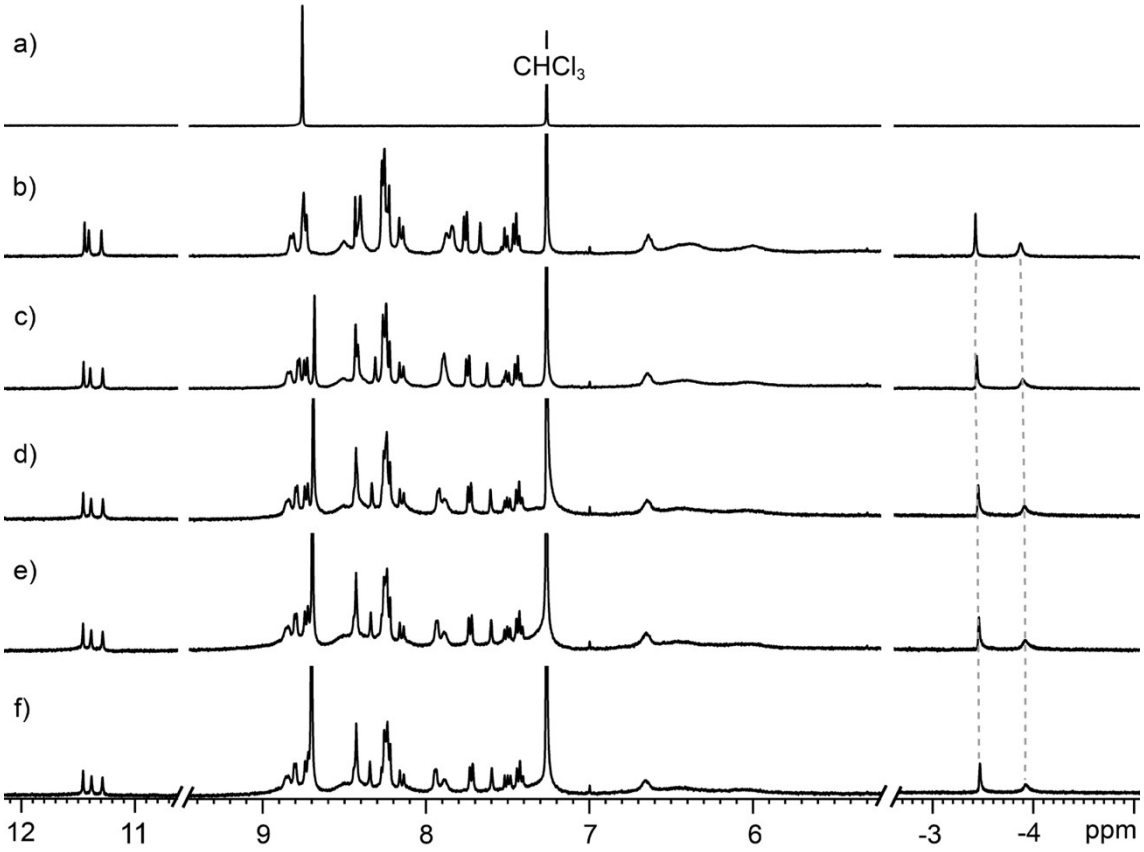


Fig. S22 The Selected region 400 MHz ^{1}H-NMR spectra of (a) **G4** (10 mM), (b) **1** (1 mM) in $CDCl_3$ and after the addition of (c) 1, (d) 2, (e) 3 and (f) 4 equivalent of guest **G4** at 298 K.

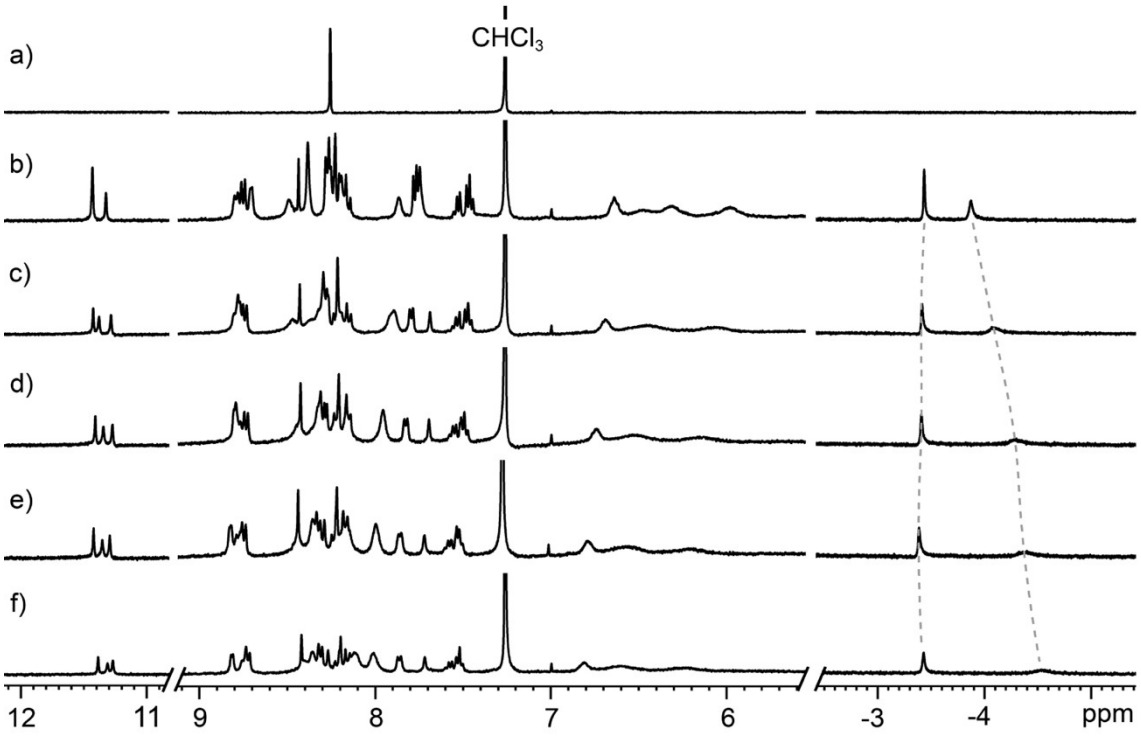


Fig. S23 The Selected region 400 MHz ^{1}H-NMR spectra of (a) **G5** (10 mM), (b) **1** (1 mM) in $CDCl_3$ and after the addition of (c) 1, (d) 2, (e) 3 and (f) 4 equivalent of guest **G5** at 298 K.

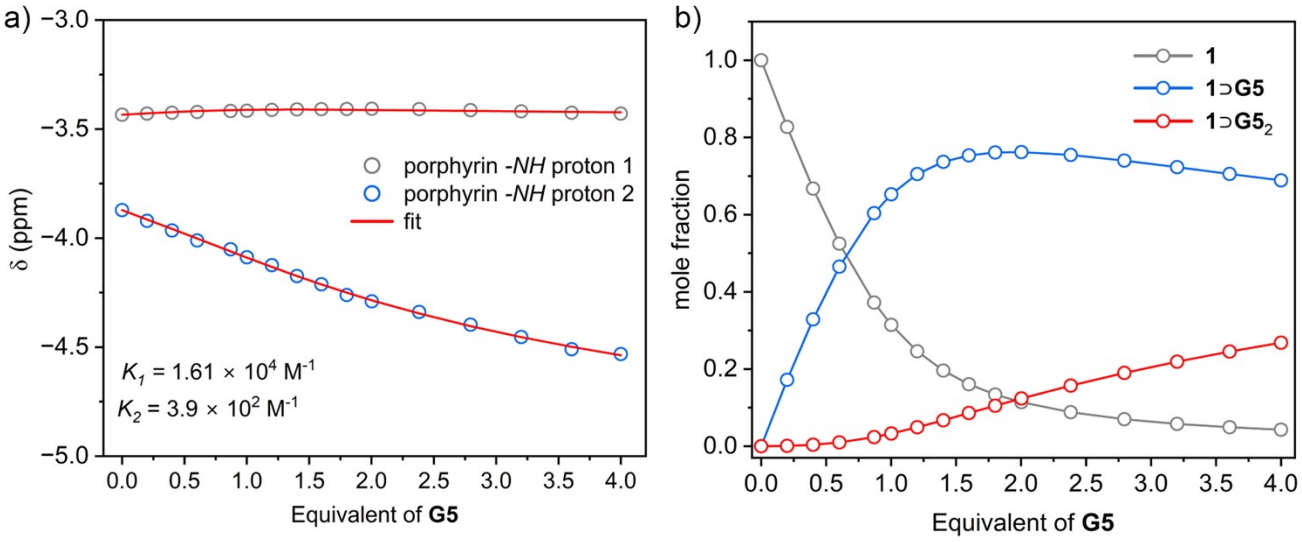


Fig. S24 (a) Variation of chemical shifts (δ) in ^{1}H-NMR (400 MHz) of two porphyrin -N*H* protons upon gradual addition of **G5** into a solution of **1** in $CDCl_3$ at 298 K. The data was fitted using a 1:2 binding model to obtain two binding constants, $K_1 = 1.61\times10^4 \pm 23$ M^{-1} and $K_2 = 3.9\times10^2 \pm 3$ M^{-1}. (b) The simulated mole fraction variation of **1**, **1⊃G5**, and **1⊃G5**$_2$ with increasing **G5** concentration. The fitting and mole fraction variation was obtained from Bindfit.

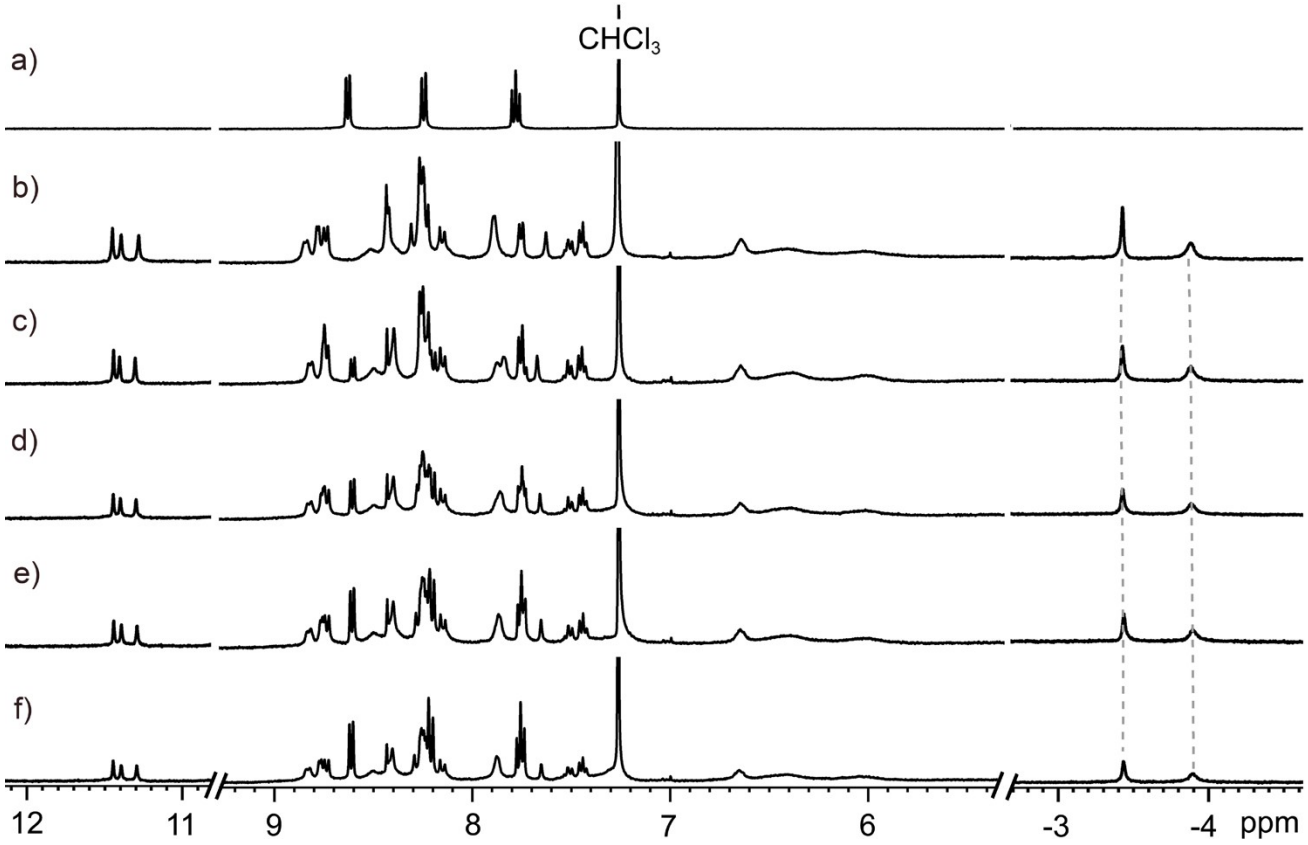


Fig. S25 The Selected region 400 MHz ^{1}H-NMR spectra of (a) **G6** (10 mM), (b) **1** (1 mM) in $CDCl_3$ and after the addition of (c) 1, (d) 2, (e) 3 and (f) 4 equivalent of guest **G6** at 298 K.

Table S1: Binding constants (K_1, K_2) of host-guest complex formation with guests **G1** – **G6** in chloroform at 298 K.

Guest	K_1	K_2
G1	$4.08 \times 10^4\ M^{-1}$	$1.43 \times 10^4\ M^{-1}$
G2	$3.16 \times 10^4\ M^{-1}$	$4.68 \times 10^3\ M^{-1}$
G3	-	-
G4	-	-
G5	$1.61 \times 10^4\ M^{-1}$	$3.9 \times 10^2\ M^{-1}$
G6	-	-

5. Computational results

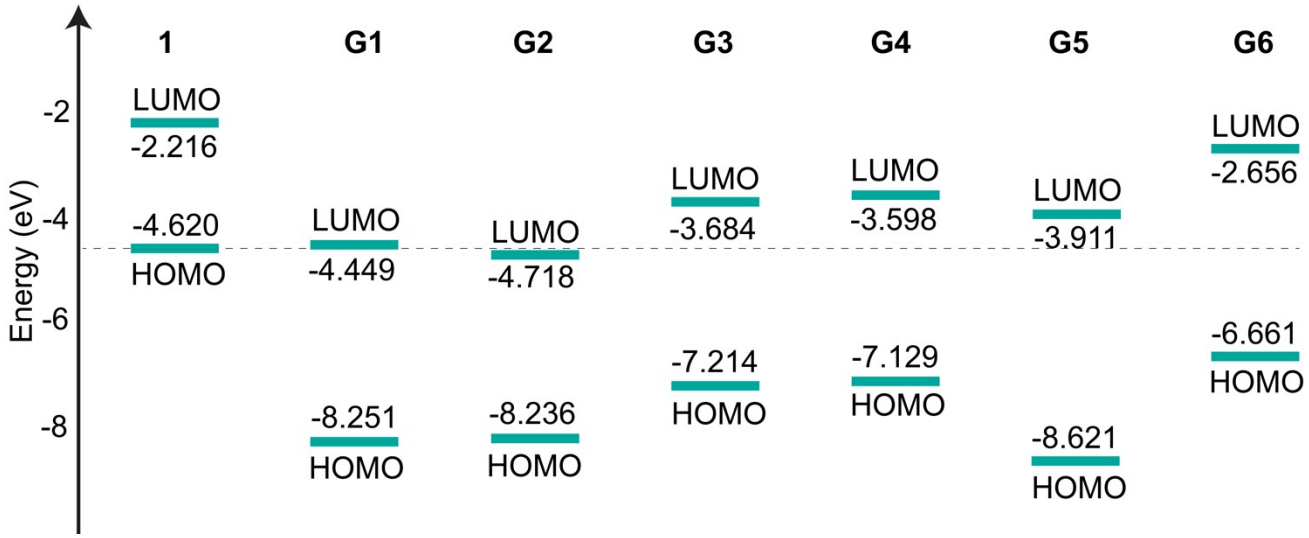


Fig. S26 The DFT calculated the HOMO and LUMO energy of the **1** and guests (**G1** – **G6**). The calculations were performed using B3LYP functional with 6-31G basis set as implemented in the Gaussian 16 Rev. C02 program.

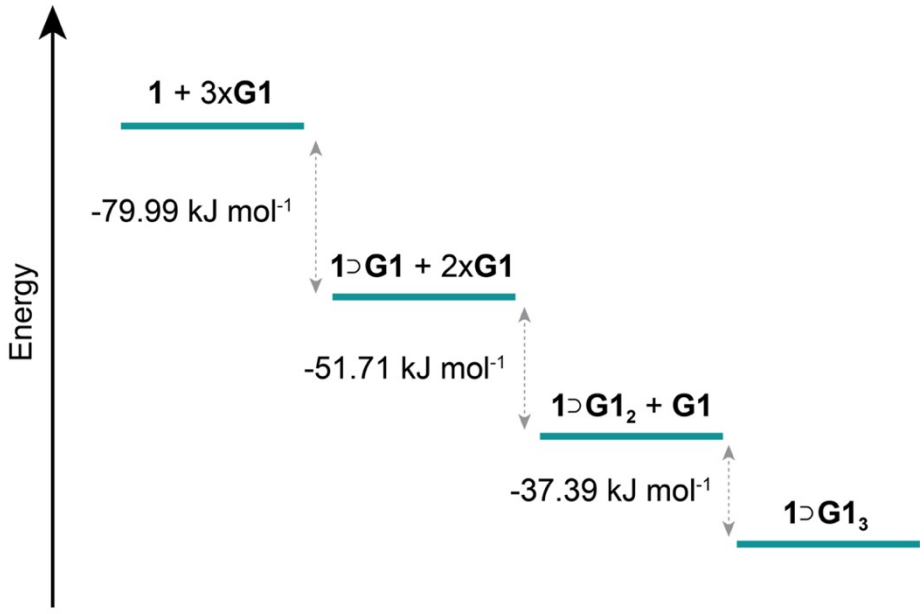


Fig. S27 Energy diagram of the gradual host-guest complexation of **1** with **G1** as estimated from the DFT calculations. The energies represent the relative stabilization of the host-guest complexes **1⊃G1**, **1⊃G1**$_2$, and **1⊃G1**$_3$ with respect to without complexation scenario. The trend is clearly indicating the third complexation is least feasible compared to the first and second binding.

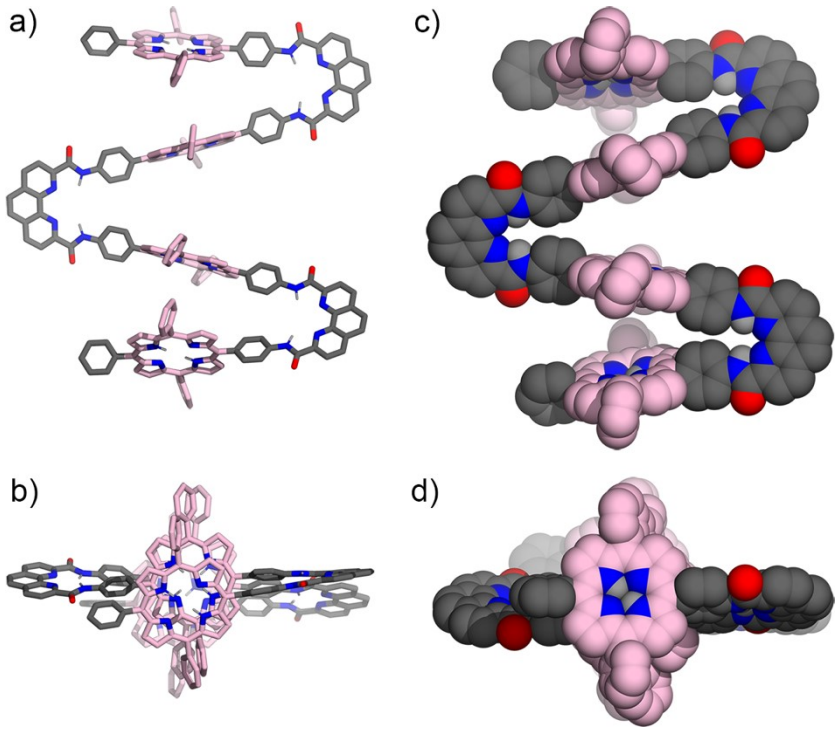


Fig. S28 Additional figure of DFT optimized structures of **1**. (a) Side view and (b) top view of the stick model of **1**. (c) Side view and (d) the top view of the corresponding space fill model shows three cleft-like cavities. Nonpolar hydrogens and side chains are omitted for clarity.

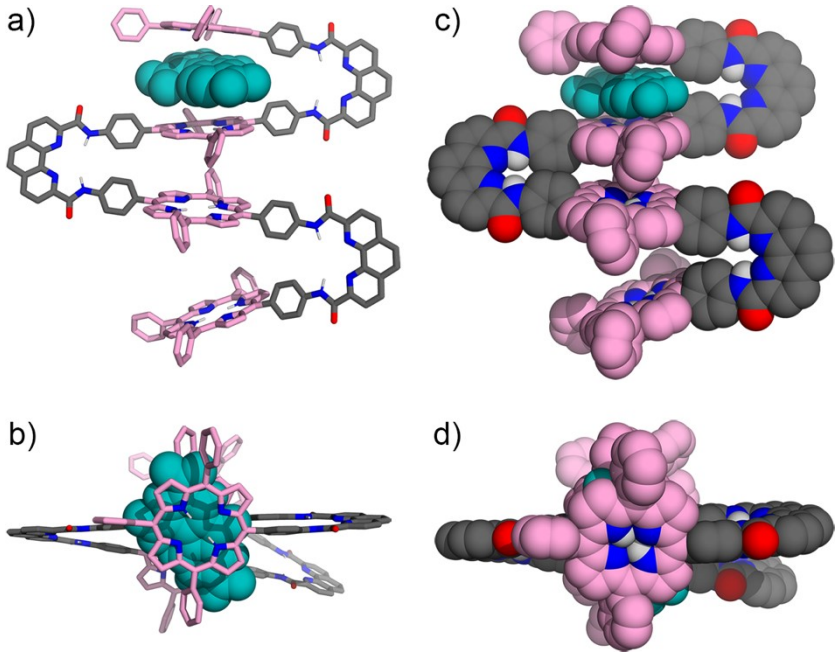


Fig. S29 DFT optimized structures of **1⊃G1**. (a) Side view and (b) top view of the stick model of **1⊃G1**. (c) The side view and (d) the top view of the corresponding space-fill model. The **G1** is represented in teal color. Nonpolar hydrogens and side chains are omitted for clarity.

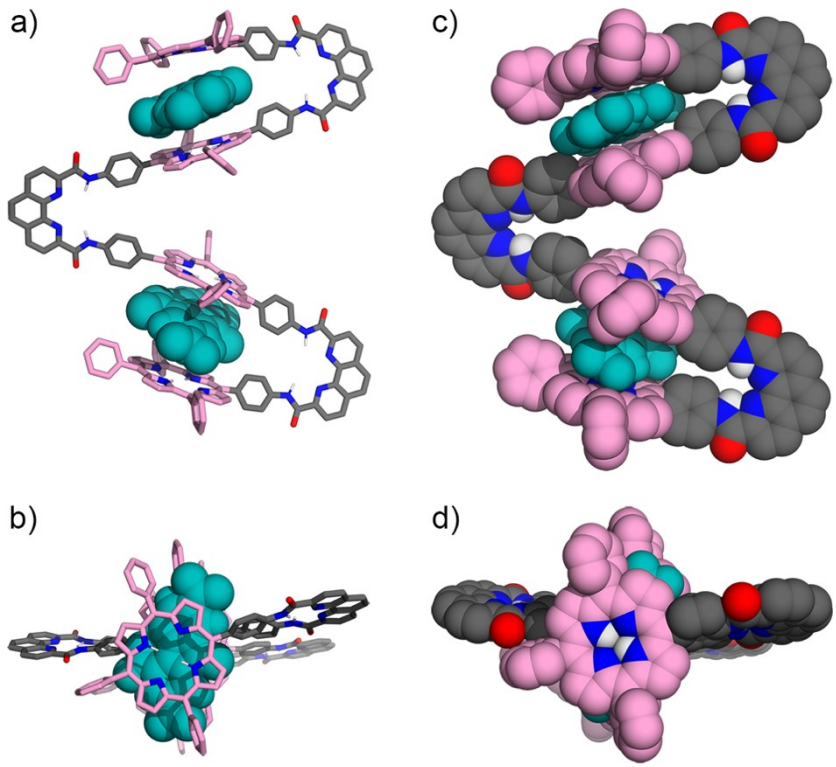


Fig. S30 Additional figure of DFT optimized structures of **1⊃G1**$_2$. (a) Side view and (b) top view of the stick model of **1⊃G1**$_2$. (c) The side view and (d) the top view of the corresponding space-fill model. The **G1** is represented in teal color. Nonpolar hydrogens and side chains are omitted for clarity.

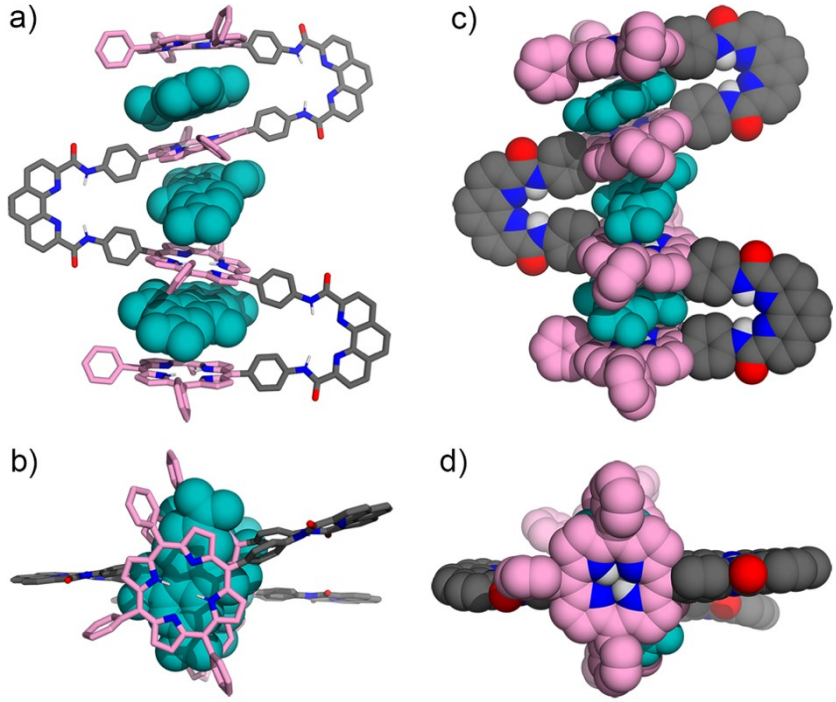


Fig. S31 DFT optimized structures of **1⊃G1**$_3$. (a) Side view and (b) top view of the stick model of **1⊃G1**$_3$. (c) The side view and (d) the top view of the corresponding space-fill model. The **G1** is represented in teal color. While two terminal guests are packed tightly between the clefts, it can be seen the central one is loosely bound. The Nonpolar hydrogens and side chains are omitted for clarity.

5.1. Geometry optimized cartesian coordinates of **1**, **G1**, **1⊃G1**, **1⊃G1$_2$**, and **1⊃G1$_3$**

Table. Cartesian coordinates of **G1**

Number of imaginary frequencies = 0
Total energy (Hartree) = -1188.52961145

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.970982	0.755292	0.025916
2	6	0	-3.232537	-0.607976	0.010405
3	6	0	-2.204052	-1.556096	-0.034492
4	6	0	-0.906791	-1.078105	-0.057724
5	6	0	-0.569200	0.305370	-0.055937
6	6	0	-1.644484	1.209361	-0.021817
7	1	0	-3.783668	1.467198	0.072885
8	1	0	-2.418264	-2.617634	-0.042685
9	6	0	0.341787	-1.895747	-0.069832
10	6	0	1.452104	-0.913653	-0.044305
11	6	0	2.811355	-1.176113	-0.012497
12	6	0	3.667507	-0.070358	0.036722
13	6	0	3.188792	1.240572	0.052876
14	6	0	1.808829	1.490868	0.011312
15	6	0	0.925797	0.407872	-0.038149
16	1	0	3.200598	-2.186337	-0.020072
17	1	0	3.897252	2.057680	0.092230
18	1	0	1.452369	2.508582	0.002851
19	8	0	0.414942	-3.132366	-0.089359
20	7	0	5.118458	-0.297696	0.074139
21	7	0	-4.628741	-1.060647	0.044051
22	7	0	-1.487440	2.668842	-0.043768
23	8	0	5.874474	0.712651	0.121524
24	8	0	5.525517	-1.492928	0.057326
25	8	0	-2.422513	3.366111	0.434342
26	8	0	-0.444325	3.149610	-0.568618
27	8	0	-5.533369	-0.181459	0.077253
28	8	0	-4.836348	-2.305456	0.037405

Table. Cartesian coordinates of **1**

Number of imaginary frequencies = 0
Total energy (Hartree) = -11766.7182533

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.647540	-14.761514	1.913177
2	6	0	-1.349337	-14.797115	1.317519
3	6	0	-0.687444	-16.029673	1.020618
4	1	0	-1.195209	-16.955064	1.259714
5	6	0	0.550644	-16.034151	0.438270
6	1	0	1.052660	-16.963205	0.201238
7	6	0	1.220353	-14.806396	0.139005
8	6	0	0.606437	-13.556742	0.440856
9	6	0	-0.727799	-13.551966	1.012603
10	7	0	-1.353718	-12.360955	1.233076
11	6	0	-2.577258	-12.372681	1.771977
12	6	0	-3.263899	-13.542596	2.145957
13	1	0	-4.245764	-13.438857	2.585127
14	7	0	1.239892	-12.370149	0.218216
15	6	0	2.463994	-12.390667	-0.319159
16	6	0	3.143643	-13.565664	-0.689941
17	6	0	2.519276	-14.780183	-0.455564
18	1	0	4.126760	-13.468944	-1.127914
19	8	0	-3.203257	-15.982400	2.211266
20	8	0	3.067528	-16.005165	-0.750696
21	6	0	4.406868	-16.074716	-1.352059
22	6	0	4.734153	-17.549069	-1.593750
23	1	0	4.405713	-15.511092	-2.294443
24	1	0	5.125884	-15.614416	-0.663033
25	6	0	3.759016	-18.189184	-2.598215
26	1	0	3.975797	-19.256482	-2.720082
27	1	0	3.849244	-17.713636	-3.583983
28	1	0	2.723270	-18.083708	-2.262834
29	6	0	6.197037	-17.678308	-2.063814
30	1	0	4.630544	-18.063909	-0.627844
31	1	0	6.457559	-18.731300	-2.214927
32	1	0	6.897234	-17.260337	-1.330719
33	1	0	6.352131	-17.157491	-3.017573
34	6	0	-4.542088	-16.042288	2.814827
35	6	0	-4.878300	-17.514049	3.060037
36	1	0	-4.535912	-15.476771	3.756056
37	1	0	-5.259265	-15.578853	2.125983
38	6	0	-6.341248	-17.633096	3.532586
39	1	0	-6.608184	-18.684117	3.686196
40	1	0	-6.491614	-17.109427	4.485535
41	1	0	-7.039941	-17.212155	2.799760
42	6	0	-3.905680	-18.158246	4.064335
43	1	0	-4.779401	-18.031506	2.095034
44	1	0	-4.129064	-19.223882	4.188783
45	1	0	-2.869801	-18.060076	3.727149
46	1	0	-3.991358	-17.680075	5.049240
47	6	0	-3.265436	-11.050558	1.962821
48	8	0	-4.385930	-10.983906	2.526638
49	7	0	-2.563554	-9.997261	1.448514
50	1	0	-1.675573	-10.274974	1.034880
51	6	0	3.161082	-11.073311	-0.511280
52	8	0	4.283716	-11.015273	-1.071774
53	7	0	2.464182	-10.014509	-0.001857
54	1	0	1.573236	-10.285697	0.409692
55	6	0	-4.425448	-0.738547	4.274943
56	6	0	-4.148105	-1.993110	3.694373
57	7	0	-4.291910	-2.324814	2.359579
58	6	0	-3.644492	-3.140669	4.452144
59	1	0	-3.412229	-3.143433	5.505033
60	6	0	-3.505013	-4.164195	3.568167
61	1	0	-3.139437	-5.159439	3.764475
62	6	0	-3.920390	-3.652861	2.260739
63	6	0	-3.904987	-4.427066	1.081618
64	6	0	-4.205199	-3.942640	-0.203529
65	6	0	-4.207836	-4.691133	-1.432313
66	1	0	-3.991554	-5.743645	-1.507839
67	6	0	-4.525404	-3.834637	-2.458678
68	1	0	-4.597993	-4.074420	-3.506347
69	6	0	-4.752947	-2.526582	-1.903103
70	7	0	-4.550135	-2.642210	-0.537122
71	1	0	-4.654856	-1.886891	0.131946
72	6	0	-5.084692	-1.359176	-2.611799
73	6	0	-5.287039	-0.085575	-2.042096
74	6	0	-5.627538	1.103882	-2.824904
75	1	0	-5.740128	1.138571	-3.896636
76	6	0	-5.766961	2.128501	-1.942402
77	1	0	-5.997236	3.158478	-2.162275
78	6	0	-5.536990	1.571803	-0.607583
79	7	0	-5.230446	0.225882	-0.695751
80	6	0	-5.629849	2.326567	0.581089
81	6	0	-5.381659	1.826321	1.873382
82	6	0	-5.550820	2.526581	3.118771
83	1	0	-5.901079	3.541173	3.207764
84	6	0	-5.214437	1.674292	4.142944
85	1	0	-5.246534	1.883231	5.199207
86	6	0	-4.827935	0.411494	3.572748
87	7	0	-4.951904	0.549417	2.198966
88	1	0	-4.795592	-0.191378	1.523916
89	6	0	-3.553517	-5.879409	1.192933
90	6	0	-4.387934	-6.768752	1.895095
91	1	0	-5.292299	-6.387951	2.358041
92	6	0	-4.092977	-8.129088	2.002198
93	1	0	-4.751433	-8.800740	2.533357
94	6	0	-2.929110	-8.636979	1.395505
95	6	0	-2.081979	-7.758547	0.693464
96	1	0	-1.183161	-8.140705	0.217225
97	6	0	-2.390524	-6.402539	0.595691

98	1	0	-1.721711	-5.739678	0.056610
99	6	0	-4.294928	-0.603937	5.763217
100	6	0	-5.138709	-1.327873	6.627405
101	1	0	-5.892884	-1.982908	6.203681
102	6	0	-5.018186	-1.202065	8.015241
103	1	0	-5.680803	-1.764495	8.665799
104	6	0	-4.051328	-0.351385	8.564168
105	1	0	-3.957394	-0.254721	9.641271
106	6	0	-3.205810	0.373165	7.715890
107	1	0	-2.449021	1.030382	8.132939
108	6	0	-3.327093	0.248948	6.327805
109	1	0	-2.663703	0.804093	5.672515
110	6	0	-6.041179	3.763418	0.488747
111	6	0	-7.300343	4.130157	-0.026094
112	1	0	-7.980393	3.359510	-0.373299
113	6	0	-7.689840	5.466622	-0.085187
114	1	0	-8.663688	5.723670	-0.491858
115	6	0	-6.834518	6.484557	0.377469
116	6	0	-5.566553	6.137703	0.879839
117	1	0	-4.898003	6.915699	1.218416
118	6	0	-5.188940	4.794238	0.927900
119	1	0	-4.205872	4.539106	1.309753
120	6	0	-5.232861	-1.502731	-4.099573
121	6	0	-6.310427	-2.224932	-4.646293
122	1	0	-7.043710	-2.668226	-3.980070
123	6	0	-6.444380	-2.370574	-6.031862
124	1	0	-7.282988	-2.930255	-6.434097
125	6	0	-5.504913	-1.792160	-6.894027
126	1	0	-5.606748	-1.906421	-7.968810
127	6	0	-4.430970	-1.068634	-6.362043
128	1	0	-3.696094	-0.620103	-7.023453
129	6	0	-4.294982	-0.926582	-4.976825
130	1	0	-3.456833	-0.372992	-4.565988
131	6	0	5.269031	-1.472913	4.040536
132	6	0	5.503160	-0.205408	3.470576
133	7	0	5.357029	0.128767	2.136771
134	6	0	5.972095	0.951310	4.236889
135	1	0	6.174910	0.960486	5.295911
136	6	0	6.095300	1.980794	3.357473
137	1	0	6.405675	2.992470	3.565117
138	6	0	5.716776	1.460488	2.042098
139	6	0	5.709855	2.242196	0.869363
140	6	0	5.326686	1.787862	-0.404453
141	6	0	5.300720	2.554051	-1.622317
142	1	0	5.575421	3.593028	-1.696573
143	6	0	4.866751	1.736292	-2.637649
144	1	0	4.723743	2.002936	-3.671506
145	6	0	4.627949	0.426090	-2.092325
146	7	0	4.913746	0.508043	-0.738801
147	1	0	4.836683	-0.262771	-0.083896
148	6	0	4.184135	-0.709239	-2.791459
149	6	0	3.959372	-1.979467	-2.222813
150	6	0	3.520085	-3.143910	-2.994444
151	1	0	3.318326	-3.154114	-4.053612
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153	1	0	3.115273	-5.192413	-2.329484
154	6	0	3.816782	-3.664797	-0.807322
155	7	0	4.135502	-2.321940	-0.894495
156	6	0	3.836120	-4.450998	0.363285
157	6	0	4.181800	-3.986371	1.644426
158	6	0	4.222156	-4.754983	2.860444
159	1	0	3.984523	-5.803421	2.928780
160	6	0	4.609581	-3.924037	3.884028
161	1	0	4.729008	-4.183028	4.922895
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164	1	0	4.645757	-1.929327	1.326964
165	6	0	6.156049	3.671461	0.962128
166	6	0	7.506283	3.990289	1.200116
167	1	0	8.226883	3.191101	1.339642
168	6	0	7.929942	5.317251	1.252358
169	1	0	8.974991	5.541490	1.446704
170	6	0	7.014118	6.369389	1.063481
171	6	0	5.656646	6.067907	0.849917
172	1	0	4.944849	6.872371	0.733885
173	6	0	5.247566	4.732975	0.800088
174	1	0	4.198631	4.509712	0.633984
175	6	0	5.488260	-1.636200	5.517458
176	6	0	6.570992	-2.391440	6.005491
177	1	0	7.256731	-2.850870	5.300737
178	6	0	6.773523	-2.542878	7.381669
179	1	0	7.616703	-3.125034	7.740594
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181	1	0	6.053966	-2.059354	9.360100
182	6	0	4.816508	-1.188138	7.818742
183	1	0	4.129762	-0.721719	8.518331
184	6	0	4.613615	-1.036598	6.442826
185	1	0	3.772418	-0.456780	6.076899
186	6	0	3.477886	-5.902800	0.249181
187	6	0	4.313046	-6.798789	-0.442879
188	1	0	5.223787	-6.425179	-0.899339
189	6	0	4.009787	-8.157593	-0.549232
190	1	0	4.667848	-8.834773	-1.073852
191	6	0	2.837982	-8.656274	0.049719
192	6	0	1.991226	-7.770830	0.743171
193	1	0	1.087192	-8.146305	1.214841
194	6	0	2.307326	-6.416306	0.839067
195	1	0	1.639861	-5.747724	1.372846
196	6	0	3.934286	-0.535194	-4.261936
197	6	0	5.001573	-0.315774	-5.153272
198	1	0	6.017141	-0.287537	-4.771312
199	6	0	4.765738	-0.143979	-6.522016
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202	1	0	3.276108	-0.057932	-8.084372
203	6	0	2.390285	-0.412313	-6.146378
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206	1	0	1.794462	-0.743898	-4.098667
207	6	0	13.563575	11.642562	0.613640
208	6	0	12.164946	11.872418	0.793925
209	6	0	11.636916	13.183737	1.010738
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211	6	0	10.290616	13.378640	1.156835
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213	6	0	9.384941	12.272515	1.116912
214	6	0	9.872326	10.946265	0.934320
215	6	0	11.296991	10.743766	0.740686
216	7	0	11.764907	9.485866	0.499723
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231	6	0	6.384012	16.260804	0.437238
232	1	0	6.299595	17.345983	0.564764
233	1	0	5.757360	15.973379	-0.417600
234	1	0	7.423092	16.022043	0.193017
235	6	0	4.464206	15.845275	2.059666
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237	1	0	4.325899	16.924766	2.182719
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239	1	0	3.790165	15.512797	1.259573
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245	1	0	18.441401	14.869010	0.718962
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252	1	0	16.368566	15.933087	-0.403776
253	6	0	13.568167	7.925286	0.030415
254	8	0	14.795301	7.686612	-0.092525
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256	1	0	11.636091	7.420002	0.047300
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261	6	0	14.397580	-2.502923	1.457528
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266	6	0	13.830676	1.057245	1.190665
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413	6	0	-13.757664	-5.414024	1.837312
414	1	0	-13.827652	-6.481616	1.971725
415	6	0	-13.413808	-4.735028	0.586131
416	7	0	-13.401297	-3.364503	0.770605
417	6	0	-13.121608	-5.416036	-0.612741
418	6	0	-12.775738	-4.806075	-1.830378
419	6	0	-12.477585	-5.469025	-3.072305
420	1	0	-12.482213	-6.537533	-3.209937
421	6	0	-12.191538	-4.511168	-4.015438
422	1	0	-11.917391	-4.672776	-5.044673
423	6	0	-12.319241	-3.217209	-3.398830
424	7	0	-12.670283	-3.446590	-2.077939
425	1	0	-12.821724	-2.718751	-1.387660
426	6	0	-12.754589	3.032903	-0.653763
427	6	0	-13.710727	3.808732	-1.333508
428	1	0	-14.531383	3.310641	-1.839450
429	6	0	-13.632490	5.202514	-1.378032
430	1	0	-14.378904	5.785276	-1.898026
431	6	0	-12.569197	5.858457	-0.730621
432	6	0	-11.618834	5.095778	-0.026166
433	1	0	-10.808520	5.595045	0.497498
434	6	0	-11.710731	3.705120	0.009094
435	1	0	-10.962009	3.132058	0.546340
436	6	0	-11.729224	-1.978128	-5.458672
437	6	0	-12.644685	-2.396677	-6.442797
438	1	0	-13.640071	-2.707879	-6.142209
439	6	0	-12.288357	-2.400492	-7.795916
440	1	0	-13.009759	-2.721003	-8.541244
441	6	0	-11.010945	-1.984379	-8.188553
442	1	0	-10.735822	-1.983918	-9.238636
443	6	0	-10.091390	-1.566048	-7.219215
444	1	0	-9.097676	-1.241433	-7.511505
445	6	0	-10.446312	-1.564872	-5.865715
446	1	0	-9.728035	-1.245204	-5.117640
447	6	0	-13.179966	-6.917018	-0.607008
448	6	0	-14.413512	-7.587408	-0.508322
449	1	0	-15.327771	-7.006583	-0.440351
450	6	0	-14.467958	-8.985384	-0.503064
451	1	0	-15.428386	-9.486175	-0.429243
452	6	0	-13.290136	-9.736178	-0.596721
453	1	0	-13.332528	-10.820840	-0.591899
454	6	0	-12.057337	-9.080557	-0.695201
455	1	0	-11.138589	-9.654966	-0.761981
456	6	0	-12.002568	-7.682398	-0.700632
457	1	0	-11.045004	-7.175922	-0.767573
458	6	0	-14.206534	-1.901126	4.202710
459	6	0	-15.461530	-1.425835	4.627206
460	1	0	-16.173654	-1.075707	3.886716
461	6	0	-15.798537	-1.412603	5.985139
462	1	0	-16.773006	-1.047186	6.294218
463	6	0	-14.886167	-1.873905	6.941187
464	1	0	-15.147551	-1.863683	7.994681
465	6	0	-13.634752	-2.348715	6.531009
466	1	0	-12.919739	-2.704513	7.266327
467	6	0	-13.297378	-2.362097	5.173391
468	1	0	-12.324440	-2.724493	4.857628

Table. Cartesian coordinates of **1⊃G1**

Number of imaginary frequencies = 0
Total energy (Hartree) = -12955.2783307

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.508287	15.508253	-1.273590
2	6	0	-4.802285	14.901876	-1.254370
3	6	0	-6.004973	15.675914	-1.284152
4	1	0	-5.920218	16.754179	-1.323785
5	6	0	-7.229677	15.064905	-1.272571
6	1	0	-8.142640	15.645400	-1.303371
7	6	0	-7.334303	13.639689	-1.206984
8	6	0	-6.161304	12.833954	-1.155995
9	6	0	-4.863066	13.479786	-1.212518
10	7	0	-3.739327	12.709586	-1.230266
11	6	0	-2.547767	13.314944	-1.264074
12	6	0	-2.373916	14.711076	-1.272864
13	1	0	-1.365904	15.100317	-1.288995
14	7	0	-6.222940	11.477345	-1.045845
15	6	0	-7.423961	10.891468	-1.004400
16	6	0	-8.643261	11.589291	-1.080901
17	6	0	-8.597304	12.971472	-1.179159
18	1	0	-9.560744	11.019143	-1.049206
19	8	0	-3.491968	16.881892	-1.296910
20	8	0	-9.704359	13.782250	-1.248460
21	6	0	-11.046454	13.183838	-1.212925
22	6	0	-12.066133	14.316711	-1.339996
23	1	0	-11.142761	12.471456	-2.042996
24	1	0	-11.165585	12.644336	-0.265109
25	6	0	-11.937693	15.046372	-2.689299
26	1	0	-12.639732	15.886176	-2.742369
27	1	0	-12.164071	14.366548	-3.521538
28	1	0	-10.924908	15.433983	-2.832134
29	6	0	-13.486376	13.752544	-1.134202
30	1	0	-11.853876	15.032329	-0.532795
31	1	0	-14.228283	14.555977	-1.193738
32	1	0	-13.592823	13.268136	-0.156237
33	1	0	-13.733339	13.014293	-1.908131
34	6	0	-2.205783	17.592633	-1.331362
35	6	0	-2.501380	19.093226	-1.324307
36	1	0	-1.613241	17.302984	-0.453431
37	1	0	-1.665147	17.297026	-2.239073
38	6	0	-1.188614	19.874534	-1.534060
39	1	0	-1.385754	20.951535	-1.560269
40	1	0	-0.482299	19.685932	-0.715212
41	1	0	-0.698529	19.599260	-2.475571
42	6	0	-3.215454	19.524586	-0.030650
43	1	0	-3.167300	19.293615	-2.175863
44	1	0	-3.464960	20.591131	-0.064780
45	1	0	-4.139913	18.958666	0.115997
46	1	0	-2.570768	19.358473	0.842735
47	6	0	-1.330172	12.434235	-1.310376
48	8	0	-0.174282	12.921799	-1.254802
49	7	0	-1.637117	11.108446	-1.430955
50	1	0	-2.640629	10.936681	-1.458841
51	6	0	-7.455439	9.396089	-0.849415
52	8	0	-8.540384	8.764562	-0.876595
53	7	0	-6.214425	8.854138	-0.669030
54	1	0	-5.473726	9.553180	-0.680130
55	6	0	2.062990	2.271988	0.744605
56	6	0	1.675187	3.551525	0.296526
57	7	0	2.147289	4.201707	-0.831925
58	6	0	0.723130	4.400949	1.011579
59	1	0	0.228298	4.143611	1.934346
60	6	0	0.623187	5.559431	0.305777
61	1	0	0.038465	6.431714	0.550803
62	6	0	1.509141	5.429066	-0.852223
63	6	0	1.690211	6.448622	-1.811260
64	6	0	2.608403	6.407279	-2.875275
65	6	0	2.808439	7.413889	-3.883976
66	1	0	2.251828	8.333750	-3.948766

67	6	0	3.812378	6.992783	-4.722638
68	1	0	4.212410	7.519337	-5.573021
69	6	0	4.258728	5.698849	-4.280260
70	7	0	3.503313	5.387195	-3.159979
71	1	0	3.597414	4.534190	-2.619672
72	6	0	5.262485	4.906950	-4.863590
73	6	0	5.668172	3.638535	-4.400746
74	6	0	6.667850	2.813275	-5.079303
75	1	0	7.192740	3.081170	-5.982289
76	6	0	6.772183	1.658111	-4.369386
77	1	0	7.397279	0.806626	-4.585512
78	6	0	5.838254	1.763357	-3.247739
79	7	0	5.170302	2.975577	-3.291897
80	6	0	5.643965	0.736750	-2.300848
81	6	0	4.709499	0.767787	-1.251007
82	6	0	4.475909	-0.260584	-0.272243
83	1	0	5.009809	-1.195179	-0.228737
84	6	0	3.470367	0.159789	0.564704
85	1	0	3.045278	-0.380055	1.394122
86	6	0	3.056522	1.474006	0.150425
87	7	0	3.831432	1.797567	-0.953046
88	1	0	3.767431	2.668653	-1.467961
89	6	0	0.841079	7.678216	-1.705033
90	6	0	1.405486	8.941118	-1.445733
91	1	0	2.478073	9.020539	-1.301496
92	6	0	0.623041	10.094606	-1.352385
93	1	0	1.071478	11.056953	-1.151743
94	6	0	-0.770428	10.001960	-1.522611
95	6	0	-1.347650	8.745995	-1.790369
96	1	0	-2.419314	8.668911	-1.948944
97	6	0	-0.554851	7.603654	-1.874634
98	1	0	-1.015625	6.644383	-2.086198
99	6	0	1.373119	1.700366	1.948612
100	6	0	2.076654	1.493380	3.150616
101	1	0	3.123142	1.775824	3.209232
102	6	0	1.436728	0.938694	4.264123
103	1	0	1.992181	0.790605	5.185278
104	6	0	0.086600	0.575682	4.190810
105	1	0	-0.407163	0.135721	5.051765
106	6	0	-0.624066	0.779179	3.001982
107	1	0	-1.665866	0.484934	2.927392
108	6	0	0.012324	1.343542	1.890910
109	1	0	-0.546886	1.496790	0.973675
110	6	0	6.486793	-0.498051	-2.417996
111	6	0	7.873866	-0.453036	-2.181468
112	1	0	8.337315	0.486572	-1.899410
113	6	0	8.658958	-1.597922	-2.305336
114	1	0	9.729415	-1.537171	-2.129298
115	6	0	8.078867	-2.828165	-2.668929
116	6	0	6.693584	-2.889946	-2.908319
117	1	0	6.246266	-3.828381	-3.202052
118	6	0	5.920469	-1.733724	-2.780446
119	1	0	4.855101	-1.788273	-2.979590
120	6	0	5.944738	5.468049	-6.077234
121	6	0	7.300677	5.843320	-6.027869
122	1	0	7.847669	5.727696	-5.097786
123	6	0	7.939385	6.365127	-7.157740
124	1	0	8.984852	6.652049	-7.100311
125	6	0	7.233757	6.521256	-8.356643
126	1	0	7.729692	6.925820	-9.233352
127	6	0	5.885224	6.151249	-8.418651
128	1	0	5.332048	6.263137	-9.346057
129	6	0	5.246207	5.629097	-7.288825
130	1	0	4.203247	5.333602	-7.342450
131	6	0	-5.231441	0.056200	3.683852
132	6	0	-4.595816	-1.122242	3.233267
133	7	0	-3.863822	-1.263061	2.063388
134	6	0	-4.642289	-2.392174	3.955656
135	1	0	-5.157561	-2.566052	4.886563
136	6	0	-3.920410	-3.287552	3.228449
137	1	0	-3.726098	-4.320685	3.466021
138	6	0	-3.430387	-2.581080	2.045959
139	6	0	-2.585584	-3.174299	1.081264
140	6	0	-2.013319	-2.501466	-0.016390
141	6	0	-1.114679	-3.051973	-0.997025
142	1	0	-0.792317	-4.079022	-1.025063
143	6	0	-0.747693	-2.048525	-1.862432
144	1	0	-0.072304	-2.125951	-2.697710
145	6	0	-1.439387	-0.846842	-1.481749
146	7	0	-2.191701	-1.168606	-0.359574
147	1	0	-2.765439	-0.509437	0.154888
148	6	0	-1.397770	0.398747	-2.136101
149	6	0	-2.184398	1.516600	-1.784981
150	6	0	-2.268969	2.726438	-2.602743
151	1	0	-1.734498	2.893340	-3.524159
152	6	0	-3.157214	3.554432	-1.989051
153	1	0	-3.493894	4.523680	-2.320406
154	6	0	-3.608792	2.870027	-0.777515
155	7	0	-3.019907	1.620048	-0.684376
156	6	0	-4.501713	3.442218	0.152295
157	6	0	-4.963764	2.814819	1.322464
158	6	0	-5.726721	3.424221	2.377582
159	1	0	-6.063479	4.447387	2.373083
160	6	0	-5.908030	2.494825	3.374755
161	1	0	-6.414616	2.641896	4.313814
162	6	0	-5.282737	1.265356	2.967085
163	7	0	-4.725082	1.506470	1.718446
164	1	0	-4.158347	0.840051	1.205198
165	6	0	-2.237035	-4.624590	1.239453
166	6	0	-3.229935	-5.622484	1.176327
167	1	0	-4.265558	-5.342280	1.015334
168	6	0	-2.897964	-6.969938	1.307264
169	1	0	-3.682483	-7.719691	1.269054
170	6	0	-1.561407	-7.368678	1.494085
171	6	0	-0.561165	-6.381797	1.581167
172	1	0	0.463906	-6.676896	1.749444
173	6	0	-0.908161	-5.034977	1.456166
174	1	0	-0.128689	-4.284277	1.536017
175	6	0	-5.892752	0.034409	5.030148
176	6	0	-7.278799	0.238606	5.168032
177	1	0	-7.884101	0.419030	4.287087
178	6	0	-7.890228	0.205359	6.425533
179	1	0	-8.963353	0.348234	6.500020
180	6	0	-7.122966	-0.024747	7.572906
181	1	0	-7.595461	-0.051920	8.549591
182	6	0	-5.741837	-0.220844	7.452821
183	1	0	-5.137704	-0.392988	8.338178
184	6	0	-5.132536	-0.193015	6.194401
185	1	0	-4.061270	-0.340889	6.106301
186	6	0	-4.968525	4.847560	-0.076604
187	6	0	-6.321388	5.132476	-0.341482
188	1	0	-7.033056	4.316806	-0.411604
189	6	0	-6.768649	6.441192	-0.540626
190	1	0	-7.809224	6.646196	-0.746874
191	6	0	-5.852930	7.507135	-0.472057
192	6	0	-4.498826	7.234067	-0.199104
193	1	0	-3.789463	8.052470	-0.118914
194	6	0	-4.063649	5.924361	-0.010665
195	1	0	-3.017473	5.731556	0.204192
196	6	0	-0.440734	0.543469	-3.284086
197	6	0	-0.600664	-0.188554	-4.476227
198	1	0	-1.447674	-0.855968	-4.594771
199	6	0	0.317660	-0.049186	-5.523005
200	1	0	0.175251	-0.617725	-6.436846
201	6	0	1.409555	0.817017	-5.394162
202	1	0	2.126103	0.916793	-6.203525
203	6	0	1.574955	1.554678	-4.215774
204	1	0	2.424299	2.219925	-4.098775
205	6	0	0.653755	1.423904	-3.171087
206	1	0	0.791749	2.000260	-2.262488
207	6	0	-3.945853	-15.527785	0.869400
208	6	0	-2.698932	-14.900455	1.173445
209	6	0	-1.537168	-15.667025	1.498541
210	1	0	-1.621324	-16.745847	1.511387
211	6	0	-0.353039	-15.047066	1.785541
212	1	0	0.532360	-15.618833	2.031033
213	6	0	-0.256639	-13.620745	1.778048
214	6	0	-1.392474	-12.814435	1.471735
215	6	0	-2.645688	-13.475477	1.144270
216	7	0	-3.737747	-12.724915	0.819962

217	6	0	-4.886420	-13.352974	0.543449
218	6	0	-5.048788	-14.749932	0.560077
219	1	0	-6.024689	-15.152207	0.328945
220	7	0	-1.331469	-11.449485	1.485568
221	6	0	-0.163608	-10.869178	1.785019
222	6	0	1.017655	-11.573220	2.084879
223	6	0	0.969907	-12.956048	2.083216
224	1	0	1.906975	-11.000762	2.305687
225	8	0	-3.951498	-16.901438	0.911135
226	8	0	2.040924	-13.770691	2.363486
227	6	0	3.337089	-13.169618	2.707932
228	6	0	4.330467	-14.307474	2.948005
229	1	0	3.665347	-12.527178	1.880108
230	1	0	3.211371	-12.554081	3.607280
231	6	0	4.550728	-15.145999	1.676003
232	1	0	5.224532	-15.986081	1.879215
233	1	0	5.003800	-14.536289	0.882834
234	1	0	3.604742	-15.545778	1.299593
235	6	0	5.656062	-13.726153	3.479568
236	1	0	3.896638	-14.954734	3.723617
237	1	0	6.370763	-14.530496	3.684015
238	1	0	5.508387	-13.163100	4.408805
239	1	0	6.114634	-13.052988	2.743665
240	6	0	-5.195655	-17.630301	0.626600
241	6	0	-4.892760	-19.126441	0.721902
242	1	0	-5.954548	-17.329871	1.359631
243	1	0	-5.545842	-17.361874	-0.378975
244	6	0	-6.207235	-19.923469	0.600889
245	1	0	-6.012545	-20.997086	0.695475
246	1	0	-6.925626	-19.641895	1.379987
247	1	0	-6.681171	-19.756436	-0.375047
248	6	0	-3.865829	-19.565997	-0.337242
249	1	0	-4.466083	-19.305111	1.719274
250	1	0	-4.265981	-19.421335	-1.349665
251	1	0	-2.940407	-18.989257	-0.251351
252	1	0	-3.622814	-20.628345	-0.221744
253	6	0	-6.080049	-12.506713	0.201039
254	8	0	-7.209500	-13.025093	0.018106
255	7	0	-5.790026	-11.175623	0.122433
256	1	0	-4.809041	-10.971408	0.304088
257	6	0	-0.095605	-9.367964	1.805205
258	8	0	0.995092	-8.784250	2.024937
259	7	0	-1.292188	-8.751679	1.572948
260	1	0	-2.059657	-9.402521	1.422580
261	6	0	-12.398970	-4.317043	2.350635
262	6	0	-11.487679	-5.245445	1.806059
263	7	0	-10.809283	-5.126142	0.605264
264	6	0	-11.078959	-6.464884	2.502418
265	1	0	-11.437267	-6.781156	3.468874
266	6	0	-10.147739	-7.072306	1.719780
267	1	0	-9.603187	-7.978480	1.929261
268	6	0	-9.993728	-6.243769	0.523061
269	6	0	-9.121977	-6.558882	-0.540880
270	6	0	-8.951361	-5.776409	-1.698021
271	6	0	-8.143501	-6.095005	-2.843334
272	1	0	-7.559196	-6.993908	-2.947501
273	6	0	-8.262116	-5.072443	-3.755753
274	1	0	-7.779809	-5.000969	-4.716363
275	6	0	-9.154692	-4.083124	-3.214166
276	7	0	-9.542548	-4.550345	-1.966209
277	1	0	-10.194350	-4.080087	-1.347397
278	6	0	-9.535017	-2.869067	-3.815505
279	6	0	-10.353339	-1.887268	-3.218567
280	6	0	-10.764627	-0.656746	-3.895811
281	1	0	-10.499248	-0.376342	-4.902377
282	6	0	-11.555600	0.026691	-3.025801
283	1	0	-12.054534	0.968558	-3.188356
284	6	0	-11.650715	-0.785038	-1.812302
285	7	0	-10.906853	-1.944804	-1.949492
286	6	0	-12.464340	-0.437231	-0.712506
287	6	0	-12.717758	-1.262570	0.396500
288	6	0	-13.570368	-0.970781	1.517922
289	1	0	-14.099893	-0.043208	1.656989
290	6	0	-13.579204	-2.063854	2.351099
291	1	0	-14.120936	-2.172788	3.275613
292	6	0	-12.708893	-3.065047	1.795231
293	7	0	-12.208019	-2.535022	0.614117
294	1	0	-11.589538	-3.024669	-0.023460
295	6	0	-8.281382	-7.793807	-0.433832
296	6	0	-8.846790	-9.080152	-0.360174
297	1	0	-9.924361	-9.190158	-0.426387
298	6	0	-8.058692	-10.223157	-0.199747
299	1	0	-8.506388	-11.204852	-0.143013
300	6	0	-6.660335	-10.093160	-0.108923
301	6	0	-6.081637	-8.816184	-0.223584
302	1	0	-5.001062	-8.713119	-0.187773
303	6	0	-6.877493	-7.685081	-0.377378
304	1	0	-6.419065	-6.704393	-0.423104
305	6	0	-13.083799	-4.673443	3.638951
306	6	0	-14.057101	-5.689818	3.664685
307	1	0	-14.306121	-6.209416	2.744820
308	6	0	-14.704748	-6.026722	4.858014
309	1	0	-15.455969	-6.810499	4.860277
310	6	0	-14.387676	-5.353642	6.043749
311	1	0	-14.889508	-5.615159	6.970181
312	6	0	-13.417459	-4.344609	6.029150
313	1	0	-13.159310	-3.825109	6.946824
314	6	0	-12.768161	-4.004619	4.837008
315	1	0	-11.999808	-3.239001	4.829306
316	6	0	-13.151437	0.897051	-0.737077
317	6	0	-14.552289	0.983538	-0.851607
318	1	0	-15.135681	0.071636	-0.930077
319	6	0	-15.190865	2.227802	-0.879985
320	1	0	-16.271301	2.275978	-0.974885
321	6	0	-14.439811	3.406027	-0.793875
322	1	0	-14.935132	4.371661	-0.815577
323	6	0	-13.046617	3.332305	-0.680578
324	1	0	-12.456042	4.240165	-0.609363
325	6	0	-12.406177	2.088654	-0.653348
326	1	0	-11.326395	2.040686	-0.556412
327	6	0	-9.022142	-2.620292	-5.203604
328	6	0	-9.423619	-3.443330	-6.273561
329	1	0	-10.119430	-4.254615	-6.085608
330	6	0	-8.946067	-3.216515	-7.568601
331	1	0	-9.270800	-3.858415	-8.381523
332	6	0	-8.057817	-2.163777	-7.817605
333	1	0	-7.685113	-1.989401	-8.821804
334	6	0	-7.652326	-1.337227	-6.763279
335	1	0	-6.960445	-0.521328	-6.947364
336	6	0	-8.130982	-1.563053	-5.468428
337	1	0	-7.810866	-0.923879	-4.652316
338	6	0	15.724467	-6.232702	-1.826110
339	6	0	14.505409	-6.752589	-2.360267
340	6	0	14.440891	-8.035956	-2.988345
341	1	0	15.349460	-8.620159	-3.055928
342	6	0	13.256578	-8.513852	-3.479609
343	1	0	13.199085	-9.488185	-3.947323
344	6	0	12.063152	-7.729790	-3.397825
345	6	0	12.089147	-6.436358	-2.801433
346	6	0	13.335300	-5.949252	-2.238627
347	7	0	13.351653	-4.744111	-1.601692
348	6	0	14.508935	-4.302908	-1.098100
349	6	0	15.727864	-4.999121	-1.194685
350	1	0	16.608953	-4.547160	-0.762101
351	7	0	10.982019	-5.642427	-2.753314
352	6	0	9.837775	-6.110058	-3.262833
353	6	0	9.694025	-7.385184	-3.840117
354	6	0	10.814732	-8.196957	-3.912528
355	1	0	8.720125	-7.668981	-4.212609
356	8	0	16.833521	-7.028986	-1.980930
357	8	0	10.827511	-9.455717	-4.463629
358	6	0	9.592333	-10.008992	-5.037068
359	6	0	9.904459	-11.416088	-5.548722
360	1	0	8.817014	-10.034564	-4.259880
361	1	0	9.258413	-9.353734	-5.851092
362	6	0	10.328215	-12.354593	-4.404487
363	1	0	10.597005	-13.342602	-4.795118
364	1	0	9.506654	-12.488918	-3.688135
365	1	0	11.189216	-11.951558	-3.863535
366	6	0	8.681786	-11.967026	-6.309758

367	1	0	10.742570	-11.323126	-6.254164
368	1	0	8.897929	-12.964008	-6.708281
369	1	0	8.402995	-11.321605	-7.151172
370	1	0	7.811552	-12.055615	-5.646578
371	6	0	18.129143	-6.579901	-1.451527
372	6	0	19.169830	-7.645854	-1.797844
373	1	0	18.386550	-5.614461	-1.906960
374	1	0	18.038852	-6.448595	-0.366073
375	6	0	20.506565	-7.297930	-1.112428
376	1	0	21.256566	-8.066750	-1.326672
377	1	0	20.899192	-6.339996	-1.477328
378	1	0	20.398115	-7.227901	-0.023518
379	6	0	19.338476	-7.800358	-3.320103
380	1	0	18.803807	-8.597820	-1.387264
381	1	0	20.048760	-8.602503	-3.550348
382	1	0	18.384243	-8.036453	-3.799776
383	1	0	19.724046	-6.872935	-3.764217
384	6	0	14.490855	-2.990572	-0.365987
385	8	0	15.552399	-2.482159	0.072446
386	7	0	13.236089	-2.467389	-0.230322
387	1	0	12.516638	-3.044331	-0.662179
388	6	0	8.641898	-5.200256	-3.233832
389	8	0	7.517077	-5.602054	-3.621659
390	7	0	8.931529	-3.944973	-2.779064
391	1	0	9.908724	-3.833179	-2.515955
392	6	0	11.646513	7.100167	1.509902
393	6	0	11.776736	5.699946	1.415002
394	7	0	11.313022	4.772300	2.330123
395	6	0	12.457961	5.026115	0.307799
396	1	0	12.918656	5.515844	-0.535178
397	6	0	12.387300	3.691640	0.557268
398	1	0	12.769990	2.886839	-0.049635
399	6	0	11.678037	3.535975	1.829131
400	6	0	11.404717	2.284948	2.420073
401	6	0	10.706242	2.095773	3.625568
402	6	0	10.419406	0.841532	4.270026
403	1	0	10.716287	-0.122086	3.890929
404	6	0	9.718163	1.098979	5.423503
405	1	0	9.342016	0.378772	6.130885
406	6	0	9.561188	2.523864	5.548863
407	7	0	10.171643	3.083550	4.437599
408	1	0	10.222218	4.078083	4.244281
409	6	0	8.906891	3.210657	6.585796
410	6	0	8.770070	4.610516	6.676861
411	6	0	8.090961	5.285545	7.785055
412	1	0	7.629928	4.796609	8.628283
413	6	0	8.160673	6.619802	7.533966
414	1	0	7.757569	7.424537	8.127759
415	6	0	8.898773	6.775798	6.278873
416	7	0	9.256480	5.538779	5.774415
417	6	0	9.171744	8.025550	5.686757
418	6	0	9.861202	8.215084	4.477276
419	6	0	10.167875	9.471069	3.845232
420	1	0	9.893470	10.435558	4.239072
421	6	0	10.851230	9.212935	2.681244
422	1	0	11.217392	9.932351	1.967782
423	6	0	11.009639	7.787973	2.556355
424	7	0	10.393732	7.227471	3.663988
425	1	0	10.337082	6.232450	3.853064
426	6	0	11.896049	1.049691	1.726305
427	6	0	13.272063	0.774908	1.624560
428	1	0	13.982344	1.470522	2.059372
429	6	0	13.750347	-0.372306	0.988005
430	1	0	14.809857	-0.574167	0.927250
431	6	0	12.838590	-1.286874	0.428663
432	6	0	11.458526	-1.026040	0.524941
433	1	0	10.745519	-1.729293	0.103656
434	6	0	10.997069	0.124523	1.162362
435	1	0	9.929964	0.312748	1.219384
436	6	0	12.225833	7.942035	0.408982
437	6	0	13.367635	8.733507	0.633740
438	1	0	13.835348	8.722770	1.613120
439	6	0	13.905506	9.518986	-0.391728
440	1	0	14.789788	10.119628	-0.202222
441	6	0	13.310099	9.526355	-1.658486
442	1	0	13.727259	10.135706	-2.454064
443	6	0	12.173793	8.743280	-1.893688
444	1	0	11.703470	8.746544	-2.872119
445	6	0	11.635774	7.957670	-0.868680
446	1	0	10.751333	7.355746	-1.050835
447	6	0	8.696030	9.263682	6.390792
448	6	0	9.284833	9.672382	7.602166
449	1	0	10.093617	9.083532	8.022784
450	6	0	8.841973	10.826047	8.258010
451	1	0	9.309699	11.128237	9.189964
452	6	0	7.803415	11.590731	7.713613
453	1	0	7.459548	12.485504	8.222926
454	6	0	7.210060	11.194390	6.509399
455	1	0	6.400247	11.778367	6.083143
456	6	0	7.652710	10.040627	5.853180
457	1	0	7.184798	9.729874	4.924521
458	6	0	8.308027	2.368455	7.675712
459	6	0	9.129985	1.675727	8.584284
460	1	0	10.208244	1.762954	8.496090
461	6	0	8.570693	0.891074	9.598826
462	1	0	9.219832	0.367540	10.293925
463	6	0	7.180338	0.785996	9.721769
464	1	0	6.746388	0.177570	10.509005
465	6	0	6.352601	1.470570	8.824048
466	1	0	5.273300	1.391956	8.910527
467	6	0	6.911470	2.254847	7.809285
468	1	0	6.268509	2.780675	7.110840
469	6	0	-8.946627	-1.325745	2.033133
470	6	0	-8.870606	-0.100768	1.388087
471	1	0	-9.453987	0.738339	1.738778
472	6	0	-8.027753	0.058860	0.276339
473	6	0	-7.254842	-1.015766	-0.206027
474	6	0	-7.398924	-2.248518	0.495613
475	6	0	-8.216717	-2.435022	1.592452
476	1	0	-8.291198	-3.395638	2.085246
477	6	0	-6.544466	-3.286115	-0.136632
478	6	0	-5.905013	-2.622507	-1.289756
479	6	0	-6.294025	-1.253914	-1.335570
480	6	0	-5.765606	-0.441061	-2.344412
481	6	0	-4.904936	-1.008415	-3.297363
482	6	0	-4.571019	-2.361647	-3.231249
483	6	0	-5.053113	-3.194875	-2.216361
484	1	0	-5.995992	0.608637	-2.398658
485	1	0	-4.489253	-0.399687	-4.089051
486	1	0	-4.773701	-4.238855	-2.168709
487	8	0	-6.401508	-4.458220	0.248147
488	7	0	-9.797409	-1.448076	3.215472
489	8	0	-9.879180	-2.583438	3.762702
490	8	0	-10.391557	-0.414223	3.636870
491	7	0	-8.024878	1.406194	-0.296416
492	8	0	-8.904735	2.225863	0.100005
493	8	0	-7.137719	1.712436	-1.137688
494	7	0	-3.694204	-2.933345	-4.254115
495	8	0	-3.395735	-4.156685	-4.164380
496	8	0	-3.286971	-2.174083	-5.182115

Table. Cartesian coordinates of **1⊃G1$_2$**

Number of imaginary frequencies = 0
Total energy (Hartree) = -14143.8276381

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.723583	-14.497400	0.306319
2	6	0	-1.350846	-14.528858	-0.088594
3	6	0	-0.674109	-15.756202	-0.373675
4	1	0	-1.229847	-16.680698	-0.285435
5	6	0	0.639049	-15.756234	-0.758028
6	1	0	1.154352	-16.680645	-0.984440
7	6	0	1.370140	-14.530979	-0.856217
8	6	0	0.739281	-13.288473	-0.560209

9	6	0	-0.667232	-13.284172	-0.201850
10	7	0	-1.297399	-12.093380	0.008797
11	6	0	-2.588122	-12.107539	0.357056
12	6	0	-3.344718	-13.280425	0.536508
13	1	0	-4.379290	-13.179404	0.831620
14	7	0	1.421716	-12.108942	-0.590161
15	6	0	2.715677	-12.127479	-0.926137
16	6	0	3.424073	-13.292437	-1.273585
17	6	0	2.747425	-14.501165	-1.235456
18	1	0	4.466714	-13.194644	-1.540127
19	8	0	-3.341056	-15.719207	0.423587
20	8	0	3.312679	-15.717517	-1.533502
21	6	0	4.730317	-15.784910	-1.916079
22	6	0	5.064346	-17.247269	-2.214617
23	1	0	4.892693	-15.154637	-2.800484
24	1	0	5.336596	-15.398496	-1.087405
25	6	0	4.252957	-17.782006	-3.408468
26	1	0	4.466331	-18.843836	-3.575589
27	1	0	4.510795	-17.239119	-4.327614
28	1	0	3.178726	-17.669036	-3.236292
29	6	0	6.581381	-17.387464	-2.452732
30	1	0	4.795819	-17.827465	-1.320185
31	1	0	6.842900	-18.434316	-2.640297
32	1	0	7.161296	-17.045751	-1.587099
33	1	0	6.898910	-16.804008	-3.326650
34	6	0	-4.757272	-15.782562	0.811935
35	6	0	-5.155417	-17.257386	0.886813
36	1	0	-4.883837	-15.289819	1.785051
37	1	0	-5.351791	-15.246704	0.061588
38	6	0	-6.675330	-17.365817	1.123100
39	1	0	-6.983025	-18.416548	1.150738
40	1	0	-6.958839	-16.911365	2.081264
41	1	0	-7.245885	-16.868967	0.329366
42	6	0	-4.359859	-18.005289	1.971843
43	1	0	-4.920852	-17.703706	-0.090191
44	1	0	-4.620780	-19.069637	1.977088
45	1	0	-3.282997	-17.915034	1.802743
46	1	0	-4.584696	-17.599659	2.967300
47	6	0	-3.274547	-10.783328	0.539583
48	8	0	-4.462203	-10.725692	0.943468
49	7	0	-2.491451	-9.715698	0.199642
50	1	0	-1.557609	-9.987029	-0.101797
51	6	0	3.457723	-10.820918	-0.898448
52	8	0	4.659342	-10.754540	-1.257529
53	7	0	2.701099	-9.783296	-0.431893
54	1	0	1.749422	-10.060397	-0.198235
55	6	0	-4.513897	-0.544011	3.212826
56	6	0	-4.148986	-1.765684	2.607029
57	7	0	-4.241984	-2.062575	1.256959
58	6	0	-3.632306	-2.920037	3.345052
59	1	0	-3.422213	-2.946998	4.401979
60	6	0	-3.450367	-3.917538	2.438069
61	1	0	-3.071758	-4.911280	2.616429
62	6	0	-3.831070	-3.378685	1.133039
63	6	0	-3.737627	-4.118762	-0.064424
64	6	0	-3.921691	-3.590355	-1.353522
65	6	0	-3.832701	-4.300332	-2.601201
66	1	0	-3.650052	-5.358352	-2.688865
67	6	0	-4.028028	-3.402793	-3.624193
68	1	0	-4.029164	-3.610390	-4.681313
69	6	0	-4.257305	-2.103498	-3.049544
70	7	0	-4.198061	-2.269656	-1.674080
71	1	0	-4.366264	-1.537039	-0.993693
72	6	0	-4.511254	-0.906846	-3.744010
73	6	0	-4.846144	0.324008	-3.140745
74	6	0	-5.060716	1.561685	-3.889695
75	1	0	-4.958022	1.674667	-4.956890
76	6	0	-5.397591	2.518583	-2.982051
77	1	0	-5.612161	3.557628	-3.172299
78	6	0	-5.385072	1.879990	-1.666578
79	7	0	-5.025888	0.547048	-1.784164
80	6	0	-5.684310	2.560917	-0.465862
81	6	0	-5.537693	2.016064	0.824464
82	6	0	-5.868683	2.645789	2.074232
83	1	0	-6.323393	3.617540	2.168162
84	6	0	-5.521317	1.792228	3.095324
85	1	0	-5.645912	1.961230	4.151890
86	6	0	-4.975977	0.592511	2.519191
87	7	0	-5.024015	0.765918	1.143412
88	1	0	-4.750675	0.065002	0.463699
89	6	0	-3.409394	-5.578917	0.028317
90	6	0	-4.331781	-6.486305	0.582119
91	1	0	-5.287780	-6.122011	0.941278
92	6	0	-4.058325	-7.853395	0.657382
93	1	0	-4.783546	-8.540044	1.068563
94	6	0	-2.832775	-8.348154	0.173916
95	6	0	-1.897385	-7.448803	-0.373104
96	1	0	-0.948603	-7.819643	-0.751436
97	6	0	-2.184120	-6.086060	-0.445087
98	1	0	-1.449834	-5.406512	-0.865692
99	6	0	-4.426147	-0.427259	4.704650
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101	1	0	-5.795226	-2.045588	5.110214
102	6	0	-5.091753	-1.159276	6.939116
103	1	0	-5.683103	-1.821084	7.563669
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105	1	0	-4.216593	-0.083826	8.595057
106	6	0	-3.527608	0.670257	6.691518
107	1	0	-2.882291	1.424787	7.130342
108	6	0	-3.604645	0.550787	5.300131
109	1	0	-3.017480	1.207256	4.666414
110	6	0	-6.199543	3.963359	-0.558376
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113	6	0	-7.893151	5.543941	-1.318340
114	1	0	-8.818877	5.735177	-1.853862
115	6	0	-7.200422	6.610944	-0.715024
116	6	0	-5.991382	6.351860	-0.043199
117	1	0	-5.441139	7.171433	0.396332
118	6	0	-5.511933	5.042078	0.030573
119	1	0	-4.574179	4.855013	0.543450
120	6	0	-4.409431	-0.962782	-5.239781
121	6	0	-5.536643	-0.743113	-6.054980
122	1	0	-6.498757	-0.532367	-5.598874
123	6	0	-5.426324	-0.797612	-7.448746
124	1	0	-6.306024	-0.628715	-8.061812
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126	1	0	-4.108641	-1.109531	-9.131715
127	6	0	-3.064188	-1.285286	-7.249244
128	1	0	-2.100838	-1.487102	-7.707160
129	6	0	-3.171640	-1.233345	-5.855651
130	1	0	-2.293311	-1.384056	-5.236224
131	6	0	7.166293	-2.060000	3.765430
132	6	0	7.123443	-0.683787	3.449591
133	7	0	6.329495	-0.085939	2.484261
134	6	0	7.959597	0.319638	4.109059
135	1	0	8.678705	0.123360	4.887935
136	6	0	7.650772	1.520689	3.549753
137	1	0	8.059044	2.486393	3.799884
138	6	0	6.625699	1.267415	2.537777
139	6	0	5.995788	2.291290	1.795010
140	6	0	4.913463	2.092918	0.915271
141	6	0	4.202496	3.097960	0.169347
142	1	0	4.448724	4.146230	0.162868
143	6	0	3.174693	2.487833	-0.510443
144	1	0	2.447226	2.960734	-1.148632
145	6	0	3.237328	1.074314	-0.252369
146	7	0	4.303545	0.882880	0.615367
147	1	0	4.579437	-0.011386	1.006951
148	6	0	2.412727	0.077914	-0.805686
149	6	0	2.597781	-1.310810	-0.639910
150	6	0	1.839598	-2.312245	-1.391869
151	1	0	1.064854	-2.096843	-2.110234
152	6	0	2.327186	-3.528981	-1.028353
153	1	0	2.029818	-4.496943	-1.398678
154	6	0	3.369209	-3.286163	-0.029898
155	7	0	3.533428	-1.926617	0.172680
156	6	0	4.067053	-4.314318	0.637412
157	6	0	5.048839	-4.107627	1.623205
158	6	0	5.644909	-5.108366	2.465597

159	1	0	5.433899	-6.162788	2.402601
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169	1	0	9.256306	5.633657	1.503668
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171	6	0	6.053907	6.029228	2.607618
172	1	0	5.389546	6.786141	2.997316
173	6	0	5.631378	4.705370	2.471856
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175	6	0	8.023397	-2.492016	4.919343
176	6	0	9.128131	-3.344523	4.735090
177	1	0	9.369193	-3.703240	3.741033
178	6	0	9.926517	-3.732367	5.816178
179	1	0	10.782356	-4.376479	5.642220
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181	1	0	10.247475	-3.578866	7.946440
182	6	0	8.528087	-2.437870	7.306546
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185	1	0	6.879457	-1.396787	6.383847
186	6	0	3.717046	-5.738478	0.331112
187	6	0	4.657427	-6.604328	-0.258446
188	1	0	5.638369	-6.224986	-0.523569
189	6	0	4.353560	-7.940230	-0.529843
190	1	0	5.084882	-8.593043	-0.983522
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193	1	0	1.149805	-7.971932	0.649711
194	6	0	2.444562	-6.256154	0.642018
195	1	0	1.704793	-5.613407	1.107591
196	6	0	1.241671	0.532567	-1.629347
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199	6	0	0.296206	1.577885	-3.616491
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207	6	0	13.315510	12.261041	0.602037
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278	6	0	10.472668	-1.102152	-4.582901
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281	1	0	9.766613	-3.651728	-5.734139
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291	1	0	15.606156	-4.530472	1.218831
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295	6	0	12.708516	3.520173	-1.279923
296	6	0	13.845795	4.338340	-1.410782
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400	6	0	-12.883137	1.367981	0.002650
401	6	0	-13.044765	1.116055	1.375588
402	6	0	-13.352268	2.084128	2.394341
403	1	0	-13.463313	3.140603	2.215993
404	6	0	-13.476695	1.425465	3.593749
405	1	0	-13.696960	1.857635	4.555690
406	6	0	-13.243329	0.024240	3.365455
407	7	0	-12.987561	-0.115056	2.009802
408	1	0	-12.800936	-0.999038	1.549537
409	6	0	-13.225124	-0.996066	4.332305
410	6	0	-12.874299	-2.338523	4.078837
411	6	0	-12.815822	-3.372599	5.113066
412	1	0	-13.037510	-3.225776	6.157973
413	6	0	-12.433072	-4.523778	4.497204
414	1	0	-12.277490	-5.492043	4.945655
415	6	0	-12.284271	-4.213768	3.074432
416	7	0	-12.543733	-2.873431	2.844816
417	6	0	-11.951295	-5.177095	2.100555
418	6	0	-11.874172	-4.941282	0.717365
419	6	0	-11.592187	-5.913347	-0.304896
420	1	0	-11.358854	-6.947674	-0.113607
421	6	0	-11.674263	-5.291392	-1.527951
422	1	0	-11.509314	-5.735872	-2.495196
423	6	0	-12.014552	-3.909455	-1.312557
424	7	0	-12.109654	-3.741379	0.061087
425	1	0	-12.352142	-2.868207	0.516148
426	6	0	-12.898048	2.809331	-0.415421
427	6	0	-13.953307	3.361974	-1.162181
428	1	0	-14.795782	2.734627	-1.435436
429	6	0	-13.950709	4.702982	-1.556278
430	1	0	-14.772176	5.119457	-2.121497
431	6	0	-12.865847	5.526804	-1.203280
432	6	0	-11.806549	4.985574	-0.450333
433	1	0	-10.968465	5.616826	-0.167599
434	6	0	-11.823577	3.648781	-0.059434
435	1	0	-11.002271	3.245031	0.524389
436	6	0	-12.121560	-3.369746	-3.724063
437	6	0	-13.078228	-4.278740	-4.218611
438	1	0	-13.862260	-4.633588	-3.557514
439	6	0	-13.035701	-4.712154	-5.547556
440	1	0	-13.786145	-5.407665	-5.910368
441	6	0	-12.035815	-4.245118	-6.408608
442	1	0	-12.003067	-4.580166	-7.440478
443	6	0	-11.080884	-3.340375	-5.931049
444	1	0	-10.301527	-2.969872	-6.589255
445	6	0	-11.122195	-2.907019	-4.601603
446	1	0	-10.377276	-2.202928	-4.248184
447	6	0	-11.713670	-6.591735	2.553747
448	6	0	-12.796723	-7.403882	2.939725
449	1	0	-13.802461	-6.996952	2.907521
450	6	0	-12.586391	-8.722425	3.356881
451	1	0	-13.432989	-9.335758	3.649723
452	6	0	-11.290146	-9.250242	3.393068
453	1	0	-11.126467	-10.273336	3.716718
454	6	0	-10.206275	-8.451563	3.011462
455	1	0	-9.197145	-8.850034	3.040618
456	6	0	-10.415323	-7.131637	2.594546
457	1	0	-9.565638	-6.518341	2.313428
458	6	0	-13.619191	-0.604440	5.727481

459	6	0	-14.951326	-0.241593	6.005597
460	1	0	-15.683219	-0.256126	5.204177
461	6	0	-15.337140	0.123059	7.299650
462	1	0	-16.369641	0.394334	7.497049
463	6	0	-14.397036	0.133080	8.336855
464	1	0	-14.695707	0.416154	9.341339
465	6	0	-13.069742	-0.222348	8.070789
466	1	0	-12.331546	-0.210985	8.866444
467	6	0	-12.681817	-0.588387	6.776968
468	1	0	-11.647305	-0.847881	6.579671
469	6	0	-8.671615	-1.943260	4.343565
470	6	0	-8.181362	-3.045762	3.659956
471	1	0	-7.898981	-3.940713	4.195659
472	6	0	-8.038204	-3.001466	2.264383
473	6	0	-8.391096	-1.848184	1.536034
474	6	0	-8.908949	-0.762084	2.302185
475	6	0	-9.059498	-0.777150	3.674242
476	1	0	-9.453190	0.078870	4.207003
477	6	0	-9.248322	0.371519	1.398492
478	6	0	-8.926450	-0.104745	0.037577
479	6	0	-8.400855	-1.425975	0.097864
480	6	0	-8.025840	-2.055825	-1.092875
481	6	0	-8.192256	-1.373548	-2.305727
482	6	0	-8.719881	-0.081979	-2.323107
483	6	0	-9.092438	0.582342	-1.150111
484	1	0	-7.602516	-3.044611	-1.097156
485	1	0	-7.901567	-1.841230	-3.236409
486	1	0	-9.511926	1.578728	-1.176785
487	8	0	-9.697199	1.476604	1.741287
488	7	0	-8.755535	-2.000259	5.801319
489	8	0	-9.317201	-1.036472	6.395990
490	8	0	-8.245734	-2.995105	6.390891
491	7	0	-7.496509	-4.226280	1.671140
492	8	0	-7.426973	-5.259211	2.401856
493	8	0	-7.103105	-4.209914	0.475656
494	7	0	-8.886878	0.600570	-3.603028
495	8	0	-9.176883	1.829260	-3.592736
496	8	0	-8.740340	-0.076858	-4.665017
497	6	0	10.584658	-2.507725	1.238747
498	6	0	9.774366	-3.490193	0.691649
499	1	0	9.937328	-4.530235	0.934315
500	6	0	8.730256	-3.139865	-0.179965
501	6	0	8.486199	-1.791863	-0.512099
502	6	0	9.373592	-0.840260	0.071761
503	6	0	10.409357	-1.154948	0.928825
504	1	0	11.055014	-0.390073	1.340119
505	6	0	9.012228	0.526077	-0.383140
506	6	0	7.868666	0.348776	-1.298637
507	6	0	7.516135	-1.028983	-1.369691
508	6	0	6.417618	-1.397200	-2.154550
509	6	0	5.730581	-0.407851	-2.875552
510	6	0	6.130015	0.926823	-2.801910
511	6	0	7.199773	1.335838	-1.998583
512	1	0	6.084299	-2.418164	-2.211084
513	1	0	4.881460	-0.672308	-3.491206
514	1	0	7.486890	2.376872	-1.934461
515	8	0	9.562104	1.586052	-0.041681
516	7	0	11.634382	-2.901107	2.176753
517	8	0	12.378160	-1.990938	2.638831
518	8	0	11.734073	-4.122933	2.488240
519	7	0	7.951703	-4.274483	-0.680089
520	8	0	8.327698	-5.442510	-0.367743
521	8	0	6.932416	-4.055769	-1.387847
522	7	0	5.412615	1.932750	-3.585650
523	8	0	5.777883	3.136860	-3.484387
524	8	0	4.466882	1.543237	-4.332665

Table. Cartesian coordinates of **1⊃G1$_3$**

Number of imaginary frequencies = 0

Total energy (Hartree) = -15332.3714923

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.340800	-14.577515	-0.506440
2	6	0	-0.952930	-14.528712	-0.839496
3	6	0	-0.197229	-15.721613	-1.061196
4	1	0	-0.704263	-16.673515	-0.972411
5	6	0	1.129263	-15.654813	-1.384692
6	1	0	1.708174	-16.552075	-1.560454
7	6	0	1.790213	-14.391588	-1.487510
8	6	0	1.079235	-13.176402	-1.259724
9	6	0	-0.339967	-13.245855	-0.952555
10	7	0	-1.051139	-12.092033	-0.785504
11	6	0	-2.352664	-12.184782	-0.490793
12	6	0	-3.044418	-13.399321	-0.327733
13	1	0	-4.095375	-13.356085	-0.080834
14	7	0	1.698683	-11.960858	-1.311791
15	6	0	3.005479	-11.924405	-1.595732
16	6	0	3.790502	-13.061102	-1.863369
17	6	0	3.178971	-14.301398	-1.808282
18	1	0	4.836912	-12.913880	-2.088671
19	8	0	-2.886534	-15.833570	-0.391364
20	8	0	3.820667	-15.495072	-2.036665
21	6	0	5.255452	-15.497275	-2.355162
22	6	0	5.680530	-16.948474	-2.584504
23	1	0	5.423643	-14.890125	-3.254528
24	1	0	5.802437	-15.049405	-1.516235
25	6	0	4.954087	-17.568167	-3.791916
26	1	0	5.231295	-18.621807	-3.910141
27	1	0	5.224052	-17.044034	-4.718442
28	1	0	3.868628	-17.508571	-3.671020
29	6	0	7.212139	-17.013112	-2.750963
30	1	0	5.402980	-17.511272	-1.681740
31	1	0	7.537598	-18.049828	-2.888113
32	1	0	7.732865	-16.610198	-1.874086
33	1	0	7.537483	-16.443534	-3.631141
34	6	0	-4.312022	-15.977327	-0.063832
35	6	0	-4.621869	-17.472362	0.026594
36	1	0	-4.512319	-15.474406	0.891543
37	1	0	-4.904096	-15.494328	-0.851085
38	6	0	-6.141421	-17.670764	0.197760
39	1	0	-6.384986	-18.737870	0.235970
40	1	0	-6.495677	-17.215449	1.131658
41	1	0	-6.704571	-17.226583	-0.631679
42	6	0	-3.832181	-18.147509	1.162439
43	1	0	-4.315967	-17.922432	-0.928716
44	1	0	-4.026851	-19.225822	1.180049
45	1	0	-2.756333	-17.993262	1.039427
46	1	0	-4.126948	-17.737206	2.137531
47	6	0	-3.139071	-10.913366	-0.343230
48	8	0	-4.352682	-10.948993	-0.020205
49	7	0	-2.419323	-9.783525	-0.610069
50	1	0	-1.448655	-9.972423	-0.850720
51	6	0	3.690655	-10.587217	-1.607956
52	8	0	4.910627	-10.498560	-1.895407
53	7	0	2.874018	-9.547552	-1.267609
54	1	0	1.916973	-9.835259	-1.074790
55	6	0	-4.107830	-0.444501	2.198648
56	6	0	-3.842963	-1.703876	1.613795
57	7	0	-4.274420	-2.120985	0.364334
58	6	0	-3.084361	-2.771039	2.268282
59	1	0	-2.606310	-2.703249	3.232097
60	6	0	-3.101983	-3.841362	1.426160
61	1	0	-2.650561	-4.809230	1.576006
62	6	0	-3.849528	-3.434585	0.238714
63	6	0	-4.097190	-4.297293	-0.846842
64	6	0	-4.746395	-3.943329	-2.040530
65	6	0	-4.997848	-4.805261	-3.164438
66	1	0	-4.742687	-5.851428	-3.196023
67	6	0	-5.597646	-4.063998	-4.153890
68	1	0	-5.910067	-4.406557	-5.126057

69	6	0	-5.732222	-2.710544	-3.686028
70	7	0	-5.222162	-2.689296	-2.394934
71	1	0	-5.244624	-1.876102	-1.789471
72	6	0	-6.242086	-1.609267	-4.395881
73	6	0	-6.372261	-0.308249	-3.862888
74	6	0	-6.821190	0.844731	-4.640544
75	1	0	-7.066067	0.833532	-5.690075
76	6	0	-6.835845	1.909668	-3.794023
77	1	0	-7.096082	2.929825	-4.024645
78	6	0	-6.394266	1.420600	-2.488157
79	7	0	-6.094205	0.068961	-2.557920
80	6	0	-6.307020	2.237444	-1.340739
81	6	0	-5.801909	1.833424	-0.090042
82	6	0	-5.811999	2.598951	1.125825
83	1	0	-6.244184	3.580185	1.225044
84	6	0	-5.202686	1.859214	2.112048
85	1	0	-5.060739	2.146231	3.140217
86	6	0	-4.786077	0.605394	1.547150
87	7	0	-5.188238	0.624162	0.217105
88	1	0	-5.106125	-0.168963	-0.409916
89	6	0	-3.648398	-5.729303	-0.739844
90	6	0	-4.550529	-6.725577	-0.327669
91	1	0	-5.560508	-6.443286	-0.048636
92	6	0	-4.175029	-8.069425	-0.263572
93	1	0	-4.878132	-8.826101	0.051148
94	6	0	-2.866904	-8.445572	-0.623327
95	6	0	-1.953670	-7.452568	-1.024293
96	1	0	-0.944915	-7.733011	-1.313571
97	6	0	-2.337732	-6.112675	-1.076903
98	1	0	-1.613174	-5.361314	-1.374176
99	6	0	-3.662746	-0.192794	3.605845
100	6	0	-4.067057	-1.037264	4.659244
101	1	0	-4.700896	-1.889849	4.444403
102	6	0	-3.666363	-0.791516	5.975997
103	1	0	-4.007403	-1.449562	6.768654
104	6	0	-2.844902	0.303962	6.266262
105	1	0	-2.533655	0.497565	7.287604
106	6	0	-2.428461	1.148724	5.230349
107	1	0	-1.786839	1.997363	5.446750
108	6	0	-2.833586	0.905365	3.913973
109	1	0	-2.504776	1.559191	3.113332
110	6	0	-6.795800	3.649646	-1.434984
111	6	0	-8.147854	3.929912	-1.713179
112	1	0	-8.842242	3.117423	-1.898193
113	6	0	-8.607713	5.243148	-1.764059
114	1	0	-9.654894	5.437230	-1.978624
115	6	0	-7.725922	6.319866	-1.550128
116	6	0	-6.366006	6.057113	-1.300415
117	1	0	-5.680411	6.881826	-1.167963
118	6	0	-5.919363	4.734922	-1.240411
119	1	0	-4.867283	4.538738	-1.058621
120	6	0	-6.637072	-1.843886	-5.823459
121	6	0	-7.972519	-1.686449	-6.241618
122	1	0	-8.732347	-1.388810	-5.526119
123	6	0	-8.330127	-1.909505	-7.575707
124	1	0	-9.364743	-1.785952	-7.879894
125	6	0	-7.361352	-2.289155	-8.511752
126	1	0	-7.640214	-2.460402	-9.546819
127	6	0	-6.029676	-2.440437	-8.107251
128	1	0	-5.269611	-2.721577	-8.829544
129	6	0	-5.667327	-2.220268	-6.774417
130	1	0	-4.630765	-2.313482	-6.468284
131	6	0	6.121648	-1.436251	3.156126
132	6	0	6.217388	-0.099879	2.710833
133	7	0	5.815869	0.384964	1.474537
134	6	0	6.799672	0.975714	3.511681
135	1	0	7.192804	0.869498	4.509778
136	6	0	6.735424	2.107192	2.759750
137	1	0	7.056410	3.098215	3.036191
138	6	0	6.122534	1.736694	1.483863
139	6	0	5.855022	2.664014	0.451217
140	6	0	5.169847	2.366836	-0.743320
141	6	0	4.865114	3.276294	-1.816823
142	1	0	5.167278	4.309400	-1.849175
143	6	0	4.135010	2.600213	-2.766086
144	1	0	3.742247	2.997492	-3.687238
145	6	0	3.989987	1.235015	-2.338185
146	7	0	4.633710	1.139824	-1.111431
147	1	0	4.694692	0.291783	-0.558291
148	6	0	3.340432	0.196808	-3.030063
149	6	0	3.307173	-1.152024	-2.617589
150	6	0	2.737855	-2.231007	-3.427955
151	1	0	2.266508	-2.106976	-4.390233
152	6	0	2.955562	-3.390050	-2.748310
153	1	0	2.689291	-4.392644	-3.043213
154	6	0	3.648554	-3.032045	-1.511063
155	7	0	3.854001	-1.663324	-1.452540
156	6	0	4.033773	-3.974548	-0.537724
157	6	0	4.676151	-3.670070	0.674056
158	6	0	4.952132	-4.586702	1.747764
159	1	0	4.725573	-5.639563	1.720990
160	6	0	5.506491	-3.880262	2.788591
161	1	0	5.797112	-4.261689	3.752887
162	6	0	5.617576	-2.502361	2.391133
163	7	0	5.106564	-2.422915	1.103298
164	1	0	5.023895	-1.564211	0.569988
165	6	0	6.303008	4.082864	0.635171
166	6	0	7.668023	4.405569	0.771890
167	1	0	8.412178	3.616655	0.746738
168	6	0	8.077456	5.729322	0.924686
169	1	0	9.133964	5.951645	1.040751
170	6	0	7.139078	6.778290	0.935528
171	6	0	5.770201	6.469585	0.821698
172	1	0	5.041330	7.265691	0.854163
173	6	0	5.373364	5.139138	0.676091
174	1	0	4.314324	4.915419	0.598926
175	6	0	6.580637	-1.758235	4.548899
176	6	0	7.702003	-2.579495	4.767545
177	1	0	8.232474	-2.996333	3.919090
178	6	0	8.141335	-2.868270	6.063607
179	1	0	9.018188	-3.492370	6.203194
180	6	0	7.456915	-2.344152	7.165827
181	1	0	7.795216	-2.564673	8.173375
182	6	0	6.330206	-1.538268	6.961662
183	1	0	5.784881	-1.140785	7.811974
184	6	0	5.892389	-1.245382	5.665611
185	1	0	5.003082	-0.643203	5.514728
186	6	0	3.729974	-5.427481	-0.772633
187	6	0	4.747998	-6.314499	-1.165402
188	1	0	5.751264	-5.933763	-1.327399
189	6	0	4.497777	-7.676364	-1.351059
190	1	0	5.286514	-8.347987	-1.656101
191	6	0	3.203391	-8.182797	-1.128593
192	6	0	2.179982	-7.301197	-0.733725
193	1	0	1.183176	-7.687017	-0.539017
194	6	0	2.436566	-5.941197	-0.564613
195	1	0	1.636919	-5.274648	-0.260671
196	6	0	2.630685	0.566488	-4.303035
197	6	0	3.338018	0.931348	-5.463124
198	1	0	4.422442	0.940146	-5.457032
199	6	0	2.653569	1.276815	-6.634389
200	1	0	3.217854	1.552868	-7.519458
201	6	0	1.254834	1.263940	-6.666959
202	1	0	0.726051	1.532478	-7.575799
203	6	0	0.539077	0.902867	-5.519216
204	1	0	-0.546608	0.894791	-5.537575
205	6	0	1.223636	0.557410	-4.349304
206	1	0	0.671928	0.284158	-3.456054
207	6	0	13.502620	12.439914	1.071504
208	6	0	12.083766	12.571260	1.173894
209	6	0	11.464658	13.841921	1.386472
210	1	0	12.099595	14.714034	1.472350
211	6	0	10.104536	13.946346	1.476943
212	1	0	9.626520	14.904383	1.634309
213	6	0	9.276223	12.785645	1.374742
214	6	0	9.850430	11.495125	1.178074
215	6	0	11.295386	11.388669	1.056177
216	7	0	11.863319	10.168689	0.832571
217	6	0	13.195952	10.090765	0.741676
218	6	0	14.063360	11.191421	0.861217

219	1	0	15.126133	11.013740	0.780199
220	7	0	9.081576	10.367922	1.107601
221	6	0	7.754128	10.497329	1.213610
222	6	0	7.088604	11.724935	1.389340
223	6	0	7.854269	12.874634	1.472714
224	1	0	6.010226	11.712978	1.454670
225	8	0	14.222578	13.603836	1.194426
226	8	0	7.342619	14.137616	1.650474
227	6	0	5.889519	14.320067	1.774725
228	6	0	5.618895	15.816983	1.933564
229	1	0	5.400718	13.924040	0.874724
230	1	0	5.537904	13.756429	2.647792
231	6	0	6.064051	16.608798	0.690800
232	1	0	5.910439	17.683263	0.842173
233	1	0	5.482429	16.307358	-0.190618
234	1	0	7.122669	16.438931	0.474377
235	6	0	4.123722	16.037214	2.239619
236	1	0	6.206674	16.160138	2.796987
237	1	0	3.916969	17.102936	2.384607
238	1	0	3.813261	15.507591	3.148183
239	1	0	3.495764	15.686602	1.410321
240	6	0	15.689860	13.560563	1.117886
241	6	0	16.207322	14.992690	1.260745
242	1	0	16.064927	12.918801	1.924707
243	1	0	15.985453	13.128644	0.152536
244	6	0	17.745992	14.973451	1.360283
245	1	0	18.132481	15.989749	1.491629
246	1	0	18.090208	14.370328	2.208883
247	1	0	18.195119	14.562702	0.446750
248	6	0	15.727079	15.887462	0.103879
249	1	0	15.801004	15.388826	2.202393
250	1	0	16.131858	15.534373	-0.853995
251	1	0	14.635570	15.887236	0.033004
252	1	0	16.063553	16.920212	0.249362
253	6	0	13.801136	8.736827	0.500074
254	8	0	15.047164	8.579018	0.484584
255	7	0	12.869490	7.757623	0.310678
256	1	0	11.913234	8.104091	0.361207
257	6	0	6.908736	9.257326	1.140867
258	8	0	5.655331	9.339399	1.169974
259	7	0	7.625467	8.097699	1.048670
260	1	0	8.632354	8.244476	1.044731
261	6	0	14.685890	-1.548041	2.765267
262	6	0	14.441132	-0.280331	2.198116
263	7	0	13.936248	-0.027219	0.934181
264	6	0	14.636009	0.971534	2.928450
265	1	0	14.994065	1.052784	3.942173
266	6	0	14.240035	1.975763	2.101773
267	1	0	14.214578	3.031735	2.315902
268	6	0	13.820944	1.351099	0.846013
269	6	0	13.360426	2.075811	-0.273896
270	6	0	12.945641	1.499365	-1.488930
271	6	0	12.551726	2.194736	-2.683595
272	1	0	12.524537	3.266695	-2.785427
273	6	0	12.237213	1.262178	-3.644642
274	1	0	11.901701	1.454780	-4.650052
275	6	0	12.432174	-0.048462	-3.085361
276	7	0	12.854790	0.145326	-1.777645
277	1	0	13.101056	-0.596959	-1.131654
278	6	0	12.213199	-1.281719	-3.726699
279	6	0	12.346146	-2.548350	-3.120203
280	6	0	12.155072	-3.811338	-3.834665
281	1	0	11.905269	-3.909599	-4.878797
282	6	0	12.383215	-4.809233	-2.939228
283	1	0	12.352597	-5.872608	-3.114629
284	6	0	12.732616	-4.168874	-1.671048
285	7	0	12.699469	-2.790911	-1.802482
286	6	0	13.123014	-4.891657	-0.523251
287	6	0	13.629097	-4.320391	0.656857
288	6	0	14.079427	-5.015794	1.833035
289	1	0	14.044069	-6.084664	1.961118
290	6	0	14.546531	-4.087577	2.732598
291	1	0	14.957541	-4.277927	3.709802
292	6	0	14.376736	-2.778050	2.162508
293	7	0	13.815242	-2.968110	0.907273
294	1	0	13.610236	-2.226148	0.246796
295	6	0	13.275285	3.567498	-0.173646
296	6	0	14.414788	4.366587	0.033510
297	1	0	15.390695	3.894767	0.083951
298	6	0	14.325779	5.753508	0.178610
299	1	0	15.209233	6.354519	0.338495
300	6	0	13.065669	6.377060	0.115812
301	6	0	11.923976	5.592431	-0.129120
302	1	0	10.952486	6.071340	-0.209535
303	6	0	12.024988	4.211063	-0.265692
304	1	0	11.131295	3.616755	-0.415606
305	6	0	15.308937	-1.601984	4.130957
306	6	0	16.656726	-1.236882	4.307267
307	1	0	17.236938	-0.917762	3.447221
308	6	0	17.249668	-1.289026	5.573242
309	1	0	18.291497	-1.007711	5.691915
310	6	0	16.503332	-1.705282	6.681955
311	1	0	16.962768	-1.745311	7.664702
312	6	0	15.160646	-2.065525	6.517392
313	1	0	14.572874	-2.379655	7.374383
314	6	0	14.564607	-2.015167	5.252245
315	1	0	13.517988	-2.271030	5.127948
316	6	0	13.035504	-6.389368	-0.569283
317	6	0	14.200657	-7.180007	-0.556971
318	1	0	15.171044	-6.695090	-0.521057
319	6	0	14.116769	-8.575511	-0.605629
320	1	0	15.025449	-9.169597	-0.601390
321	6	0	12.867042	-9.203342	-0.666793
322	1	0	12.801825	-10.286228	-0.704088
323	6	0	11.702156	-8.427344	-0.680363
324	1	0	10.728534	-8.905132	-0.723643
325	6	0	11.784155	-7.031418	-0.633126
326	1	0	10.876374	-6.436937	-0.634382
327	6	0	11.814237	-1.222981	-5.172096
328	6	0	12.700158	-0.709966	-6.139279
329	1	0	13.682001	-0.367171	-5.829296
330	6	0	12.331884	-0.651807	-7.487475
331	1	0	13.030396	-0.257946	-8.219090
332	6	0	11.071122	-1.104314	-7.893622
333	1	0	10.784423	-1.056963	-8.939224
334	6	0	10.181816	-1.618252	-6.942742
335	1	0	9.200760	-1.967576	-7.249050
336	6	0	10.550663	-1.677735	-5.594713
337	1	0	9.857633	-2.072650	-4.859343
338	6	0	-14.506905	11.199676	-1.761970
339	6	0	-13.116057	11.516256	-1.851164
340	6	0	-12.652341	12.840868	-2.129481
341	1	0	-13.387683	13.620413	-2.281309
342	6	0	-11.312378	13.115162	-2.186680
343	1	0	-10.956764	14.118290	-2.383490
344	6	0	-10.345627	12.077402	-1.998598
345	6	0	-10.767116	10.740202	-1.751418
346	6	0	-12.185843	10.460137	-1.636171
347	7	0	-12.587505	9.199898	-1.309974
348	6	0	-13.897042	8.950054	-1.211443
349	6	0	-14.900487	9.908593	-1.443951
350	1	0	-15.932238	9.601093	-1.350148
351	7	0	-9.878303	9.715930	-1.626037
352	6	0	-8.571670	9.986580	-1.706199
353	6	0	-8.046249	11.276773	-1.902868
354	6	0	-8.939426	12.326274	-2.058504
355	1	0	-6.972271	11.391857	-1.938606
356	8	0	-15.373234	12.239623	-1.997591
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358	6	0	-7.147427	13.979803	-2.372955
359	6	0	-7.049324	15.489858	-2.595041
360	1	0	-6.644877	13.684402	-1.442373
361	1	0	-6.704283	13.424247	-3.208756
362	6	0	-7.625296	16.276856	-1.404057
363	1	0	-7.593798	17.354278	-1.601885
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365	1	0	-8.663301	15.992190	-1.209434
366	6	0	-5.581002	15.872349	-2.869741
367	1	0	-7.644413	15.722557	-3.489707
368	1	0	-5.496039	16.947711	-3.059154

369	1	0	-5.180700	15.344186	-3.743326
370	1	0	-4.944026	15.635324	-2.007719
371	6	0	-16.822805	12.010780	-1.912592
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373	1	0	-17.102679	11.222128	-2.623533
374	1	0	-17.066862	11.677072	-0.896382
375	6	0	-19.039071	13.177804	-2.003722
376	1	0	-19.554330	14.121552	-2.211852
377	1	0	-19.470661	12.411741	-2.660852
378	1	0	-19.256779	12.897318	-0.966256
379	6	0	-17.225973	13.777659	-3.690058
380	1	0	-17.131590	14.086534	-1.556169
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383	1	0	-17.623009	13.052632	-4.413037
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385	8	0	-15.512428	7.227865	-0.751180
386	7	0	-13.237857	6.771417	-0.471329
387	1	0	-12.343981	7.247064	-0.581827
388	6	0	-7.624844	8.823442	-1.599574
389	8	0	-6.383086	8.997344	-1.543546
390	7	0	-8.268728	7.617765	-1.597084
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392	6	0	-13.204338	-3.073683	-0.566885
393	6	0	-13.273462	-1.679940	-0.350839
394	7	0	-12.950802	-1.023178	0.825147
395	6	0	-13.678259	-0.715187	-1.374337
396	1	0	-14.006754	-0.956516	-2.372222
397	6	0	-13.555495	0.522186	-0.821018
398	1	0	-13.750407	1.473343	-1.289563
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407	7	0	-12.420500	0.045293	3.522794
408	1	0	-12.431857	-0.877665	3.103107
409	6	0	-11.903739	-0.665099	5.858050
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411	6	0	-11.355564	-3.009716	6.651496
412	1	0	-11.213877	-2.784065	7.696182
413	6	0	-11.243575	-4.219392	6.039118
414	1	0	-10.986919	-5.165307	6.488748
415	6	0	-11.561952	-4.009889	4.625900
416	7	0	-11.829960	-2.672874	4.386659
417	6	0	-11.606893	-5.052189	3.677951
418	6	0	-11.984926	-4.912232	2.331772
419	6	0	-12.095459	-5.965126	1.357763
420	1	0	-11.851803	-6.997434	1.547083
421	6	0	-12.556511	-5.421045	0.182540
422	1	0	-12.740529	-5.937746	-0.744579
423	6	0	-12.753631	-4.009429	0.382696
424	7	0	-12.379857	-3.745706	1.692273
425	1	0	-12.424297	-2.830393	2.126602
426	6	0	-13.055519	2.792649	0.974249
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429	6	0	-14.389783	4.656536	0.113956
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431	6	0	-13.229670	5.445762	0.005133
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434	6	0	-11.903654	3.597344	0.870515
435	1	0	-10.941760	3.191297	1.168148
436	6	0	-13.638990	-3.622029	-1.894313
437	6	0	-14.737367	-4.502027	-1.967883
438	1	0	-15.266548	-4.765009	-1.057689
439	6	0	-15.158031	-5.022822	-3.195697
440	1	0	-16.010579	-5.693956	-3.231083
441	6	0	-14.489166	-4.673825	-4.374738
442	1	0	-14.816128	-5.076589	-5.328112
443	6	0	-13.398463	-3.798937	-4.316370
444	1	0	-12.872715	-3.519266	-5.223704
445	6	0	-12.976385	-3.278470	-3.088416
446	1	0	-12.131953	-2.599029	-3.061012
447	6	0	-11.278261	-6.445516	4.139666
448	6	0	-12.193446	-7.167953	4.928202
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473	6	0	-8.276385	-2.044225	1.646119
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485	1	0	-9.443606	-2.346892	-2.992938
486	1	0	-10.149073	1.272585	-0.771002
487	8	0	-9.359269	1.340551	2.050758
488	7	0	-7.280143	-1.994127	5.807820
489	8	0	-7.593938	-0.979221	6.492027
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496	8	0	-10.652705	-0.620093	-4.183837
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507	6	0	-0.193878	-0.044618	0.667080
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509	6	0	1.022856	0.700793	2.612131
510	6	0	1.514461	-0.592634	2.794042
511	6	0	1.198017	-1.641264	1.922298
512	1	0	-0.228507	1.982698	1.424776
513	1	0	1.316892	1.476672	3.306349
514	1	0	1.610399	-2.631692	2.064903
515	8	0	0.163372	-3.445494	-0.381924
516	7	0	-2.650772	-1.098496	-4.397760
517	8	0	-2.579617	-2.299703	-4.784572
518	8	0	-3.122161	-0.156300	-5.095136

519	7	0	-2.150326	2.177428	-0.821320
520	8	0	-2.601651	3.008405	-1.657401
521	8	0	-2.010656	2.431259	0.407934
522	7	0	2.394930	-0.859038	3.933605
523	8	0	2.779594	-2.046730	4.120212
524	8	0	2.724115	0.115219	4.672172
525	6	0	10.263491	-2.256771	1.950123
526	6	0	9.651567	-3.282693	1.244971
527	1	0	9.697450	-4.299131	1.609149
528	6	0	8.960786	-3.001538	0.055658
529	6	0	8.890394	-1.688622	-0.446833
530	6	0	9.554777	-0.689016	0.321233
531	6	0	10.235490	-0.932981	1.497911
532	1	0	10.728817	-0.138242	2.042190
533	6	0	9.409311	0.631081	-0.346091
534	6	0	8.662942	0.362892	-1.592612
535	6	0	8.320091	-1.016377	-1.661060
536	6	0	7.594152	-1.474753	-2.765261
537	6	0	7.260552	-0.569684	-3.784323
538	6	0	7.634526	0.771718	-3.688378
539	6	0	8.332667	1.269786	-2.583025
540	1	0	7.278423	-2.501147	-2.843448
541	1	0	6.708141	-0.903267	-4.652425
542	1	0	8.606159	2.314343	-2.516861
543	8	0	9.827166	1.721444	0.075564
544	7	0	10.934376	-2.570070	3.211057
545	8	0	11.519579	-1.626598	3.812532
546	8	0	10.880994	-3.758716	3.639378
547	7	0	8.331197	-4.163010	-0.575773
548	8	0	8.696379	-5.314442	-0.204878
549	8	0	7.430429	-3.971449	-1.438983
550	7	0	7.294619	1.687276	-4.777741
551	8	0	7.627320	2.899218	-4.662118
552	8	0	6.690039	1.215627	-5.786353

6. Reference:

1. Gaussian 16, Revision C.02, M. J. Frisch et. al. Gaussian, Inc., Wallingford CT, 2019.
2. M. H. Lee, J. W. Kim and C. Y. Lee, *J. Organomet. Chem.,* 2014, **761**, 20-27.
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5. R. Luguya, L. Jaquinod, F. R Fronczek, M.G. H Vicente and K. M Smith, *Tetrahedron,* 2004, **60**, 2757-2763.
6. http://supramolecular.org
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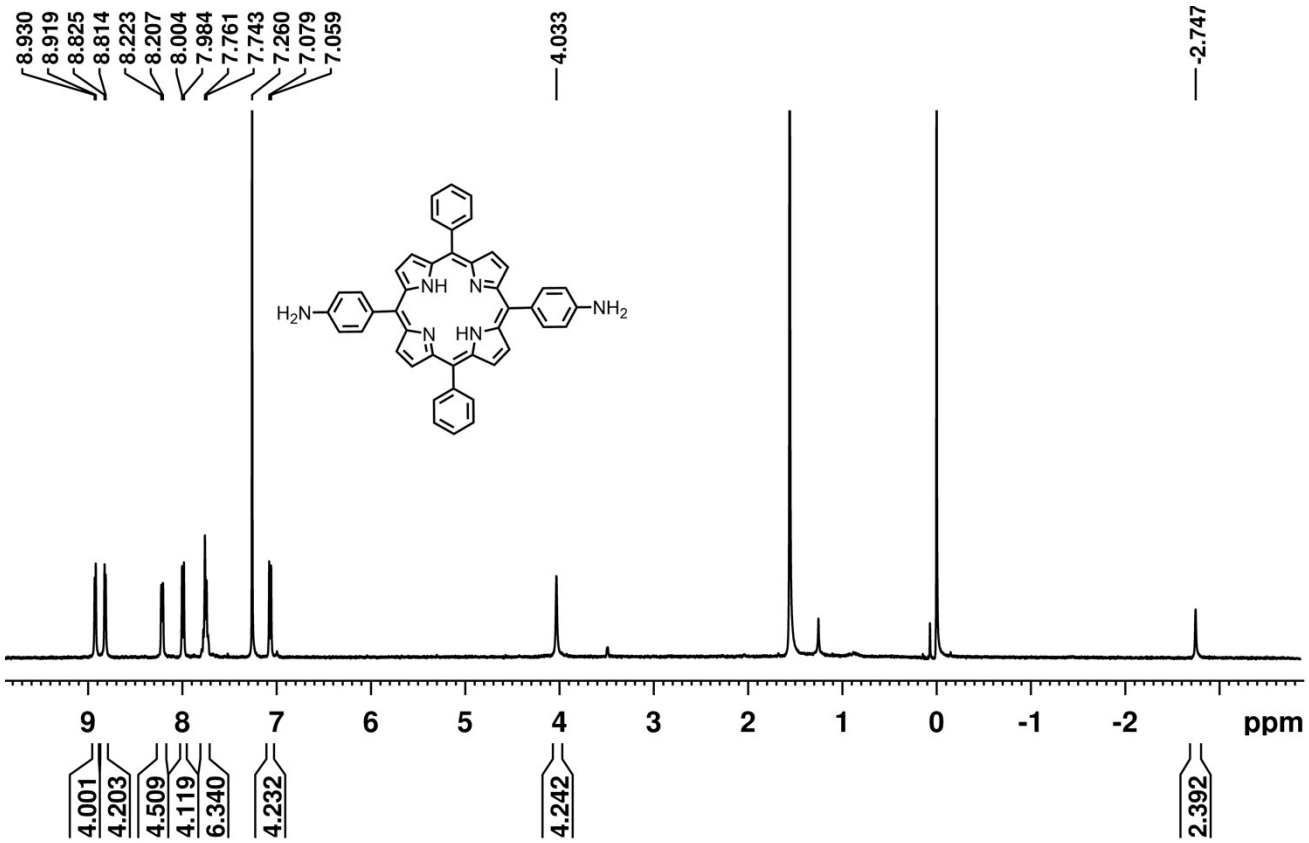
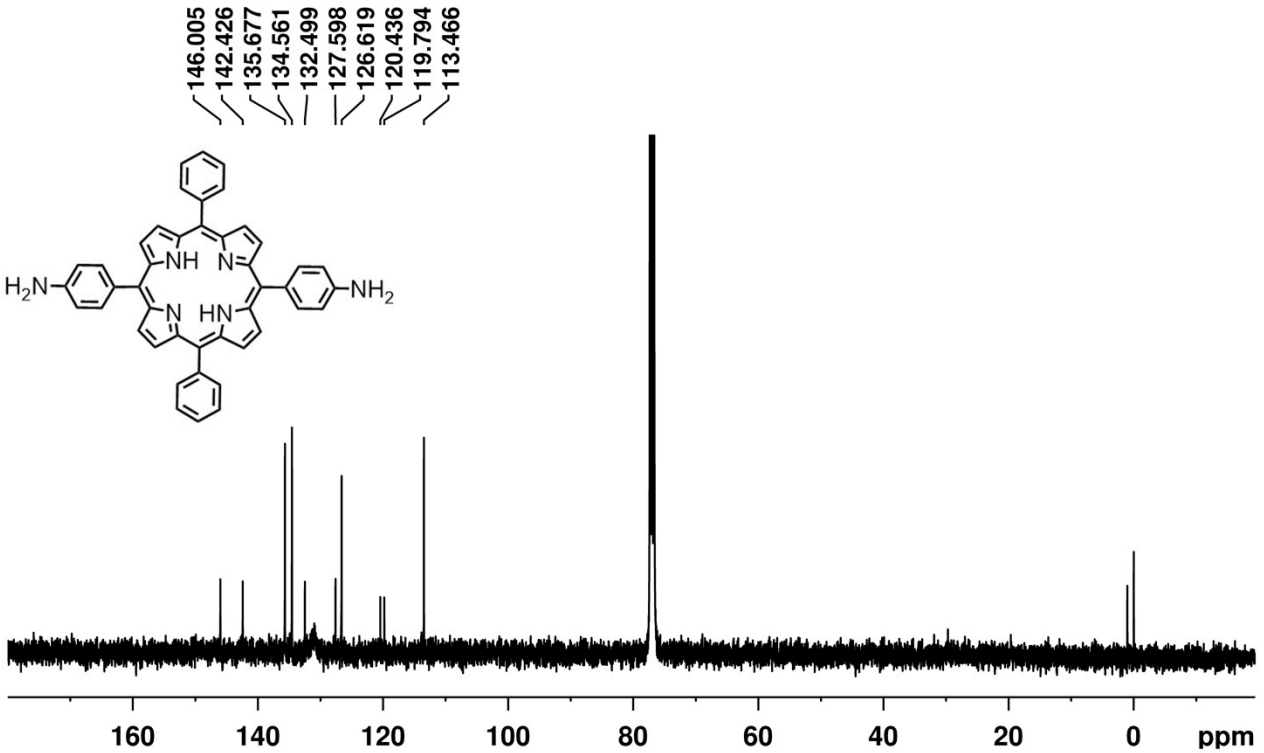
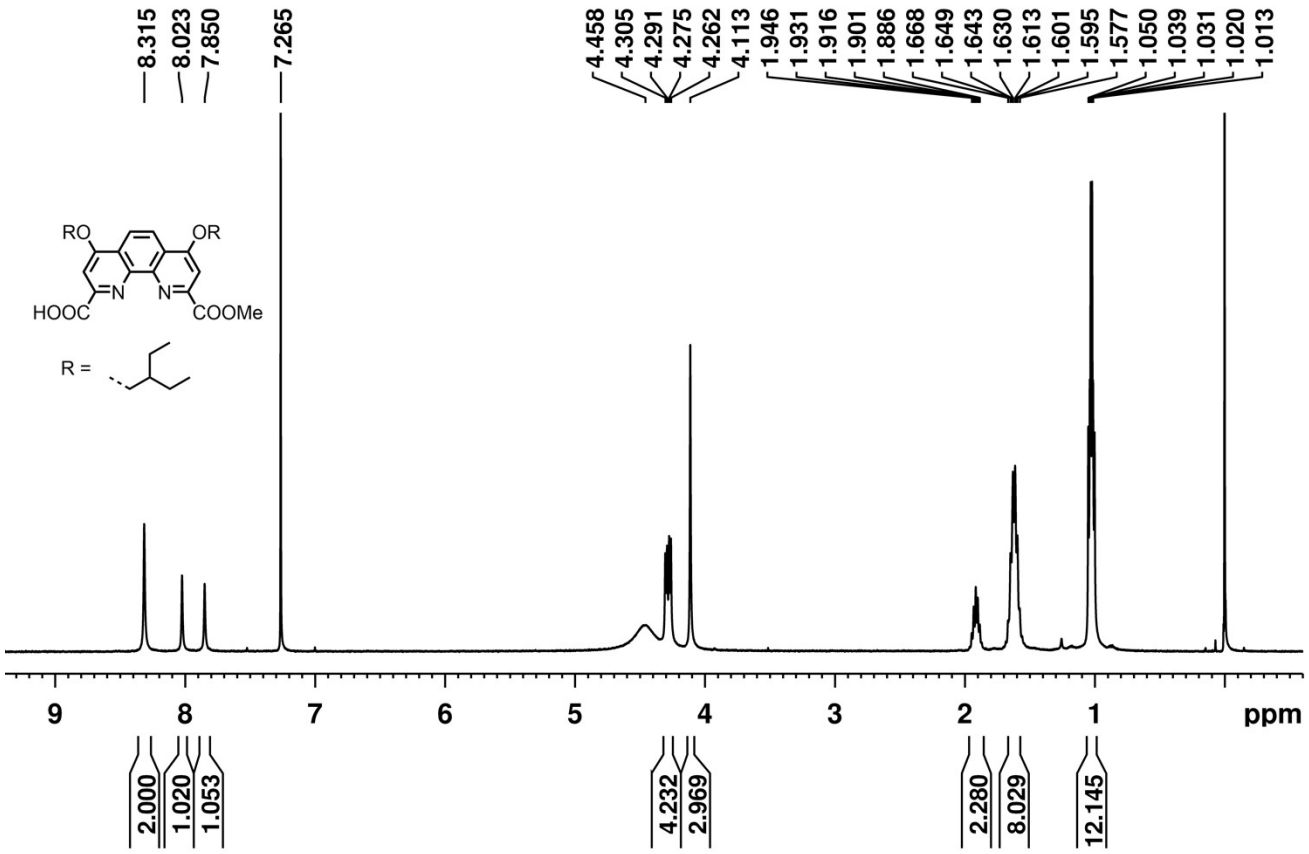
7. NMR spectra of the synthesized compounds



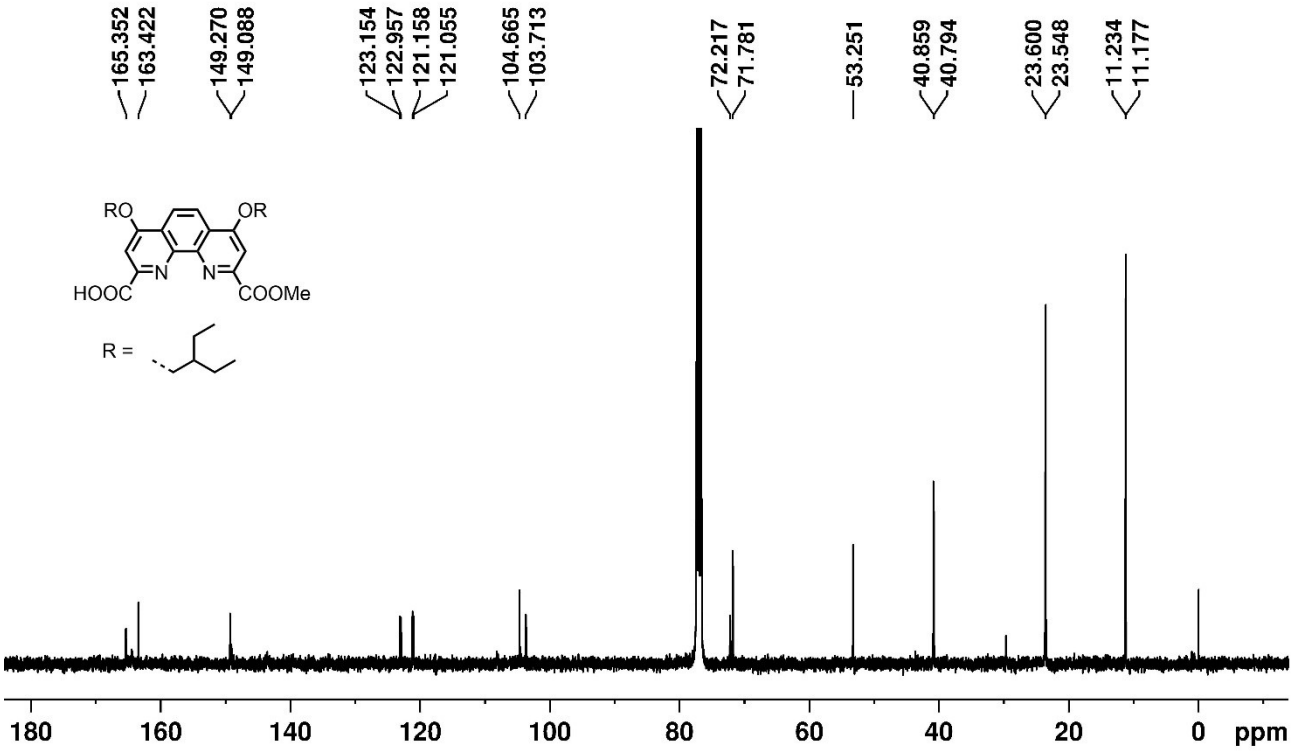
400 MHz ^{1}H-NMR of **3** in $CDCl_3$ at 298 K.



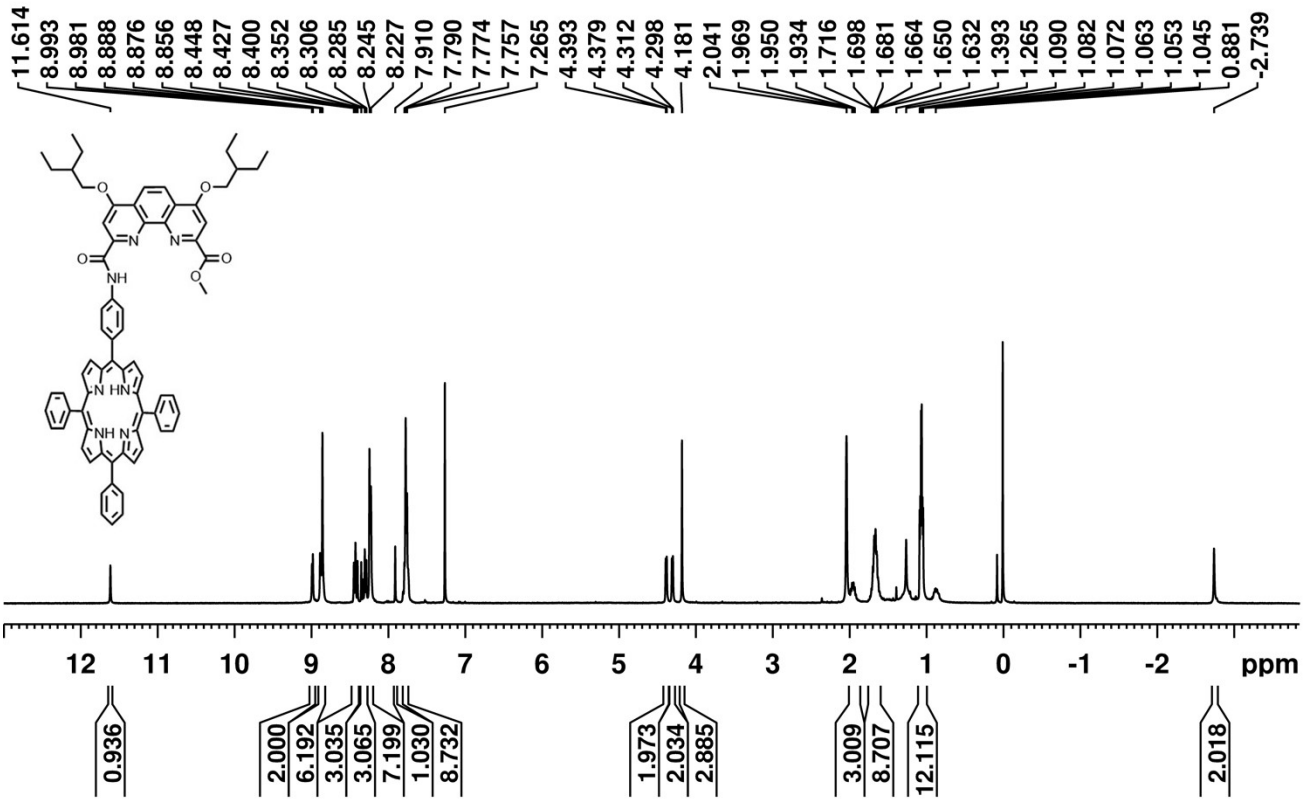
100 MHz ^{13}C-NMR of **3** in $CDCl_3$ at 298 K.



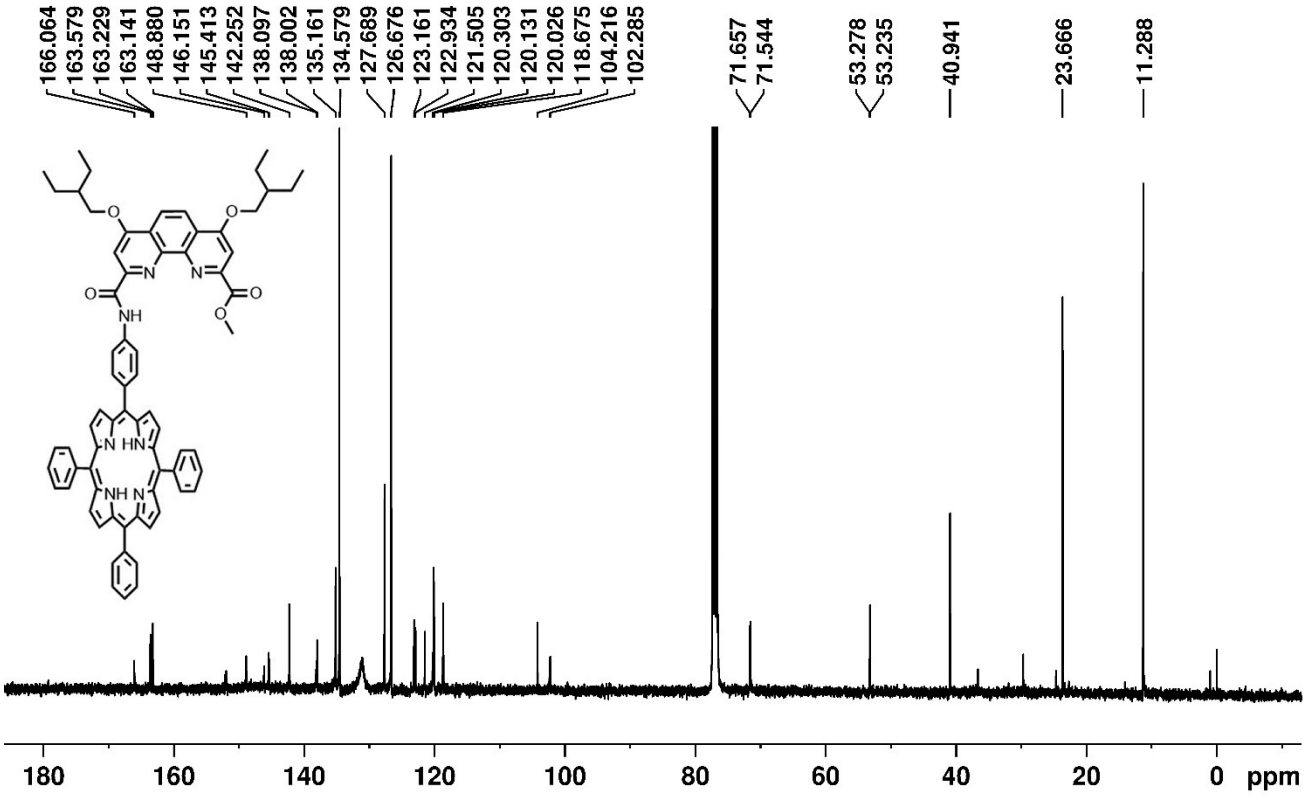
400 MHz ^{1}H-NMR of **5** in $CDCl_3$ at 298 K.



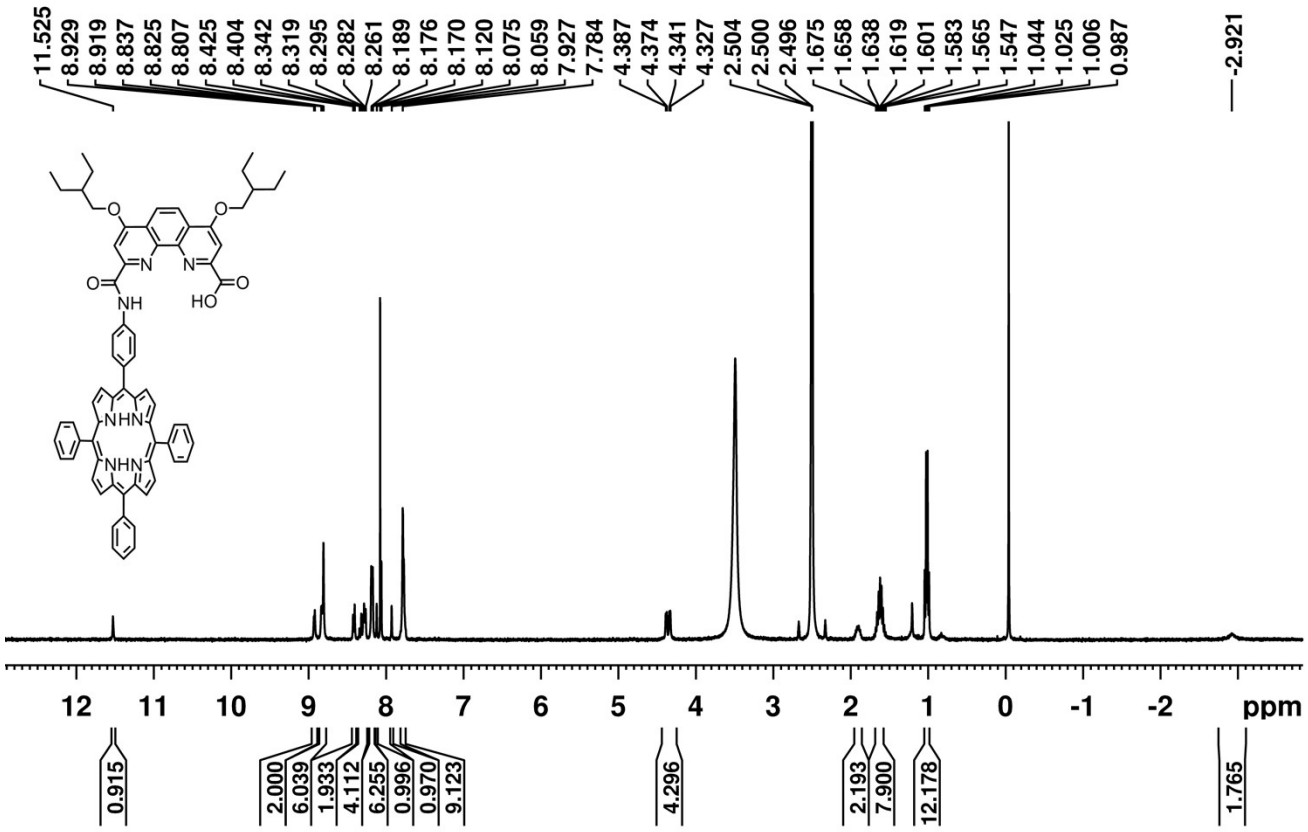
100 MHz ^{13}C-NMR of **5** in $CDCl_3$ at 298 K.



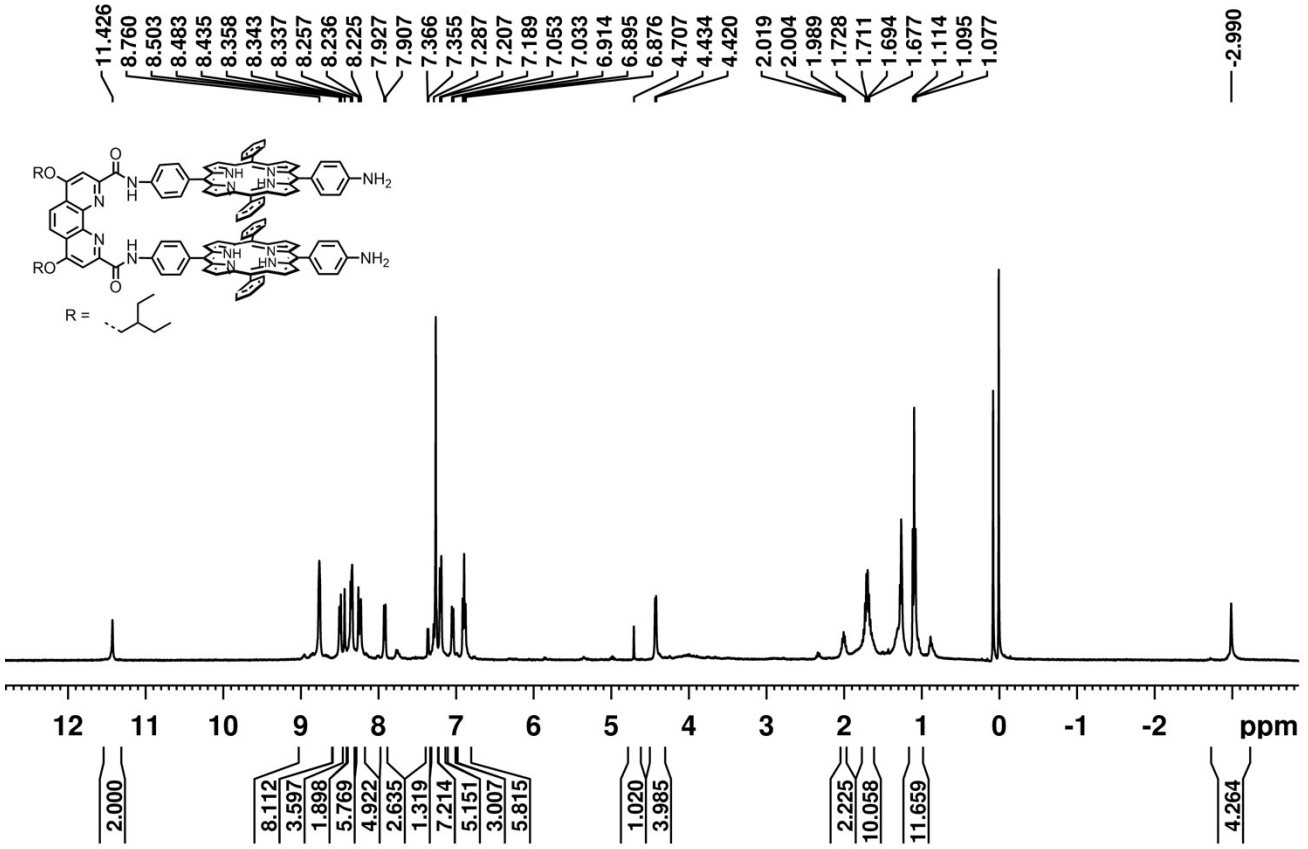
400 MHz ^{1}H-NMR of **6** in $CDCl_3$ at 298 K.



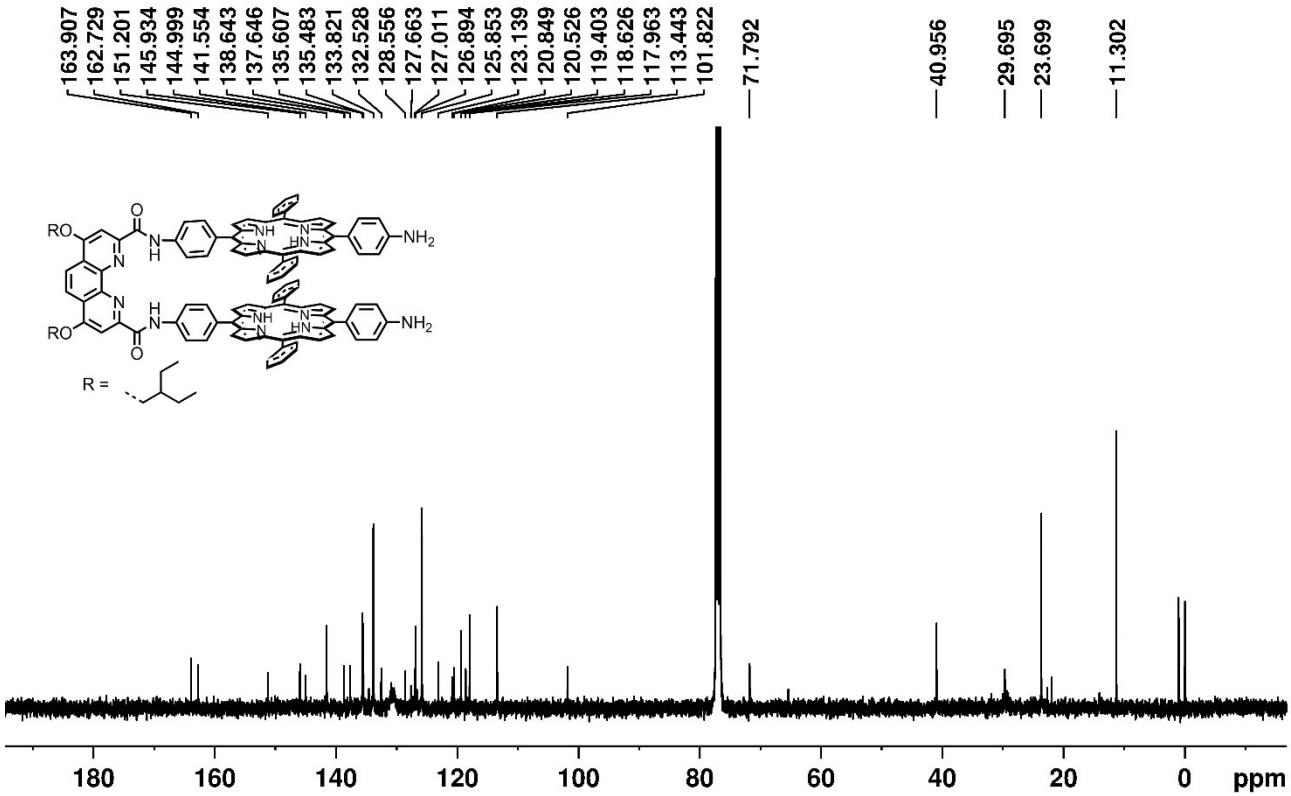
100 MHz ^{13}C-NMR of **6** in $CDCl_3$ at 298 K.



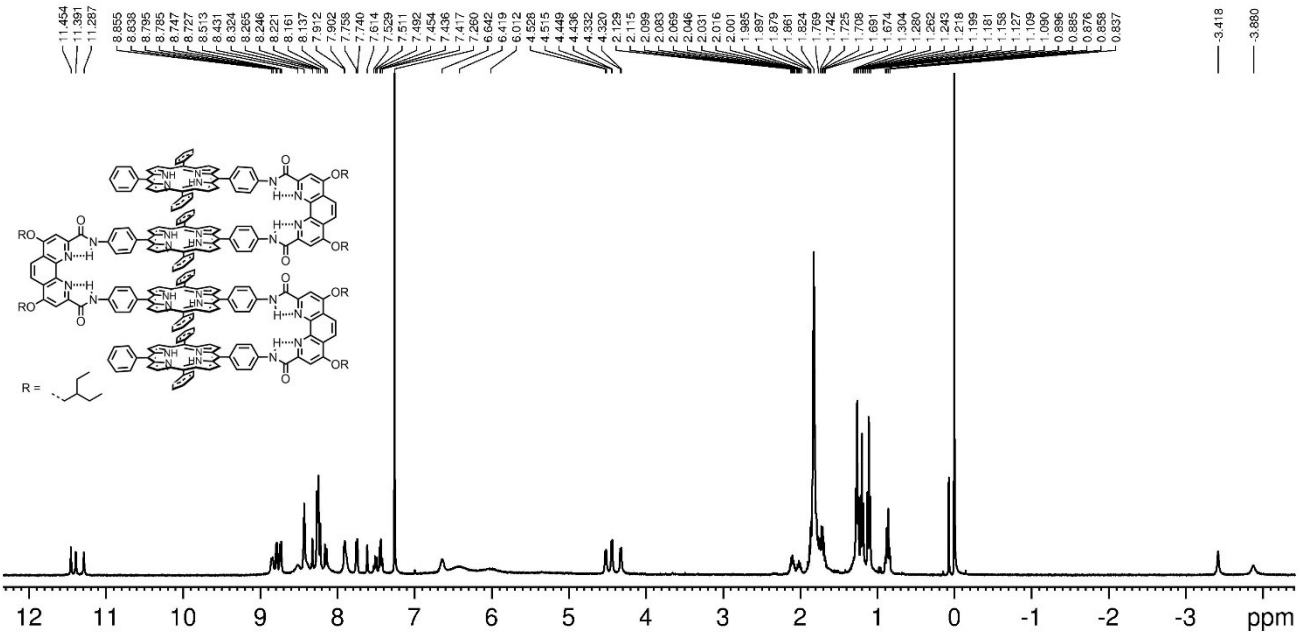
400 MHz ^{1}H-NMR of **6** in DMSO-d_6 : $CDCl_3$ (1:1) at 298 K.



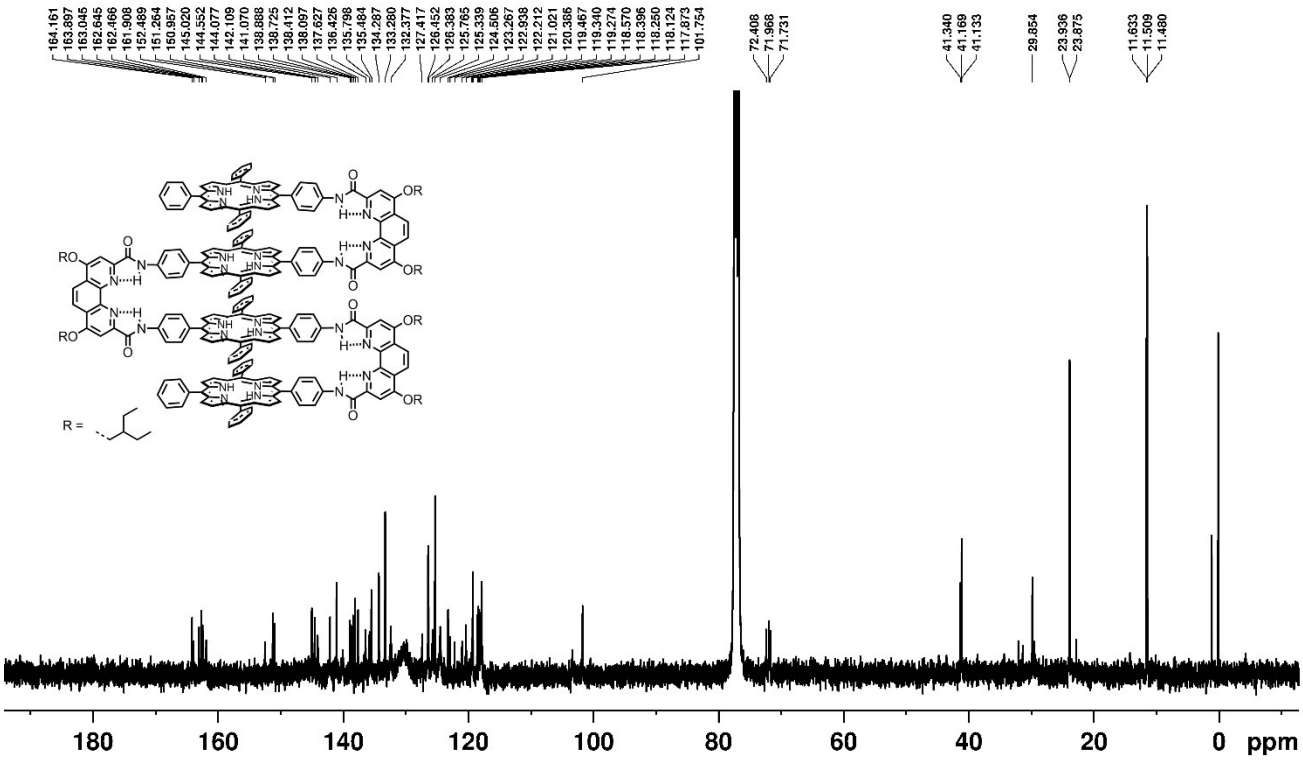
400 MHz ^{1}H-NMR of **8** in $CDCl_3$ at 298 K.



100 MHz ^{13}C-NMR of **8** in $CDCl_3$ at 298 K.



400 MHz ^{1}H-NMR of **1** in $CDCl_3$ at 298 K.



100 MHz ^{13}C-NMR of **1** in $CDCl_3$ at 298 K.