Electronic Supplementary Information

for

Triply stranded metallo-supramolecular helicate based on triptycene with efficient encapsulation to bulky guest molecules

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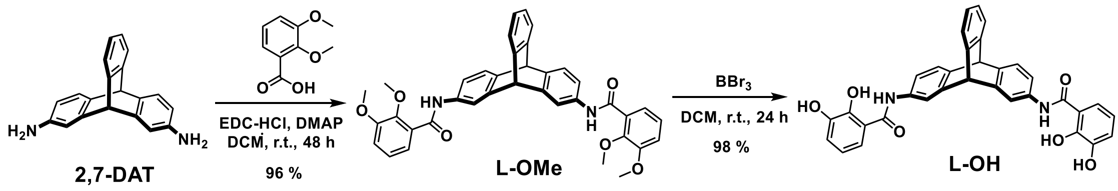
Contents

1. General information

The commercially available reagents were used without further purification. Solvents were employed as purchased or dried with Molecular Sieves. ^{1}H NMR spectra, ^{13}C NMR spectra, 2D NOESY spectra, DOSY experiments were recorded on a Bruker 700 MHz spectrometer (or other Bruker NMR spectrometers). High-resolution mass spectrum (HRMS) was obtained on a Bruker mass spectrometer and an auto-flex TOF/TOF mass spectrometer. Circular dichroism spectroscopy was recorded on a J-815 spectrometer. The UV-vis spectra were recorded on PerkinElmer® UV/Vis/NIR spectrometer (Lambda 950). Preparative silica gel plates separation and normal TLC analysis were performed on pre-coated, glass-backed silica gel plates. The energy-minimized structures of the 2,7-T based [$\mathbf{Ga_2L_3}$]$^{6-}$, [Me_4N^+@$\mathbf{Ga_2L_3}$]$^{5-}$, [Et_4N^+@$\mathbf{Ga_2L_3}$]$^{5-}$, and 2,6-T based chiral [$\mathbf{Ga_2L_3}$]$^{6-}$ were optimized using the Gaussian 16 program,[S1] based on the density functional theory (DFT) using the B3LYP functional and 6–31G(d) basis set.

2. Synthesis and characterizations

2.1 Synthesis of the 2,7-triptycene-based ligands



Scheme S1. Synthetic routes of achiral ligand.

2.1.1 Synthesis of **L-OMe**

To a 10 mL flask was added 2,7-**DAT** (114 mg, 0.40 mmol), DMAP (56 mg, 0.46 mmol), EDC·HCl (382 mg, 2.0 mmol), 2,3-dimethoxybenzoic acid (160 mg, 0.88 mmol) and dried DCM (6.0 mL). The reaction was kept stirring at room temperature for 48 hours. Then a saturated solution of potassium hydroxide (2.0 mL) was added to the flask with stirring heavily for 10 minutes. The organic phase was collected and dried by anhydrous magnesium sulfate, and concentrated under reduced pressure. The white solid was subjected to silica gel column chromatography using DCM/MeOH (100:1, v/v) as the eluent to afford the **L-OMe** as a white powder (236 mg, 96%). M.p.: 155.9-157.2 °C. ^{1}H NMR (300 MHz, $CDCl_3$, 298 K): δ 9.90 (s, NH, 2H), 7.87 (s, 2H), 7.75 (d, *J* = 7.8 Hz, 2H), 7.45-7.28 (m, 4H), 7.20 (dd, *J* = 15.9, 7.9 Hz, 4H), 7.07 (d, *J* = 7.9 Hz, 2H), 7.03-6.94 (m, 2H), 5.46 (s, 1H), 5.39 (s, 1H), 3.94 (s, 6H), 3.91 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$, 298 K): δ 163.1, 152.8, 147.4, 146.3, 145.5, 145.0, 141.6, 135.7, 127.2, 125.6, 125.4, 125.0, 124.1, 124.0, 123.6, 123.2, 116.9, 116.7, 115.9, 61.9, 56.4, 54.5, 53.3. HR-ESI-MS: *m/z* calculated for $[M+H]^+$ $C_{38}H_{33}O_6N_2^+$, 613.2333; found 613.2328.

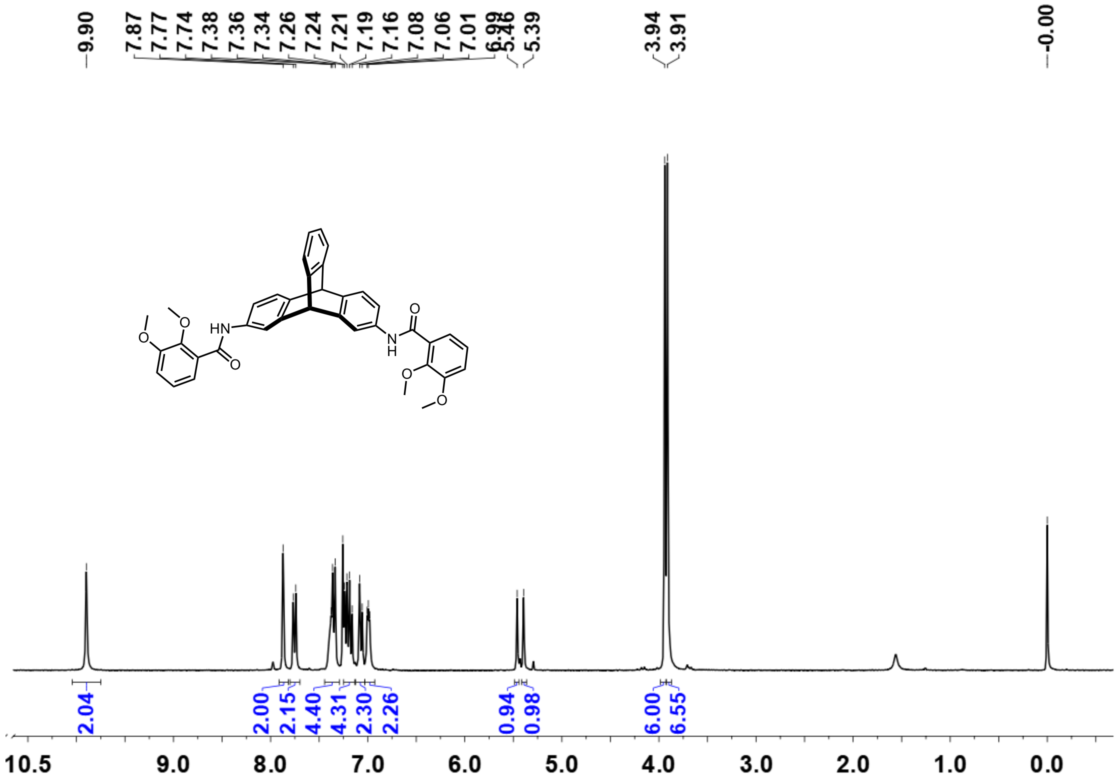


Fig. S1 ^{1}H NMR (300 MHz, $CDCl_3$, 298 K) spectrum of **L-OMe**.

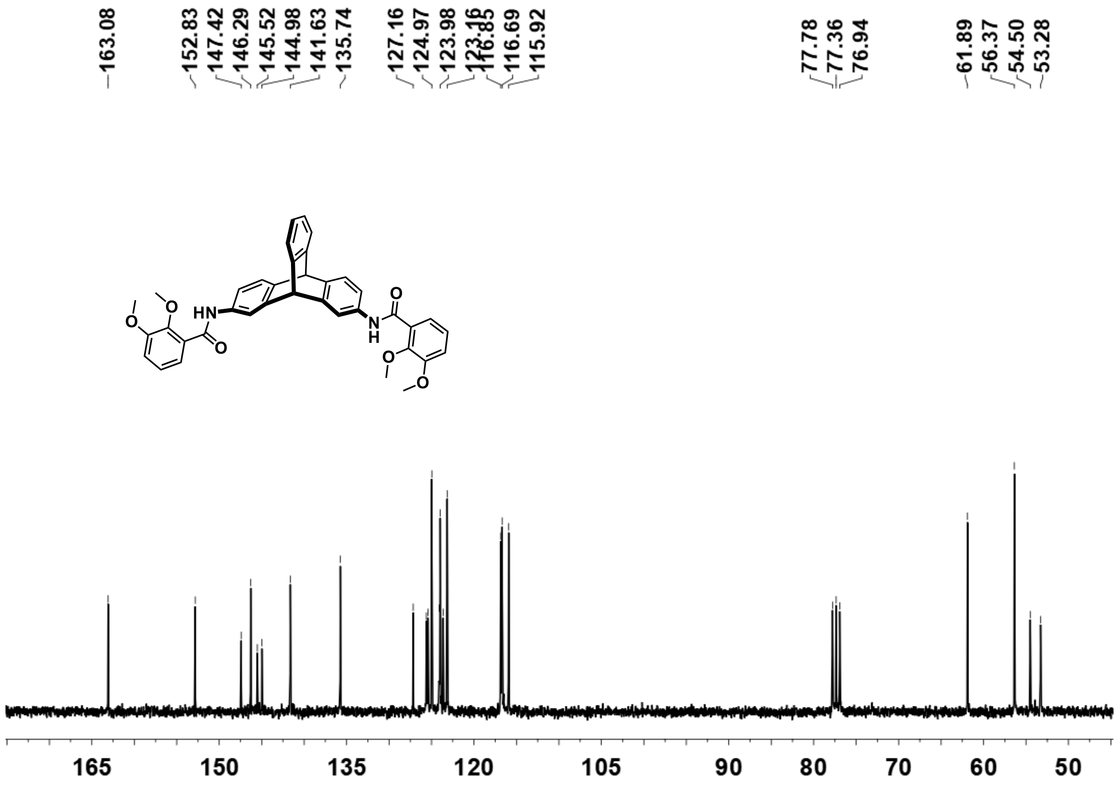


Fig. S2 ^{13}C NMR (75 MHz, $CDCl_3$, 298 K) spectrum of **L-OMe**.

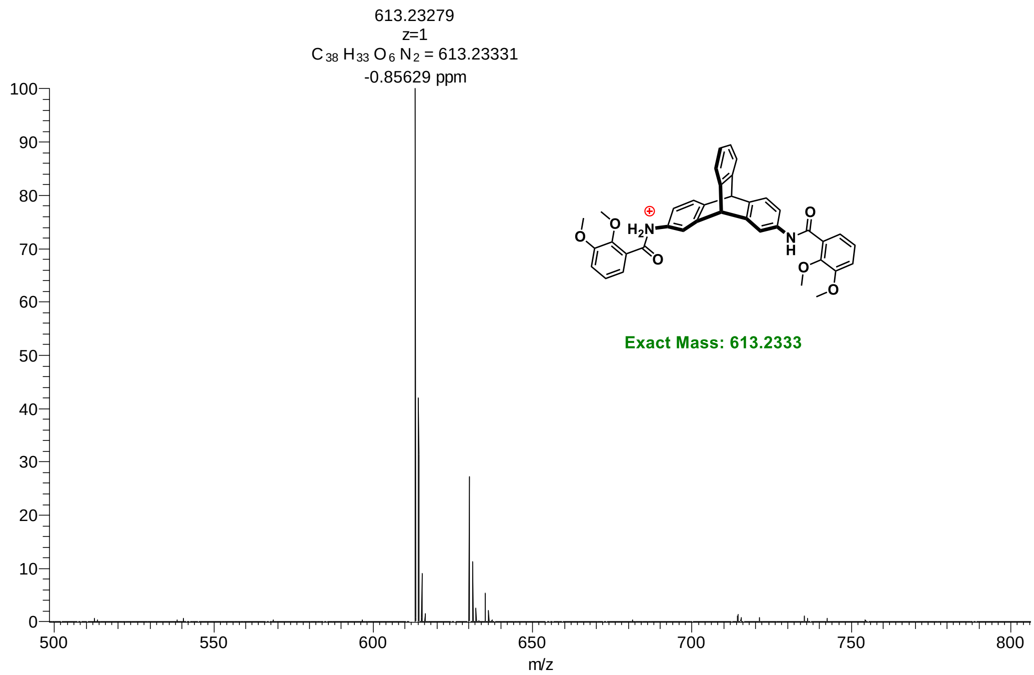


Fig. S3 HR-ESI-MS (positive mode) of **L-OMe**.

2.1.2 Synthesis of **L-OH**

To a 25 mL round-bottom bottle was added **L-OMe** (91.8 mg, 0.15 mmol) and dried DCM (10.0 mL). The solution was stirred at 0 °C for several minutes, then BBr_3 (0.3 mL) was added. The reaction was kept at room temperature 24 hours, then 10 mL methanol was added with stirring heavily 6 hours. The mixture was concentrated under reduced pressure. The grey red fibrous solid was subjected to a silica gel column chromatography using DCM/MeOH (25:1, v/v) as the eluent to afford the **L-OH** as a white fibrous solid (83 mg, 98%). M.p.: 203.6-205.2 °C. ^{1}H NMR (500 MHz, DMSO-d_6, 298 K): δ 11.77 (s, 2H), 10.29 (s, 2H), 9.37 (s, 2H), 7.88 (s, 2H), 7.51-7.44 (m, 2H), 7.42 (d, *J* = 8.0 Hz, 4H), 7.25 (d, *J* = 7.9 Hz, 2H), 7.06-6.99 (m, 2H), 6.97 (d, *J* = 7.8 Hz, 2H), 6.76 (t, *J* = 7.9 Hz, 2H), 5.71 (s, 1H), 5.62 (s, 1H). ^{13}C NMR (126 MHz, DMSO-d_6, 298 K): δ 168.1, 149.0, 146.7, 146.2, 145.9, 145.5, 142.0, 135.2, 125.6, 125.4, 124.2, 124.0, 123.9, 119.5, 118.8, 118.7, 118.2, 118.1, 117.2, 53.2, 52.1. HR-ESI-MS: *m/z* calculated for $[M-H]^-$ $C_{34}H_{23}O_6N_2^-$, 555.1562; found 555.1557; $[M-2H]^{2-}$ $C_{34}H_{22}O_6N_2^{2-}$, 277.0745; found 277.0739.

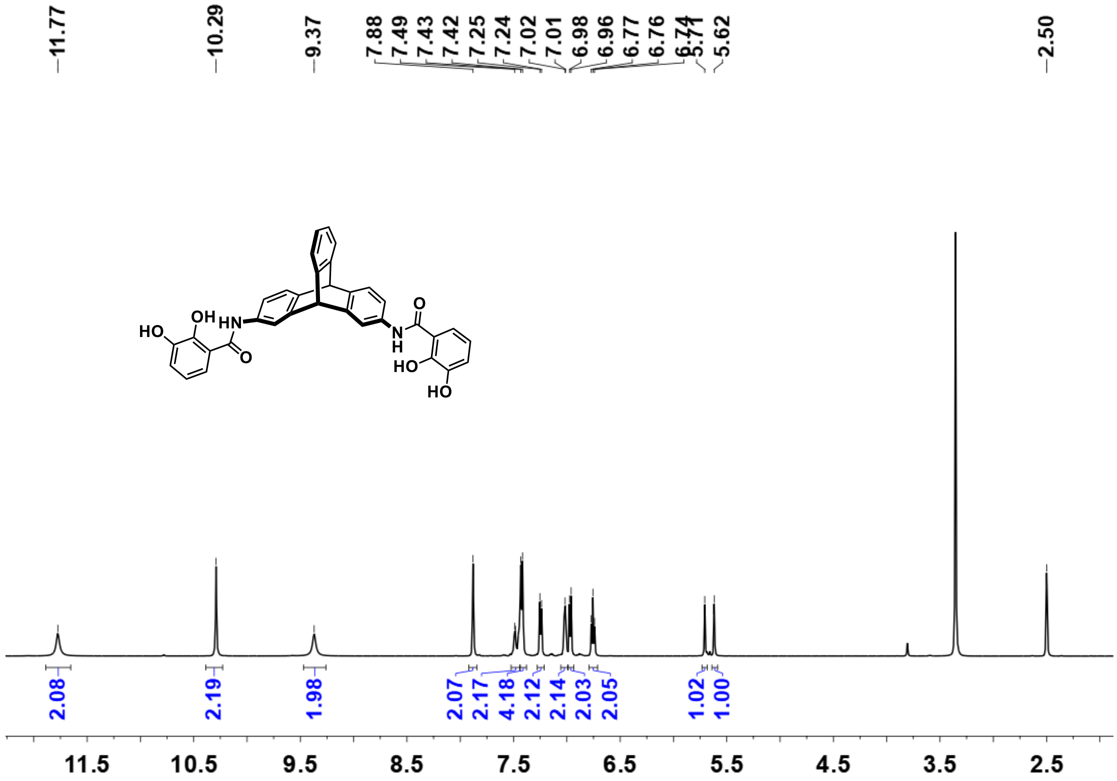


Fig. S4 ^{1}H NMR (500 MHz, DMSO-d_6, 298 K) spectrum of **L-OH**.

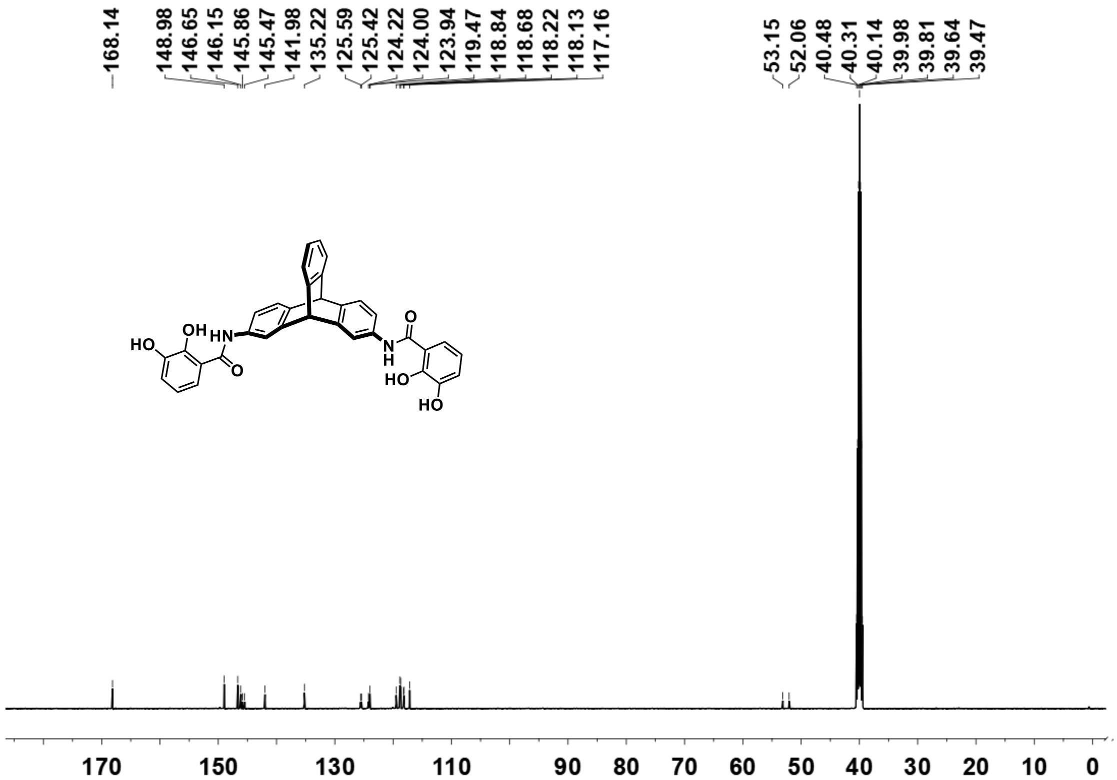


Fig. S5 ^{13}C NMR (126 MHz, DMSO-d_6, 298 K) spectrum of **L-OH**.

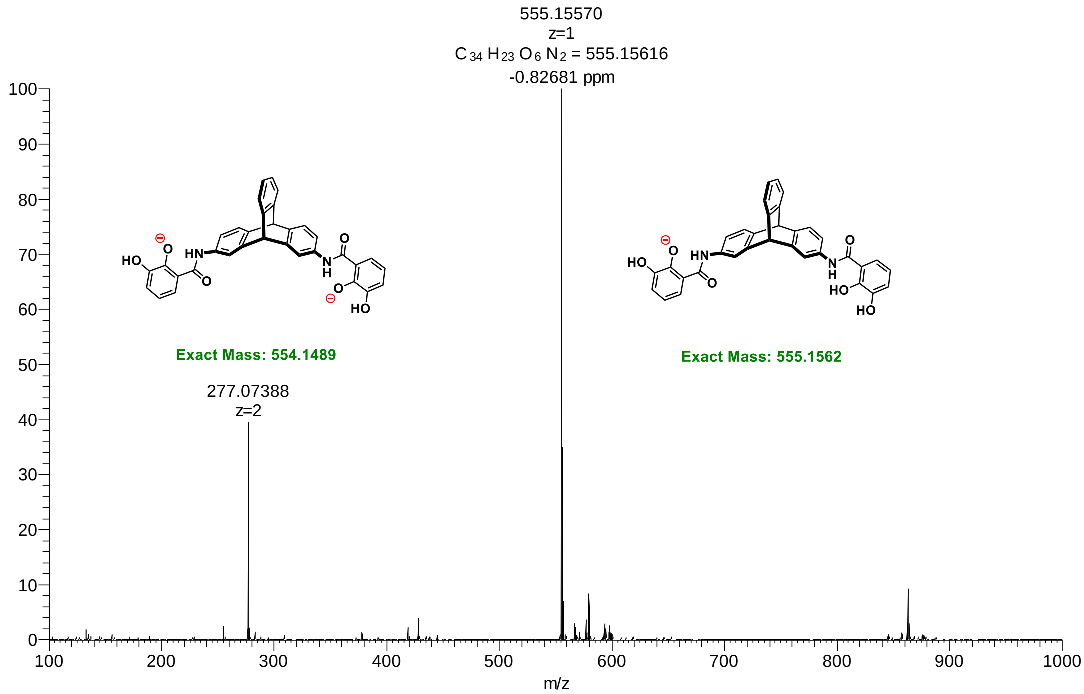
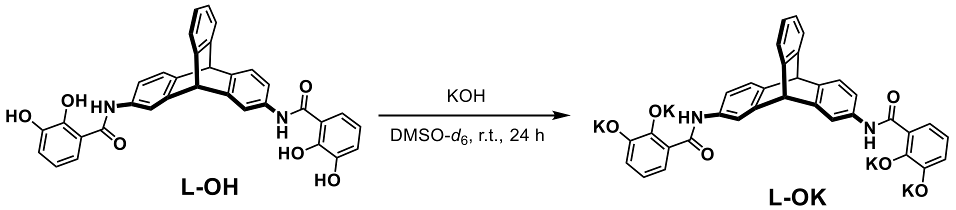


Fig. S6 HR-ESI-MS (negative mode) of **L-OH**.

2.1.3 Synthesis of **L-OK**



To an NMR tube with L-OH (11.4 mg, 0.02 mmol) in DMSO-d_6 was added KOH (9.2 mg, 0.16 mmol). The solution was subjected to the ultrasonic treatment for 10 minutes at room temperature and NMR analysis directly. ^{1}H NMR (500 MHz, DMSO-d_6, 298 K): δ 12.57 (s, 2H), 7.89 (s, 2H), 7.44 (d, *J* = 25.6 Hz, 2H), 7.34 (d, *J* = 7.2 Hz, 2H), 7.25 (dd, *J* = 14.8, 7.7 Hz, 4H), 7.00 (d, *J* = 3.1 Hz, 2H), 6.71 (d, *J* = 6.8 Hz, 2H), 6.41-6.23 (m, 2H), 5.60 (s, 1H), 5.52 (s, 1H). ^{13}C NMR (126 MHz, DMSO-d_6, 298 K): δ 167.6, 148.4, 146.3, 146.2, 145.8, 141.5, 140.5, 136.9, 125.4, 125.2, 124.1, 123.9, 123.7, 119.1, 116.9, 116.6, 116.3, 114.7, 113.1, 53.4, 52.0.

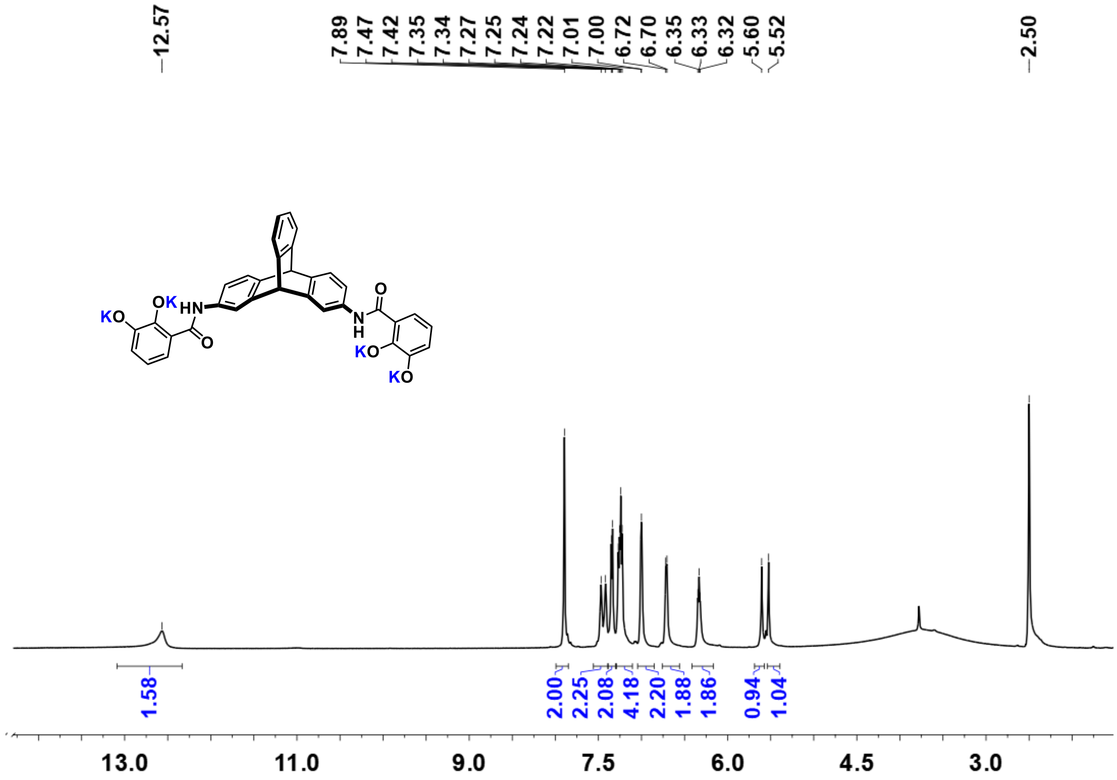


Fig. S7 ^{1}H NMR (500 MHz, DMSO-d_6, 298 K) spectrum of **L-OK**.

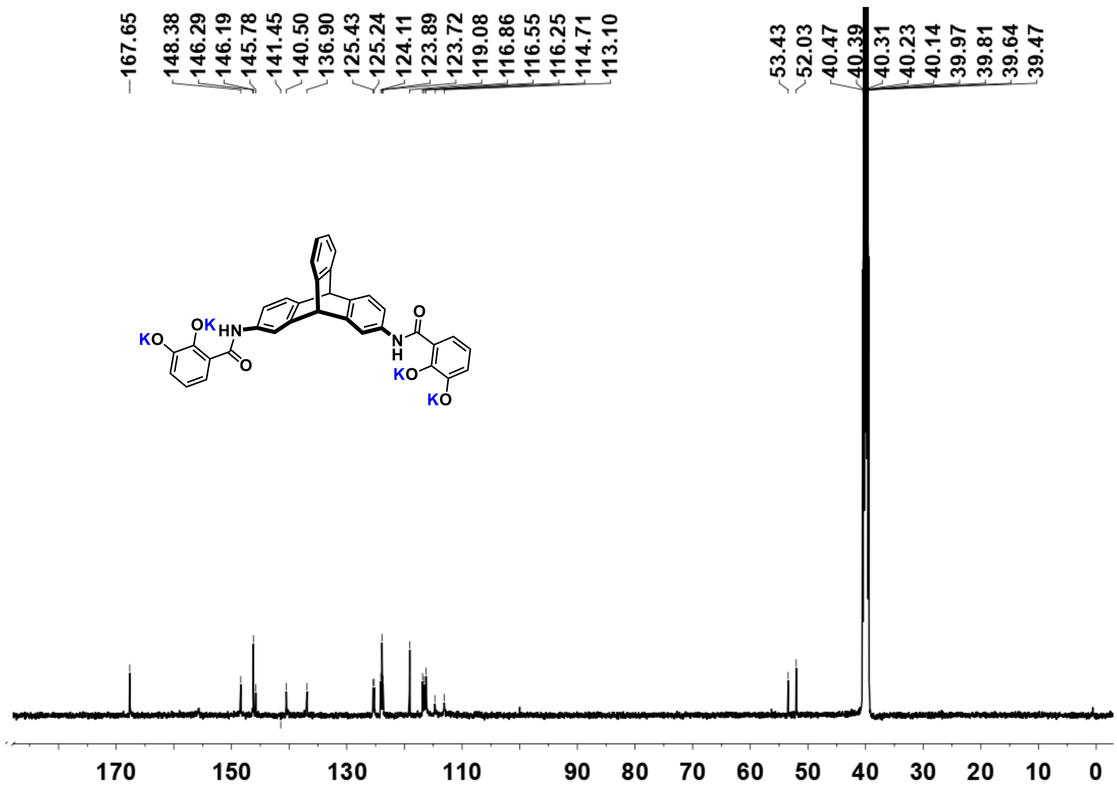
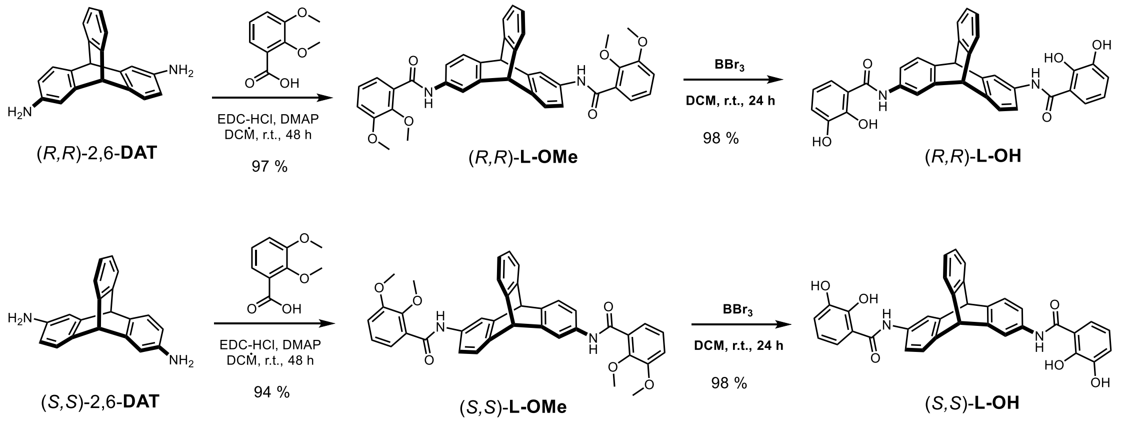


Fig. S8 ^{13}C NMR (126 MHz, DMSO-d_6, 298 K) spectrum of **L-OK**.

2.2 Synthesis of the 2,6-triptycene-based ligands



Scheme S2. Synthetic routes of chiral ligands.

2.2.1 Synthesis of (R,R)/(S,S)-**L-OMe**

To a 10 mL flask was added (*R,R*)-2,6-**DAT** (56.8 mg, 0.20 mmol), DMAP (28 mg, 0.23 mmol), EDC·HCl (191 mg, 1.0 mmol), 2,3-dimethoxybenzoic acid (80 mg, 0.44 mmol) and dried DCM (4.0 mL). The reaction was kept stir at room temperature for 48 hours. Then a saturated solution of potassium hydroxide (2.0 mL) was added to the flask with stirring heavily for 10 minutes. The organic phase was collected and dried by anhydrous magnesium sulfate, and concentrated under reduced pressure. The white solid was subjected to silica gel column chromatography using DCM/MeOH (100:1, v/v) as the eluent to afford the (*R*,*R*)-**L-OMe** as a white powder (118 mg, 97%). M.p.: 143.4-145.1 °C. ^{1}H NMR (300 MHz, $CDCl_3$, 298 K): δ 9.90 (s, NH, 2H), 7.98 (s, 2H), 7.75 (d, *J* = 7.9 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 4H), 7.19 (t, *J* = 8.0 Hz, 2H), 7.09 (dd, *J* = 14.7, 8.0 Hz, 4H), 7.03-6.95 (m, 2H), 5.43 (s, 2H), 3.93 (s, 6H), 3.91 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$, 298 K): δ 163.1, 152.8, 147.4, 146.6, 145.3, 141.4, 135.9, 127.2, 125.5, 125.0, 124.2, 123.9, 123.2, 116.6, 116.5, 115.9, 61.9, 56.4, 53.9. HR-ESI-MS: *m/z* calculated for $[M+H]^+$ $C_{38}H_{33}O_6N_2^+$, 613.2333; found 613.2328.

The synthetic procedures for (*S,S*)-**L-OMe** were completely same as (*R*,*R*)-**L-OMe**, and the isolated yield was 94 %. M.p.: 144.2-145.3 °C. ^{1}H NMR (300 MHz, $CDCl_3$, 298 K): δ 9.90 (s, 2H), 7.97 (d, *J* = 1.7 Hz, 2H), 7.75 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.42-7.37 (m, 2H), 7.35 (d, *J* = 7.7 Hz, 2H), 7.19 (t, *J* = 8.0 Hz, 2H), 7.12 (dd, *J* = 7.9, 2.0 Hz, 2H), 7.07 (dd, *J* = 8.1, 1.3 Hz, 2H), 7.03-6.95 (m, 2H), 5.43 (s, 2H), 3.93 (s, 6H), 3.91 (s, 6H).

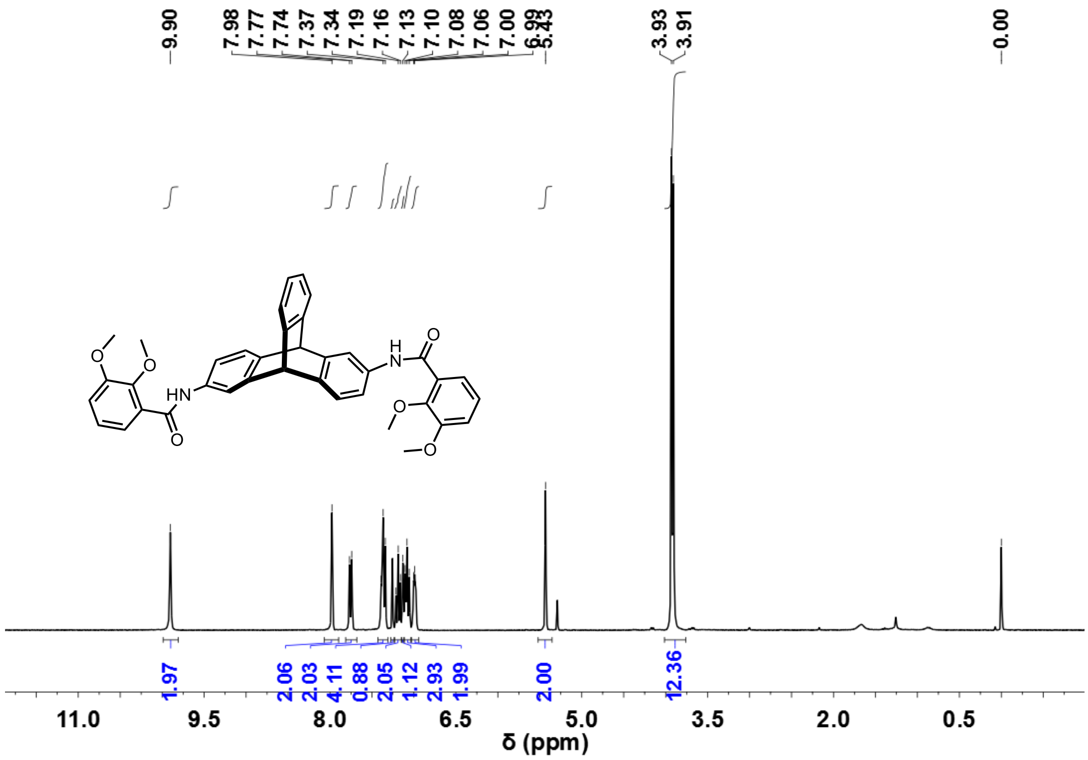


Fig. S9 ^{1}H NMR (300 MHz, $CDCl_3$, 298 K) spectrum of (*R,R*)-**L-OMe**.

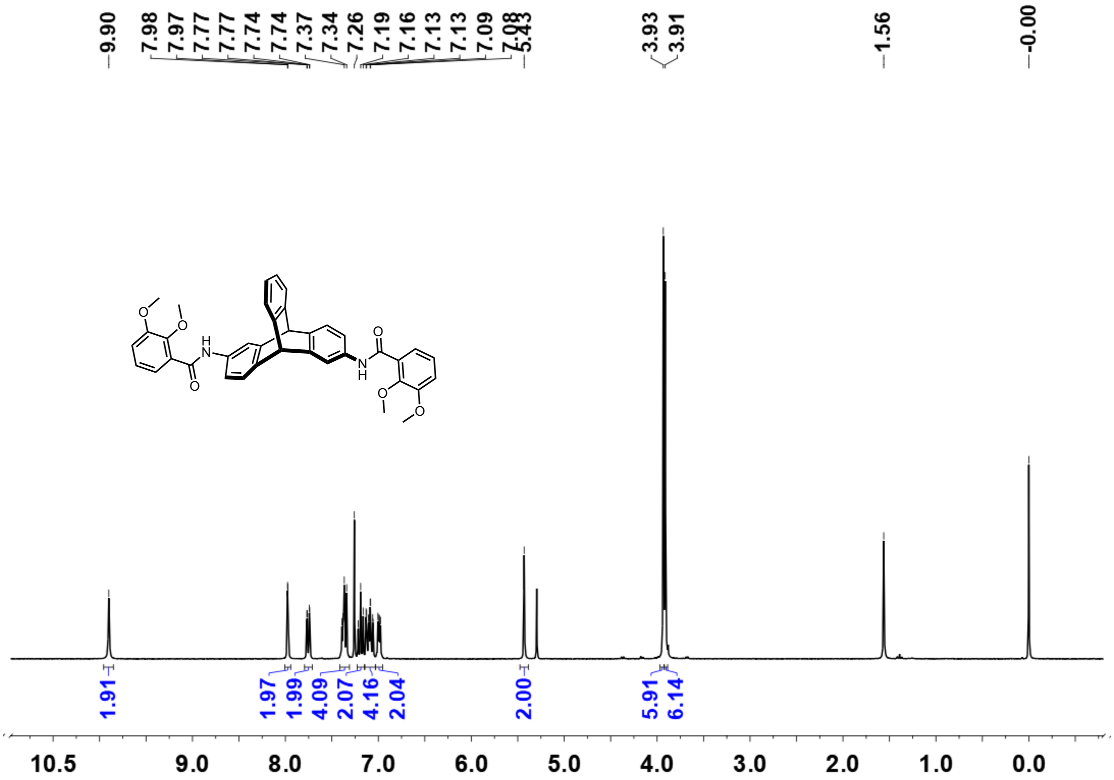


Fig. S10 ^{1}H NMR (300 MHz, $CDCl_3$, 298 K) spectrum of (*S,S*)-**L-OMe**.

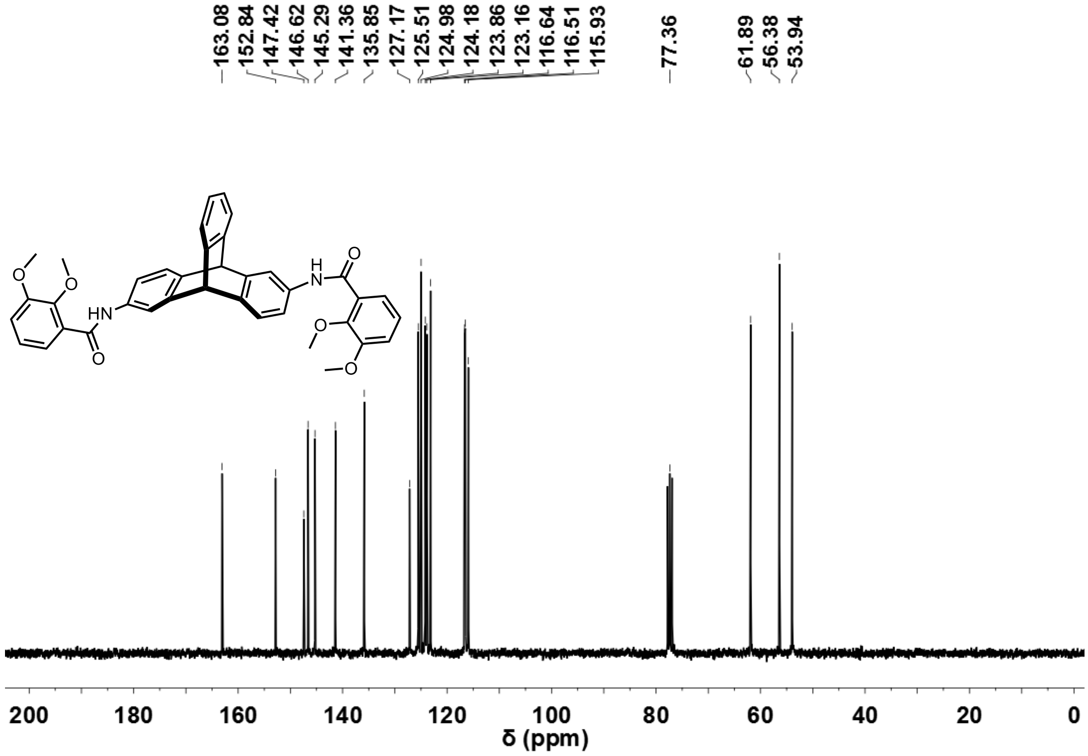


Fig. S11 ^{13}C NMR (75 MHz, $CDCl_3$, 298 K) spectrum of (*R,R*)-**L-OMe**.

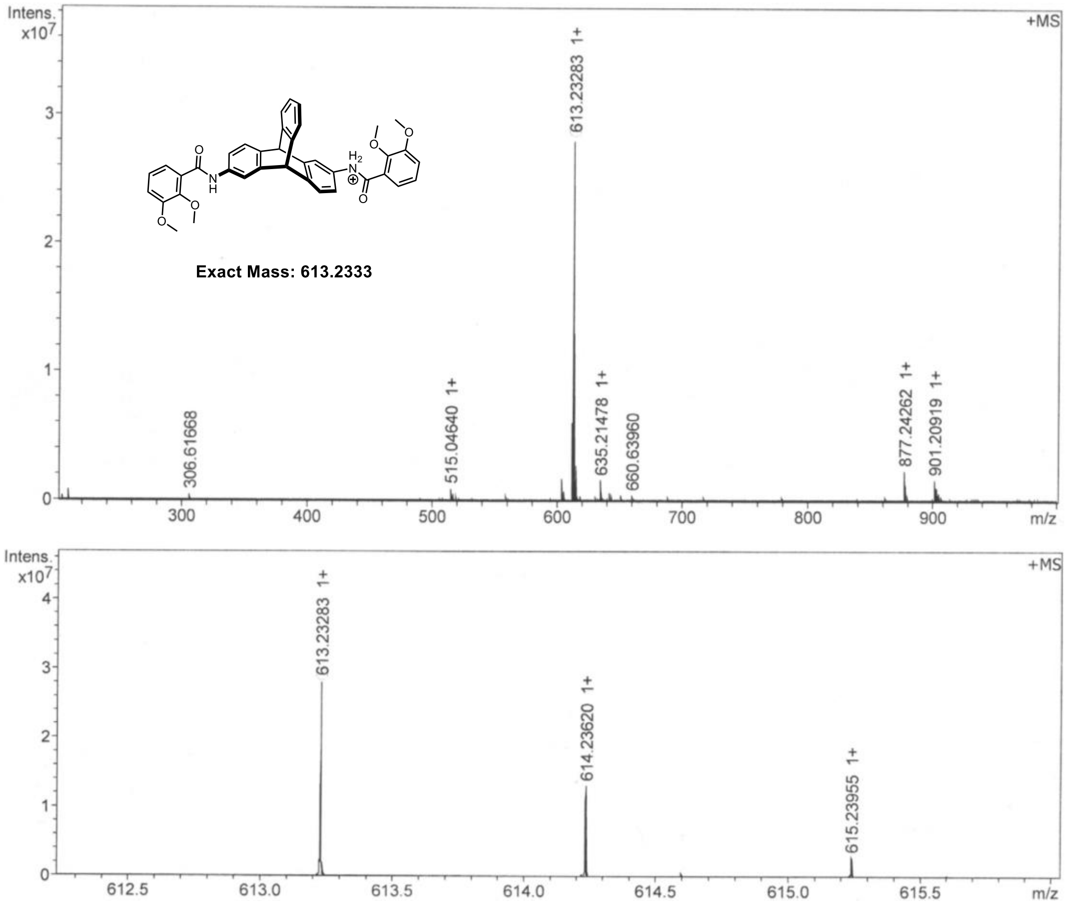


Fig. S12 HR-ESI-MS of (*R,R*)-**L-OMe**.

2.2.2 Synthesis of (R,R)/(S,S)-**L-OH**

To a 25 mL round-bottom bottle was added (R,R)-**L-OMe** (91.8 mg, 0.15 mmol) and dried DCM (10.0 mL). The solution was stirred at 0 °C for several minutes, then BBr_3 (0.3 mL) was added. The reaction was kept at room temperature 24 hours, then 10 mL methanol was added with stirring heavily 6 hours. The mixture was concentrated under reduced pressure. The grey red fibrous solid was subjected to a silica gel column chromatography using DCM/MeOH (25:1, v/v) as the eluent to afford the (R,R)-**L-OH** as a grey red fibrous solid (83 mg, 98%). M.p.: 186.5-188.4 °C. **^{1}H NMR** (400 MHz, DMSO-d_6, 298 K): δ 11.81 (s, 2H), 10.34 (s, 2H), 9.43 (s, 2H), 7.92 (s, 2H), 7.50 (dt, *J* = 16.9, 6.1 Hz, 6H), 7.30 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.10-7.04 (m, 2H), 7.02 (d, *J* = 7.8 Hz, 2H), 6.81 (t, *J* = 7.9 Hz, 2H), 5.70 (s, 2H). **^{13}C NMR** (101 MHz, DMSO-d_6, 298 K): δ 168.1, 149.0, 146.7, 146.4, 145.7, 141.8, 135.3, 125.5, 124.2, 124.1, 119.5, 118.9, 118.7, 118.1, 117.9, 117.2, 55.4, 52.6. **HR-ESI-MS**: *m/z* calculated for $[M+H]^+$ $C_{34}H_{25}O_6N_2^+$, 557.1707; found 557.1702; $[M+Na]^+$ $C_{34}H_{24}O_6N_2Na^+$, 579.1532; found 559.1521.

The synthetic procedures for (*S*,*S*)-**L-OH** were completely same as (*R*,*R*)-**L-OH**, and the isolated yield was 98 %. M.p.: 187.2-188.6 °C. ^{1}H NMR (300 MHz, DMSO-d_6, 298 K): δ 11.74 (s, 2H), 10.28 (s, 2H), 9.36 (s, 2H), 7.86 (s, 2H), 7.50-7.46 (m, 2H), 7.44 (d, *J* = 7.9 Hz, 2H), 7.41 (d, *J* = 10.0 Hz, 2H), 7.24 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.02 (dd, *J* = 5.0, 3.3 Hz, 2H), 6.96 (d, *J* = 7.6 Hz, 2H), 6.75 (t, *J* = 8.0 Hz, 2H), 5.66 (s, 2H).

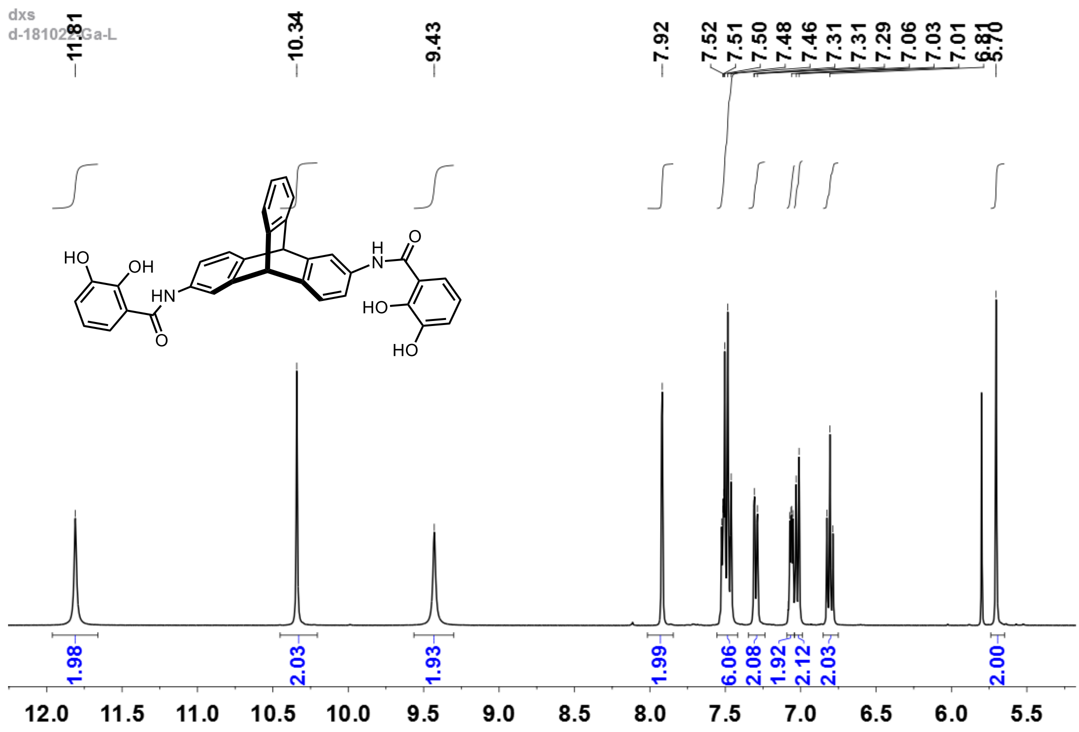


Fig. S13 [1]H NMR (400 MHz, DMSO-d_6, 298 K) spectrum of (*R,R*)-**L-OH**.

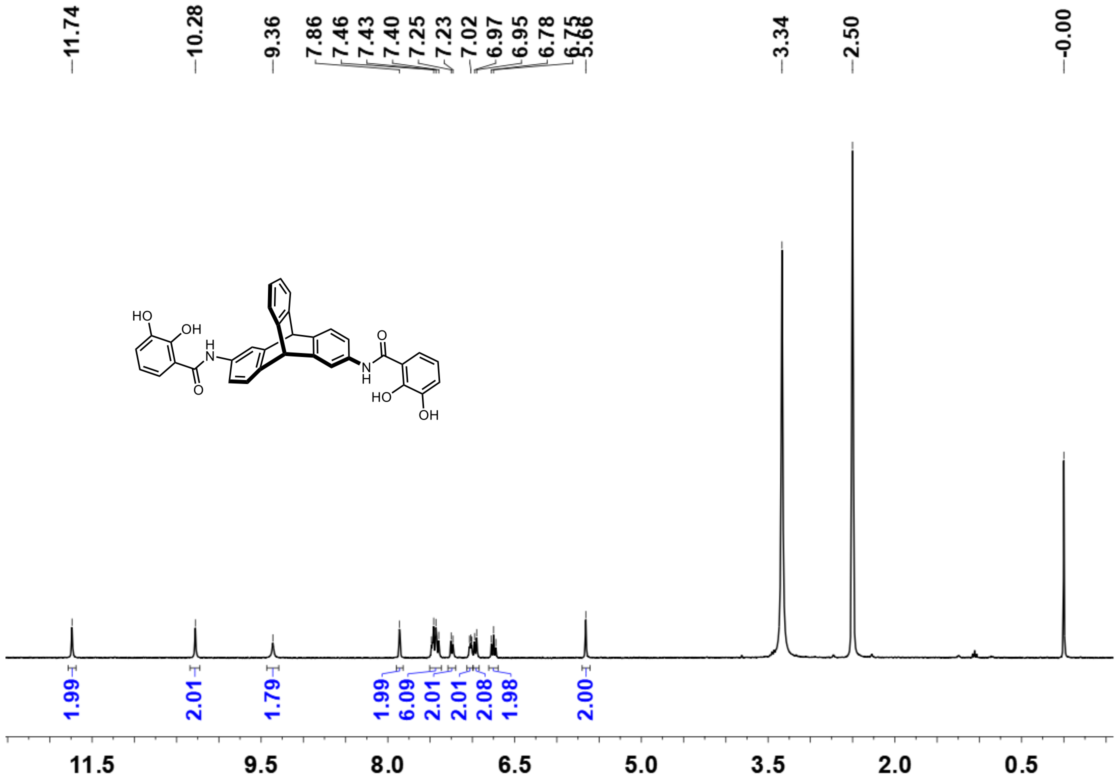


Fig. S14 [1]H NMR (300 MHz, DMSO-d_6, 298 K) spectrum of (*S,S*)-**L-OH**.

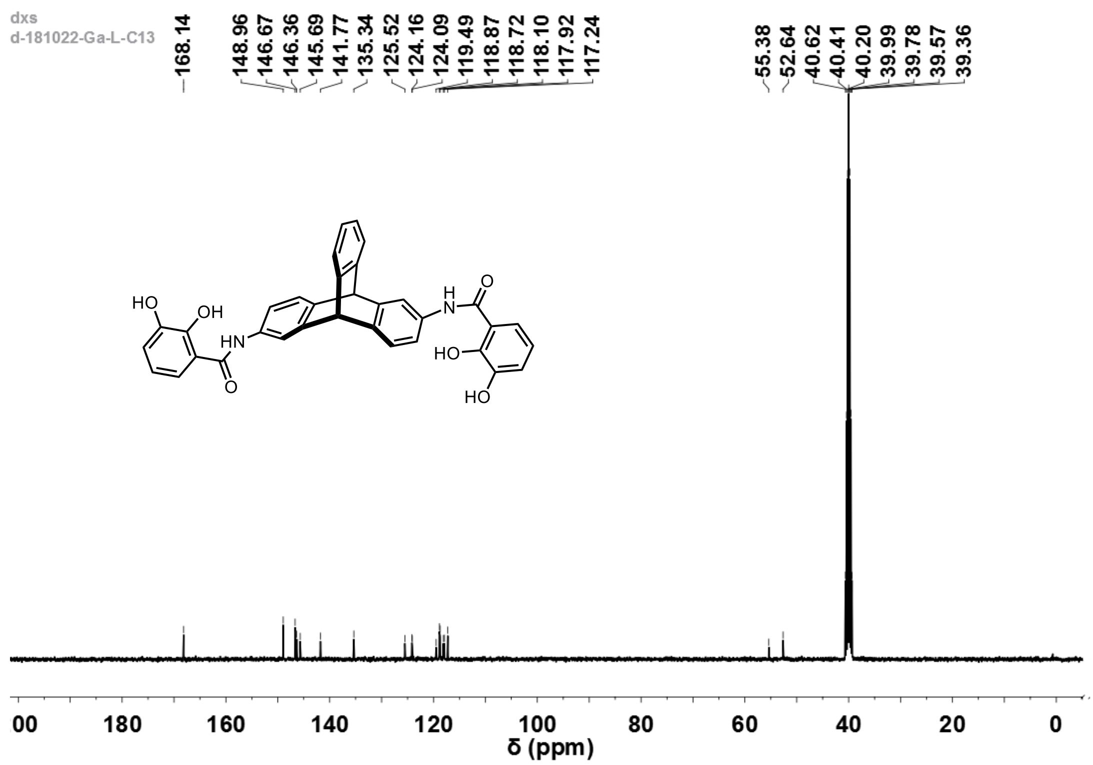


Fig. S15 ^{13}C NMR (100 MHz, DMSO-d_6, 298 K) spectrum of (*R,R*)-**L-OH**.

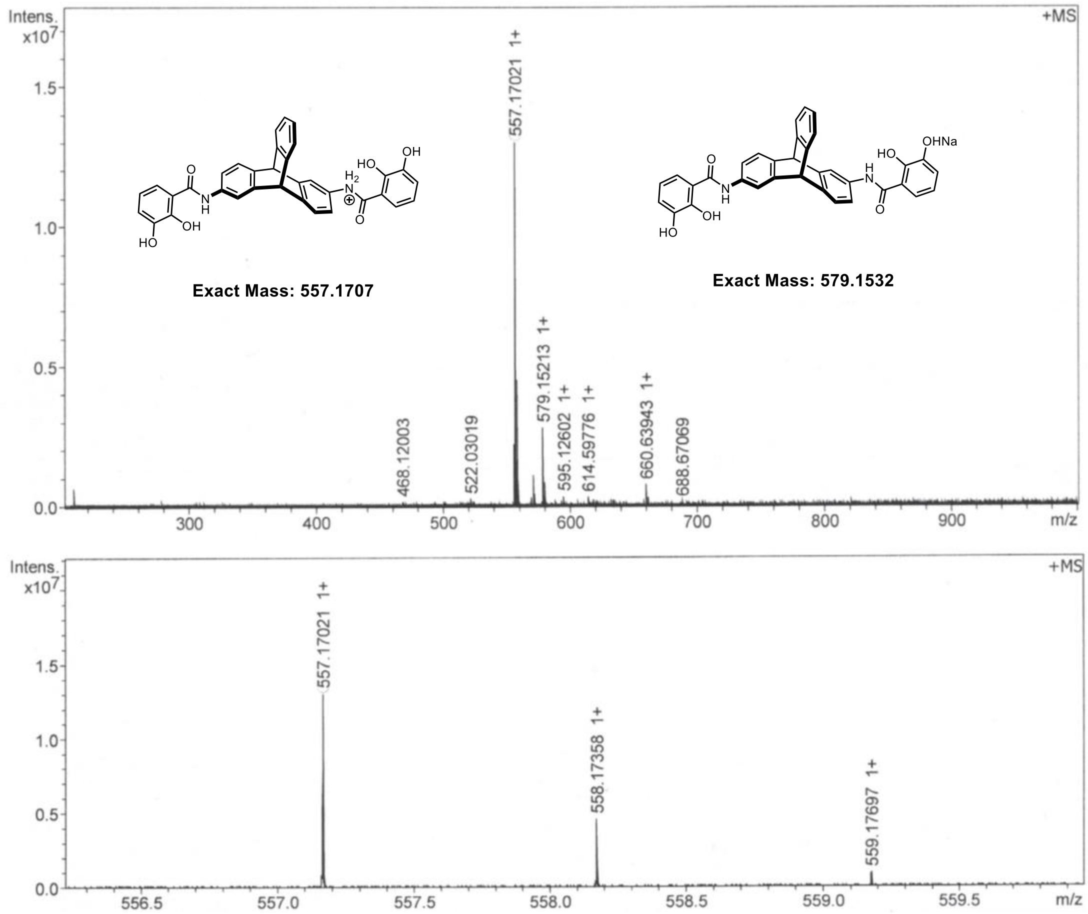
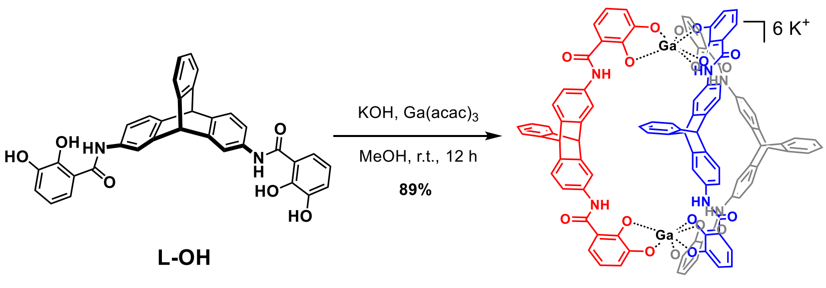


Fig. S16 HR-ESI-MS of (*R,R*)-**L-OH**.

2.3 Synthesis of the 2,7-triptycene-based helicates

2.3.1 Synthesis of K_6[**Ga₂L₃**]



To a 15 mL tube was added **L-OH** (41.7 mg, 0.075 mmol), KOH (8.4 mg, 0.15 mmol) and dried methanol (3.0 mL). Keep the mixture stirred for 30 minutes at room temperature, and then the solution of $Ga(acac)_3$ (18.4 mg, 0.05 mmol) in methanol (1.0 mL) was added by syringe, and kept at room temperature for 12 hours. Then 10 mL diethyl ether was added to produce brown precipitate, which was filtered and washed with diethyl ether three times. The pale-yellow powder was subjected to NMR analysis. ^{1}H NMR (700 MHz, DMSO-d_6, 298 K): δ 13.86 (s, NH, 6H), 8.38 (s, 6H), 7.36 (dd, J = 40.0, 6.0 Hz, 6H), 6.89-6.86 (m, 6H), 6.79 (dd, J = 8.2, 1.2 Hz, 6H), 6.74 (d, J = 7.9 Hz, 6H), 6.22 (dd, J = 7.2, 1.2 Hz, 6H), 6.08-6.01 (m, 12H), 5.31 (s, 3H), 5.06 (s, 3H). ^{13}C NMR (176 MHz, DMSO-d_6, 298 K): δ 166.9, 158.9, 157.2, 147.3, 146.8, 145.6, 138.6, 137.9, 124.8, 124.6, 123.7, 123.5, 123.3, 115.7, 114.6, 113.1, 112.5, 112.4, 54.4, 52.5.

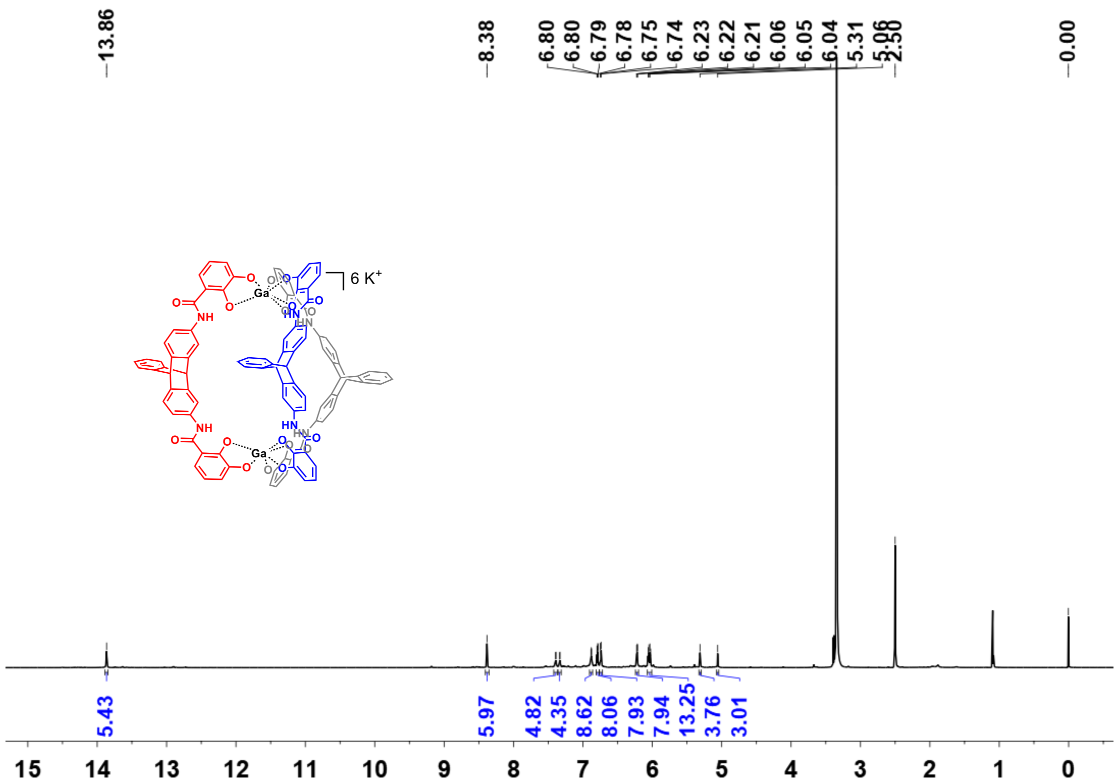


Fig. S17 ^{1}H NMR (700 MHz, DMSO-d_6, 298 K) spectrum of K_6[$\mathbf{Ga_2L_3}$].

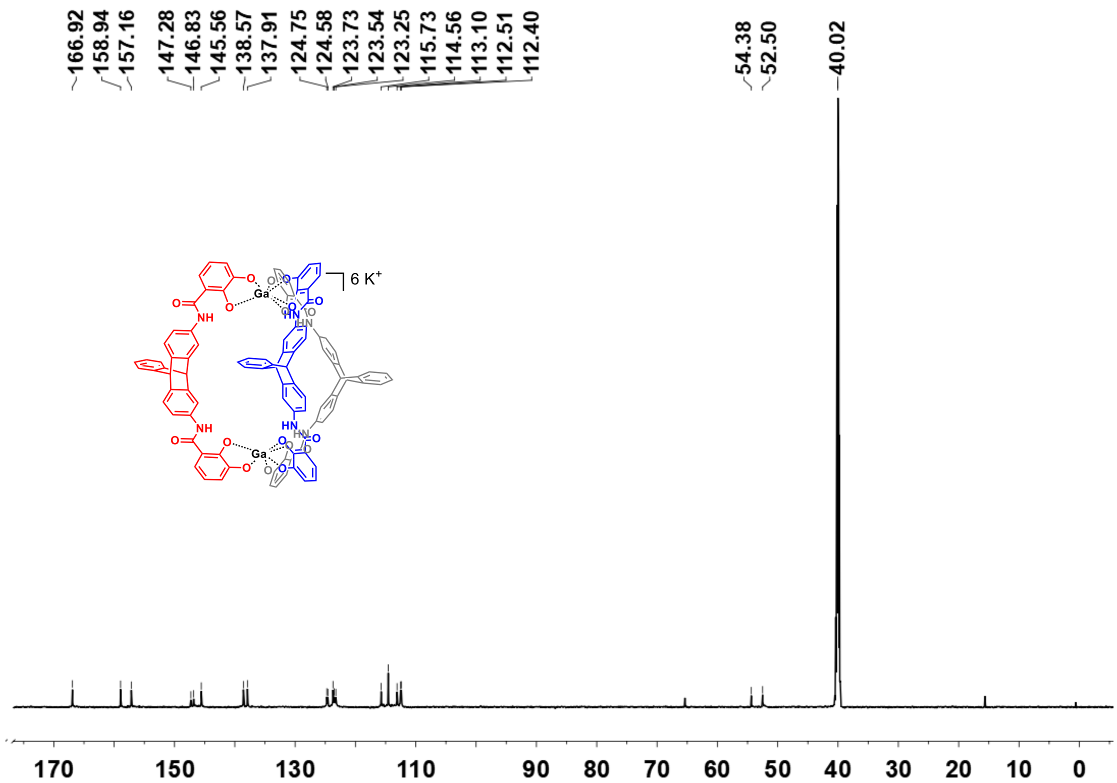


Fig. S18 ^{13}C NMR (176 MHz, DMSO-d_6, 298 K) spectrum of K_6[$\mathbf{Ga_2L_3}$].

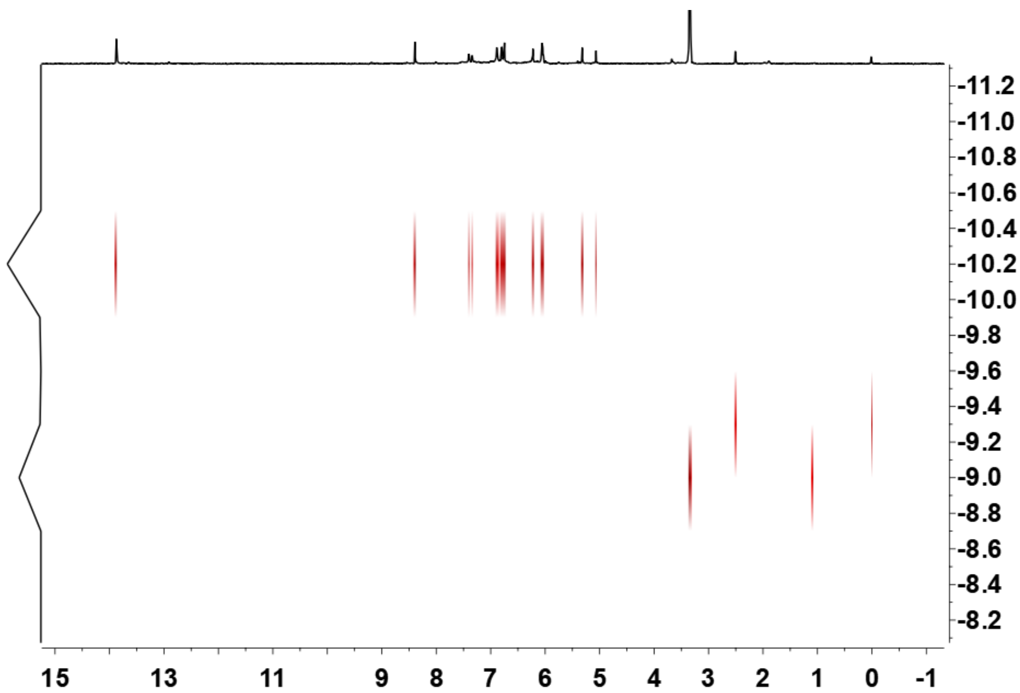
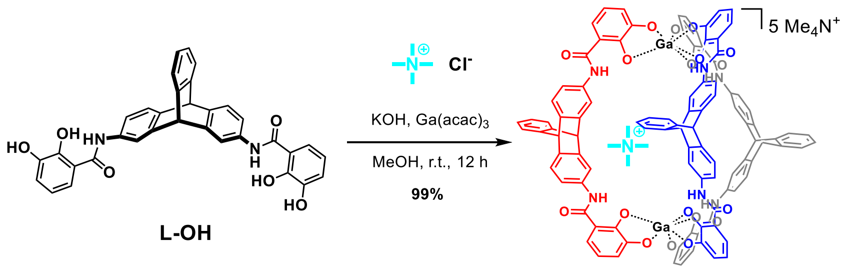


Fig. S19 DOSY (700 MHz, DMSO-d_6, 298 K) spectrum of K_6[**Ga_2L_3**].

2.3.2 Synthesis of $(Me_4N)_6$[**Ga_2L_3**]



To a 15 mL tube was added **L-OH** (41.7 mg, 0.075 mmol), KOH (8.4 mg, 0.15 mmol) and dried methanol (3.0 mL). Keep the mixture stirred for 30 minutes and the solution of Me_4NCl (22.3 mg, 0.20 mmol) in methanol (1.0 mL) was added by syringe. After 10 minutes the solution of $Ga(acac)_3$ (18.4 mg, 0.05 mmol) in methanol (1.0 mL) was added by syringe, and kept at room temperature for 12 hours. Then 10 mL diethyl ether was added to produce white precipitate, which was filtered and washed with diethyl ether three times. The final white powder was used without further purification. ^{1}H NMR (700 MHz, DMSO-d_6, 298 K): δ 14.12 (s, 6H), 8.59 (s, 6H), 7.41 (d, J = 38.0 Hz, 6H), 6.95 (s, 6H), 6.88 (d, J = 7.4 Hz, 6H), 6.83 (d, J = 7.5 Hz, 6H), 6.24 (d, J = 5.9 Hz, 6H), 6.07 (t, J = 7.2 Hz, 6H), 5.99 (d, J = 7.3 Hz, 6H), 5.46 (s, 3H), 5.40 (s, 3H), 3.05 (s, Me_4N^+ as counter cation, 60H), -0.06 (s, encapsulated Me_4N^+, 12H). ^{13}C NMR (176 MHz, DMSO-d_6, 298 K): δ 167.4, 159.1, 157.2, 146.9, 146.2, 145.5, 138.9, 138.8, 125.3, 125.1, 124.0, 123.8, 123.6, 114.9, 114.6, 114.2, 112.9, 112.7, 54.8, 53.9, 52.6, 51.4. HR-ESI-MS: *m/z* calculated for $[(\mathbf{Ga_2L_3})+K+H+2Me_4N]^{2-}$ $(C_{110}H_{85}Ga_2N_8O_{18}K)^{2-}$, 991.2071; found 991.2075; $[(\mathbf{Ga_2L_3})+K+H+Me_4N]^{2-}$ $(C_{106}H_{73}Ga_2N_7O_{18}K)^{3-}$, 636.1059; found 636.1052; $[(\mathbf{Ga_2L_3})+2H]^{4-}$ $(C_{102}H_{62}Ga_2N_6O_{18})^{4-}$, 449.0664; found 449.0666.

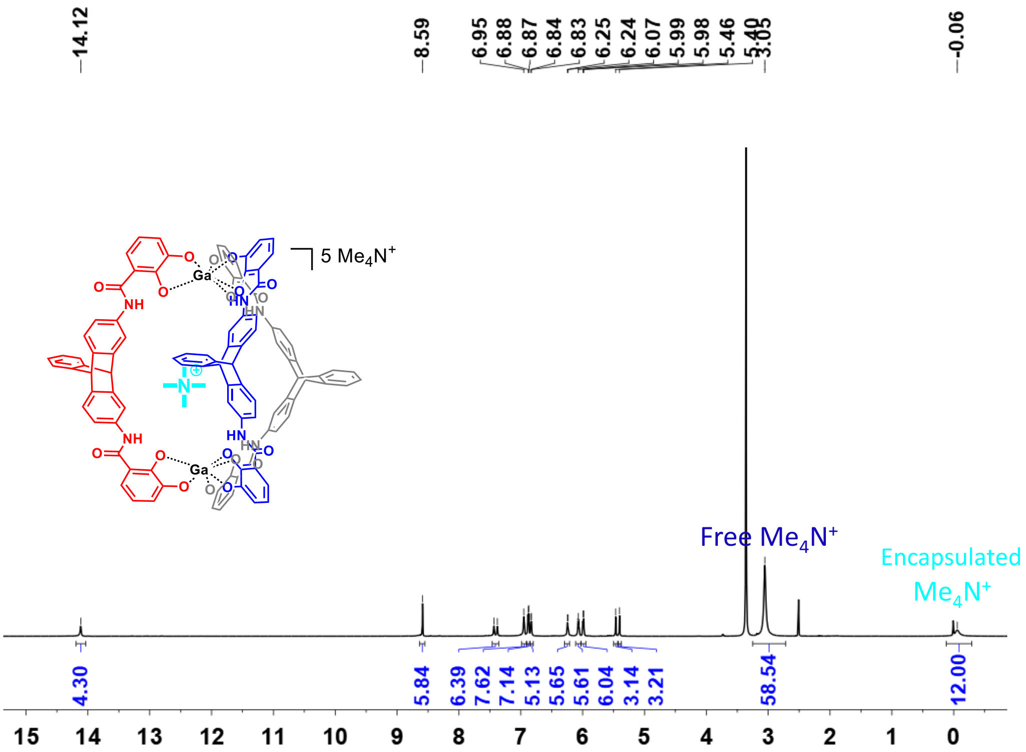


Fig. S20 ^{1}H NMR (700 MHz, DMSO-d_6, 298 K) spectrum of $(Me_4N)_5[Me_4N@\mathbf{Ga_2L_3}]$.

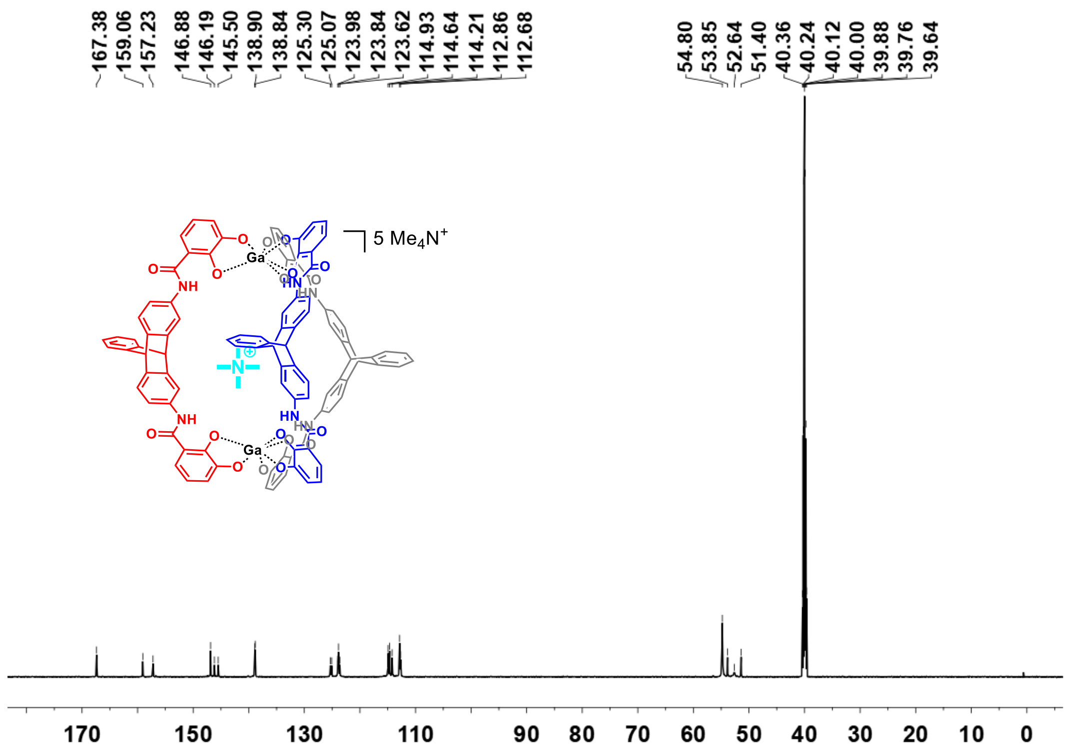


Fig. S21 ^{13}C NMR (176 MHz, DMSO-d_6, 298 K) spectrum of $(Me_4N)_5[Me_4N@\mathbf{Ga_2L_3}]$.

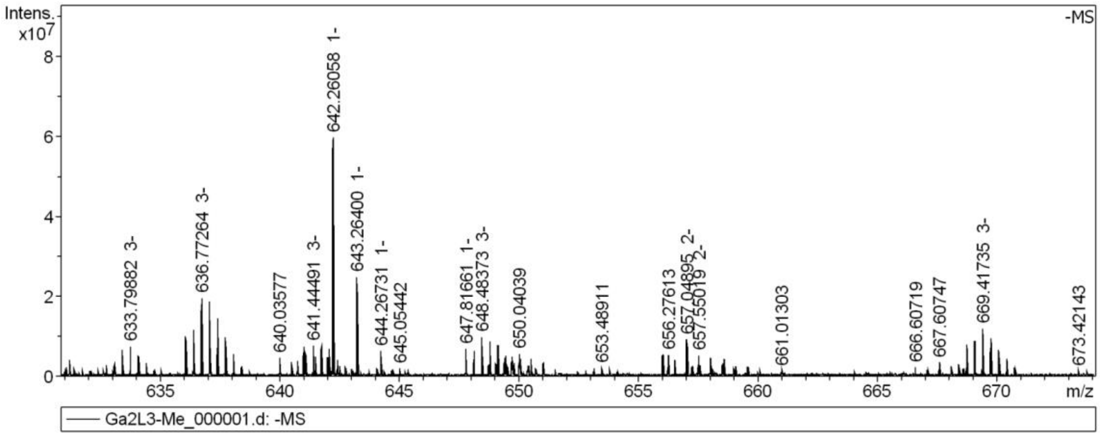


Fig. S22 HR-ESI-MS of $(Me_4N)_5[Me_4N@\mathbf{Ga_2L_3}]$.

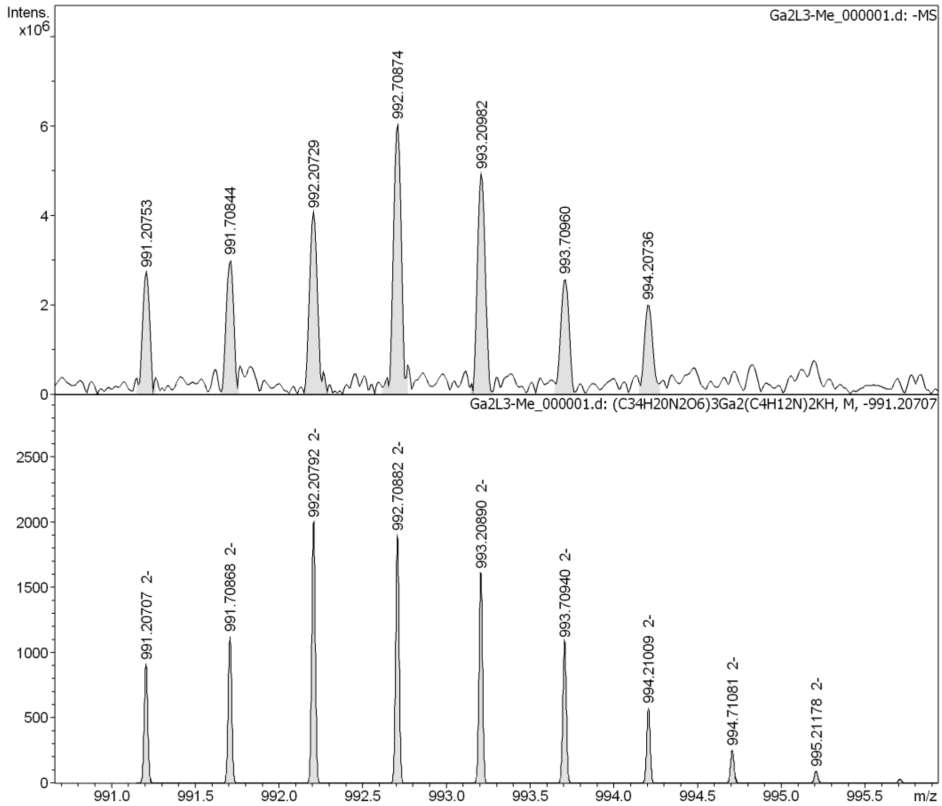


Fig. S23 HR-ESI-MS of $(Me_4N)_5[Me_4N@\mathbf{Ga_2L_3}]$. Exact mass of $[(\mathbf{Ga_2L_3})+K+H+2Me_4N]^{2-}$ was calculated 991.2071, and found 991.2075.

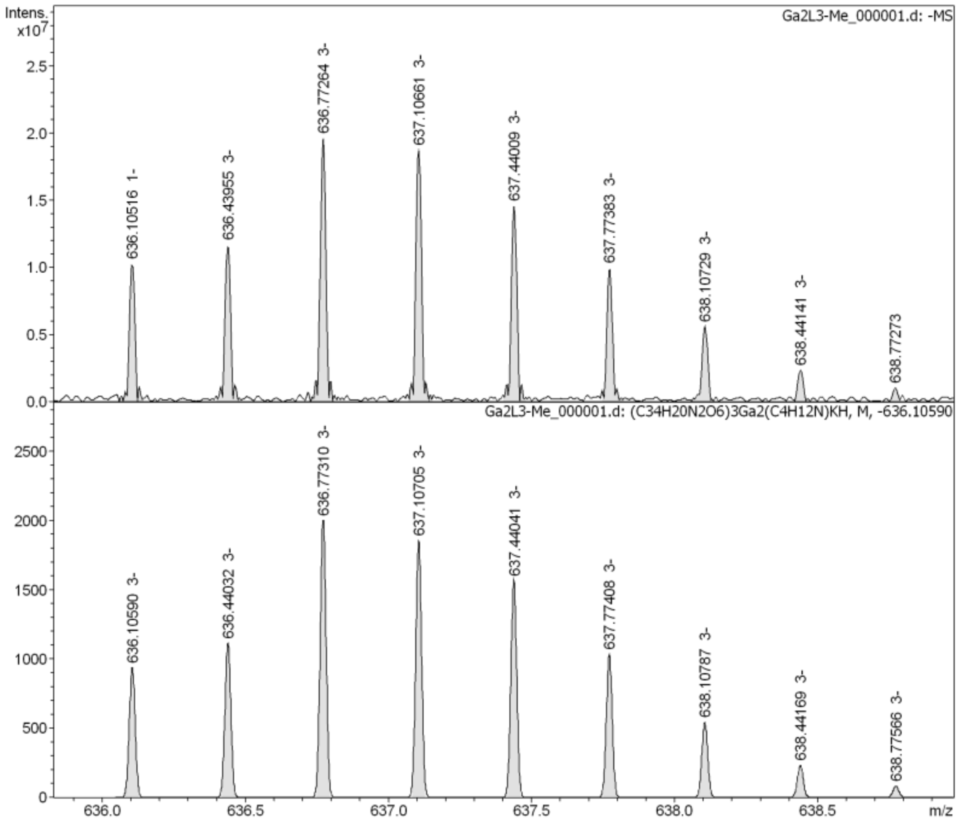


Fig. S24 HR-ESI-MS of $(Me_4N)_5[Me_4N@\mathbf{Ga_2L_3}]$. Exact mass of $[(\mathbf{Ga_2L_3})+K+H+Me_4N]^{3-}$ was calculated 636.1059, and found 636.1052.

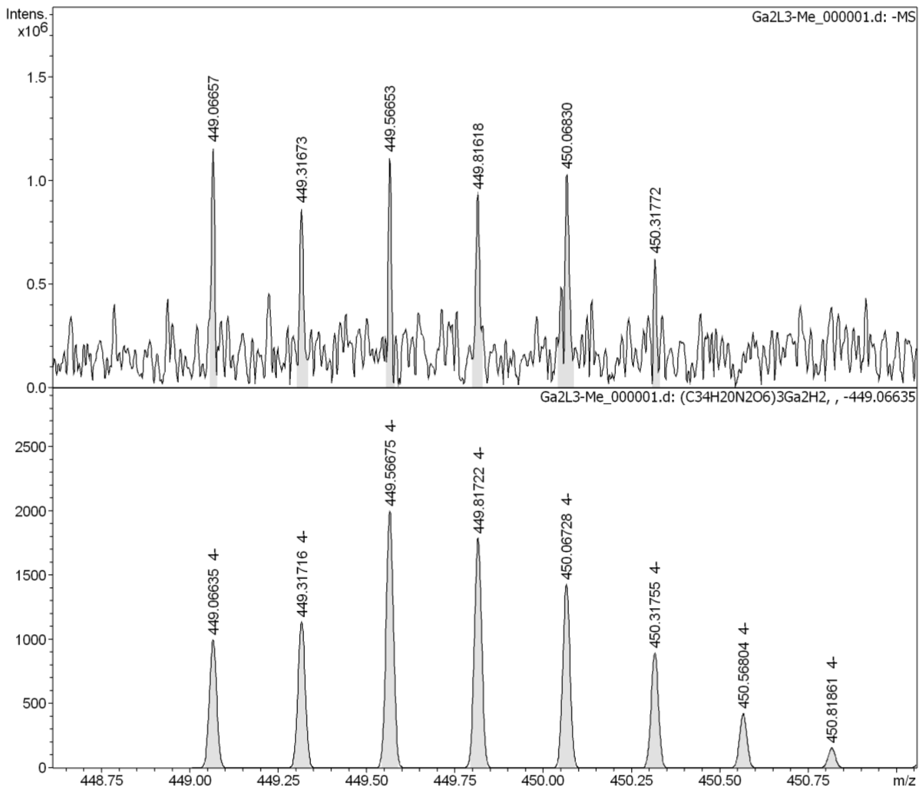


Fig. S25 HR-ESI-MS of $(Me_4N)_5[Me_4N@\mathbf{Ga_2L_3}]$. Exact mass of $[(\mathbf{Ga_2L_3})+2H]^{4-}$ was calculated 449.0664, and found 449.0666.

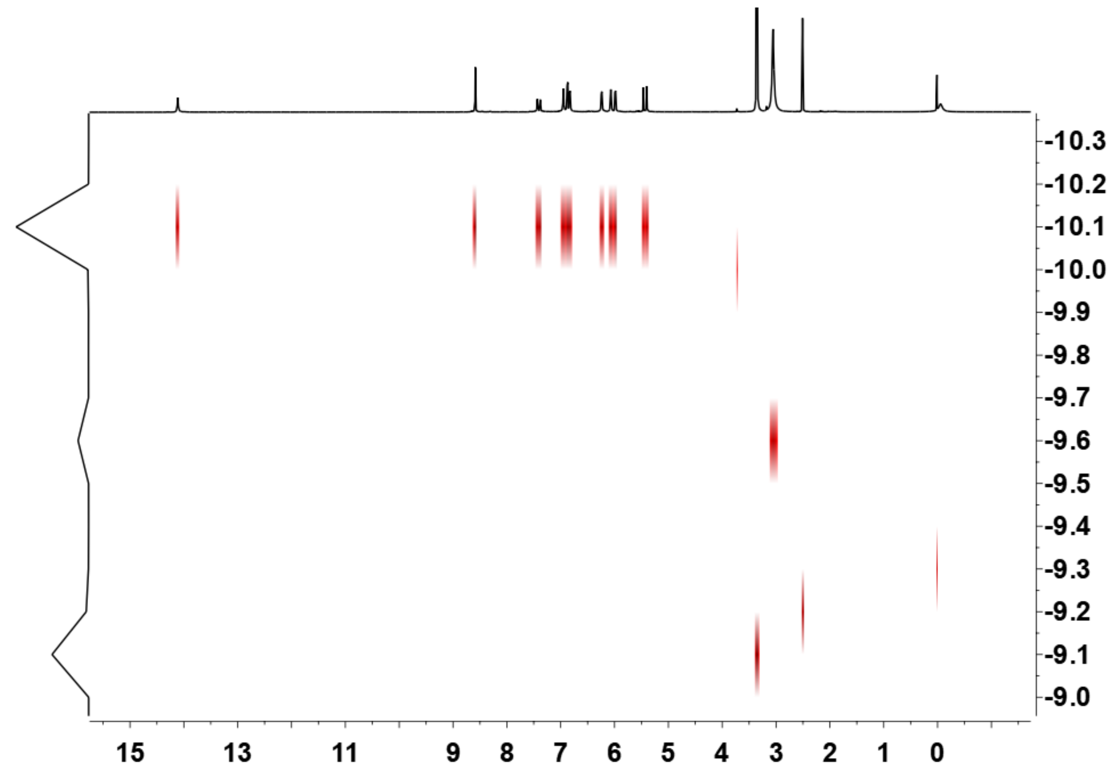


Fig. S26 DOSY (700 MHz, DMSO-d_6, 298 K) spectrum of $(Me_4N)_5[Me_4N@\mathbf{Ga_2L_3}]$.

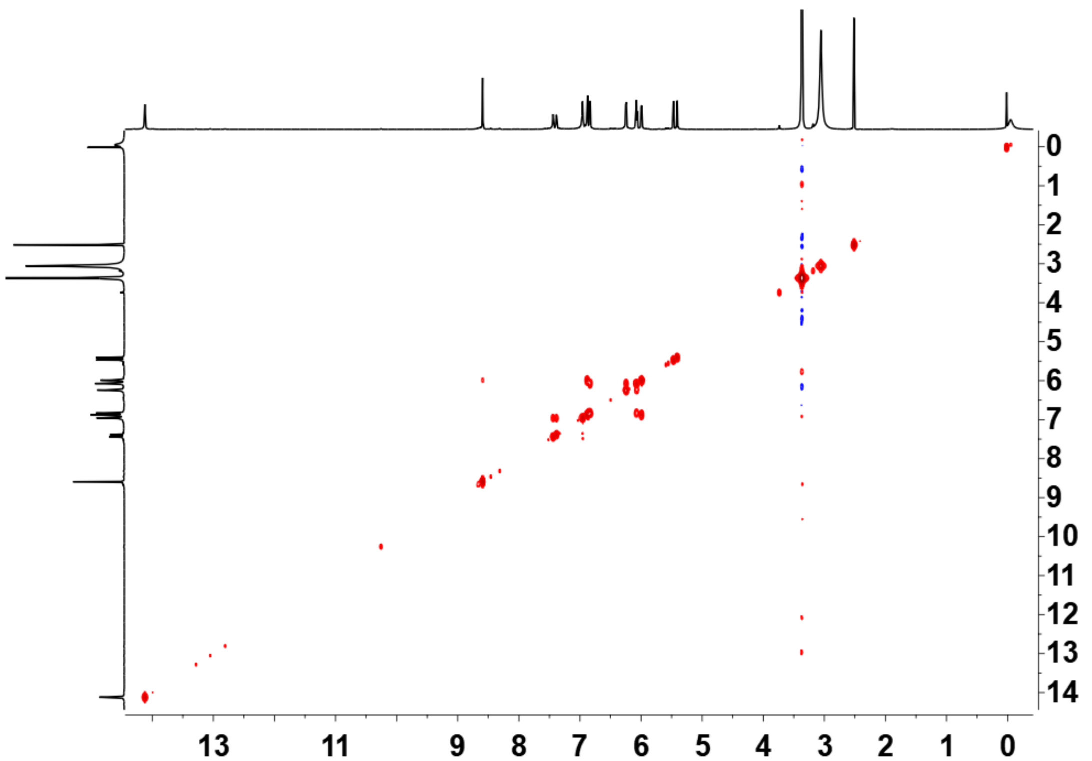


Fig. S27 ^1H-^1H COSY (700 MHz, DMSO-d_6, 298 K) spectrum of $(Me_4N)_5[Me_4N@\mathbf{Ga_2L_3}]$.

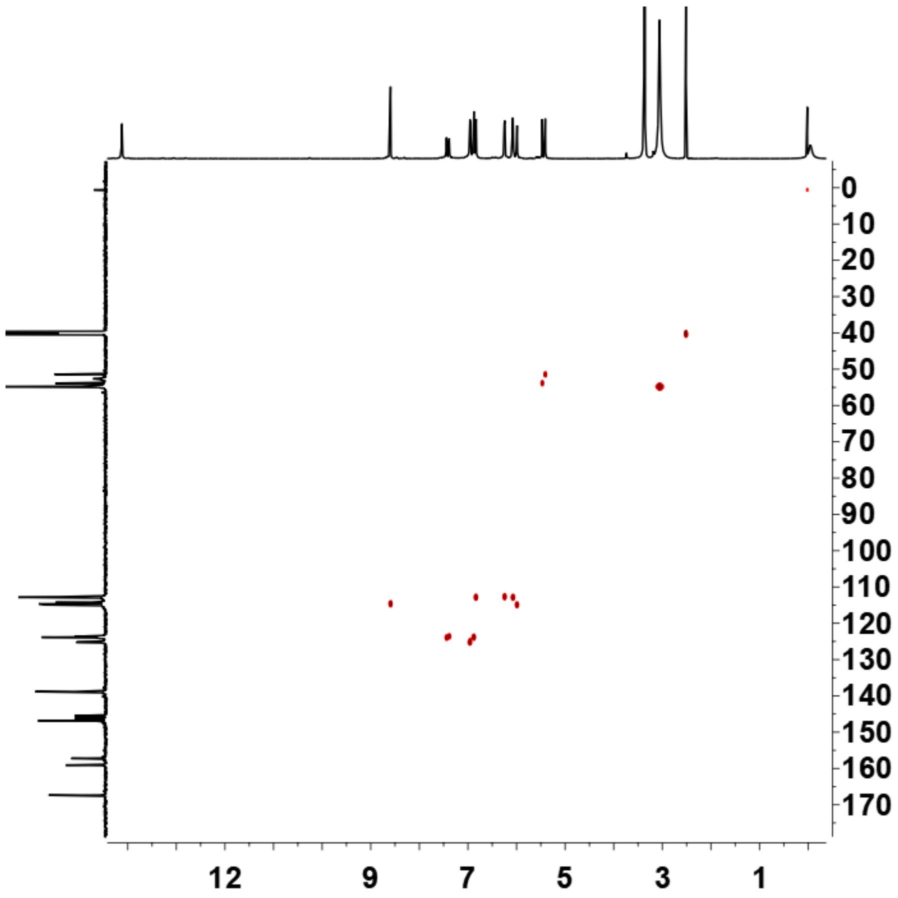


Fig. S28 ^{1}H-^{13}C HSQC (700 MHz, DMSO-d_6, 298 K) spectrum of $(Me_4N)_5[Me_4N@$**Ga_2L_3**$]$.

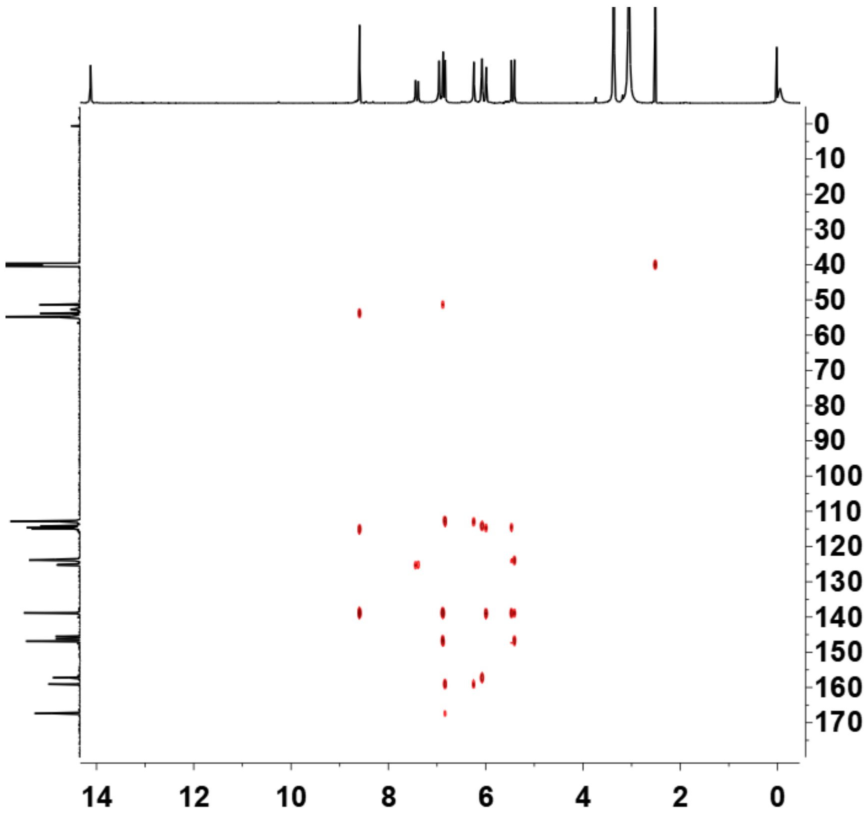


Fig. S29 ^{1}H-^{13}C HMBC (700 MHz, DMSO-d_6, 298 K) spectrum of $(Me_4N)_5[Me_4N@$**Ga_2L_3**$]$.

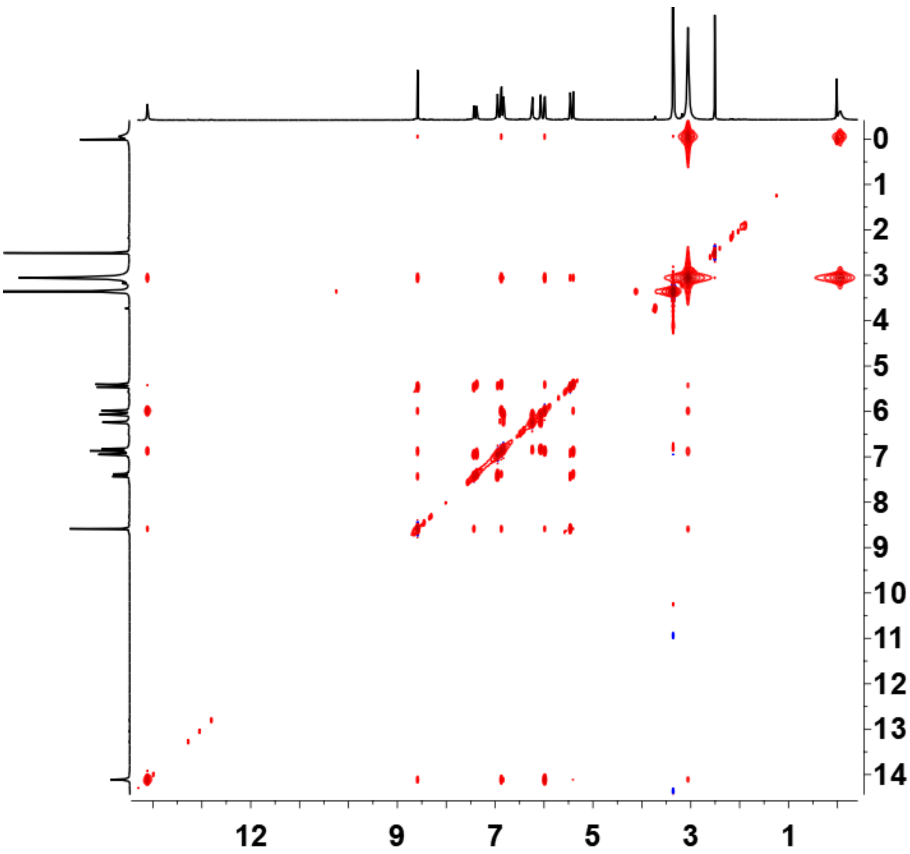
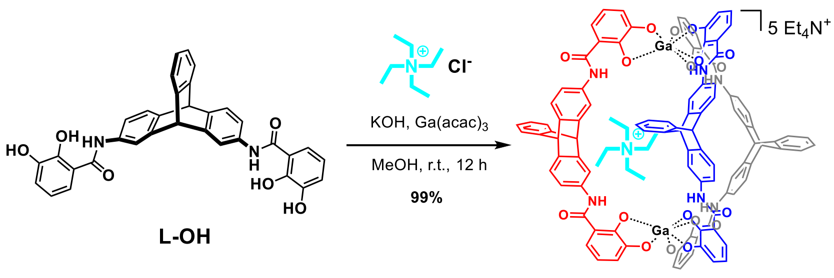


Fig. S30 2D NOESY (700 MHz, DMSO-d_6, 298 K) spectrum of $(Me_4N)_5[Me_4N@$**Ga_2L_3**$]$.

2.3.3 Synthesis of $(Et_4N)_6[$**Ga_2L_3**$]$



To a 15 mL tube was added **L-OH** (41.7 mg, 0.075 mmol), KOH (8.4 mg, 0.15 mmol) and dried methanol (3.0 mL). Keep the mixture stirred for 30 minutes and the solution of Et_4NCl (33.3 mg, 0.2 mmol) in methanol (1.0 mL) was added by syringe. After 10 minutes the solution of $Ga(acac)_3$ (18.4 mg, 0.05 mmol) in methanol (1.0 mL) was added by syringe, and kept at room temperature for 12 hours. Then 10 mL diethyl ether was added to produce light yellow precipitate, which was filtered and washed with diethyl ether three times. The final light-yellow powder was used without further purification. ^1H NMR (500 MHz, DMSO-d_6, 298 K): δ 13.58 (s, 6H), 8.48 (s, 6H), 7.51-7.45 (m, 3H), 7.45-7.39 (m, 3H), 7.03 (d, J = 7.8 Hz, 6H), 7.00-6.95

(m, 6H), 6.79 (d, J = 7.9 Hz, 6H), 6.22 (d, J = 7.0 Hz, 6H), 6.06 (t, J = 7.7 Hz, 6H), 5.98 (d, J = 7.5 Hz, 6H), 5.54 (s, 3H), 5.42 (s, 3H), 3.13 (q, J = 7.5 Hz, 14.5 Hz, Et_4N^+ as counter cation, 40H), 1.10 (t, J = 6.2 Hz, Et_4N^+ as counter cation, 60H), 0.18-0.02 (m, encapsulated Et_4N^+, 8H), -0.29 (t, J = 6.3 Hz, encapsulated Et_4N^+, 12H). ^{13}C NMR (126 MHz, DMSO-d_6, 298 K): δ 166.8, 158.7, 157.0, 146.04, 145.97, 145.3, 138.7, 137.5, 124.8, 124.6, 123.5, 123.1, 115.4, 115.2, 113.8, 112.5, 112.3, 112.2, 53.4, 51.4, 51.34, 51.32, 49.2, 7.0, 6.0. HR-ESI-MS: m/z calculated for $[(\mathbf{Ga_2L_3})+NH_4+H+2Et_4N]^{2-}$ $(C_{110}H_{85}Ga_2N_8O_{18}K)^{2-}$, 1035.2814; found 1035.3014; $[(\mathbf{Ga_2L_3})+NH_4+H+Et_4N]^{3-}$ $(C_{110}H_{85}Ga_2N_8O_{18})^{3-}$, 646.8012; found 646.8142; $[(\mathbf{Ga_2L_3})+2NH_4]^{4-}$ $(C_{118}H_{105}Ga_2N_9O_{18})^{4-}$, 456.0651; found 456.0746.

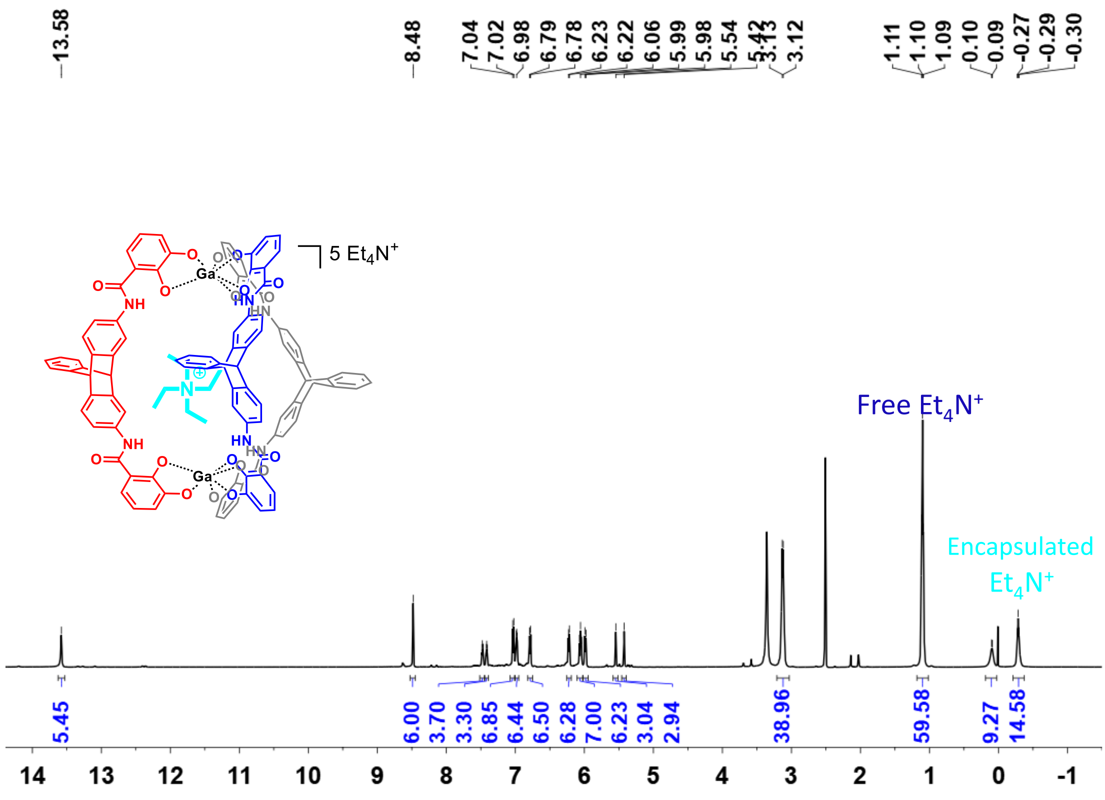


Fig. S31 ^1H NMR (500 MHz, DMSO-d_6, 298 K) spectrum of $(Et_4N)_5[Et_4N@\mathbf{Ga_2L_3}]$.

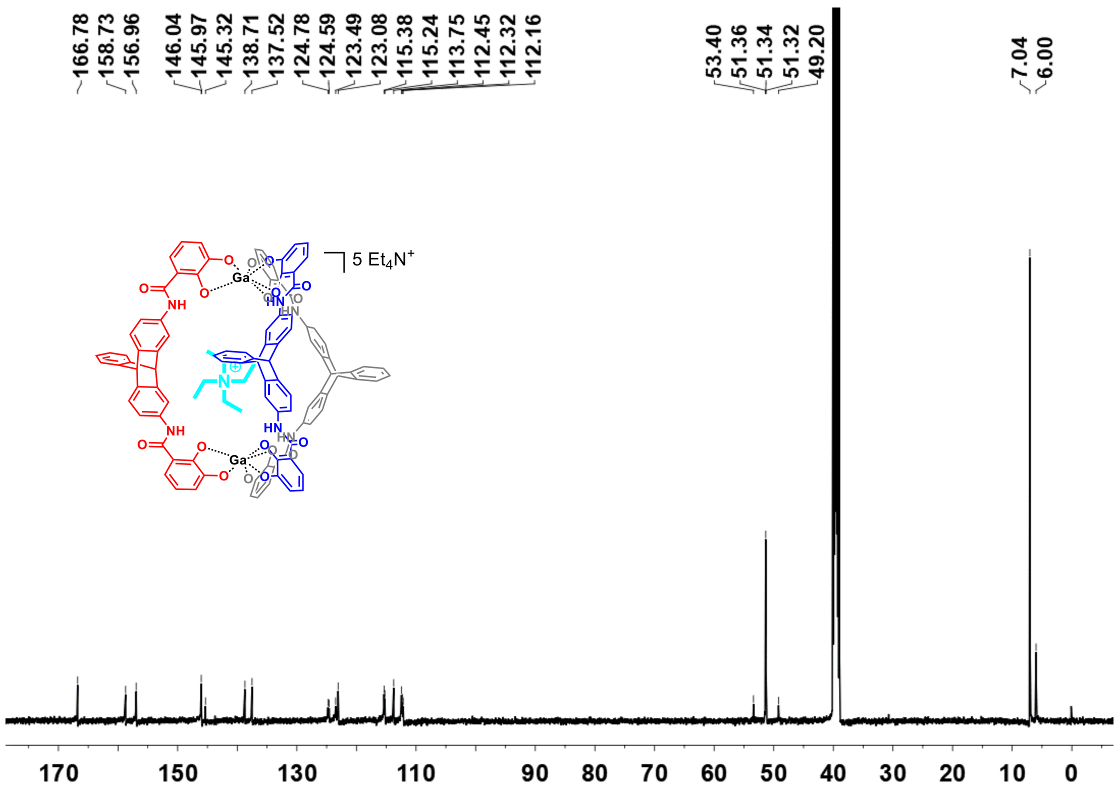


Fig. S32 ^{13}C NMR (126 MHz, DMSO-d_6, 298 K) spectrum of $(Et_4N)_5[Et_4N@\mathbf{Ga_2L_3}]$.

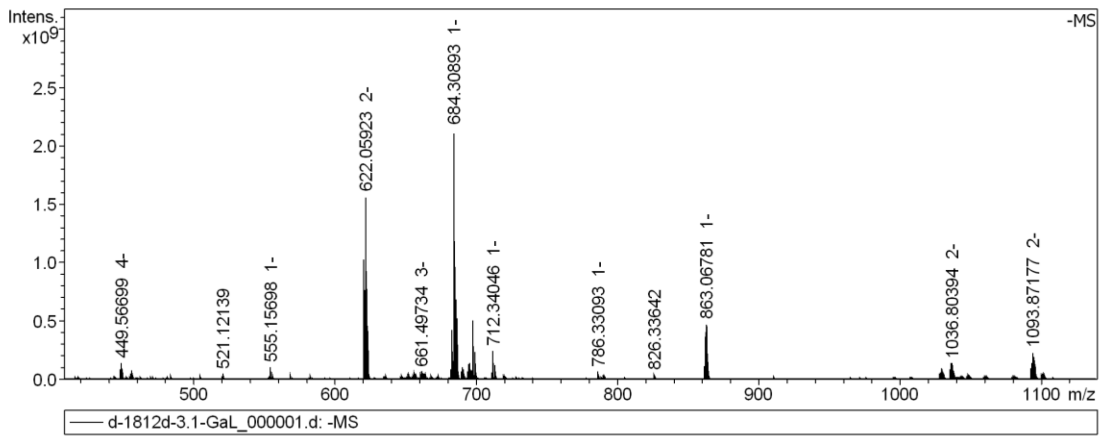


Fig. S33 HR-ESI-MS of $(Et_4N)_5[Et_4N@\mathbf{Ga_2L_3}]$.

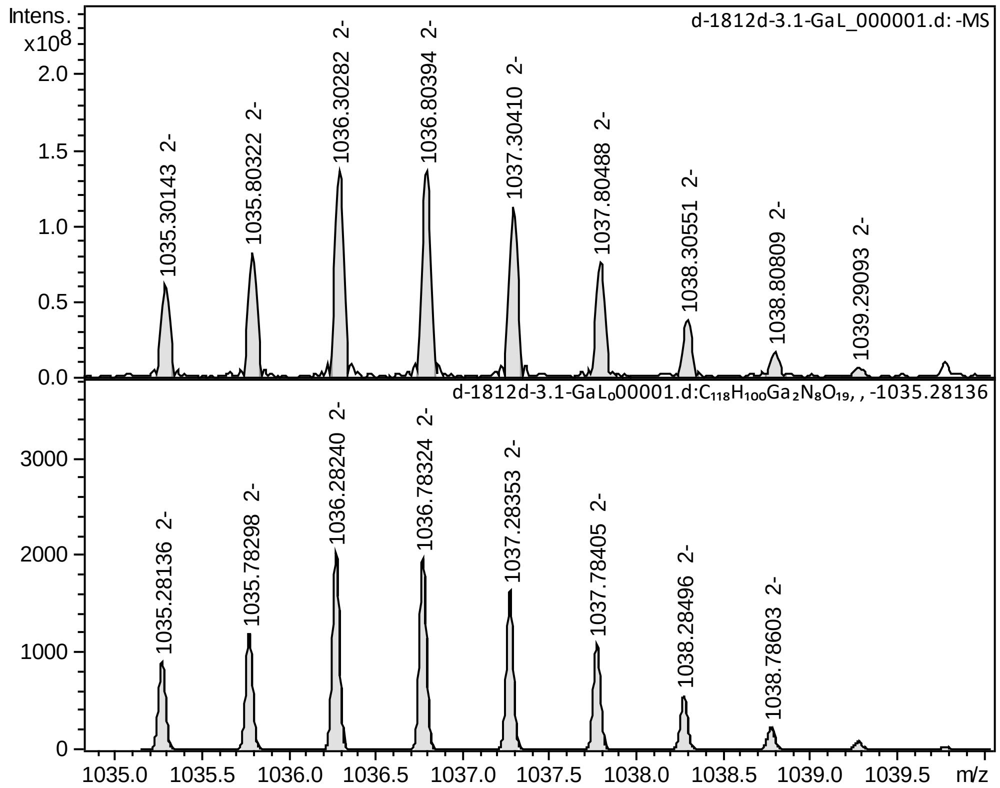


Fig. S34 HR-ESI-MS of $(Et_4N)_5[Et_4N@\mathbf{Ga_2L_3}]$. Exact mass of $[(\mathbf{Ga_2L_3})+NH_4+H+2Et_4N]^{2-}$ was calculated 1035.2814, and found 1035.3014.

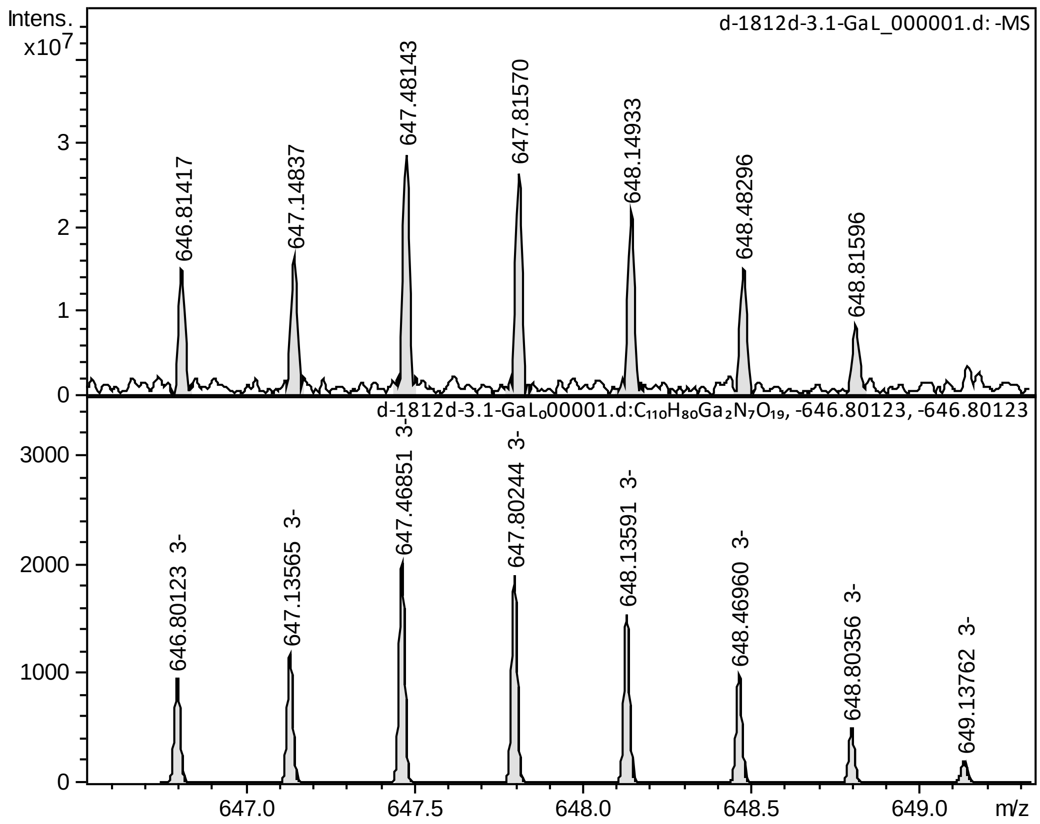


Fig. S35 HR-ESI-MS of $(Et_4N)_5[Et_4N@\mathbf{Ga_2L_3}]$. Exact mass of $[(\mathbf{Ga_2L_3})+NH_4+H+Et_4N]^{3-}$ was calculated 646.8012, and found 646.8142.

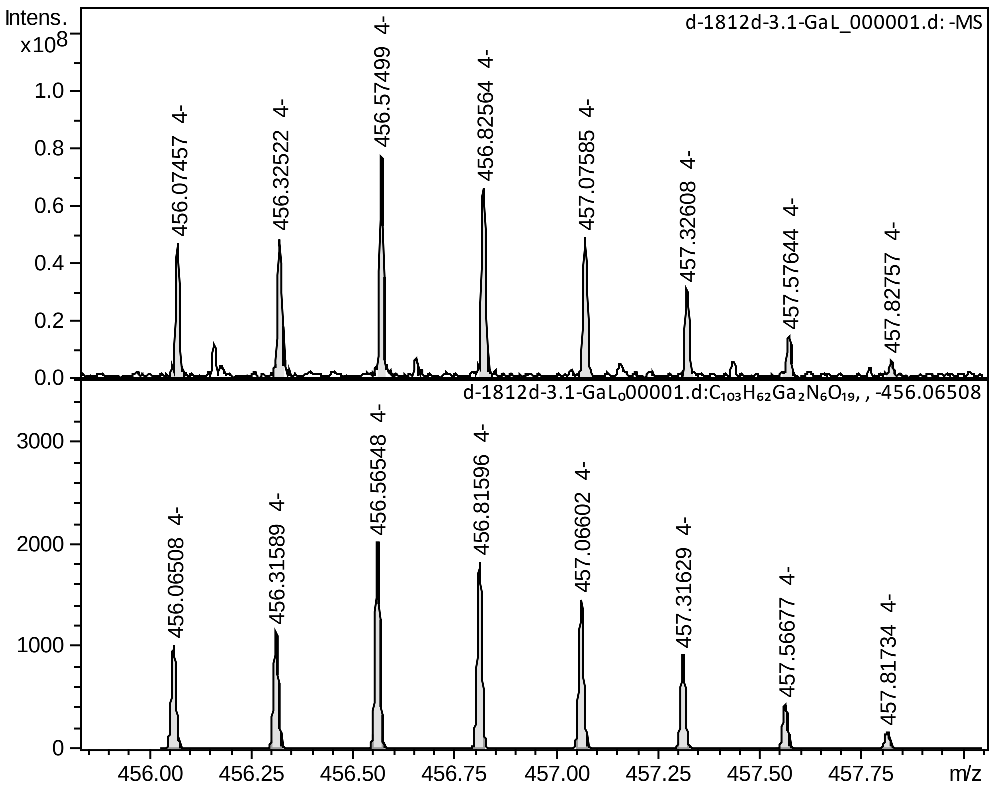


Fig. S36 HR-ESI-MS of $(Et_4N)_5[Et_4N@\mathbf{Ga_2L_3}]$. The exact mass of $[(\mathbf{Ga_2L_3})+2NH_4]^{4-}$ was calculated 456.0651, and found 456.0746.

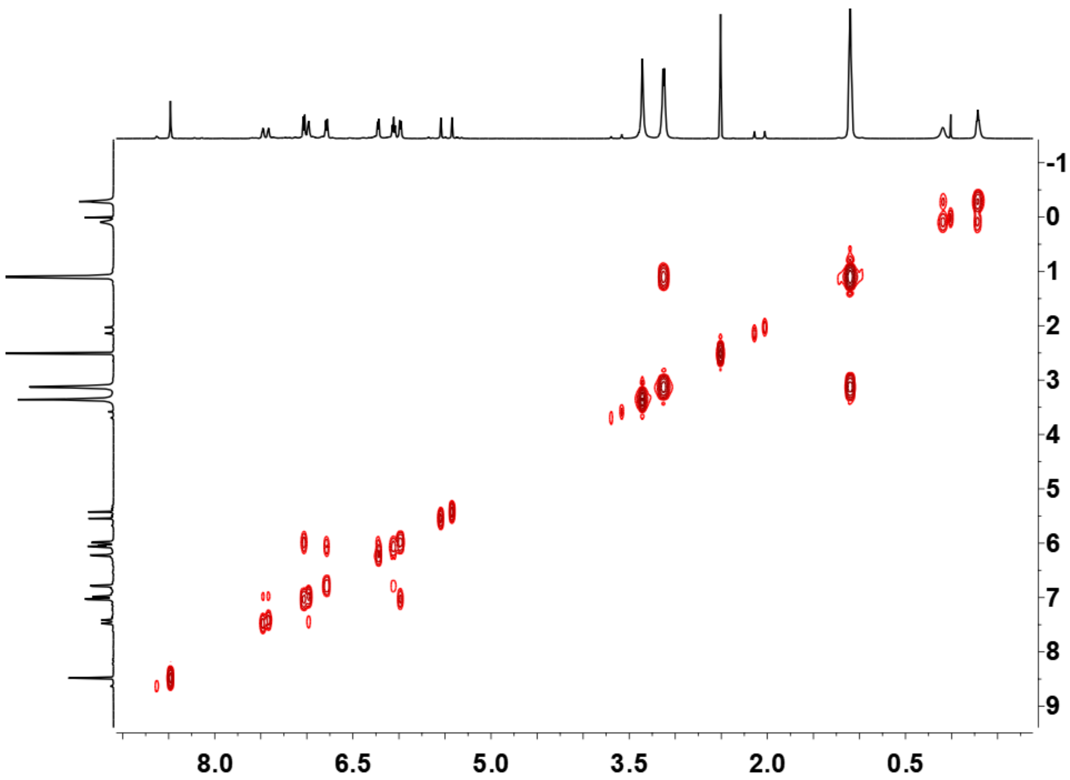


Fig. S37 ^1H-^1H COSY (500 MHz, DMSO-d_6, 298 K) spectrum of $(Et_4N)_5[Et_4N@\mathbf{Ga_2L_3}]$.

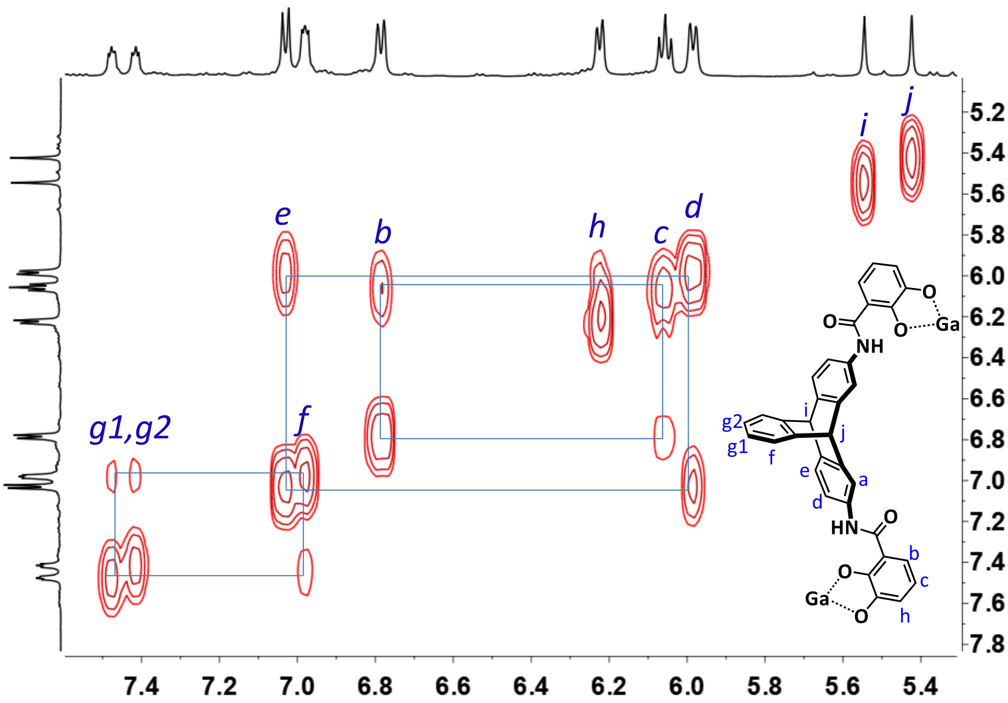


Fig. S38 Partial ^1H-^1H COSY (500 MHz, DMSO-d_6, 298 K) spectrum of $(Et_4N)_5[Et_4N@\mathbf{Ga_2L_3}]$.

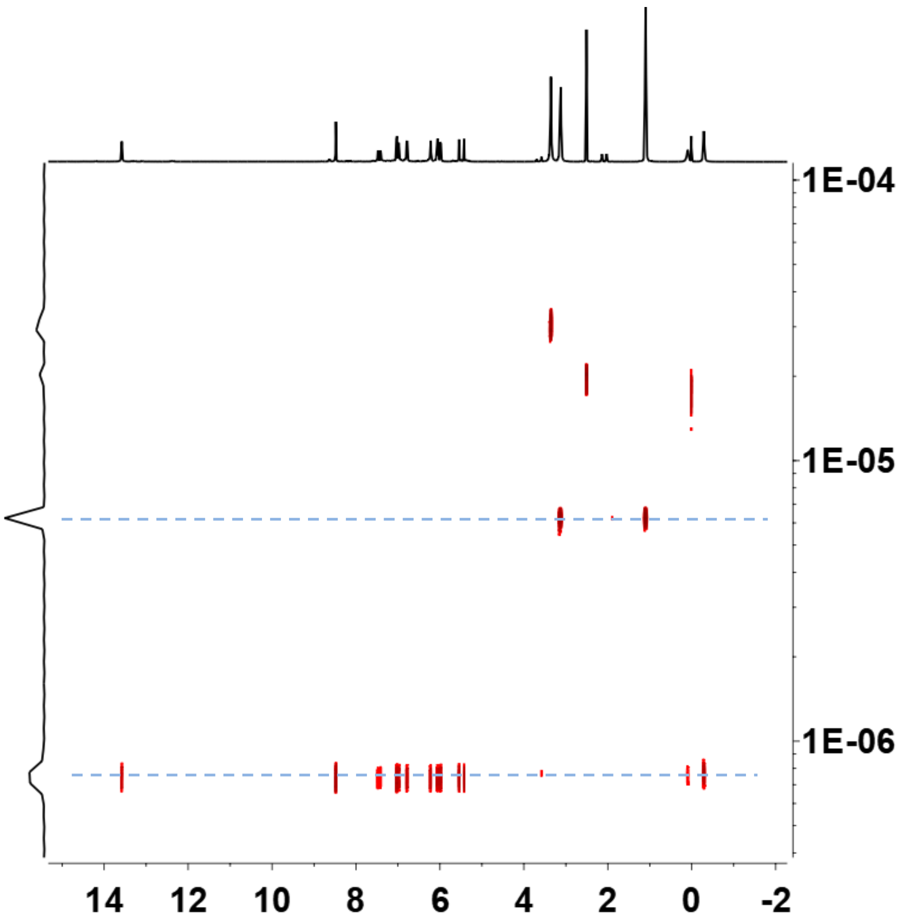


Fig. S39 DOSY (500 MHz, DMSO-d_6, 298 K) spectrum of $(Et_4N)_5[Et_4N@\mathbf{Ga_2L_3}]$.

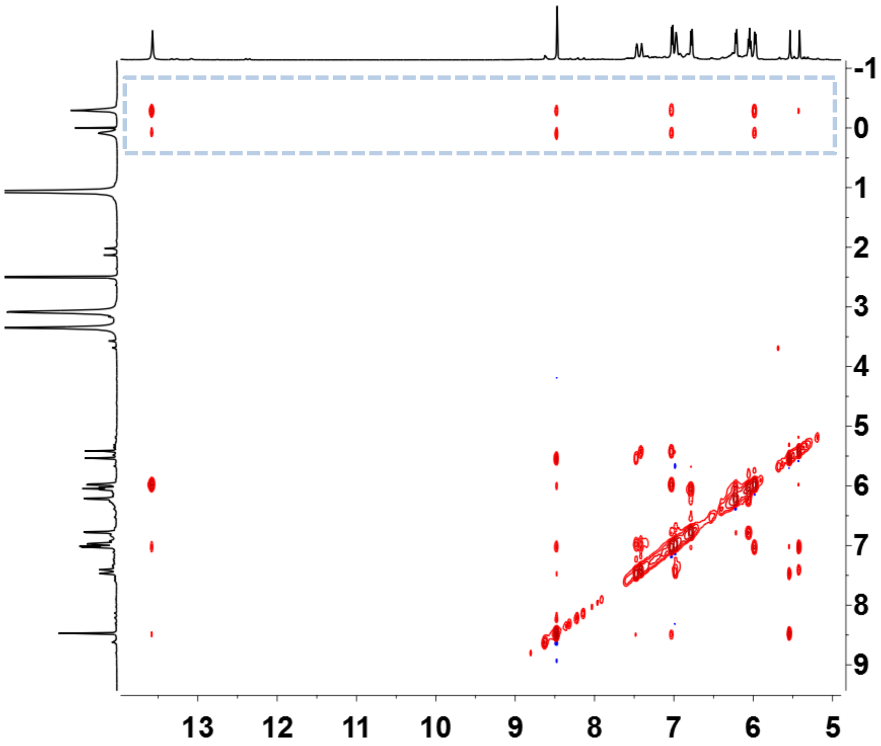


Fig. S40 2D NOESY (500 MHz, DMSO-d_6, 298 K) spectrum of $(Et_4N)_5[Et_4N@\mathbf{Ga_2L_3}]$.

2.3.4 Synthesis of $(Pr_4N)_6[\mathbf{Ga_2L_3}]$

The synthetic procedures are same as $(Et_4N)_6[\mathbf{Ga_2L_3}]$. The ^1H NMR shows no Pr_4N^+ encapsulated is found. The poor solubility of $(Pr_4N)_6[\mathbf{Ga_2L_3}]$ in DMSO-d_6 induces a set of broaden peaks that are hard to be distinguished.

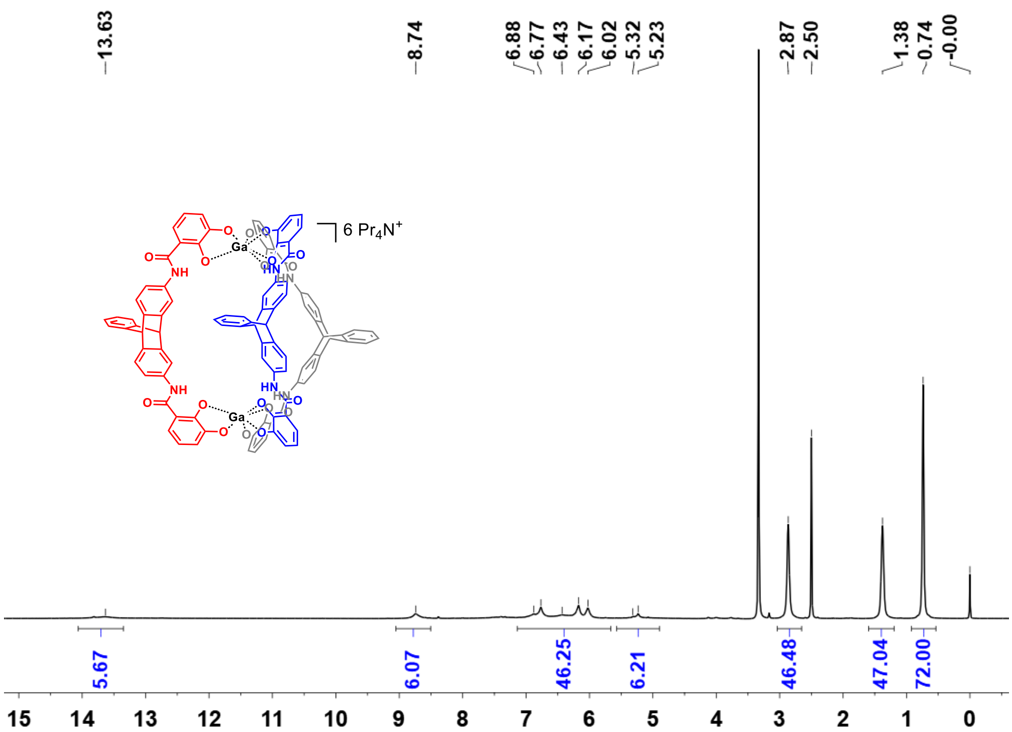


Fig. S41 ^1H NMR (700 MHz, DMSO-d_6, 298 K) spectrum of $(Pr_4N)_6[\mathbf{Ga_2L_3}]$.

2.3.5 Synthesis of $(Bu_4N)_6$[$\mathbf{Ga_2L_3}$]

The synthetic procedures are same as $(Et_4N)_6$[$\mathbf{Ga_2L_3}$]. The ^{1}H NMR shows no Bu_4N^+ encapsulated is found. The solubility of $(Bu_4N)_6$[$\mathbf{Ga_2L_3}$] in DMSO-d_6 is slightly poor compared with $(Et_4N)_6$[$\mathbf{Ga_2L_3}$]. HR-ESI-MS revealed that the core structure is still the helicate [$\mathbf{Ga_2L_3}$]$^{6-}$.

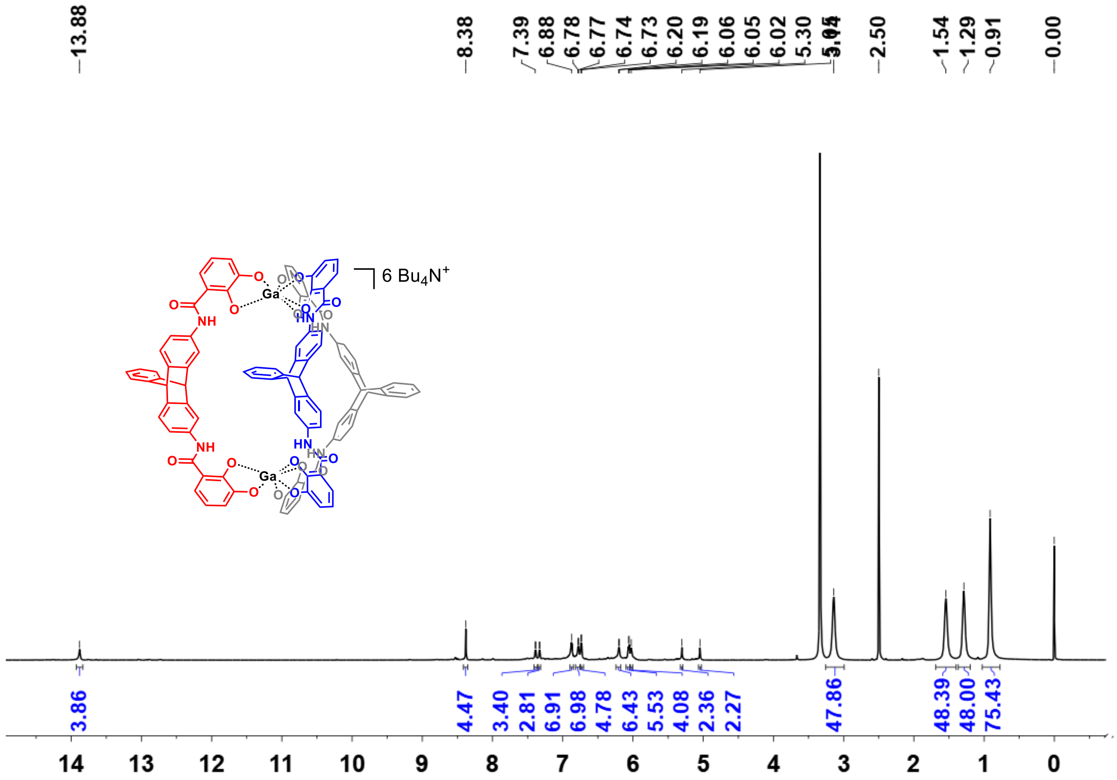


Fig. S42 ^{1}H NMR (700 MHz, DMSO-d_6, 298 K) spectrum of $(Bu_4N)_6$[$\mathbf{Ga_2L_3}$].

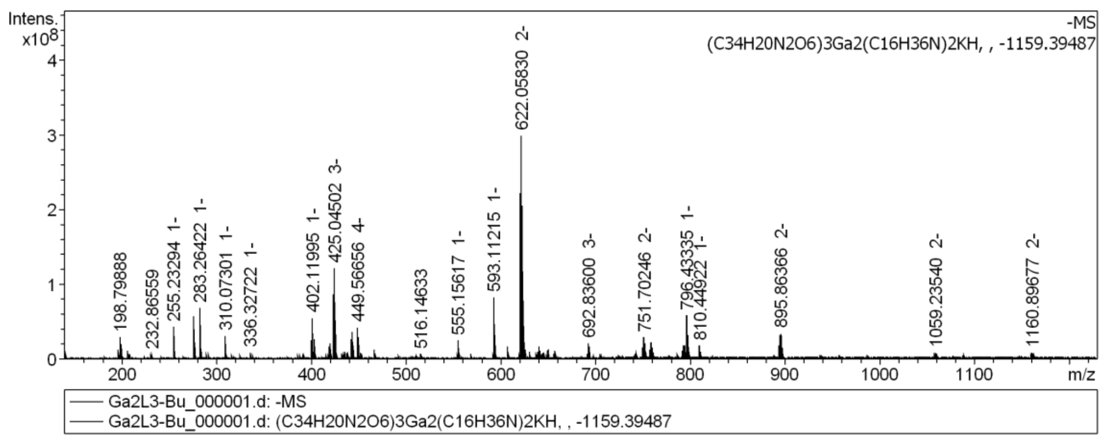


Fig. S43 HR-ESI-MS of $(Bu_4N)_6$[$\mathbf{Ga_2L_3}$].

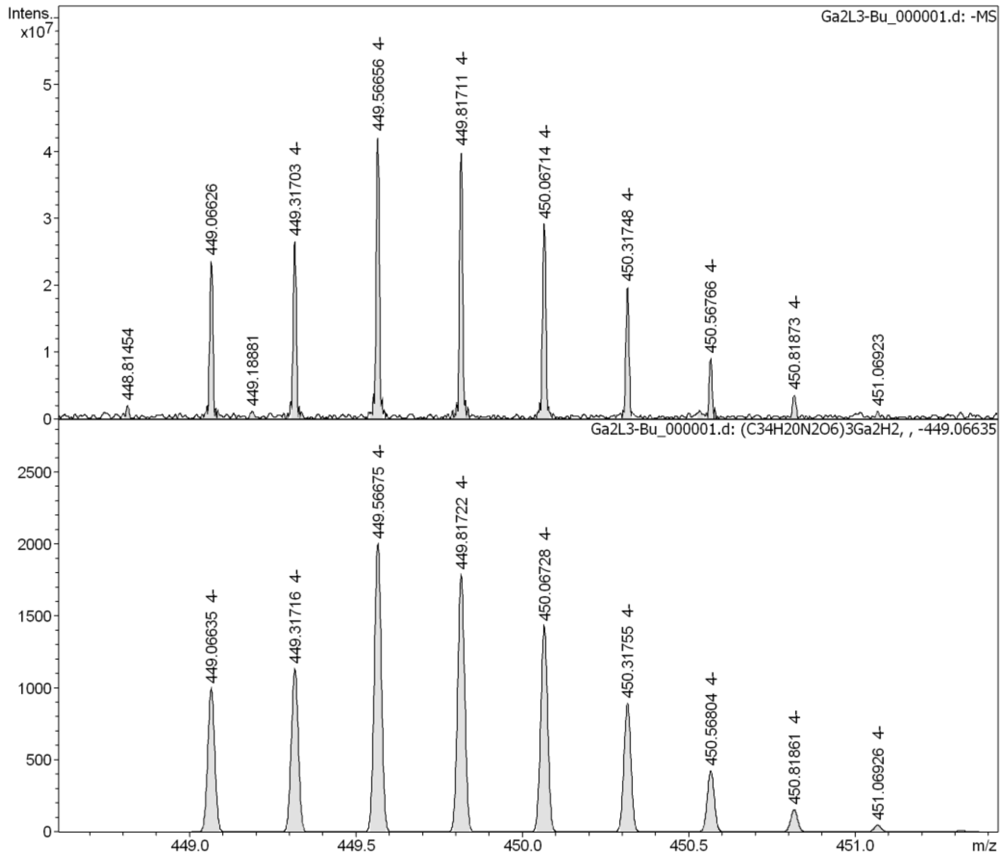


Fig. S44 HR-ESI-MS of $(Bu_4N)_6$[$\mathbf{Ga_2L_3}$].

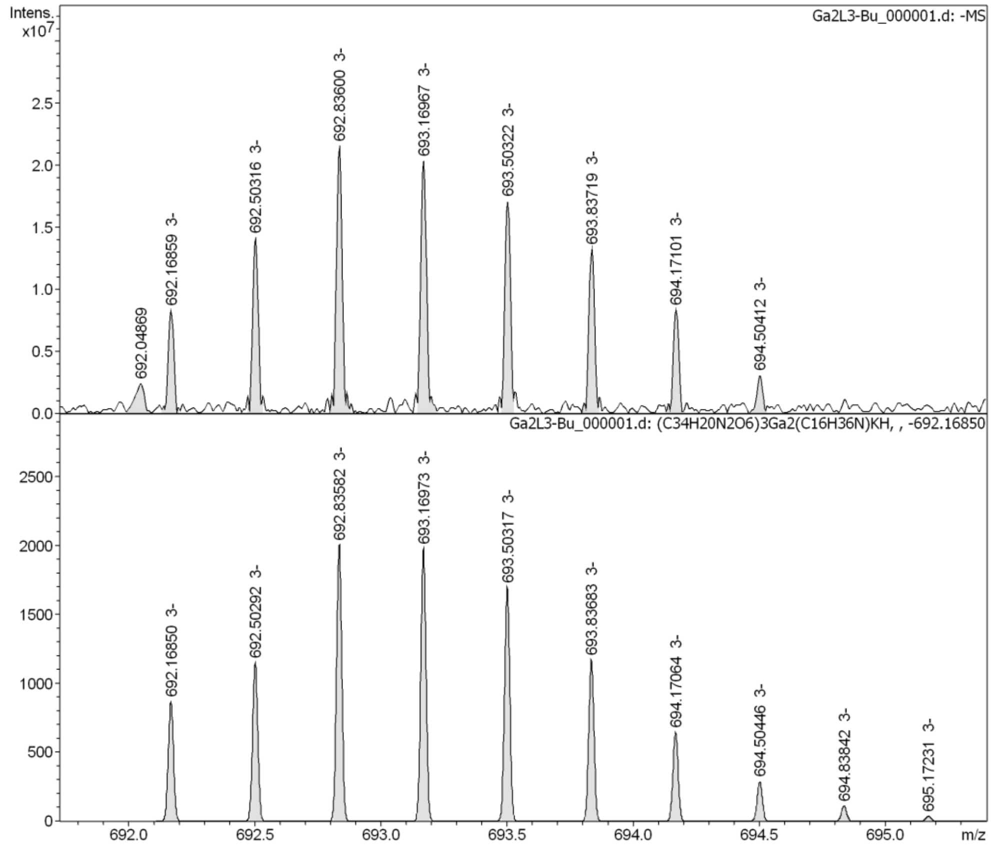


Fig. S45 HR-ESI-MS of $(Bu_4N)_6$[$\mathbf{Ga_2L_3}$].

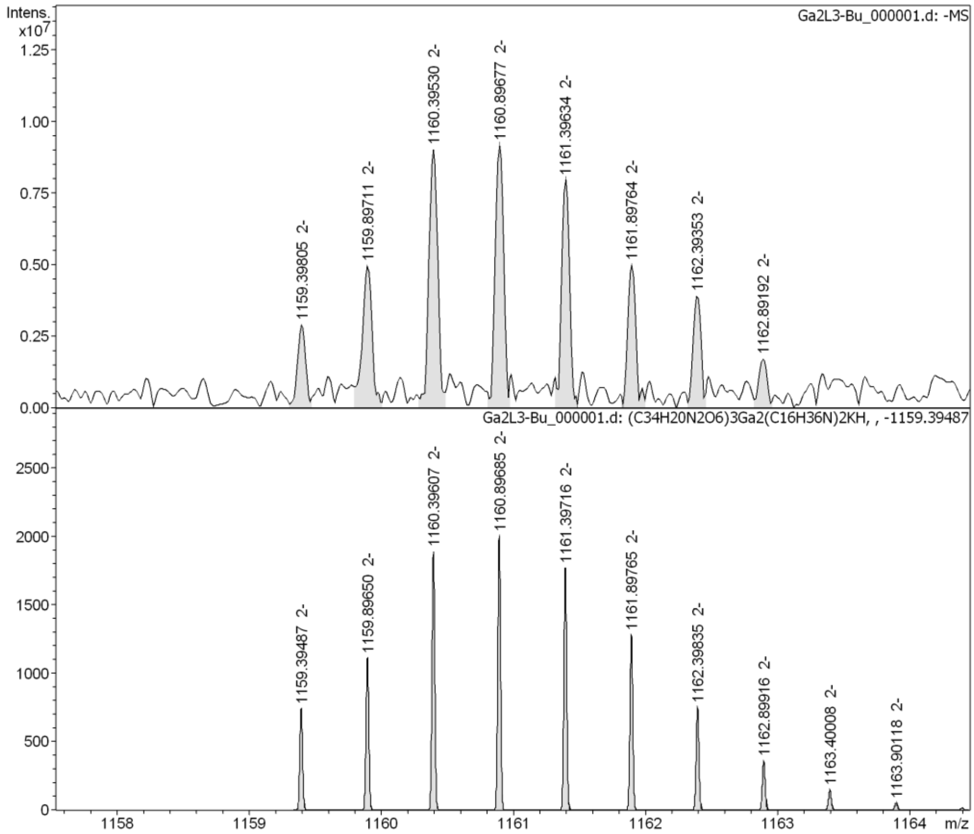


Fig. S46 HR-ESI-MS of $(Bu_4N)_6$[$\mathbf{Ga_2L_3}$].

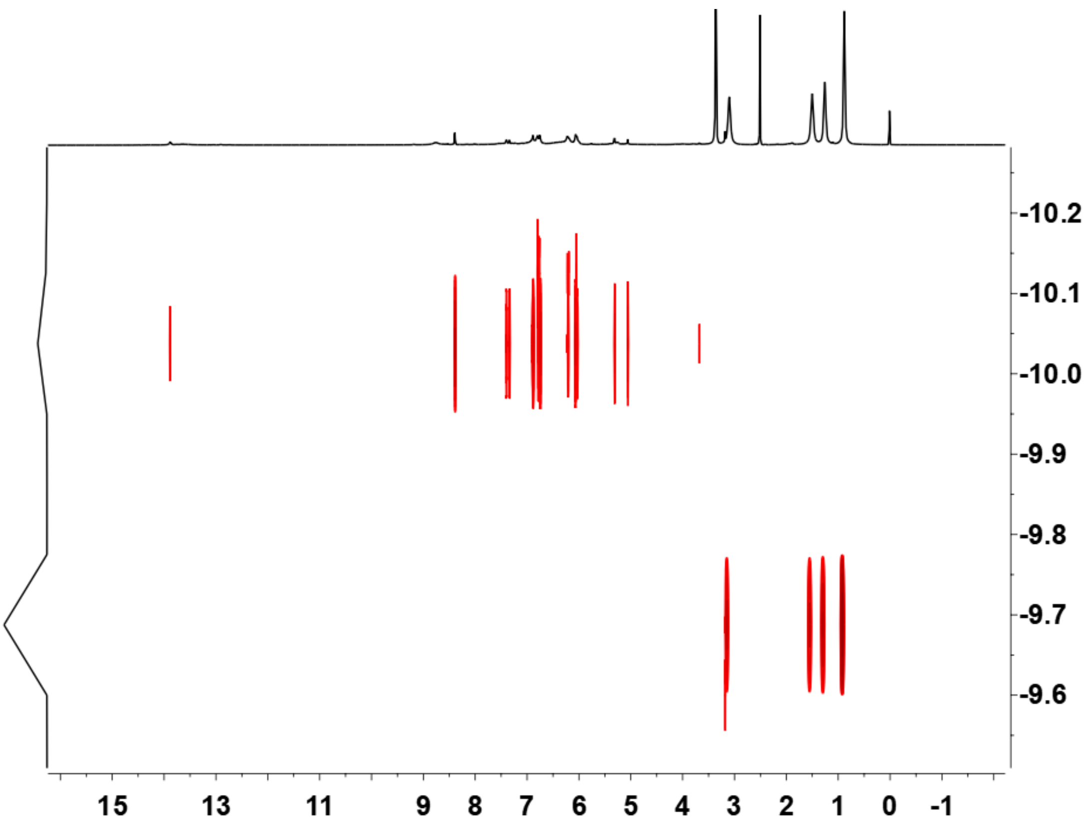
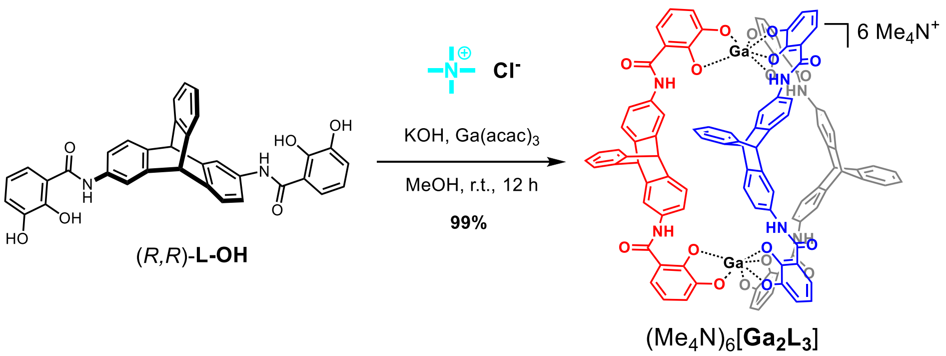


Fig. S47 DOSY (700 MHz, DMSO-d_6, 298 K) spectrum of $(Bu_4N)_6$[$\mathbf{Ga_2L_3}$].

2.4 Synthesis of the 2,6-triptycene-based helicates

2.4.1 Synthesis of chiral $(Me_4N)_6$[**Ga_2L_3**]



To a 15 mL tube was added **L-OH** (41.7 mg, 0.075 mmol), KOH (8.4 mg, 0.15 mmol) and dried methanol (3.0 mL). Keep the mixture stirred for 30 minutes and the solution of Me_4NCl (22.3 mg, 0.20 mmol) in methanol (1.0 mL) was added by syringe. After 10 minutes the solution of $Ga(acac)_3$ (18.4 mg, 0.05 mmol) in methanol (1.0 mL) was added by syringe, and kept at room temperature for 12 hours. Then 10 mL diethyl ether was added to produce white precipitate, which was filtered and washed with diethyl ether three times. The final white powder was used without further purification.^{1}H NMR (700 MHz, DMSO-d_6, 298 K): δ 13.99 (s, 3H), 13.55 (s, 3H), 8.85 (s, 3H), 8.49 (d, J = 7.9 Hz, 3H), 7.45 (s, 3H), 7.40 (d, J = 8.0 Hz, 3H), 7.28 (d, J = 20.08 Hz, 3H), 6.84-6.81 (m, 6H), 6.74 (d, J = 8.0 Hz, 3H), 6.66 (d, J = 8.0 Hz, 3H), 6.17 (d, J = 6.9 Hz, 4H), 6.07 (dd, J = 19.4, 7.1 Hz, 10H), 5.97 (t, J = 7.6 Hz, 3H), 5.35 (s, 3H), 5.15 (d, J = 7.6 Hz, 3H), 4.53 (s, 3H), 2.98 (s, Me_4N^+, 72H). ^{13}C NMR (176 MHz, DMSO-d_6, 298 K): δ 168.0, 167.7, 159.3, 158.9, 158.0, 157.9, 147.3, 146.3, 146.0, 145.9, 139.2, 138.4, 137.7, 125.1, 124.6, 124.2, 123.7, 123.1, 114.5, 114.1, 114.0, 113.8, 112.9, 112.61, 112.55, 112.3, 112.0, 111.7, 54.8, 53.5, 52.5.

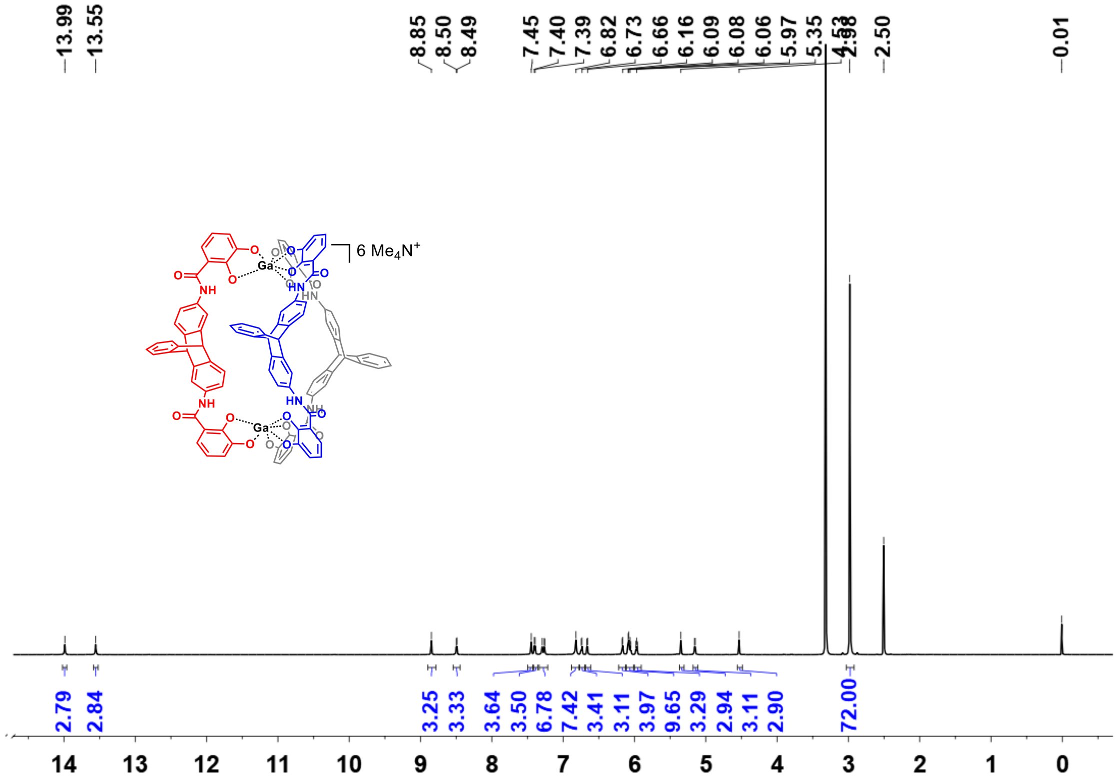


Fig. S48 ^{1}H NMR (700 MHz, DMSO-d_6, 298 K) spectrum of chiral $(Me_4N)_6$[$\mathbf{Ga_2L_3}$].

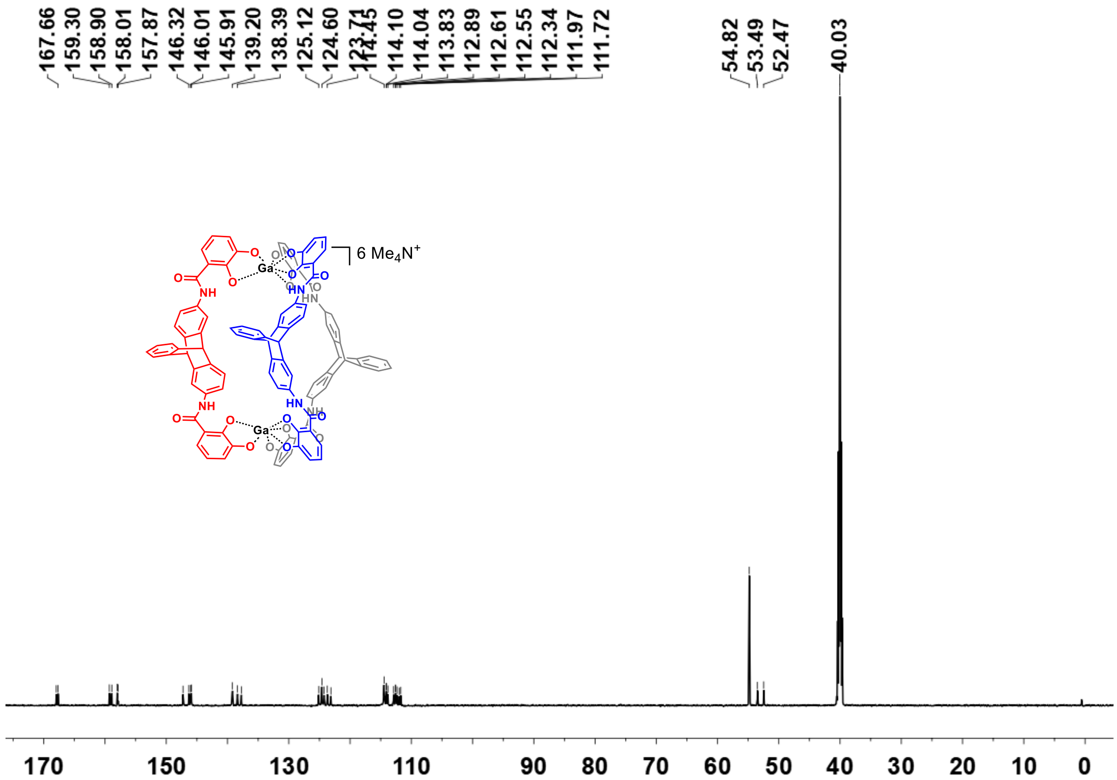


Fig. S49 ^{13}C NMR (176 MHz, DMSO-d_6, 298 K) spectrum of chiral $(Me_4N)_6$[$\mathbf{Ga_2L_3}$].

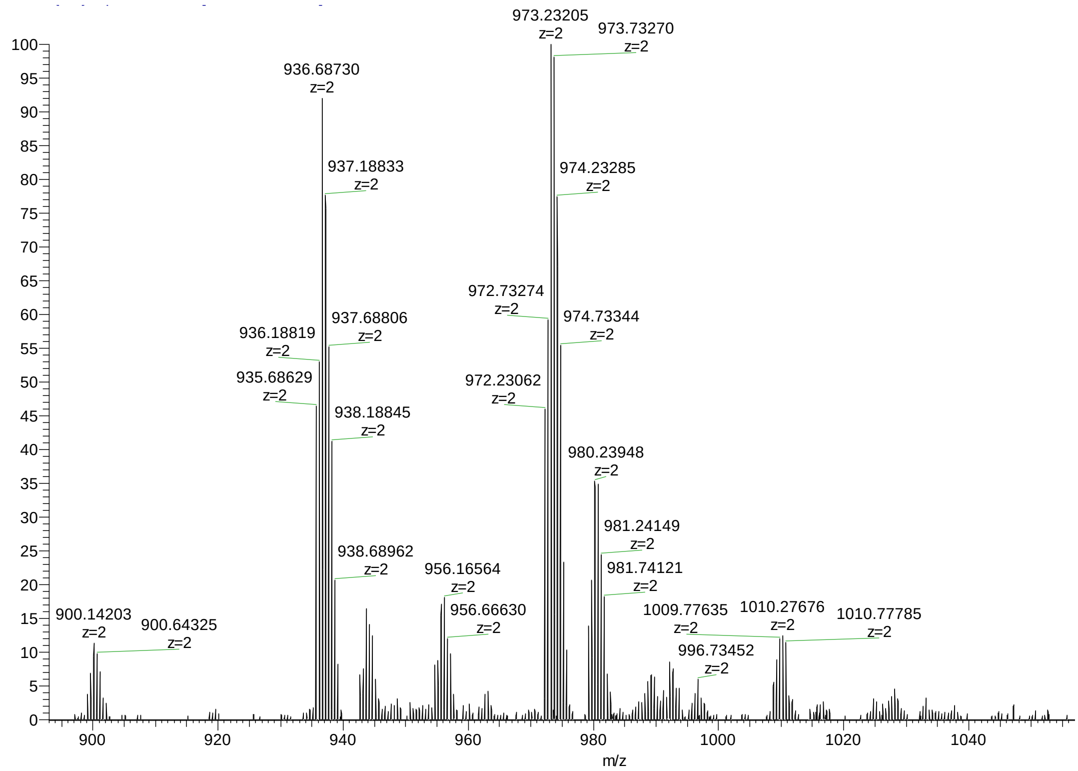


Fig. S50 HR-ESI-MS of chiral $(Me_4N)_6[\mathbf{Ga_2L_3}]$.

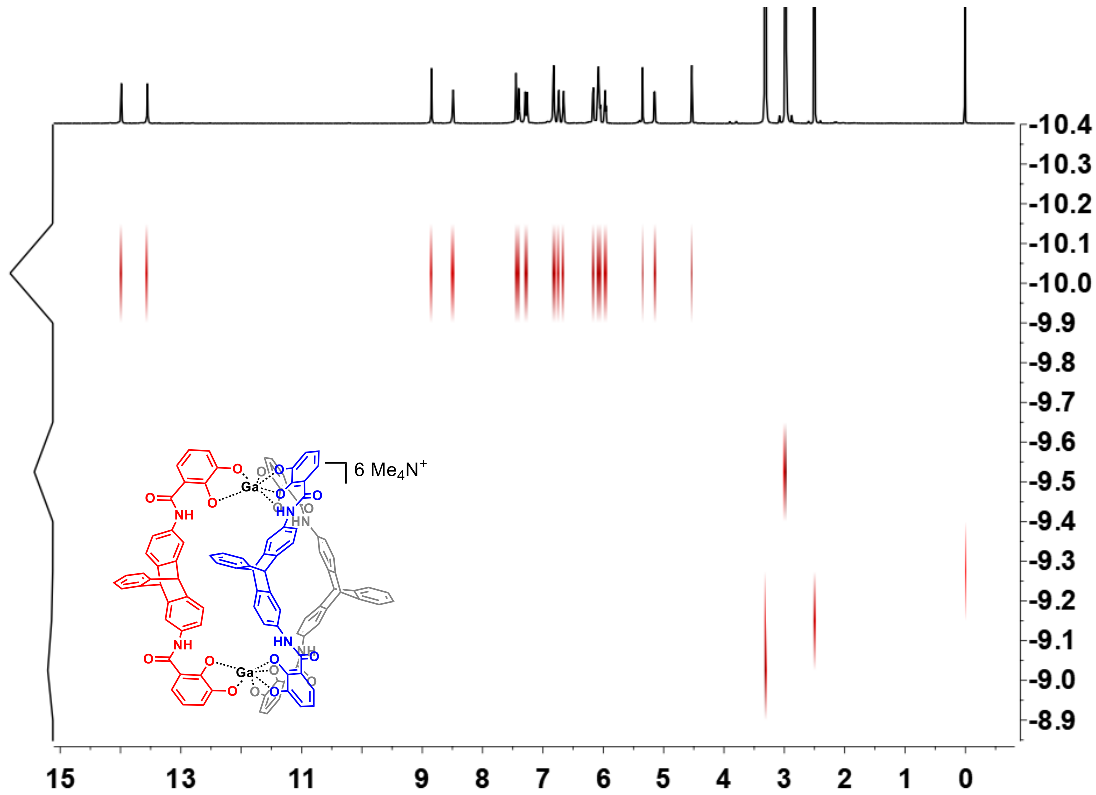
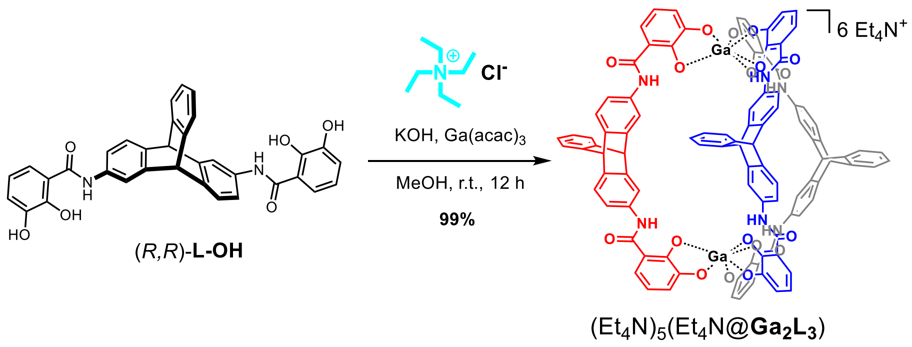


Fig. S51 DOSY (500 MHz, DMSO-*d*$_6$, 298 K) spectrum of chiral $(Me_4N)_6[\mathbf{Ga_2L_3}]$.

2.4.2 Synthesis of chiral $(Et_4N)_6$[**Ga_2L_3**]



The synthetic procedures are same as chiral $(Me_4N)_6$[**Ga_2L_3**]. The ^{1}H NMR shows no Et_4N^+ encapsulated is found. The DOSY spectrum of $(Et_4N)_6$[**Ga_2L_3**] shows a high purity. And HR-ESI-MS revealed that the core structure is still the chiral helicate [**Ga_2L_3**]$^{6-}$.

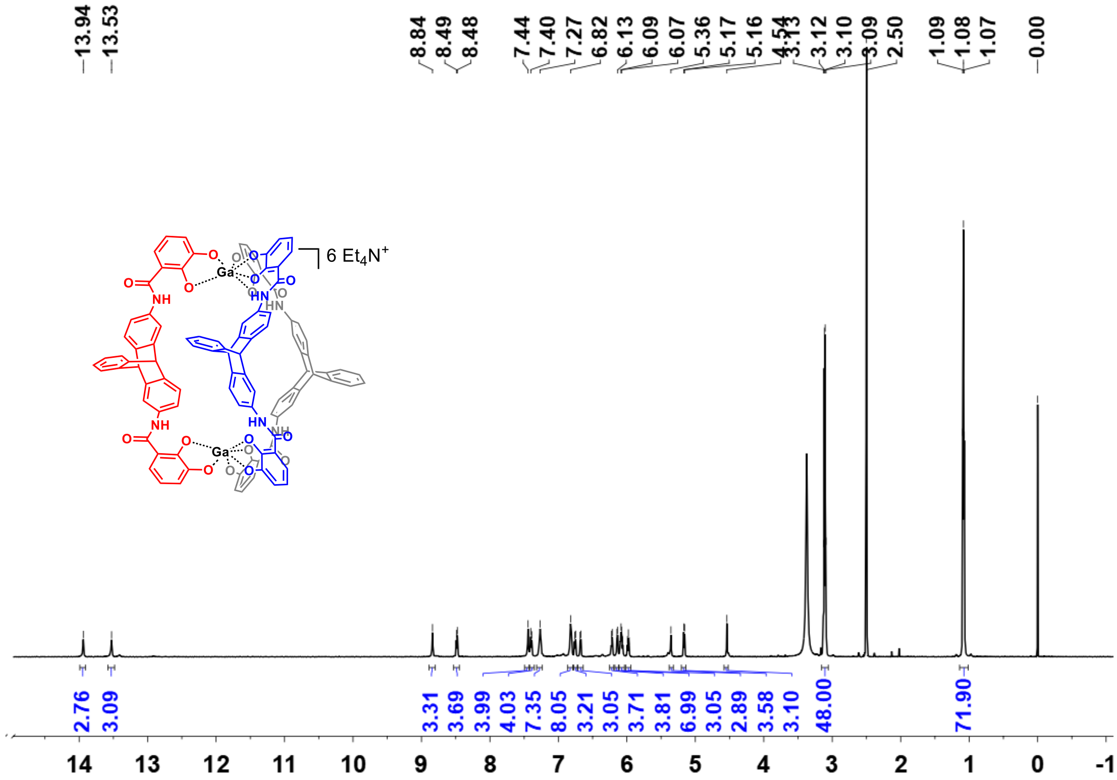


Fig. S52 ^{1}H NMR (600 MHz, DMSO-d_6, 298 K) spectrum of chiral $(Et_4N)_6$[**Ga_2L_3**].

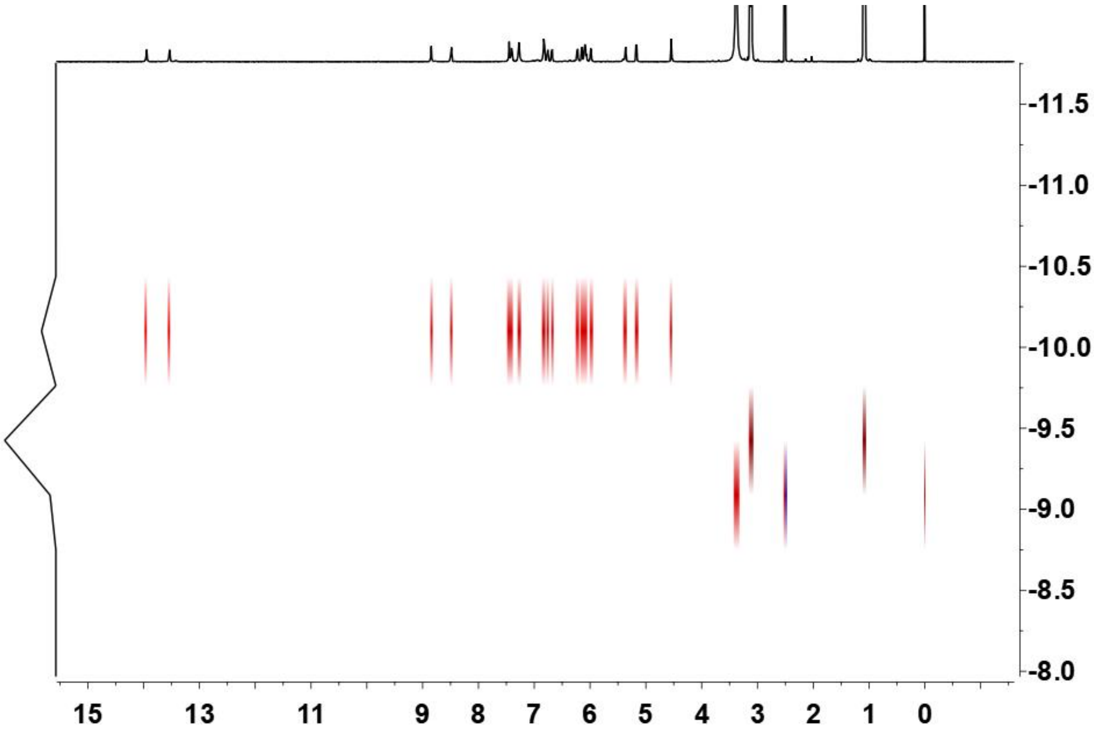


Fig. S53 DOSY (600 MHz, DMSO-d_6, 298 K) spectrum of chiral $(Et_4N)_6$[$\mathbf{Ga_2L_3}$].

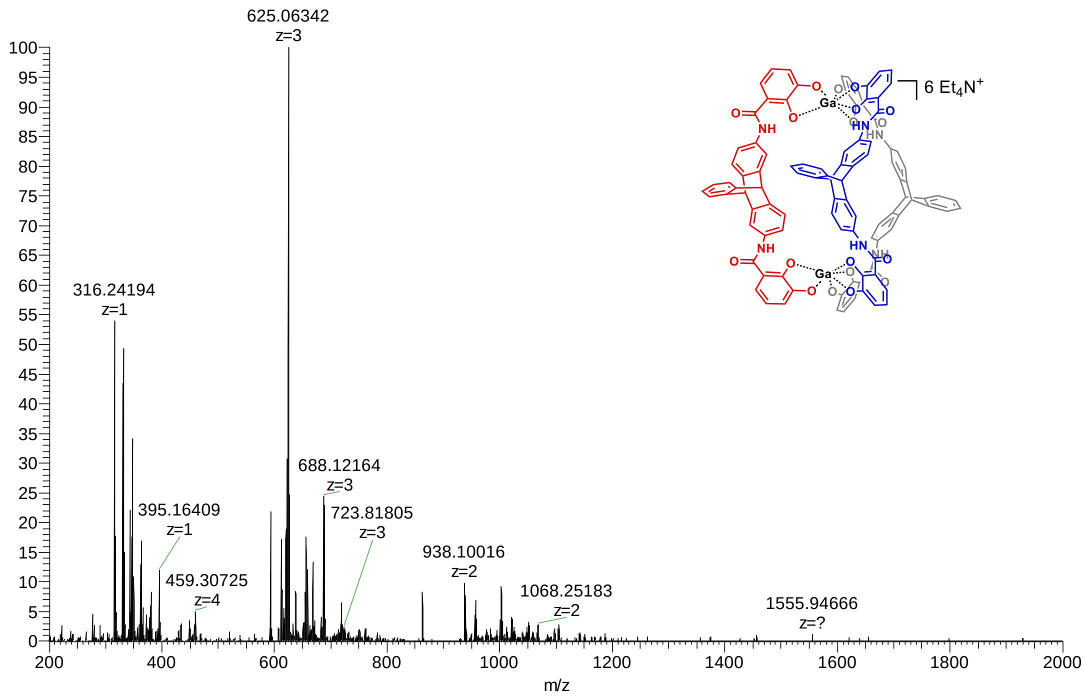


Fig. S54 HR-ESI-MS of chiral $(Et_4N)_6$[$\mathbf{Ga_2L_3}$].

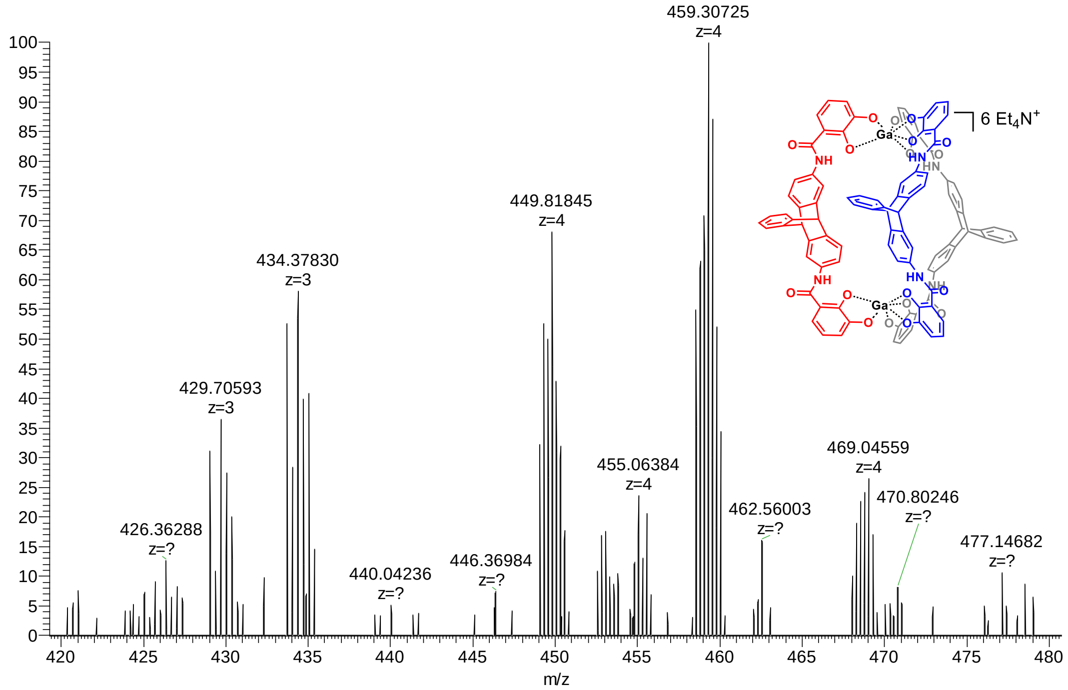


Fig. S55 HR-ESI-MS of chiral $(Et_4N)_6$[$\mathbf{Ga_2L_3}$].

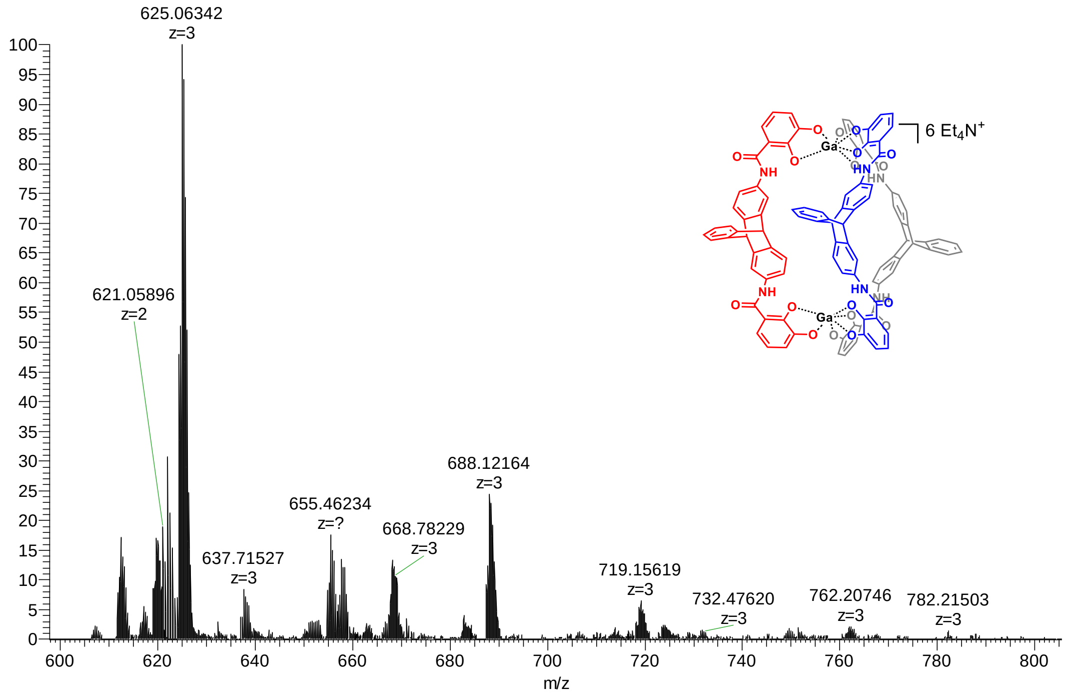


Fig. S56 HR-ESI-MS of chiral $(Et_4N)_6$[$\mathbf{Ga_2L_3}$].

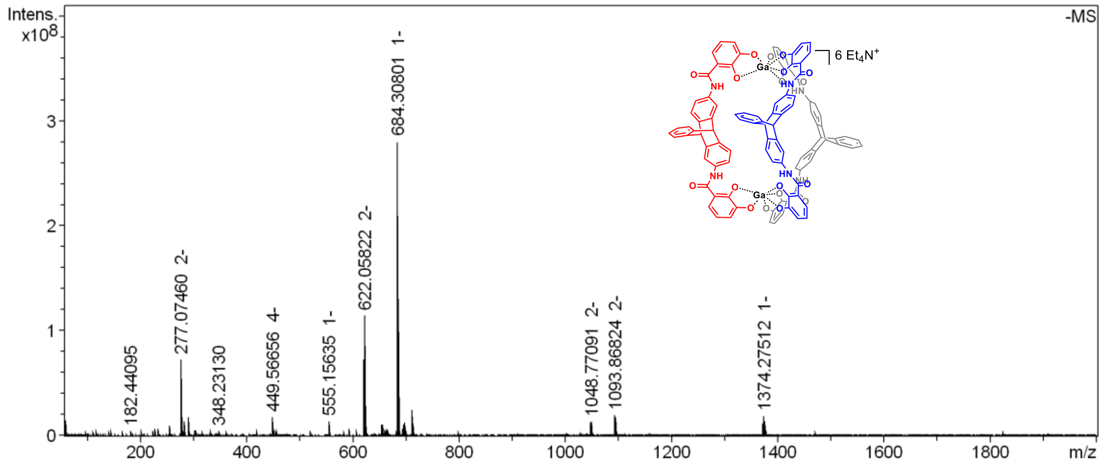


Fig. S57 HR-ESI-MS of chiral $(Et_4N)_6$[**Ga_2L_3**].

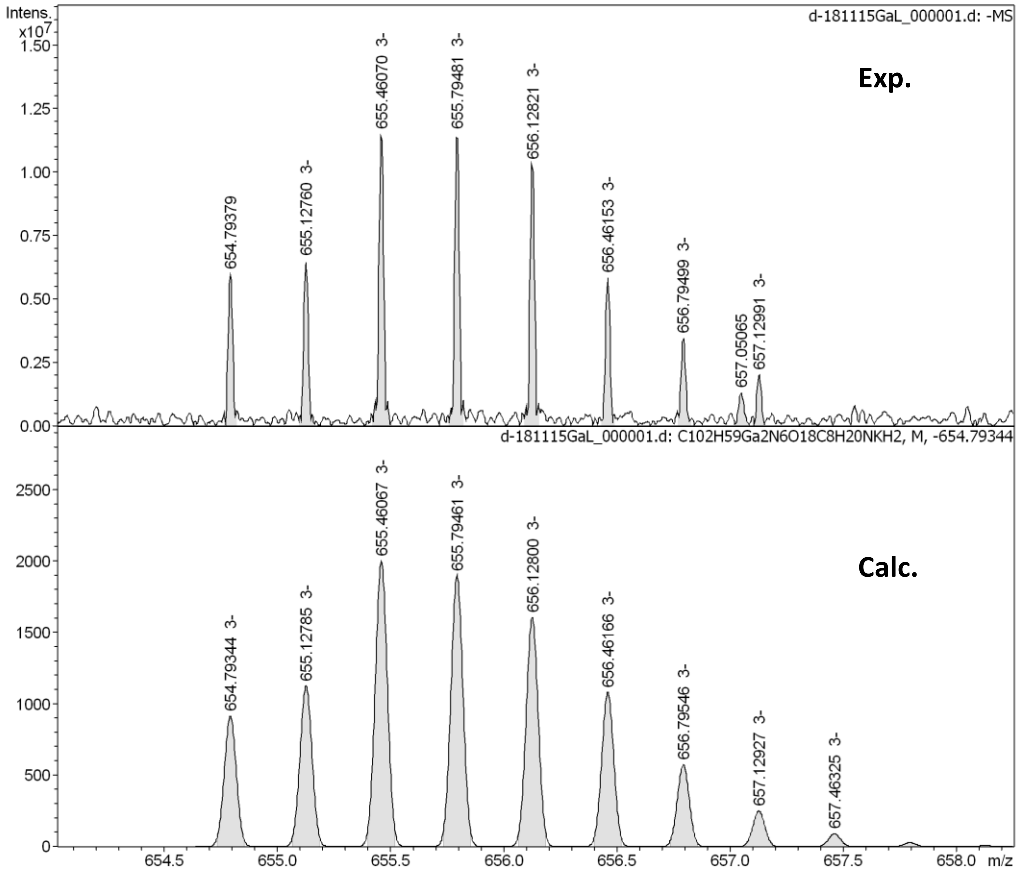


Fig. S58 HR-ESI-MS of chiral $(Et_4N)_6$[**Ga_2L_3**].

3. Photophysical properties

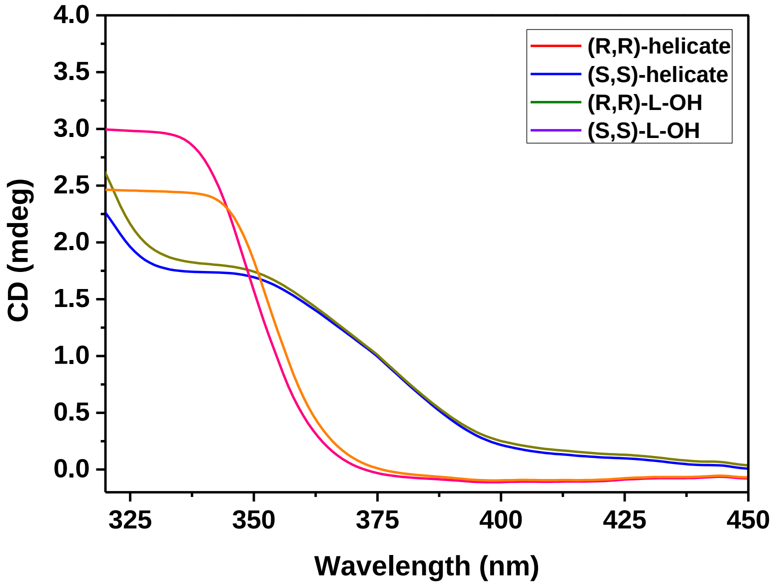


Fig. S59 UV-vis absorption spectra of $(Et_4N)_6$[$\mathbf{Ga_2L_3}$] and the corresponding ligands in DMSO, [$\mathbf{Ga_2L_3}$] = [**L-OH**] = 1.0×10^{-5} M.

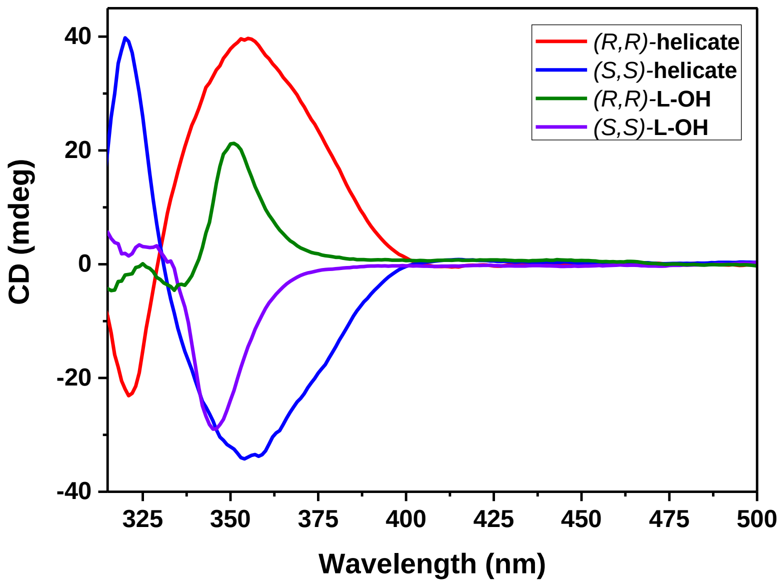


Fig. S60 CD spectra of $(Et_4N)_6$[$\mathbf{Ga_2L_3}$] and the corresponding ligands in DMSO, [$\mathbf{Ga_2L_3}$] = [**L-OH**] = 1.0×10^{-5} M.

4. Theoretical calculations

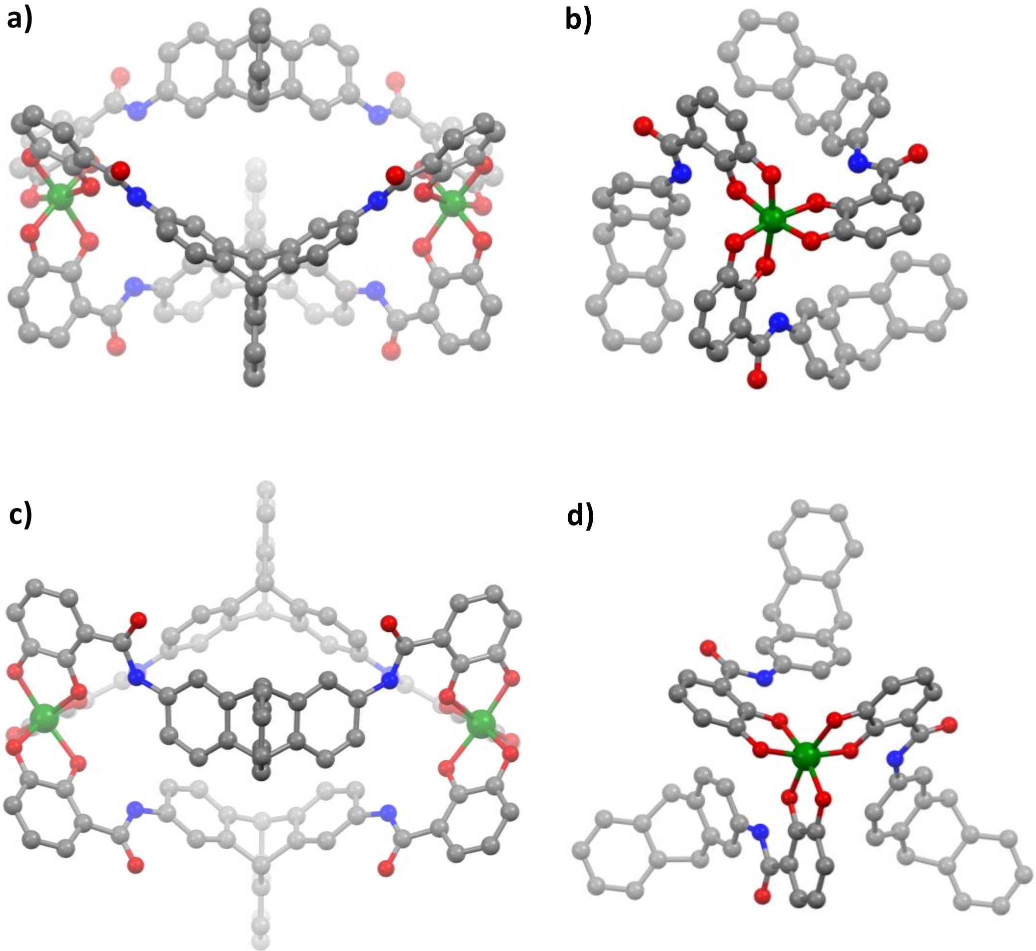


Fig. S61 Energy minimized structure of the [$\mathbf{Ga_2L_3}$]$^{6-}$, a) and b) the top and side views by using model 1; c) and d) the top and side views by using model 2.

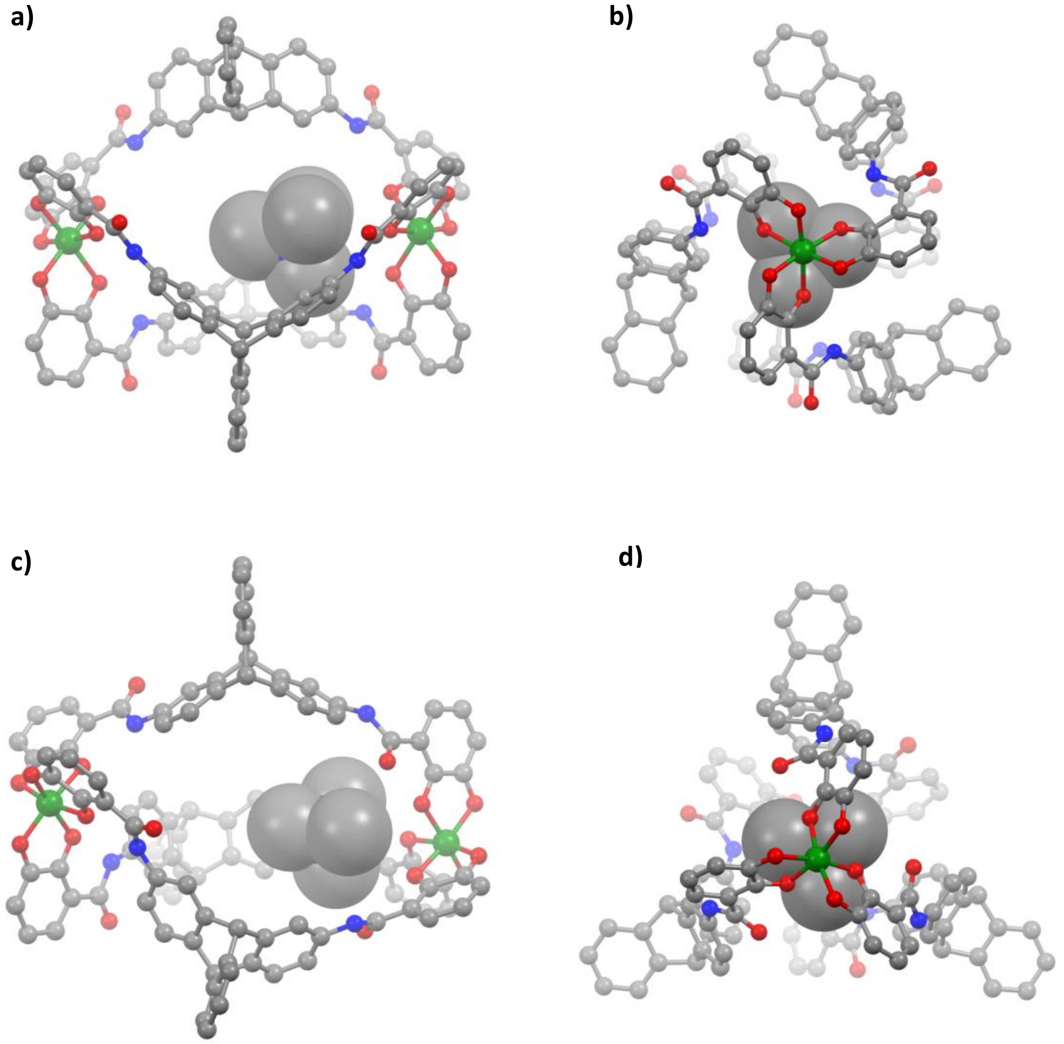


Fig. S62 Energy minimized structure of the $[Me_4N@\mathbf{Ga_2L_3}]^{5-}$, a) and b) the top and side views by using model 1; c) and d) the top and side views by using model 2.

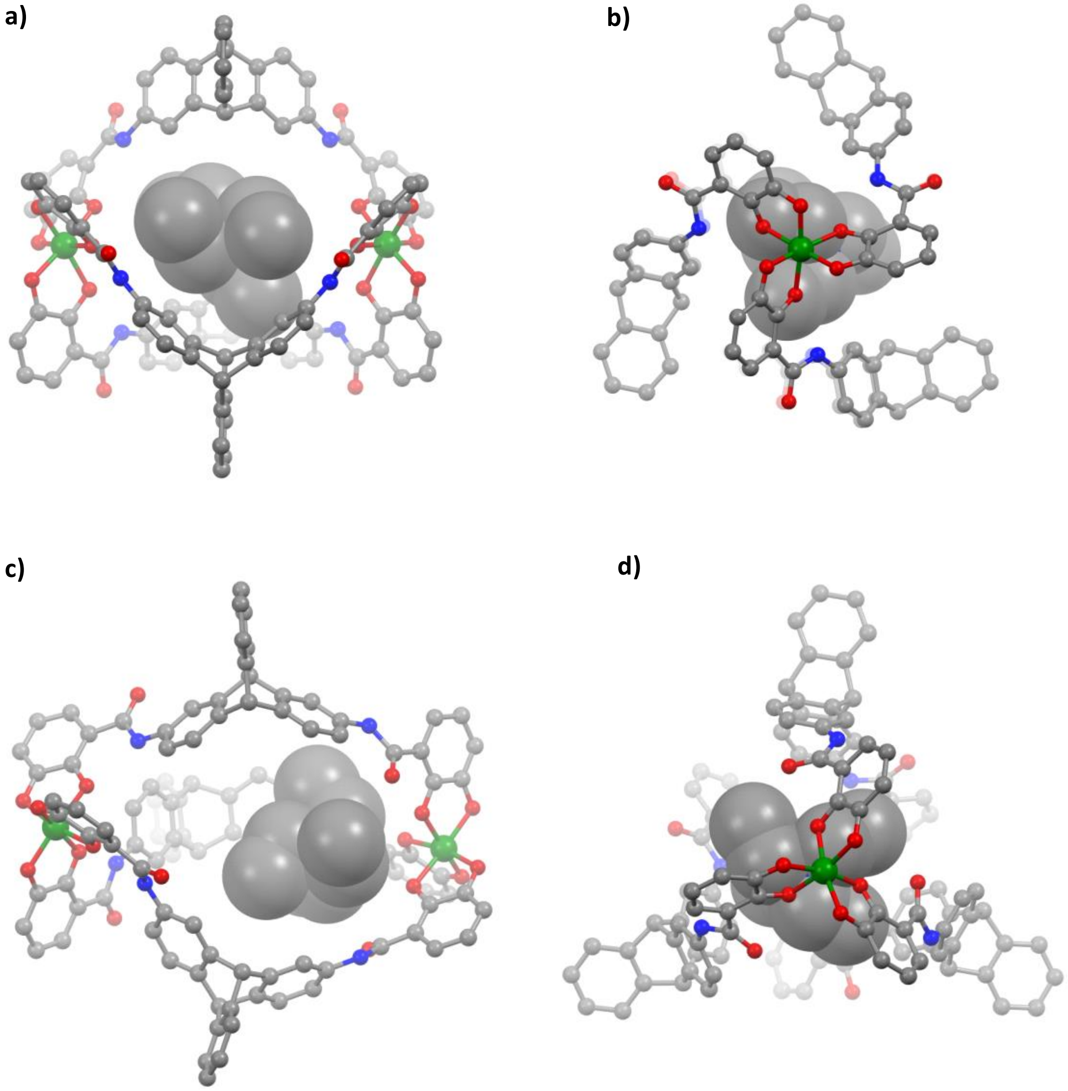


Fig. S63 Energy minimized structure of the $[Et_4N@\mathbf{Ga_2L_3}]^{5-}$, a) and b) the top and side views by using model 1; c) and d) the top and side views by using model 2.

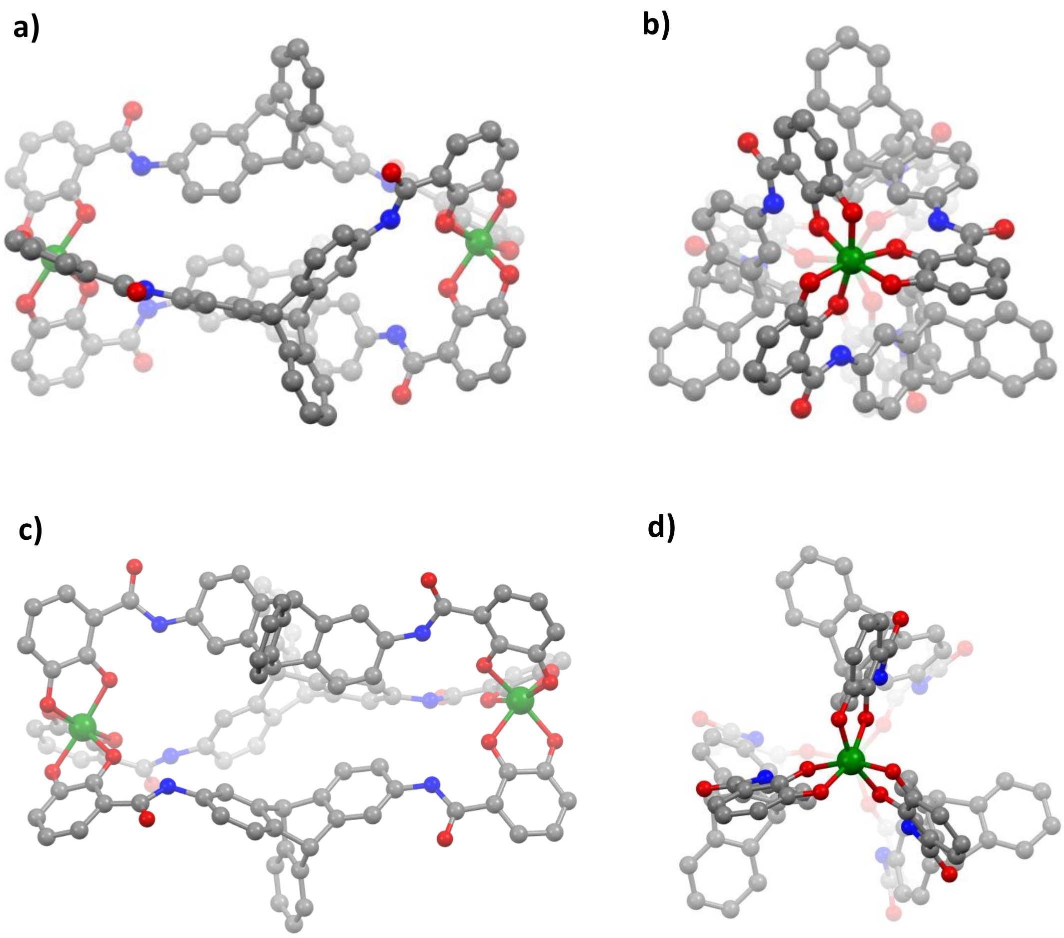


Fig. S64 Energy minimized structure of the chiral [$\mathbf{Ga_2L_3}$]$^{6-}$, a) and b) the top and side views by using model 1; c) and d) the top and side views by using model 2.

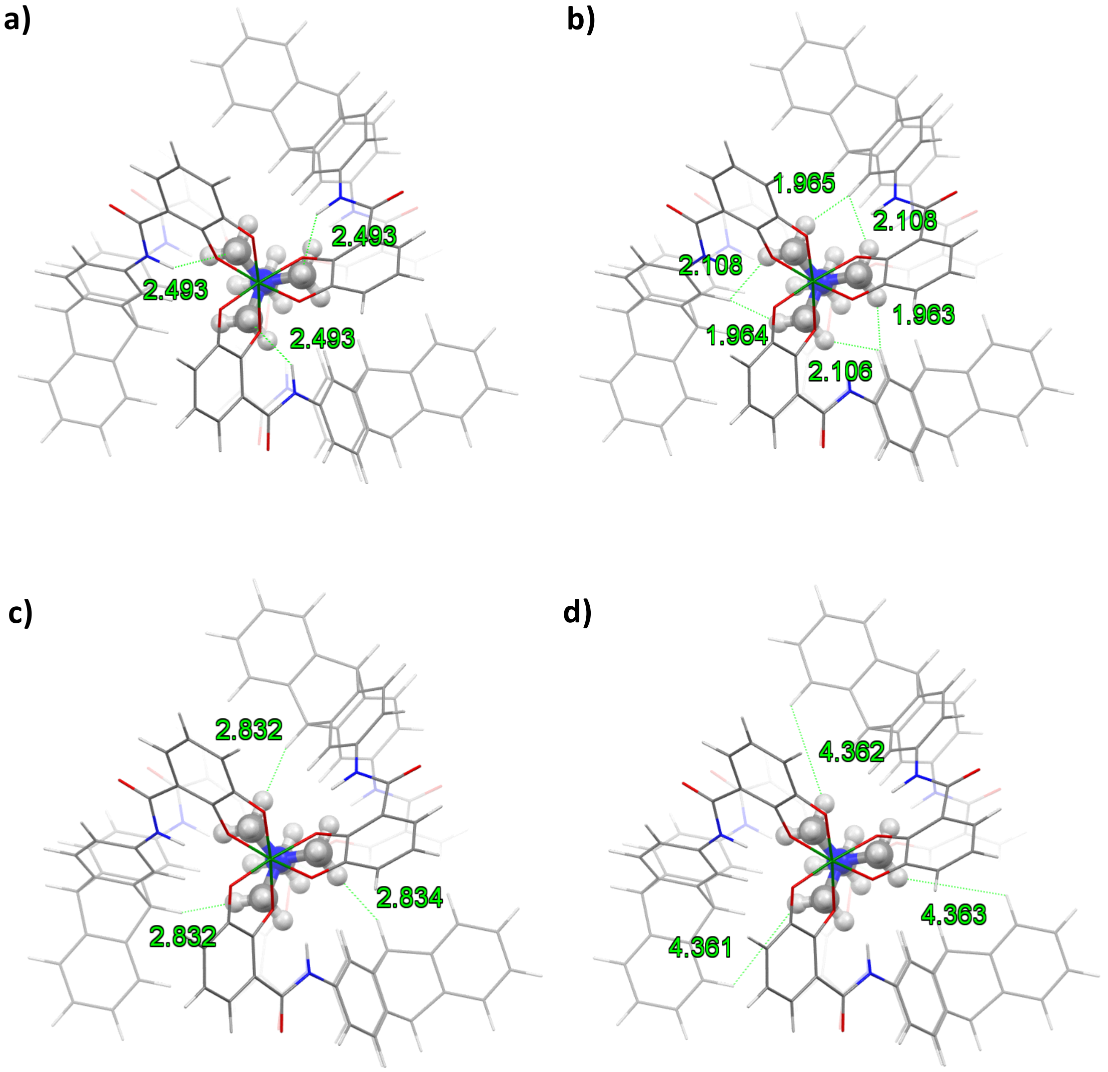


Fig. S65 The shortest distance measurements between guest Me_4N^+ and helicate [**Ga_2L_3**]$^{6-}$ according to model 1. (a) the shortest contact of amide NH and CH_3 of the Me_4N^+; (b) the shortest contact of aromatic CH and CH_3 of the Me_4N^+; (c) the shortest contact of bridged CH and CH_3 of the Me_4N^+; (d) the shortest contact of outside unsubstituted aromatic CH and CH_3 of the Me_4N^+.

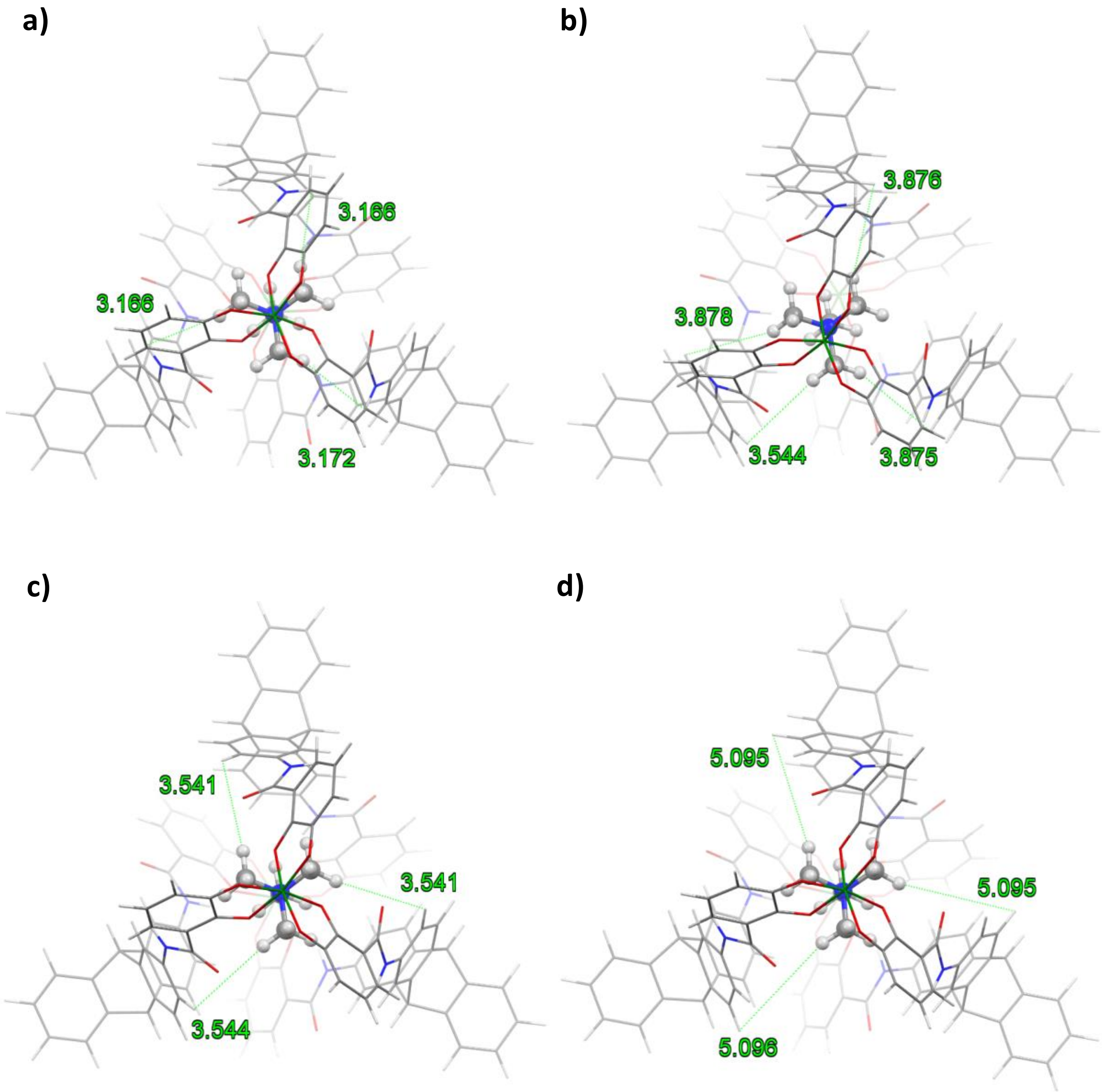


Fig. S66 The shortest distance measurements between guest Me_4N^+ and helicate [$\mathbf{Ga_2L_3}$]$^{6-}$ according to model 2. (a) the shortest contact of amide NH and CH_3 of the Me_4N^+; (b) the shortest contact of aromatic CH and CH_3 of the Me_4N^+; (c) the shortest contact of bridged CH and CH_3 of the Me_4N^+; (d) the shortest contact of outside unsubstituted aromatic CH and CH_3 of the Me_4N^+.

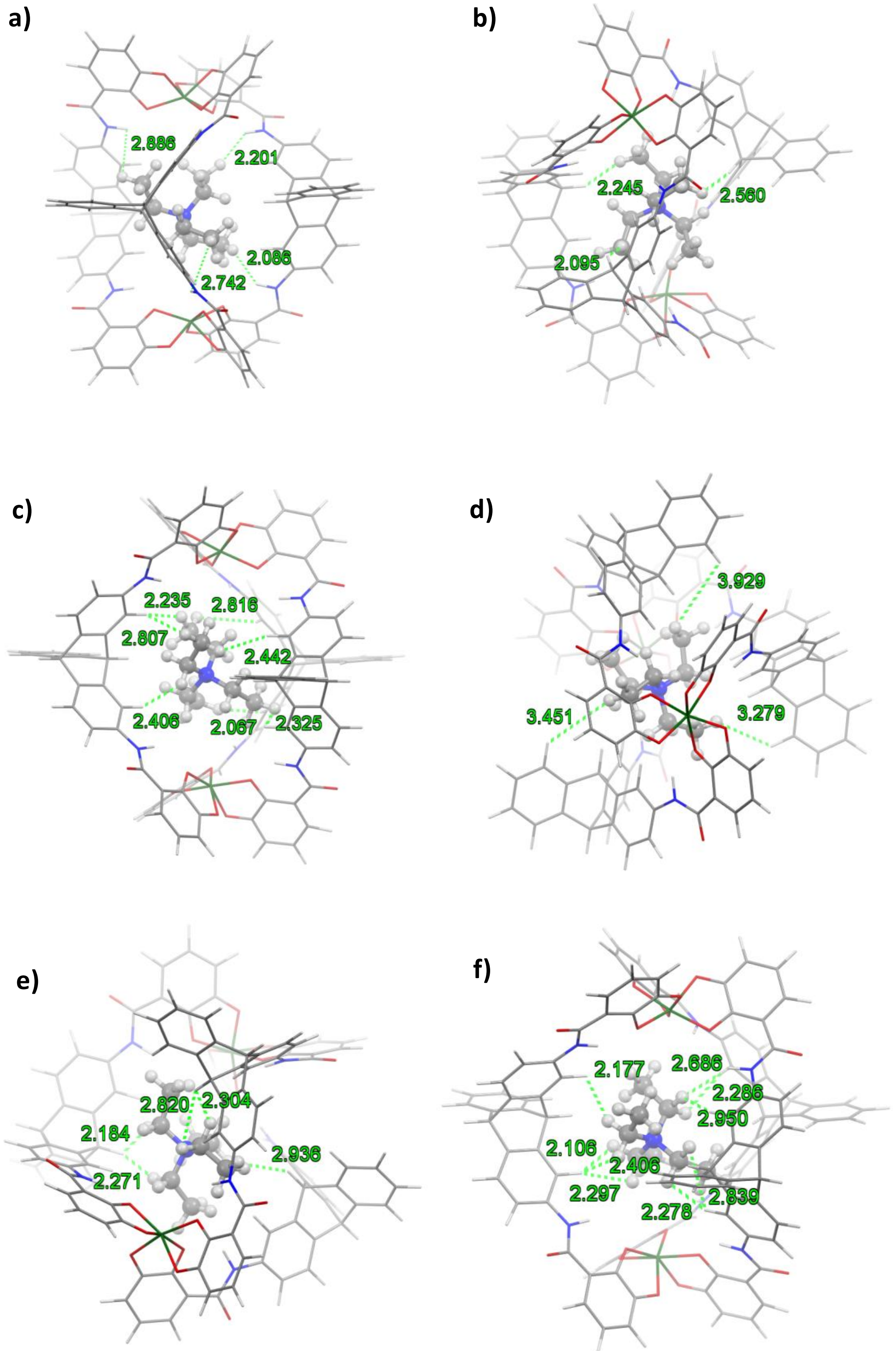


Fig. S67 The shortest distance measurements between guest Et_4N^+ and helicate [$\mathbf{Ga_2L_3}$]$^{6-}$ according to model 1. (a) the shortest contact of amide NH and CH_3 of the Et_4N^+; (b) the shortest contact of bridged CH and CH_3 of the Et_4N^+; (c) the shortest contact of aromatic CH and CH_3 of the Et_4N^+; (d) the shortest contact of outside unsubstituted aromatic CH and CH_3 of the Et_4N^+; (e) the shortest contact of bridged CH and CH_2 of the Et_4N^+; (f) the shortest contact of aromatic CH and CH_2 of the Et_4N^+.

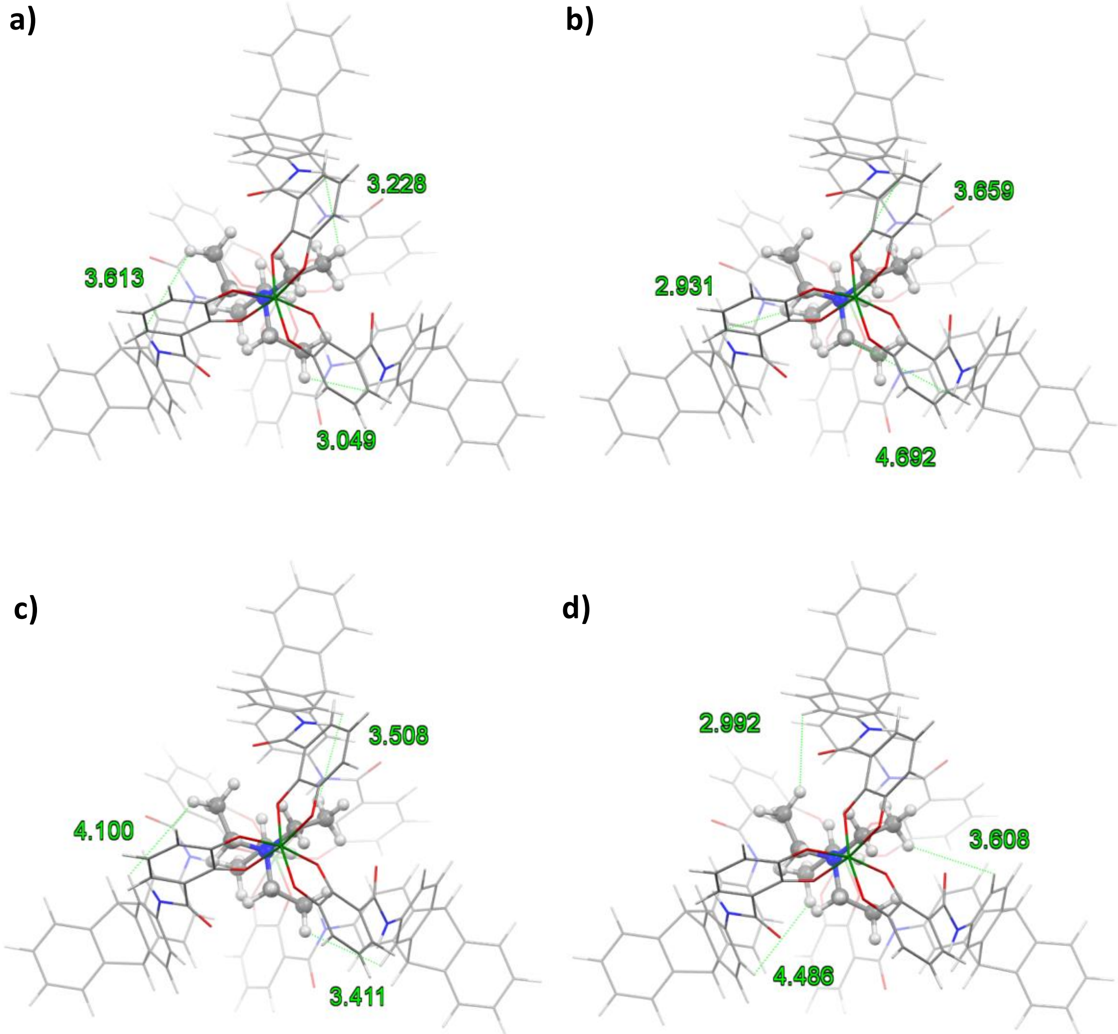


Fig. S68 The shortest distance measurements between guest Et_4N^+ and helicate [$\mathbf{Ga_2L_3}$]$^{6-}$ according to model 2. (a) the shortest contact of amide NH and CH_3 of the Et_4N^+; (b) the shortest contact of amide NH and CH_2 of the Et_4N^+; (c) the shortest contact of aromatic CH and CH_3 of the Et_4N^+; (d) the shortest contact of aromatic CH and CH_3 of the Et_4N^+.

Table S1. Summary of calculated energies.

Energy (Hartree/Particle)	Thermal Correction to Gibbs Free Energy	Sum of electronic and thermal Free Energies
$[Ga_2L_3]^{6-}$ (model 1)	1.251196	−9450.498829
$[Ga_2L_3]^{6-}$ (model 2)	1.253772	−9450.532545
$[Me_4N@Ga_2L_3]^{6-}$ (model 1)	1.487498	−9666.622038
$[Me_4N@Ga_2L_3]^{6-}$ (model 2)	1.408219	−9664.914315
$[Et_4N@Ga_2L_3]^{6-}$ (model 1)	1.519466	−9822.041156
$[Et_4N@Ga_2L_3]^{6-}$ (model 2)	1.517000	−9822.057932
Chiral $[Ga_2L_3]^{6-}$ (model 1)	1.257302	−9450.540073
Chiral $[Ga_2L_3]^{6-}$ (model 2)	1.253257	−9450.490857

5. Energies and cartesian coordinates

$[\mathbf{Ga_2L_3}]^{6-}$ (model 1)

```
Zero-point correction=                           1.387149 (Hartree/Particle)
 Thermal correction to Energy=                    1.483685
 Thermal correction to Enthalpy=                  1.484629
 Thermal correction to Gibbs Free Energy=         1.251196
 Sum of electronic and zero-point Energies=          -9450.362877
 Sum of electronic and thermal Energies=             -9450.266341
 Sum of electronic and thermal Enthalpies=           -9450.265396
 Sum of electronic and thermal Free Energies=        -9450.498829
 ----------------
```

Charge = -6 Multiplicity = 1

C	-5.26	-0.6593	-3.1076
C	-3.9945	-1.1146	-3.0713
C	-3.1163	-0.5491	-2.2207
C	-3.515	0.4266	-1.3901
C	-4.7804	0.8824	-1.4526
C	-5.6565	0.3424	-2.3088
C	-3.2119	5.1618	-1.0606
C	-1.9547	4.6967	-0.9751
C	-1.7321	3.3954	-0.7338
C	-2.7724	2.5638	-0.5794
C	-4.0326	3.0299	-0.6641
C	-4.2552	4.3306	-0.9053
C	-5.2466	0.4671	2.9466

C	-3.9823	0.0237	3.0696
C	-3.1087	0.2436	2.068
C	-3.5104	0.8591	0.9453
C	-4.7754	1.3096	0.8457
C	-5.6469	1.1161	1.8433
C	-5.1123	1.9831	-0.4676
C	-2.6673	1.0781	-0.3047
N	-3.5274	-2.0991	-3.8638
C	-4.1719	-3.0099	-4.6447
C	-3.4042	-3.6285	-5.5905
O	-5.324	-3.3052	-4.4291
C	-2.2181	-3.1363	-6.0079
C	-1.5222	-3.7419	-6.9872
C	-1.968	-4.8743	-7.549
C	-3.1321	-5.3874	-7.1272
C	-3.8428	-4.7633	-6.1738
O	-1.7155	-2.0947	-5.596
O	-0.4867	-3.1961	-7.3565
N	-3.5112	-0.6143	4.1591
C	-4.1508	-1.1816	5.2194
O	-5.3085	-1.519	5.1357
C	-3.3748	-1.4362	6.3147
C	-2.176	-0.8484	6.5177
C	-1.4717	-1.0807	7.6403
C	-1.9219	-1.9329	8.5719
C	-3.0991	-2.5416	8.3722
C	-3.8172	-2.2834	7.2671
O	-0.4231	-0.4587	7.7813
O	-1.6671	-0.0287	5.7585
C	2.0375	-4.8098	-2.4132
C	1.7975	-3.5145	-2.6869
C	1.0254	-2.7968	-1.8483
C	0.5366	-3.3604	-0.7329
C	0.7683	-4.6635	-0.4862
C	1.5199	-5.3915	-1.3213
C	-3.5936	-5.1435	0.8008
C	-3.8077	-3.8367	0.5752
C	-2.7696	-2.9992	0.4258
C	-1.5192	-3.4769	0.5028
C	-1.3039	-4.7864	0.7298
C	-2.3416	-5.6232	0.8792
C	2.0556	-3.7479	3.6746
C	1.8201	-2.4357	3.4927
C	1.0434	-2.0436	2.4643
C	0.5455	-2.9512	1.6104
C	0.7753	-4.2613	1.8191
C	1.531	-4.6645	2.848
C	0.1574	-5.1891	0.7951
C	-0.2602	-2.6487	0.3532
N	2.261	-2.881	-3.782
C	3.2152	-3.2294	-4.6888
C	3.1803	-2.5505	-5.8738
O	4.0834	-4.0197	-4.4015
C	2.0902	-1.8767	-6.2996
C	2.0743	-1.2734	-7.502
C	3.1548	-1.2912	-8.2951
C	4.2518	-1.9364	-7.8747
C	4.2552	-2.5672	-6.689
O	1.0306	-1.8107	-5.6829
O	1.0242	-0.7382	-7.8449
N	2.2925	-1.4681	4.3028

C	3.2516	-1.4892	5.2694
O	4.11	-2.3401	5.2717
C	3.2345	-0.4397	6.144
C	2.1573	0.3573	6.3124
C	2.1612	1.3426	7.2287
C	3.2484	1.5853	7.9743
C	4.3325	0.8165	7.8014
C	4.3164	-0.1877	6.9098
O	1.1225	1.9815	7.3673
O	1.0928	0.2215	5.7158
C	1.9238	3.4687	-3.9018
C	0.9174	2.5845	-3.7773
C	0.8541	1.8108	-2.6764
C	1.7623	1.9535	-1.6988
C	2.7744	2.8286	-1.8494
C	2.8585	3.5896	-2.9477
C	5.654	-0.2812	-0.1312
C	4.6333	-1.1379	0.0381
C	3.3665	-0.6991	-0.0258
C	3.1285	0.5995	-0.2601
C	4.1511	1.4587	-0.4291
C	5.4171	1.0199	-0.365
C	1.9998	4.5679	2.1702
C	0.9916	3.7033	2.3853
C	0.9044	2.5938	1.6262
C	1.7901	2.3786	0.6413
C	2.8029	3.2455	0.4523
C	2.9113	4.3417	1.2129
C	3.7389	2.8961	-0.6848
C	1.7547	1.2292	-0.3583
N	-0.0347	2.3953	-4.7118
C	-0.389	3.1344	-5.7994
C	-1.1414	2.4856	-6.7372
O	-0.1275	4.313	-5.8584
C	-1.2148	1.1393	-6.8142
C	-1.9199	0.539	-7.7904
C	-2.6001	1.2611	-8.6918
C	-2.5539	2.5983	-8.6136
C	-1.8234	3.1968	-7.6588
O	-0.6157	0.3691	-6.0692
O	-1.8883	-0.6873	-7.8324
N	0.0602	3.8592	3.3466
C	-0.2706	4.9334	4.1158
O	0.0011	6.0562	3.7603
C	-1.0127	4.6604	5.2301
C	-1.101	3.4251	5.7689
C	-1.7966	3.2118	6.9009
C	-2.4517	4.2127	7.5057
C	-2.3903	5.4395	6.9697
C	-1.6698	5.6579	5.8576
O	-1.7805	2.0753	7.3639
O	-0.5249	2.4341	5.3291
Ga	-0.3598	1.0494	6.6225
Ga	-0.4392	-1.3744	-6.8084
H	-6.0045	-1.0636	-3.81
H	-2.0745	-0.9067	-2.1671
H	-6.6927	0.7151	-2.3496
H	-3.3884	6.2323	-1.259
H	-1.1012	5.3837	-1.1029
H	-0.7034	3.0142	-0.663
H	-5.2864	4.7123	-0.9748

H	-5.988	0.3449	3.7506
H	-2.0677	-0.1131	2.1406
H	-6.6824	1.4816	1.7527
H	-6.1499	2.3707	-0.5375
H	-1.6307	0.6882	-0.2343
H	-2.5234	-2.1584	-3.7992
H	-1.3971	-5.3671	-8.3531
H	-3.5162	-6.3149	-7.585
H	-4.802	-5.2284	-5.89
H	-2.5083	-0.6997	4.1117
H	-1.3439	-2.119	9.4919
H	-3.487	-3.2401	9.133
H	-4.7862	-2.803	7.1775
H	2.6316	-5.4469	-3.0857
H	0.8169	-1.7324	-2.0473
H	1.7111	-6.4558	-1.1093
H	-4.451	-5.8265	0.9229
H	-4.838	-3.448	0.5124
H	-2.9432	-1.9291	0.2417
H	-2.1665	-6.6949	1.0648
H	2.6529	-4.1212	4.5201
H	0.8376	-0.9743	2.2901
H	1.72	-5.7381	3.0092
H	0.3306	-6.2691	0.983
H	-0.4323	-1.5687	0.1654
H	1.82	-1.9803	-3.8823
H	3.138	-0.7986	-9.2811
H	5.1465	-1.9666	-8.5195
H	5.1832	-3.0967	-6.4146
H	1.8558	-0.5853	4.0896
H	3.2474	2.3913	8.7264
H	5.2326	0.9987	8.4129
H	5.2351	-0.7936	6.8341
H	2.0395	4.0973	-4.7977
H	0.0368	1.082	-2.5471
H	3.6854	4.3089	-3.0611
H	6.6927	-0.6482	-0.0773
H	4.8338	-2.2053	0.2304
H	2.5301	-1.3994	0.1133
H	6.2544	1.7224	-0.5032
H	2.1362	5.4694	2.7864
H	0.0855	1.871	1.7781
H	3.7391	5.0502	1.0486
H	4.5847	3.6013	-0.823
H	0.9077	0.5259	-0.2204
H	-0.5777	1.5725	-4.5022
H	-3.175	0.7666	-9.4919
H	-3.1026	3.2064	-9.3527
H	-1.8133	4.2999	-7.6647
H	-0.4883	3.0196	3.4465
H	-3.0186	4.0352	8.4343
H	-2.9182	6.2752	7.4598
H	-1.647	6.6949	5.4821

$[Ga_2L_3]^{6-}$ (model 2)

Zero-point correction= 1.388857 (Hartree/Particle)

Thermal correction to Energy= 1.485200
Thermal correction to Enthalpy= 1.486144
Thermal correction to Gibbs Free Energy= 1.253772
Sum of electronic and zero-point Energies= -9450.397460
Sum of electronic and thermal Energies= -9450.301117
Sum of electronic and thermal Enthalpies= -9450.300173
Sum of electronic and thermal Free Energies= -9450.532545

Charge = -6 Multiplicity = 1

C	-1.835	-5.5355	3.2961
C	-1.4316	-4.328	3.7347
C	-0.1279	-4.0024	3.6269
C	0.7628	-4.9037	3.1798
C	0.3423	-6.125	2.8024
C	-0.9593	-6.4347	2.8251
C	3.4187	-8.0358	5.4918
C	3.8489	-6.8193	5.866
C	3.5108	-5.7312	5.1556
C	2.7386	-5.8715	4.0681
C	2.307	-7.0923	3.6917
C	2.6456	-8.1777	4.403
C	3.5344	-6.2551	-0.5292
C	4.0522	-5.0731	-0.1438
C	3.6637	-4.5503	1.0352
C	2.7715	-5.1938	1.8047
C	2.3066	-6.3972	1.4236
C	2.6705	-6.924	0.2485
C	1.4388	-7.0999	2.4421
C	2.2775	-4.7358	3.1676
N	-2.2466	-3.4245	4.3209
C	-3.3788	-3.6585	5.0485
C	-3.8681	-2.5809	5.7251
O	-3.7551	-4.7837	5.282
C	-3.8203	-1.3168	5.2506
C	-4.3249	-0.3179	6.0003
C	-4.8415	-0.5323	7.22
C	-4.8873	-1.784	7.6909
C	-4.4146	-2.7907	6.9415
O	-3.4241	-0.9948	4.1252
O	-4.3177	0.8067	5.5104
N	4.9859	-4.3942	-0.8426
C	5.4154	-4.5538	-2.1266
O	4.7184	-5.1257	-2.9314
C	6.6096	-3.9569	-2.4237
C	7.4433	-3.5116	-1.4609
C	8.6318	-2.9602	-1.7633
C	9.0275	-2.8229	-3.0381
C	8.2079	-3.243	-4.0133
C	7.0299	-3.8029	-3.6974
O	8.4429	-3.1159	-5.2184
O	6.3844	-4.1036	-4.6935
C	-4.8261	1.3798	-2.8474
C	-4.7898	0.3028	-2.0407
C	-4.1528	-0.8071	-2.4628
C	-3.6415	-0.8631	-3.7037
C	-3.7233	0.2125	-4.508
C	-4.2882	1.3462	-4.0752
C	-5.4984	-2.327	-7.7808
C	-5.4207	-3.4076	-6.9864

C	-4.6551	-3.3858	-5.8834
C	-3.9688	-2.2734	-5.5831
C	-4.0458	-1.1886	-6.3805
C	-4.8116	-1.2126	-7.4814
C	0.4065	-0.8108	-6.3309
C	0.4889	-1.9542	-5.6239
C	-0.6038	-2.3889	-4.9678
C	-1.7512	-1.695	-5.0221
C	-1.8296	-0.5892	-5.7839
C	-0.7458	-0.1297	-6.4211
C	-3.2166	0.	-5.9152
C	-3.0625	-2.1025	-4.3737
N	-5.3929	0.2413	-0.8349
C	-6.5135	0.8981	-0.4148
C	-7.0031	0.4752	0.7846
O	-7.1538	1.5952	-1.1672
C	-6.2117	0.0972	1.812
C	-6.7811	-0.3155	2.9619
C	-8.1138	-0.3948	3.1017
C	-8.8975	-0.0207	2.083
C	-8.3415	0.4204	0.945
O	-4.9791	0.1825	1.8135
O	-6.0361	-0.5882	3.8991
N	1.584	-2.7416	-5.577
C	2.8583	-2.5065	-6.0002
O	3.2542	-1.3684	-6.1053
C	3.6059	-3.6202	-6.2823
C	3.1537	-4.8731	-6.0562
C	3.8987	-5.962	-6.3197
C	5.1476	-5.8417	-6.7939
C	5.5863	-4.5999	-7.0364
C	4.8681	-3.4932	-6.7789
O	6.725	-4.2676	-7.3213
O	5.2828	-2.4056	-7.2354
C	1.1093	3.8489	3.7561
C	0.0704	3.8154	2.9007
C	0.306	3.9479	1.5805
C	1.5497	4.1984	1.1382
C	2.5684	4.2614	2.0155
C	2.3598	4.0602	3.322
C	3.866	8.2225	0.2951
C	2.8528	8.1736	-0.5857
C	2.2026	7.0202	-0.8095
C	2.5754	5.917	-0.1442
C	3.5929	5.9654	0.7393
C	4.2405	7.1187	0.9618
C	5.3624	2.2618	-1.0602
C	4.4124	2.2854	-2.0146
C	3.2942	3.0038	-1.8018
C	3.1326	3.6793	-0.6532
C	4.1225	3.6995	0.2577
C	5.2303	2.9723	0.0698
C	3.9035	4.6412	1.4209
C	1.9373	4.5449	-0.2947
N	-1.2148	3.6935	3.2942
C	-1.7762	4.1323	4.4583
C	-3.1328	4.0291	4.52
O	-1.1429	4.7913	5.25
C	-3.8233	3.0145	3.9616
C	-5.1614	2.9857	4.0853
C	-5.8484	3.9511	4.7101

C	-5.165	4.9696	5.2476
C	-3.8256	4.9935	5.1622
O	-3.3448	2.0145	3.4225
O	-5.7072	1.9857	3.6402
N	4.5462	1.6739	-3.2096
C	5.4422	0.7261	-3.601
O	5.9369	-0.0084	-2.778
C	5.6732	0.6585	-4.9474
C	5.2603	1.6277	-5.7898
C	5.5618	1.5874	-7.0994
C	6.2902	0.5838	-7.6125
C	6.695	-0.4042	-6.7996
C	6.3765	-0.3552	-5.4952
O	7.3376	-1.3881	-7.1835
O	6.7575	-1.3397	-4.876
Ga	6.7552	-2.8299	-6.0715
Ga	-4.4992	0.5101	3.6347
H	-2.8915	-5.843	3.3139
H	0.2365	-3.0283	3.9924
H	-1.298	-7.4346	2.5092
H	3.7015	-8.9236	6.0821
H	4.4835	-6.7131	6.7618
H	3.8629	-4.7329	5.4607
H	2.2918	-9.1747	4.0957
H	3.8475	-6.7615	-1.4544
H	4.0828	-3.594	1.3888
H	2.3022	-7.919	-0.0497
H	1.0866	-8.1076	2.1382
H	2.6324	-3.7302	3.4748
H	-1.8125	-2.5186	4.4107
H	-5.2464	0.3018	7.8167
H	-5.318	-1.9822	8.6868
H	-4.4721	-3.7974	7.3898
H	5.3751	-3.6405	-0.2979
H	7.2041	-3.6013	-0.3886
H	9.2952	-2.6114	-0.9534
H	9.9946	-2.353	-3.28
H	-5.2997	2.3242	-2.5383
H	-4.1281	-1.7116	-1.8331
H	-4.3542	2.2227	-4.7397
H	-6.1302	-2.3546	-8.6845
H	-5.9885	-4.3183	-7.2409
H	-4.5896	-4.2711	-5.231
H	-4.8754	-0.3258	-8.1319
H	1.2462	-0.4277	-6.9298
H	-0.5766	-3.3318	-4.3974
H	-0.8185	0.7654	-7.0599
H	-3.2839	0.8893	-6.5758
H	-2.9976	-2.9945	-3.7167
H	-5.093	-0.5583	-0.2984
H	-8.5616	-0.7348	4.0502
H	-9.9946	-0.068	2.1864
H	-9.0363	0.7079	0.1373
H	1.3682	-3.6299	-5.1545
H	2.1544	-5.0737	-5.6388
H	3.5011	-6.9674	-6.0993
H	5.7979	-6.7185	-6.9391
H	0.9768	3.7053	4.8397
H	-0.5287	3.9465	0.8607
H	3.1989	4.114	4.0342
H	4.3937	9.1747	0.4724

H	2.5528	9.0857	-1.1285
H	1.3719	6.9781	-1.5318
H	5.0706	7.158	1.685
H	6.3182	1.7335	-1.1983
H	2.506	3.0547	-2.5706
H	6.0451	3.0026	0.8112
H	4.7423	4.6874	2.1462
H	1.0997	4.5027	-1.0215
H	-1.8348	3.47	2.5311
H	-6.945	3.895	4.8058
H	-5.7042	5.7739	5.7758
H	-3.3208	5.8566	5.6291
H	3.8486	1.9815	-3.8688
H	4.6931	2.5072	-5.4436
H	5.2219	2.4	-7.7641
H	6.5354	0.5616	-8.6868

$[Me_4N@\mathbf{Ga_2L_3}]^{5-}$ (model 1)

```
Zero-point correction=                           1.608303 (Hartree/Particle)
 Thermal correction to Energy=                    1.700506
 Thermal correction to Enthalpy=                  1.701450
 Thermal correction to Gibbs Free Energy=         1.487498
 Sum of electronic and zero-point Energies=          -9666.501233
 Sum of electronic and thermal Energies=             -9666.409031
 Sum of electronic and thermal Enthalpies=           -9666.408087
 Sum of electronic and thermal Free Energies=        -9666.622038
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```

Charge = -5 Multiplicity = 1

H	-1.1789	-0.9912	-1.7688
C	-0.1011	-1.0928	-1.5111
N	0.3708	0.0764	-0.667
C	-0.4137	0.092	0.6284
C	1.8497	-0.0562	-0.3569
H	2.209	0.7741	0.2877
H	-0.178	0.9812	1.2449
C	0.1395	1.3676	-1.4271
H	0.6795	1.3667	-2.4008
H	0.456	-1.1479	-2.4713
H	0.0319	-2.0581	-0.9717
H	-1.5079	0.1236	0.4395
H	-0.1742	-0.8063	1.2378
H	2.4651	-0.024	-1.2799
H	2.0644	-1.0124	0.1668
H	0.5156	2.2304	-0.8367
H	-0.9414	1.5323	-1.6354
C	2.7272	-3.0978	-2.4662
C	2.7303	-4.4188	-2.2061
C	3.1422	-5.2467	-3.1864
C	3.5016	-4.7875	-4.396
C	3.4442	-3.4741	-4.6473
C	3.0546	-2.6258	-3.6784
C	6.3346	0.2974	-4.9101

C	6.7338	-0.5532	-5.8703
C	5.9422	-1.5696	-6.2491
C	4.7479	-1.7279	-5.6596
C	4.3486	-0.8747	-4.698
C	5.1393	0.1402	-4.3191
C	3.7542	-2.8258	-5.9839
C	2.9807	-1.1729	-4.1205
C	0.5473	-1.6072	-7.4958
C	0.1184	-0.757	-6.5432
C	0.9013	-0.5682	-5.4623
C	2.0538	-1.2407	-5.3229
C	2.4563	-2.0975	-6.279
C	1.7058	-2.2746	-7.3732
N	2.3197	-4.775	-0.9676
C	1.9791	-5.9983	-0.4694
C	1.7904	-6.1209	0.8809
O	1.8777	-6.9474	-1.2125
C	1.7598	-5.0962	1.7662
C	1.6309	-5.3622	3.0793
C	1.4985	-6.6052	3.5597
C	1.4926	-7.6206	2.6906
C	1.6442	-7.3696	1.3819
O	1.8429	-3.8932	1.5104
O	1.6552	-4.4077	3.8424
N	-1.0337	-0.0515	-6.5538
C	-2.1319	-0.108	-7.361
C	-3.0829	0.8654	-7.2078
O	-2.2453	-0.9902	-8.1801
C	-3.0379	1.8527	-6.2837
C	-3.9937	2.7994	-6.2513
C	-5.0333	2.7896	-7.0953
C	-5.1085	1.801	-7.9939
C	-4.1444	0.8685	-8.0458
O	-2.1681	2.0096	-5.4282
O	-3.8592	3.6883	-5.4197
C	1.9222	2.6854	2.6092
C	3.124	2.5726	3.2052
C	3.5981	3.6516	3.8579
C	2.9279	4.8159	3.8727
C	1.762	4.9198	3.2218
C	1.2488	3.8446	2.5971
C	-2.9637	5.0538	3.9686
C	-2.4482	6.1222	4.5993
C	-1.1938	6.5256	4.3398
C	-0.4564	5.8504	3.4456
C	-0.9736	4.7776	2.8185
C	-2.2277	4.376	3.0734
C	0.9645	6.1996	3.0464
C	-0.0386	4.1151	1.832
C	1.4178	7.242	-0.5362
C	0.8942	6.1786	-1.1742
C	0.3558	5.1922	-0.4326
C	0.4008	5.2354	0.9053
C	0.9323	6.302	1.5299
C	1.43	7.3137	0.8057
N	3.7272	1.3712	3.0556
C	5.019	0.9867	3.2683
C	5.3472	-0.3241	3.0446
O	5.8507	1.8076	3.5803
C	4.4659	-1.3107	2.7573
C	4.8956	-2.5786	2.6095

C	6.1899	-2.9112	2.6939
C	7.0754	-1.9393	2.9399
C	6.6503	-0.6792	3.1202
O	3.2441	-1.1965	2.6527
O	4.0354	-3.4313	2.4271
N	0.8473	5.9573	-2.5048
C	1.4461	6.5683	-3.5659
C	1.0939	6.1222	-4.8118
O	2.2519	7.452	-3.389
C	0.2147	5.1221	-5.0502
C	-0.1456	4.8049	-6.3069
C	0.391	5.4194	-7.3688
C	1.3042	6.3744	-7.1516
C	1.6324	6.7221	-5.8966
O	-0.3691	4.4477	-4.2037
O	-1.0203	3.9527	-6.4187
C	-2.885	-1.9112	2.3192
C	-2.9711	-1.9357	3.6634
C	-4.2002	-1.9168	4.2144
C	-5.3079	-1.8272	3.4609
C	-5.1941	-1.7396	2.1301
C	-3.9791	-1.7857	1.555
C	-5.6832	-4.3142	-1.865
C	-6.8955	-4.2759	-1.2874
C	-7.1543	-3.392	-0.3102
C	-6.1908	-2.5465	0.0849
C	-4.9768	-2.5861	-0.4943
C	-4.7178	-3.4686	-1.4705
C	-6.3433	-1.5015	1.171
C	-3.9874	-1.5777	0.0471
C	-6.0384	2.068	0.0843
C	-4.8321	2.0529	-0.5145
C	-4.1753	0.8811	-0.6087
C	-4.687	-0.2298	-0.0553
C	-5.8937	-0.1947	0.542
C	-6.5768	0.9547	0.6047
N	-1.7842	-1.96	4.3096
C	-1.4615	-1.7921	5.6246
C	-0.1448	-1.9231	5.9771
O	-2.3217	-1.5541	6.4403
C	0.8831	-2.0724	5.1079
C	2.1333	-2.2551	5.5755
C	2.4157	-2.2589	6.8847
C	1.4142	-2.0716	7.7508
C	0.1624	-1.9167	7.2943
O	0.8035	-2.0751	3.8782
O	3.019	-2.4499	4.7524
N	-4.2322	3.1385	-1.0483
C	-4.4859	4.46	-0.828
C	-4.0496	5.367	-1.7552
O	-5.1019	4.7902	0.1598
C	-3.3101	5.059	-2.8459
C	-3.0229	6.0131	-3.753
C	-3.4023	7.2875	-3.588
C	-4.0905	7.6128	-2.4883
C	-4.4146	6.6597	-1.602
O	-2.8641	3.9418	-3.105
O	-2.4063	5.683	-4.7589
Ga	2.3281	-2.8291	3.018
Ga	-2.0548	3.8131	-4.8246
H	2.2058	-3.9666	-0.3789

H	-1.0471	0.5848	-5.7759
H	3.1039	0.7137	2.6173
H	0.3048	5.1305	-2.6812
H	-1.0353	-2.0586	3.6458
H	-3.4489	2.8769	-1.6216
H	2.4092	-2.3892	-1.6899
H	3.2216	-6.3343	-3.0494
H	3.8257	-5.4838	-5.1866
H	6.9916	1.1292	-4.6049
H	7.7174	-0.4166	-6.3503
H	6.2689	-2.2678	-7.0362
H	4.8097	0.8361	-3.531
H	4.081	-3.5308	-6.7762
H	2.6509	-0.4574	-3.3433
H	-0.0158	-1.7917	-8.4211
H	0.5889	0.1191	-4.6587
H	2.0358	-2.9743	-8.1582
H	1.3981	-6.7907	4.6417
H	1.3866	-8.6559	3.0567
H	1.6591	-8.2715	0.7469
H	-5.8051	3.5756	-7.0556
H	-5.9538	1.7704	-8.7022
H	-4.2764	0.1089	-8.8347
H	1.504	1.8307	2.0647
H	4.5544	3.64	4.3996
H	3.3503	5.6971	4.3826
H	-3.9964	4.7323	4.1844
H	-3.0603	6.6744	5.3321
H	-0.7736	7.4052	4.8532
H	-2.6488	3.5017	2.5511
H	1.3907	7.0861	3.56
H	-0.4672	3.2354	1.3111
H	1.8532	8.0929	-1.0794
H	-0.0838	4.308	-0.9186
H	1.8764	8.1835	1.3144
H	6.518	-3.9567	2.5755
H	8.1484	-2.1845	3.0168
H	7.4502	0.048	3.3398
H	0.0821	5.1553	-8.3933
H	1.7586	6.8979	-8.0099
H	2.3622	7.5447	-5.8096
H	-1.9037	-1.9352	1.8252
H	-4.3675	-1.961	5.299
H	-6.3035	-1.7794	3.9313
H	-5.4792	-5.0433	-2.6671
H	-7.683	-4.9741	-1.6174
H	-8.1484	-3.3601	0.1636
H	-3.7227	-3.4976	-1.9426
H	-7.3448	-1.4661	1.6476
H	-2.9861	-1.6175	-0.4266
H	-6.6447	2.984	0.1534
H	-3.1855	0.8345	-1.0895
H	-7.561	0.9861	1.0996
H	3.4461	-2.4167	7.2436
H	1.6201	-2.0714	8.8347
H	-0.6022	-1.8008	8.0809
H	-3.1559	8.0547	-4.3404
H	-4.4145	8.6559	-2.3331
H	-5.0196	7.0074	-0.7477

$[Me_4N@\mathbf{Ga_2L_3}]^{5-}$ (model 2)

```
Zero-point correction=                           1.552881 (Hartree/Particle)
 Thermal correction to Energy=                    1.658324
 Thermal correction to Enthalpy=                  1.659268
 Thermal correction to Gibbs Free Energy=         1.408219
 Sum of electronic and zero-point Energies=          -9664.769654
 Sum of electronic and thermal Energies=             -9664.664211
 Sum of electronic and thermal Enthalpies=           -9664.663266
 Sum of electronic and thermal Free Energies=        -9664.914315
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```

Charge = -5 Multiplicity = 1

C	-1.8186	-5.4868	3.2919
C	-1.4083	-4.2875	3.7467
C	-0.0979	-3.9777	3.662
C	0.7916	-4.8869	3.225
C	0.3608	-6.0997	2.8321
C	-0.9449	-6.3923	2.8296
C	3.3552	-8.0747	5.5671
C	3.7995	-6.8677	5.9558
C	3.4918	-5.7699	5.2461
C	2.7371	-5.8916	4.1441
C	2.292	-7.1033	3.7538
C	2.5986	-8.1987	4.4645
C	3.6033	-6.2603	-0.4472
C	4.1362	-5.0899	-0.0466
C	3.7495	-4.5774	1.1377
C	2.83	-5.2063	1.8879
C	2.3498	-6.3984	1.4905
C	2.7228	-6.9234	0.3172
C	1.4488	-7.0899	2.4876
C	2.311	-4.7438	3.2413
N	-2.2304	-3.3843	4.3255
C	-3.3742	-3.621	5.0365
C	-3.8803	-2.5496	5.7112
O	-3.752	-4.7473	5.2624
C	-3.8369	-1.2833	5.2426
C	-4.3524	-0.288	5.9893
C	-4.8842	-0.5078	7.2014
C	-4.9315	-1.7619	7.6666
C	-4.443	-2.764	6.92
O	-3.4291	-0.9491	4.1252
O	-4.3393	0.8363	5.4982
N	5.0648	-4.4048	-0.7474
C	5.4364	-4.5214	-2.0557
O	4.6989	-5.064	-2.8461
C	6.6242	-3.9263	-2.3884
C	7.4996	-3.5244	-1.4441
C	8.6899	-2.994	-1.7731
C	9.0493	-2.8517	-3.0576
C	8.1918	-3.225	-4.0204
C	6.9991	-3.746	-3.6762
O	8.4343	-3.0896	-5.2239
O	6.2673	-3.9959	-4.6301

C	-4.8788	1.4158	-2.8264
C	-4.843	0.3403	-2.0177
C	-4.2031	-0.7705	-2.4321
C	-3.689	-0.8287	-3.6711
C	-3.7672	0.245	-4.4782
C	-4.3347	1.3795	-4.0513
C	-5.5351	-2.2953	-7.7515
C	-5.4622	-3.3747	-6.9551
C	-4.7	-3.3533	-5.8497
C	-4.0118	-2.2423	-5.5482
C	-4.0835	-1.1591	-6.3483
C	-4.8459	-1.1826	-7.4516
C	0.3724	-0.786	-6.2631
C	0.4497	-1.9227	-5.5446
C	-0.6476	-2.3549	-4.8951
C	-1.7951	-1.6638	-4.9699
C	-1.868	-0.5619	-5.7379
C	-0.7791	-0.1058	-6.3682
C	-3.2536	0.0283	-5.8824
C	-3.1111	-2.071	-4.334
N	-5.4501	0.278	-0.8146
C	-6.5701	0.934	-0.3928
C	-7.0524	0.5067	0.8075
O	-7.2107	1.634	-1.1417
C	-6.2528	0.1114	1.8216
C	-6.8076	-0.3116	2.9732
C	-8.1385	-0.3791	3.1319
C	-8.9324	0.0157	2.1284
C	-8.3888	0.463	0.9863
O	-5.0198	0.1798	1.8142
O	-6.0404	-0.6029	3.8861
N	1.5437	-2.7099	-5.4818
C	2.8179	-2.48	-5.9068
O	3.2126	-1.3422	-6.017
C	3.5578	-3.5983	-6.1927
C	3.0947	-4.8464	-5.9628
C	3.8239	-5.9435	-6.2331
C	5.0673	-5.8328	-6.7222
C	5.518	-4.5968	-6.9712
C	4.8155	-3.48	-6.7056
O	6.6582	-4.2985	-7.283
O	5.2174	-2.3817	-7.1488
C	1.0574	3.8763	3.7764
C	0.0154	3.8422	2.9247
C	0.2433	3.9718	1.6031
C	1.4848	4.2211	1.1555
C	2.5083	4.2814	2.0271
C	2.3061	4.0833	3.335
C	3.8098	8.2377	0.3013
C	2.7923	8.1927	-0.5749
C	2.1369	7.0417	-0.7964
C	2.5091	5.9369	-0.1333
C	3.5318	5.9808	0.7443
C	4.184	7.1319	0.9649
C	5.2569	2.247	-1.0575
C	4.2977	2.2761	-2.0027
C	3.1894	3.0075	-1.7873
C	3.0467	3.6917	-0.6417
C	4.0438	3.7069	0.2618
C	5.1424	2.9667	0.0686
C	3.8412	4.655	1.4234

C	1.8626	4.5684	-0.2793
N	-1.2687	3.7232	3.3213
C	-1.8293	4.1647	4.4841
C	-3.1853	4.0588	4.5403
O	-1.1968	4.8246	5.2753
C	-3.8687	3.0447	3.9736
C	-5.2063	3.0084	4.0853
C	-5.9021	3.9675	4.7101
C	-5.2263	4.9858	5.2581
C	-3.8863	5.017	5.1825
O	-3.3869	2.0487	3.432
O	-5.7362	2.0064	3.6263
N	4.4166	1.6566	-3.1948
C	5.2996	0.6934	-3.5759
O	5.7656	-0.0553	-2.7482
C	5.5645	0.6408	-4.9171
C	5.223	1.6491	-5.7452
C	5.5926	1.6388	-7.0381
C	6.337	0.6385	-7.5351
C	6.6678	-0.3898	-6.7377
C	6.2549	-0.3882	-5.4569
O	7.328	-1.3581	-7.1296
O	6.5122	-1.4079	-4.825
Ga	6.742	-2.8343	-6.0696
Ga	-4.5275	0.5306	3.6243
H	-2.8792	-5.7819	3.2893
H	0.2705	-3.0099	4.0397
H	-1.2913	-7.3855	2.5005
H	3.6158	-8.9711	6.1546
H	4.4233	-6.7777	6.8613
H	3.8558	-4.7791	5.5624
H	2.2353	-9.1884	4.143
H	3.9079	-6.7574	-1.381
H	4.1808	-3.6303	1.5003
H	2.3344	-7.9062	0.0039
H	1.0856	-8.0899	2.1714
H	2.6747	-3.7452	3.5614
H	-1.7967	-2.4801	4.4301
H	-5.2997	0.323	7.7953
H	-5.3745	-1.9653	8.6561
H	-4.5015	-3.7718	7.365
H	5.4744	-3.6658	-0.1968
H	7.2954	-3.6389	-0.367
H	9.3904	-2.6834	-0.9779
H	10.0284	-2.4165	-3.3181
H	-5.3557	2.3597	-2.521
H	-4.1792	-1.673	-1.7996
H	-4.3979	2.2544	-4.7182
H	-6.1658	-2.3217	-8.6561
H	-6.0332	-4.2834	-7.2093
H	-4.6404	-4.2375	-5.1952
H	-4.9059	-0.2963	-8.1031
H	1.2157	-0.4074	-6.8597
H	-0.6247	-3.2929	-4.3163
H	-0.847	0.7843	-7.0144
H	-3.3149	0.9163	-6.5454
H	-3.0517	-2.9612	-3.674
H	-5.1507	-0.5224	-0.2789
H	-8.576	-0.7266	4.0823
H	-10.0284	-0.0219	2.2461
H	-9.0909	0.7654	0.1909

H	1.3252	-3.5938	-5.0517
H	2.0975	-5.0384	-5.5379
H	3.4174	-6.9452	-6.0125
H	5.7043	-6.7171	-6.8802
H	0.9281	3.7348	4.8607
H	-0.5951	3.9706	0.8876
H	3.1491	4.1351	4.0428
H	4.341	9.1884	0.4775
H	2.4919	9.1065	-1.1146
H	1.3011	7.0034	-1.5133
H	5.0178	7.1678	1.6842
H	6.2066	1.7079	-1.2016
H	2.3955	3.0603	-2.5504
H	5.9636	2.9946	0.8029
H	4.6853	4.6969	2.1429
H	1.0196	4.5297	-1.0001
H	-1.8895	3.4987	2.559
H	-6.999	3.907	4.7964
H	-5.7725	5.7857	5.7857
H	-3.3874	5.8795	5.6561
H	3.727	1.97	-3.8594
H	4.672	2.5385	-5.3963
H	5.3156	2.4827	-7.6939
H	6.6561	0.6522	-8.5913
N	1.0457	-1.7584	-0.3828
C	1.8119	-2.7488	-1.3473
C	0.2185	-0.644	-1.126
C	1.7027	-1.3299	0.9949
C	-0.0711	-2.6765	0.1327
H	2.1401	-3.6565	-0.7954
H	2.7222	-2.2585	-1.772
H	1.1638	-3.0613	-2.1987
H	-0.7684	-2.1463	0.8195
H	0.3354	-3.5494	0.6908
H	-0.687	-3.0875	-0.6972
H	0.9714	-0.7847	1.6372
H	2.5679	-0.6458	0.8209
H	2.0868	-2.2172	1.5484
H	-0.4586	-0.1148	-0.4168
H	-0.3868	-1.084	-1.9517
H	0.9053	0.1139	-1.575

[Et_4N@$\mathbf{Ga_2L_3}$]$^{5-}$ (model 1)

```
Zero-point correction=                           1.669216 (Hartree/Particle)
 Thermal correction to Energy=                    1.779093
 Thermal correction to Enthalpy=                  1.780037
 Thermal correction to Gibbs Free Energy=         1.519466
 Sum of electronic and zero-point Energies=          -9821.891406
 Sum of electronic and thermal Energies=             -9821.781529
 Sum of electronic and thermal Enthalpies=           -9821.780585
 Sum of electronic and thermal Free Energies=        -9822.041156
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```

Charge = -5 Multiplicity = 1

C	1.8844	0.8391	2.1629
C	0.6662	1.3366	1.4022
N	0.0709	0.4115	0.3303
C	-0.3354	-0.8976	1.0016
C	-1.1886	1.143	-0.1824
C	-1.6717	0.8308	-1.5905
C	-1.202	-1.8586	0.1965
C	1.0862	0.1106	-0.7704
C	1.7608	1.3176	-1.4047
H	2.1818	1.6455	2.8397
H	1.6673	-0.0318	2.7825
H	2.7619	0.6413	1.5402
H	0.9007	2.2689	0.8911
H	-0.165	1.5423	2.0824
H	0.5932	-1.3873	1.294
H	-0.8615	-0.599	1.9101
H	-0.953	2.2018	-0.1002
H	-1.9724	0.929	0.5498
H	-1.0682	1.3204	-2.3583
H	-2.7087	1.1757	-1.6677
H	-1.6971	-0.2331	-1.8088
H	-0.744	-2.1362	-0.755
H	-1.2921	-2.7722	0.7898
H	-2.2166	-1.4906	0.0239
H	0.5456	-0.4652	-1.5191
H	1.8446	-0.5365	-0.3241
H	1.0487	2.093	-1.6996
H	2.2788	0.9772	-2.3037
H	2.5345	1.7371	-0.7612
C	-2.1235	4.697	0.4421
C	-3.0169	4.9189	1.5164
C	-2.9962	6.1825	2.1438
C	-2.0727	7.155	1.757
C	-1.143	6.8941	0.7591
C	-1.1752	5.6535	0.1033
C	-0.0287	7.783	-3.9413
C	-0.0088	9.0154	-3.2909
C	0.0199	9.0721	-1.8902
C	0.0279	7.8934	-1.1538
C	0.0077	6.6486	-1.8122
C	-0.0204	6.5928	-3.2005
C	0.0591	7.7555	0.363
C	0.0183	5.4643	-0.8515
C	3.1816	6.1577	1.9974
C	3.148	4.8869	1.3879
C	2.1947	4.6646	0.3661
C	1.2509	5.6364	0.0572
C	1.268	6.8815	0.7048
C	2.2511	7.1388	1.6507
N	-3.8626	3.8867	1.928
C	-4.4114	3.7608	3.2058
C	-5.3238	2.6211	3.4198
O	-4.1757	4.5995	4.0896
C	-5.6347	1.6293	2.4533
C	-6.7861	0.7743	2.6985
C	-7.4221	0.8149	3.9398
C	-7.0195	1.733	4.9318
C	-6.0078	2.6305	4.6723
O	-4.9937	1.4348	1.3083
O	-7.1739	0.0032	1.7165

N	4.	3.8462	1.7771
C	4.5781	3.7199	3.0427
C	5.4748	2.5649	3.25
O	4.3747	4.5682	3.9249
C	5.7422	1.5485	2.2958
C	6.8727	0.6649	2.5359
C	7.5398	0.7162	3.7602
C	7.185	1.6661	4.7401
C	6.1901	2.5833	4.4852
O	5.0712	1.3441	1.1694
O	7.2123	-0.1434	1.566
C	-2.3143	-2.0801	-3.8281
C	-3.257	-1.398	-4.6352
C	-3.2529	-1.6538	-6.0218
C	-2.2997	-2.5049	-6.585
C	-1.3287	-3.1044	-5.795
C	-1.3435	-2.8849	-4.4082
C	-0.0573	-7.3626	-3.7099
C	-0.0543	-7.5801	-5.0864
C	-0.0708	-6.4926	-5.9713
C	-0.0908	-5.1973	-5.4683
C	-0.0946	-4.9787	-4.0773
C	-0.0776	-6.0567	-3.2005
C	-0.1091	-3.8995	-6.2663
C	-0.1193	-3.4993	-3.7049
C	2.9824	-1.5871	-6.0133
C	2.975	-1.3269	-4.6288
C	2.0319	-2.0084	-3.8229
C	1.0868	-2.8448	-4.4038
C	1.0859	-3.0708	-5.7899
C	2.0467	-2.4546	-6.5792
N	-4.1285	-0.484	-4.0366
C	-4.7581	0.5797	-4.6808
C	-5.5857	1.4644	-3.8314
O	-4.6499	0.7519	-5.9049
C	-5.7649	1.3167	-2.4342
C	-6.8019	2.0959	-1.779
C	-7.4727	3.0838	-2.5024
C	-7.2125	3.28	-3.8744
C	-6.3068	2.4755	-4.5317
O	-5.0738	0.4908	-1.6519
O	-7.053	1.8174	-0.5256
N	3.8495	-0.4083	-4.0352
C	4.4463	0.6731	-4.6852
C	5.3591	1.5034	-3.871
O	4.2348	0.902	-5.8859
C	5.6656	1.2687	-2.5085
C	6.7608	2.0074	-1.9011
C	7.3752	3.0304	-2.6258
C	6.9963	3.3066	-3.9563
C	6.025	2.5495	-4.5746
O	5.0466	0.3921	-1.7249
O	7.1149	1.6601	-0.6905
C	-2.224	-2.8189	3.4665
C	-3.226	-3.7793	3.182
C	-3.214	-4.9856	3.9146
C	-2.2072	-5.2422	4.8464
C	-1.1876	-4.3257	5.0624
C	-1.2023	-3.1088	4.3622
C	0.2704	-0.8882	8.2405
C	0.2714	-2.0956	8.9361

C	0.2047	-3.3105	8.2389
C	0.1374	-3.3041	6.8511
C	0.1362	-2.0833	6.1489
C	0.2024	-0.8797	6.84
C	0.0614	-4.5127	5.9247
C	0.056	-2.2648	4.6348
C	3.1395	-5.1296	3.6546
C	3.1499	-3.9218	2.925
C	2.1911	-2.9346	3.2593
C	1.238	-3.1733	4.2418
C	1.2328	-4.3861	4.9497
C	2.1909	-5.3463	4.6553
N	-4.1647	-3.5068	2.1857
C	-4.9319	-4.4572	1.5102
C	-5.8595	-3.9439	0.4837
O	-4.8547	-5.6643	1.7901
C	-6.0084	-2.5796	0.1223
C	-7.1375	-2.2124	-0.72
C	-7.9381	-3.2135	-1.272
C	-7.7143	-4.5724	-0.9704
C	-6.7104	-4.9304	-0.0987
O	-5.2215	-1.5851	0.517
O	-7.3511	-0.9373	-0.9121
N	4.057	-3.6604	1.8979
C	4.8141	-4.6105	1.2133
C	5.7668	-4.0911	0.2124
O	4.7066	-5.8222	1.4625
C	5.9707	-2.7189	-0.089
C	7.1045	-2.3608	-0.9293
C	7.8674	-3.3679	-1.5211
C	7.5961	-4.7288	-1.2701
C	6.5803	-5.0838	-0.411
O	5.2311	-1.7116	0.357
O	7.3573	-1.0865	-1.0817
Ga	-6.1257	0.209	0.087
Ga	6.1651	0.0685	-0.0595
H	-4.0717	3.0957	1.3072
H	4.1927	3.0563	1.1513
H	-4.2709	-0.491	-3.0189
H	4.0936	-0.4784	-3.0383
H	-4.2873	-2.5511	1.8271
H	4.2112	-2.6992	1.5663
H	-2.1678	3.7531	-0.0895
H	-3.6761	6.3595	2.9628
H	-2.062	8.1134	2.2744
H	-0.0508	7.7391	-5.0271
H	-0.0154	9.9365	-3.8701
H	0.0357	10.033	-1.3791
H	-0.0358	5.6324	-3.7085
H	0.076	8.7217	0.8768
H	0.0016	4.5046	-1.3732
H	3.9071	6.3356	2.776
H	2.1851	3.7111	-0.1489
H	2.2792	8.1018	2.1589
H	-8.2543	0.1333	4.1028
H	-7.5285	1.7448	5.8965
H	-5.7145	3.3896	5.3888
H	8.3559	0.0146	3.9196
H	7.718	1.6864	5.6915
H	5.9322	3.3629	5.193
H	-2.3375	-1.9367	-2.7527

H	-3.9712	-1.137	-6.6393
H	-2.3022	-2.6673	-7.6622
H	-0.0431	-8.2053	-3.0238
H	-0.038	-8.5957	-5.4768
H	-0.0676	-6.6587	-7.0471
H	-0.079	-5.8891	-2.1271
H	-0.1038	-4.0662	-7.3481
H	-0.1222	-3.3437	-2.624
H	3.6969	-1.0635	-6.6299
H	2.0357	-1.844	-2.749
H	2.0568	-2.6216	-7.6555
H	-8.2188	3.6767	-1.977
H	-7.749	4.0582	-4.4192
H	-6.1226	2.5672	-5.5963
H	8.1701	3.5898	-2.1366
H	7.4909	4.112	-4.5011
H	5.7454	2.7059	-5.6106
H	-2.255	-1.8645	2.9505
H	-3.9761	-5.7188	3.7019
H	-2.2115	-6.1886	5.3858
H	0.3228	0.0534	8.7806
H	0.3246	-2.0972	10.0229
H	0.2058	-4.2553	8.7794
H	0.2021	0.0628	6.2993
H	0.063	-5.4632	6.4674
H	0.0533	-1.3099	4.1058
H	3.8604	-5.8891	3.3944
H	2.2094	-1.9946	2.7185
H	2.1955	-6.2925	5.1951
H	-8.7523	-2.9041	-1.924
H	-8.3513	-5.3375	-1.4166
H	-6.541	-5.9613	0.1912
H	8.6889	-3.0638	-2.1667
H	8.2041	-5.4986	-1.7475
H	6.3718	-6.1186	-0.1635

[Et_4N@$\mathbf{Ga_2L_3}$]$^{5-}$ (model 2)

Zero-point correction= 1.667525 (Hartree/Particle)
Thermal correction to Energy= 1.778132
Thermal correction to Enthalpy= 1.779076
Thermal correction to Gibbs Free Energy= 1.517000
Sum of electronic and zero-point Energies= -9821.907407
Sum of electronic and thermal Energies= -9821.796800
Sum of electronic and thermal Enthalpies= -9821.795856
Sum of electronic and thermal Free Energies= -9822.057932

Charge = -5 Multiplicity = 1

C	3.7743	2.3362	0.0911
C	3.6018	2.1952	1.4853
C	2.58	2.9384	2.1267
C	1.8021	3.8092	1.3717
C	2.0193	3.9849	-0.0026

C	2.9976	3.2295	-0.6427
C	1.8315	8.6358	0.6028
C	1.5902	8.4503	1.9621
C	1.2036	7.1902	2.4439
C	1.0634	6.1275	1.5604
C	1.3086	6.3147	0.1838
C	1.6892	7.5635	-0.2912
C	-2.6045	3.9387	-0.8299
C	-2.8647	3.7463	0.539
C	-1.8289	3.9919	1.4714
C	-0.5752	4.4031	1.0349
C	-0.3274	4.5931	-0.3347
C	-1.3419	4.3594	-1.2531
C	1.1032	5.0367	-0.6303
C	0.6593	4.6926	1.9024
N	4.4611	1.3263	2.1455
C	4.8225	1.3356	3.4864
C	6.0266	0.5261	3.7987
O	4.2138	2.0077	4.3347
C	6.7363	-0.2262	2.8272
C	7.9823	-0.8806	3.187
C	8.4314	-0.7836	4.5043
C	7.6995	-0.0532	5.4704
C	6.5271	0.5904	5.1297
O	6.36	-0.3848	1.5758
O	8.6106	-1.5219	2.2275
N	-4.1235	3.3378	1.0033
C	-5.0482	2.5102	0.31
O	-4.7985	2.1364	-0.8329
C	-6.2641	2.1891	1.0807
C	-6.8669	3.1874	1.9081
C	-8.0578	2.9283	2.5592
C	-8.6891	1.6702	2.4335
C	-8.1285	0.6553	1.6547
C	-6.8667	0.9093	0.9651
O	-8.6493	-0.5341	1.4979
O	-6.3546	-0.1108	0.3352
C	3.9919	-4.0555	-2.7222
C	3.821	-2.8028	-3.3496
C	2.8246	-2.6665	-4.3469
C	2.0581	-3.7745	-4.6916
C	2.2665	-5.0263	-4.0943
C	3.228	-5.1579	-3.0971
C	2.1219	-7.0404	-8.3316
C	1.8925	-5.797	-8.9158
C	1.5008	-4.7071	-8.123
C	1.3434	-4.8719	-6.7527
C	1.5763	-6.1313	-6.1602
C	1.9624	-7.209	-6.9474
C	-2.3595	-5.6689	-3.6435
C	-2.6118	-4.4201	-4.2394
C	-1.5679	-3.7792	-4.9461
C	-0.3156	-4.3741	-5.0396
C	-0.0782	-5.626	-4.4496
C	-1.0997	-6.2606	-3.7546
C	1.353	-6.1211	-4.6479
C	0.9296	-3.8056	-5.7379
N	4.6539	-1.771	-2.9329
C	4.9997	-0.6126	-3.6118
C	6.1428	0.1252	-3.0138
O	4.4285	-0.2534	-4.6544

C	6.8058	-0.2868	-1.8291
C	7.9903	0.4215	-1.3769
C	8.4296	1.5235	-2.1114
C	7.7456	1.939	-3.2782
C	6.6308	1.2577	-3.724
O	6.4348	-1.2988	-1.0728
O	8.5762	-0.0382	-0.2937
N	-3.8747	-3.8163	-4.1743
C	-4.7714	-3.8833	-3.0678
O	-4.4642	-4.5469	-2.0796
C	-6.0102	-3.1118	-3.2488
C	-6.5559	-2.9225	-4.5591
C	-7.7419	-2.2391	-4.7348
C	-8.4328	-1.6972	-3.6265
C	-7.9407	-1.8441	-2.3296
C	-6.685	-2.5669	-2.1216
O	-8.5251	-1.37	-1.2595
O	-6.2636	-2.6098	-0.8926
C	3.8958	-3.5217	4.1366
C	3.7763	-4.5968	3.2303
C	2.7643	-5.5636	3.4465
C	1.9418	-5.4449	4.5603
C	2.1092	-4.4082	5.4903
C	3.0777	-3.4355	5.2614
C	1.8491	-7.5564	8.964
C	1.653	-8.5717	8.0307
C	1.3063	-8.2562	6.7078
C	1.1601	-6.9271	6.3314
C	1.3601	-5.8982	7.276
C	1.7013	-6.2131	8.5855
C	-2.5441	-3.7854	5.7849
C	-2.7537	-4.7961	4.8285
C	-1.6891	-5.6789	4.5263
C	-0.4586	-5.5358	5.1552
C	-0.2592	-4.5185	6.1031
C	-1.302	-3.6554	6.41
C	1.1539	-4.5047	6.6812
C	0.7962	-6.3973	4.9434
N	4.6698	-4.6374	2.1664
C	5.1008	-5.7529	1.4612
C	6.3025	-5.5191	0.6213
O	4.5513	-6.8609	1.5691
C	6.9353	-4.2556	0.4943
C	8.1726	-4.1389	-0.2579
C	8.6983	-5.2819	-0.8611
C	8.0465	-6.5319	-0.7429
C	6.8772	-6.6526	-0.0198
O	6.4893	-3.1342	1.0212
O	8.7211	-2.9461	-0.3115
N	-3.9873	-4.9745	4.1889
C	-4.986	-3.994	3.9654
O	-4.8242	-2.8431	4.3726
C	-6.1693	-4.4878	3.2431
C	-6.6723	-5.7985	3.516
C	-7.8246	-6.2482	2.9021
C	-8.5078	-5.4327	1.9711
C	-8.0392	-4.1587	1.648
C	-6.8317	-3.6553	2.3001
O	-8.6082	-3.3576	0.7829
O	-6.4261	-2.4822	1.9115
Ga	-7.5375	-1.7447	0.4057

Ga	7.6265	-1.5486	0.528
H	4.5472	1.7575	-0.4071
H	2.4493	2.8228	3.1945
H	3.1705	3.3331	-1.7112
H	2.1349	9.6126	0.2315
H	1.7051	9.2815	2.6547
H	1.0199	7.0417	3.5056
H	1.881	7.7056	-1.3526
H	-3.3874	3.7254	-1.5425
H	-2.0152	3.8334	2.5324
H	-1.155	4.4947	-2.3166
H	1.29	5.1819	-1.6978
H	0.4748	4.5497	2.97
H	5.0732	0.7172	1.5742
H	9.362	-1.2838	4.767
H	8.0727	0.0009	6.4943
H	5.9589	1.1718	5.8489
H	-4.271	3.3803	2.0018
H	-6.4214	4.1795	1.9515
H	-8.5254	3.706	3.1643
H	-9.6234	1.4611	2.9514
H	4.7484	-4.1617	-1.9496
H	2.696	-1.7029	-4.8219
H	3.3943	-6.1134	-2.6055
H	2.429	-7.8837	-8.9472
H	2.0201	-5.6665	-9.9885
H	1.3258	-3.734	-8.5763
H	2.1448	-8.1785	-6.4888
H	-3.1474	-6.1439	-3.0773
H	-1.7452	-2.8015	-5.3908
H	-0.9194	-7.2237	-3.2813
H	1.532	-7.097	-4.1883
H	0.7532	-2.8307	-6.1991
H	5.2292	-1.9226	-2.0862
H	9.3141	2.0535	-1.7618
H	8.1094	2.8076	-3.8294
H	6.1	1.5484	-4.6251
H	-4.0171	-3.0165	-4.7746
H	-6.0706	-3.398	-5.4088
H	-8.1608	-2.128	-5.7358
H	-9.3639	-1.1497	-3.7618
H	4.6575	-2.7667	3.9625
H	2.6704	-6.3814	2.7444
H	3.2092	-2.6085	5.9554
H	2.1211	-7.8027	9.9885
H	1.7719	-9.6126	8.3243
H	1.1577	-9.0472	5.9764
H	1.8574	-5.4185	9.3121
H	-3.35	-3.0997	5.9997
H	-1.8358	-6.4577	3.7801
H	-1.1542	-2.8606	7.1385
H	1.3043	-3.7069	7.414
H	0.6482	-7.1961	4.2126
H	5.2371	-3.7955	1.9671
H	9.6234	-5.1834	-1.4267
H	8.4775	-7.4072	-1.2315
H	6.3665	-7.6033	0.0958
H	-4.0794	-5.7987	3.6122
H	-6.1829	-6.4045	4.2762
H	-8.2185	-7.2363	3.1431
H	-9.4072	-5.7888	1.4719

N	-2.7948	-1.2149	0.6497
C	-3.444	-0.2629	1.662
C	-3.4725	-2.6042	0.8163
C	-1.2956	-1.2945	0.8547
C	-3.1509	-0.6408	-0.7238
H	-3.1844	0.7424	1.3306
C	-3.0433	-0.457	3.1171
H	-4.5188	-0.3977	1.5211
C	-2.5795	-1.4073	-1.9044
H	-2.8103	0.3945	-0.7306
H	-4.2422	-0.6134	-0.7502
H	-0.9163	-2.016	0.1329
H	-1.1432	-1.7219	1.8465
C	-0.5422	0.0242	0.7157
C	-2.6082	-3.8373	0.5871
H	-4.3274	-2.6064	0.1369
H	-3.8813	-2.6127	1.8231
H	-3.6395	0.2543	3.6985
H	-1.9882	-0.2358	3.3055
H	-3.2917	-1.4451	3.5079
H	-3.2877	-4.6886	0.6864
H	-1.8083	-3.9524	1.3244
H	-2.1884	-3.9009	-0.418
H	-2.9659	-0.9329	-2.8115
H	-2.904	-2.4469	-1.9174
H	-1.4869	-1.3717	-1.955
H	0.5143	-0.1655	0.9251
H	-0.8831	0.7883	1.4175
H	-0.6036	0.4372	-0.2933

Chiral [**Ga_2L_3**]$^{6-}$ (model 1)

```
Zero-point correction=                           1.390018 (Hartree/Particle)
 Thermal correction to Energy=                    1.485966
 Thermal correction to Enthalpy=                  1.486910
 Thermal correction to Gibbs Free Energy=         1.257302
 Sum of electronic and zero-point Energies=          -9450.407357
 Sum of electronic and thermal Energies=             -9450.311409
 Sum of electronic and thermal Enthalpies=           -9450.310465
 Sum of electronic and thermal Free Energies=        -9450.540073
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```

Charge = -6 Multiplicity = 1

C	2.051	2.3771	2.4764
C	1.85	3.005	3.6525
C	2.2813	2.4117	4.7808
C	2.8964	1.2196	4.748
C	3.0816	0.6059	3.5726
C	2.6474	1.176	2.4339
C	6.5611	0.0927	0.3675
C	7.0118	-0.439	1.516
C	6.16	-0.7179	2.5162
C	4.8547	-0.4499	2.363
C	4.4062	0.0982	1.2173
C	5.2543	0.3572	0.2124

C	3.7763	-0.7276	3.3956
C	2.9126	0.3535	1.1819
C	1.3986	-3.425	2.3049
C	0.9953	-2.8714	1.1434
C	1.4475	-1.6761	0.7317
C	2.3253	-1.0112	1.4938
C	2.7604	-1.5636	2.6406
C	2.2948	-2.7527	3.049
N	1.2474	4.2102	3.5854
C	0.8002	5.0784	4.5375
C	0.4508	6.3255	4.0973
O	0.6342	4.7227	5.6804
C	0.8513	6.8365	2.9116
C	0.4997	8.0817	2.5379
C	-0.2723	8.8418	3.3279
C	-0.6827	8.347	4.5032
C	-0.3176	7.1115	4.8805
O	1.5806	6.2409	2.1245
O	0.9153	8.5046	1.4625
N	0.8261	-4.6088	2.6101
C	0.9598	-5.4712	3.6581
C	0.0352	-6.4782	3.7623
O	1.8601	-5.3394	4.4538
C	-1.0141	-6.6511	2.9252
C	-1.8987	-7.6497	3.1092
C	-1.7646	-8.5172	4.1214
C	-0.73	-8.3668	4.9577
C	0.1444	-7.364	4.7774
O	-1.2593	-5.9465	1.9508
O	-2.8254	-7.7414	2.3093
C	-1.6311	3.6354	0.8624
C	-2.2189	4.3859	-0.0913
C	-3.56	4.3588	-0.198
C	-4.3059	3.5985	0.6179
C	-3.7059	2.8511	1.5528
C	-2.3656	2.8571	1.6718
C	-2.7461	3.0836	6.2092
C	-4.0837	3.1166	6.0881
C	-4.6705	2.7662	4.932
C	-3.9079	2.3924	3.8938
C	-2.5665	2.3742	4.0116
C	-1.9828	2.7061	5.1715
C	-4.4298	1.9567	2.5364
C	-1.8293	1.9392	2.7616
C	-3.7922	-1.6659	1.7693
C	-2.4574	-1.6729	1.9637
C	-1.7793	-0.5618	2.2938
C	-2.4472	0.5894	2.4435
C	-3.7856	0.6022	2.3087
C	-4.451	-0.51	1.966
N	-1.3909	5.1317	-0.8514
C	-1.5904	5.918	-1.9479
C	-0.5383	6.7116	-2.3144
O	-2.6015	5.834	-2.6042
C	0.4839	7.02	-1.4856
C	1.4877	7.8223	-1.8881
C	1.5035	8.3274	-3.1301
C	0.4986	8.029	-3.9644
C	-0.5073	7.2393	-3.5561
O	0.5547	6.6355	-0.3224
O	2.3793	8.0849	-1.0854

N	-4.3264	-2.8409	1.3723
C	-5.5934	-3.2401	1.0571
C	-5.7335	-4.4896	0.5108
O	-6.53	-2.4855	1.1745
C	-4.7605	-5.4295	0.4838
C	-4.9536	-6.6161	-0.1236
C	-6.1289	-6.9154	-0.6943
C	-7.1136	-6.0094	-0.6533
C	-6.9102	-4.82	-0.0656
O	-3.6581	-5.2898	1.0037
O	-4.0257	-7.4194	-0.1429
C	1.5112	2.5994	-1.7207
C	2.8329	2.7287	-1.9554
C	3.3634	2.082	-3.0098
C	2.6072	1.3125	-3.8076
C	1.2994	1.1836	-3.552
C	0.7476	1.8216	-2.5037
C	-2.8146	3.0174	-5.0931
C	-2.2436	2.4108	-6.1471
C	-1.2294	1.5489	-5.9679
C	-0.7833	1.3065	-4.7264
C	-1.3463	1.9269	-3.6719
C	-2.371	2.7723	-3.8502
C	0.3384	0.3473	-4.3709
C	-0.7423	1.5643	-2.3305
C	-0.8296	-2.6561	-2.4331
C	-1.4377	-2.0059	-1.4206
C	-1.456	-0.666	-1.3424
C	-0.8529	0.051	-2.2988
C	-0.282	-0.5792	-3.3412
C	-0.2621	-1.9187	-3.4047
N	3.5094	3.5288	-1.1048
C	4.8341	3.8206	-0.956
C	5.1366	4.8352	-0.0893
O	5.687	3.1487	-1.4864
C	4.2386	5.7566	0.3252
C	4.5957	6.7465	1.1657
C	5.8524	6.8361	1.6244
C	6.7533	5.9282	1.2264
C	6.3977	4.9504	0.3783
O	3.0714	5.7865	-0.0521
O	3.7438	7.5692	1.4906
N	-0.8429	-4.0031	-2.3375
C	-0.3659	-5.0024	-3.1339
C	-0.3593	-6.2705	-2.612
O	0.0991	-4.7541	-4.2216
C	-0.9672	-6.6397	-1.4593
C	-0.8545	-7.8983	-0.9916
C	-0.168	-8.8324	-1.6642
C	0.4153	-8.4929	-2.8197
C	0.3217	-7.2333	-3.2728
O	-1.6559	-5.8959	-0.7659
O	-1.3971	-8.1761	0.0731
Ga	-2.4721	-6.7498	0.725
Ga	2.0854	7.2725	0.6087
H	1.1072	4.4659	2.6205
H	0.1662	-4.8395	1.8894
H	-0.4464	5.0402	-0.5115
H	-3.5812	-3.506	1.264
H	2.8651	3.9501	-0.4546
H	-1.2748	-4.2563	-1.4671

H	1.7222	2.8377	1.5307
H	2.1789	2.8832	5.7685
H	3.2601	0.7518	5.6772
H	7.2645	0.3079	-0.4543
H	8.0863	-0.6578	1.6345
H	6.5273	-1.1662	3.4531
H	4.8755	0.7782	-0.7307
H	4.1489	-1.1843	4.336
H	2.5388	0.809	0.2424
H	0.2626	-3.3986	0.5083
H	1.0988	-1.2351	-0.2148
H	2.6703	-3.1214	4.0116
H	-0.5603	9.8611	3.0219
H	-1.316	8.9635	5.1636
H	-0.6896	6.7722	5.862
H	-2.4877	-9.3369	4.2644
H	-0.6035	-9.0697	5.7988
H	0.9599	-7.3118	5.5183
H	-0.536	3.6408	0.9846
H	-4.1031	4.9702	-0.9325
H	-5.4043	3.5928	0.5287
H	-2.2717	3.3621	7.1651
H	-4.7046	3.4241	6.9463
H	-5.7678	2.7821	4.8361
H	-0.8877	2.6629	5.2672
H	-5.5358	1.968	2.4451
H	-0.7242	1.9264	2.8513
H	-1.8851	-2.6068	1.8264
H	-0.6851	-0.5852	2.4186
H	-5.5351	-0.4065	1.8373
H	2.3253	8.9838	-3.4607
H	0.499	8.4406	-4.988
H	-1.3004	7.0374	-4.2958
H	-6.286	-7.8883	-1.1887
H	-8.0863	-6.2398	-1.1204
H	-7.7646	-4.1232	-0.101
H	1.0391	3.1213	-0.8727
H	4.4257	2.1667	-3.2784
H	3.0534	0.7933	-4.6711
H	-3.6549	3.7151	-5.2468
H	-2.6164	2.614	-7.1651
H	-0.7692	1.0418	-6.8309
H	-2.8436	3.254	-2.9812
H	0.797	-0.1656	-5.2417
H	-1.2002	2.0745	-1.4591
H	-1.923	-2.5824	-0.6155
H	-1.9405	-0.1545	-0.4965
H	0.2589	-2.358	-4.2642
H	6.1447	7.6463	2.3126
H	7.7913	5.9919	1.5949
H	7.1932	4.2406	0.095
H	-0.0826	-9.8611	-1.2768
H	0.9868	-9.2482	-3.3856
H	0.856	-7.0359	-4.2175

Chiral [$\mathbf{Ga_2L_3}$]$^{6-}$ (model 2)

Zero-point correction= 1.389174 (Hartree/Particle)
Thermal correction to Energy= 1.485515
Thermal correction to Enthalpy= 1.486459
Thermal correction to Gibbs Free Energy= 1.253257
Sum of electronic and zero-point Energies= -9450.354939
Sum of electronic and thermal Energies= -9450.258598
Sum of electronic and thermal Enthalpies= -9450.257654
Sum of electronic and thermal Free Energies= -9450.490857

Charge = -6 Multiplicity = 1

C	-1.1266	-3.61	3.9988
C	-0.1807	-2.6632	4.1649
C	1.1169	-2.9381	3.9726
C	1.4651	-4.1669	3.5745
C	0.5243	-5.0811	3.2735
C	-0.7698	-4.8165	3.5207
C	2.789	-8.3037	5.4869
C	3.7138	-7.4002	5.8524
C	3.7865	-6.2154	5.2253
C	2.9257	-5.9415	4.2345
C	1.9963	-6.8465	3.8702
C	1.9253	-8.0313	4.4951
C	2.9936	-5.9992	-0.4943
C	3.943	-5.1239	-0.1112
C	3.9274	-4.6804	1.1576
C	2.9874	-5.0999	2.0104
C	2.0502	-5.9874	1.6341
C	2.0551	-6.4335	0.3685
C	1.084	-6.3919	2.7435
C	2.8944	-4.6463	3.444
N	-2.3484	-3.2061	4.3987
C	-3.4596	-3.8841	4.8044
C	-4.2363	-3.0873	5.5944
O	-3.5541	-5.0842	4.7164
C	-4.3679	-1.7597	5.3916
C	-5.0335	-0.9993	6.2744
C	-5.598	-1.5314	7.3672
C	-5.4989	-2.8551	7.5607
C	-4.8282	-3.6199	6.6824
O	-3.9547	-1.1451	4.4091
O	-5.0885	0.1955	6.0062
N	4.9644	-4.6254	-0.8377
C	5.3119	-4.7049	-2.1519
O	4.5246	-5.1118	-2.9722
C	6.5595	-4.2067	-2.4206
C	7.4587	-3.9448	-1.4472
C	8.6829	-3.4617	-1.7193
C	9.0619	-3.2188	-2.9821
C	8.1902	-3.4781	-3.9657
C	6.9696	-3.9631	-3.6824
O	8.4215	-3.2453	-5.1507
O	6.2613	-4.0991	-4.6715
C	-4.5767	-0.9724	-1.3807
C	-4.2424	-2.2576	-1.1495
C	-3.7298	-3.0338	-2.1168
C	-3.5164	-2.5091	-3.3304
C	-3.7401	-1.1996	-3.5441

C	-4.2917	-0.4414	-2.5839
C	-5.7958	-2.0841	-7.4793
C	-5.6196	-3.4002	-7.2751
C	-4.7511	-3.8337	-6.3469
C	-4.0594	-2.9403	-5.6238
C	-4.2355	-1.6205	-5.8312
C	-5.1039	-1.188	-6.7574
C	0.271	-1.0679	-5.7759
C	0.4456	-2.392	-5.6018
C	-0.6129	-3.123	-5.2056
C	-1.8009	-2.5459	-4.9886
C	-1.9706	-1.2261	-5.181
C	-0.9242	-0.4852	-5.572
C	-3.3885	-0.7261	-4.944
C	-3.0435	-3.2832	-4.546
N	-5.2164	-0.3667	-0.3581
C	-6.0641	0.7039	-0.337
C	-6.8479	0.7016	0.7787
O	-6.288	1.3706	-1.3185
C	-6.4001	0.3253	1.993
C	-7.2438	0.2376	3.0335
C	-8.544	0.5334	2.9074
C	-8.9906	0.9411	1.7108
C	-8.1525	1.0235	0.6639
O	-5.2263	0.1051	2.2846
O	-6.7321	-0.1018	4.0943
N	1.5684	-3.1153	-5.7986
C	2.8516	-2.7885	-6.1265
O	3.1955	-1.6298	-6.1547
C	3.6654	-3.8547	-6.425
C	3.2659	-5.135	-6.2509
C	4.0577	-6.188	-6.515
C	5.3118	-5.999	-6.9445
C	5.708	-4.733	-7.1309
C	4.9407	-3.6553	-6.8692
O	6.8478	-4.3907	-7.3932
O	5.3128	-2.5173	-7.2406
C	-0.5732	3.602	2.2125
C	-1.0944	3.7275	0.9758
C	-0.3445	4.1191	-0.0655
C	0.9591	4.3595	0.1235
C	1.5136	4.1362	1.3294
C	0.7492	3.7867	2.3758
C	3.897	7.9918	1.0484
C	3.3276	8.2577	-0.1389
C	2.6794	7.293	-0.8115
C	2.6055	6.0606	-0.2868
C	3.1774	5.7937	0.9034
C	3.824	6.7585	1.5747
C	4.8625	1.9257	-0.8306
C	4.3351	2.2331	-2.0309
C	3.3943	3.1917	-2.0939
C	2.9883	3.8136	-0.9803
C	3.5406	3.5262	0.2122
C	4.4775	2.5701	0.2854
C	3.0149	4.3589	1.3734
C	1.9141	4.8756	-0.9368
N	-1.48	3.3326	3.1743
C	-1.456	3.5401	4.5233
C	-2.7185	3.5595	5.0378
O	-0.4777	3.9548	5.0972

C	−3.7013	2.7409	4.6103
C	−4.9538	2.8933	5.0676
C	−5.2635	3.8363	5.9674
C	−4.2832	4.6285	6.4249
C	−3.029	4.4893	5.9639
O	−3.5594	1.7847	3.8498
O	−5.7758	2.1052	4.6164
N	4.6763	1.6982	−3.2205
C	5.4465	0.627	−3.5565
O	5.6785	−0.2387	−2.7461
C	5.8517	0.623	−4.8645
C	5.7519	1.7243	−5.6402
C	6.2126	1.7479	−6.9022
C	6.8142	0.6731	−7.4314
C	6.9217	−0.4319	−6.6814
C	6.4305	−0.4568	−5.4309
O	7.4321	−1.4714	−7.0941
O	6.5132	−1.5529	−4.8898
Ga	6.8015	−2.98	−6.1175
Ga	−4.9173	0.4751	4.1287
H	1.8935	−2.1876	4.1862
H	−1.5032	−5.6148	3.3388
H	2.7369	−9.2732	6.0104
H	4.4147	−7.6317	6.6736
H	4.5416	−5.4719	5.5215
H	1.1634	−8.7702	4.2013
H	2.9745	−6.4117	−1.5147
H	4.6849	−3.965	1.517
H	1.2979	−7.1672	0.0456
H	0.3209	−7.1365	2.4369
H	3.6589	−3.9026	3.7519
H	−2.3082	−2.2259	4.63
H	−6.1362	−0.8941	8.0873
H	−5.9455	−3.3084	8.4637
H	−4.7341	−4.6938	6.9171
H	5.5513	−4.0601	−0.2433
H	7.2486	−4.1229	−0.3803
H	9.3868	−3.2535	−0.8949
H	10.0577	−2.8016	−3.2024
H	−2.175	3.574	0.8085
H	−3.5298	−4.1013	−1.9325
H	−4.5039	0.6077	−2.8302
H	−6.5115	−1.7372	−8.2436
H	−6.1916	−4.129	−7.8739
H	−4.6062	−4.913	−6.1808
H	−5.2467	−0.1083	−6.9235
H	1.0851	−0.4133	−6.1189
H	−0.5232	−4.2119	−5.055
H	−1.0542	0.5962	−5.7413
H	−3.5263	0.3614	−5.1172
H	−2.9068	−4.3712	−4.3747
H	−5.2089	−0.9602	0.4584
H	−9.2236	0.4597	3.7719
H	−10.0577	1.1897	1.5855
H	−8.5856	1.3213	−0.306
H	1.3539	−4.0879	−5.6568
H	2.2708	−5.4062	−5.8666
H	3.6959	−7.2152	−6.3357
H	5.9987	−6.8458	−7.1011
H	−0.4465	−1.66	4.5466
H	−0.7988	4.2758	−1.0568

H	1.2449	3.6626	3.3483
H	4.4281	8.7905	1.5934
H	3.3937	9.2732	-0.5645
H	2.2138	7.5096	-1.7861
H	4.2913	6.54	2.5482
H	5.6566	1.1705	-0.7278
H	2.9374	3.4732	-3.0571
H	4.939	2.3295	1.257
H	3.4928	4.1365	2.35
H	1.4379	5.0994	-1.9139
H	-2.3796	3.1432	2.7576
H	-6.2983	3.9471	6.33
H	-4.5172	5.4138	7.163
H	-2.2725	5.2004	6.337
H	4.2362	2.2093	-3.97
H	5.3193	2.6708	-5.277
H	6.1177	2.6662	-7.5066
H	7.1997	0.6944	-8.4637
H	-4.4576	-2.7221	-0.1712

6. References and notes

S1. Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.