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Supporting Information

Remote Control of the Synthesis of a [2]Rotaxane and its Shuttling via Metal-Ion Translocation

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Table of Contents

1. Synthesis

1.1 General Remarks

All solvents were dried by distillation prior to use while commercial reagents (**7**, hexacyclen) were used without any further purification. Bruker Avance (400 MHz) and JEOL (500 MHz) spectrometers were used to measure ^{1}H and ^{13}C NMR spectra using a deuterated solvent as the lock and residual protiated solvent as internal reference ($CDCl_3$: δ_H 7.26 ppm, δ_C 77.0 ppm; CD_2Cl_2: δ_H 5.32 ppm, δ_C 53.8 ppm, THF-d_8: δ_H 1.72 ppm, 3.58 ppm, δ_C 25.3 ppm, 67.2 ppm). The following abbreviations were used to define NMR peak patterns: s = singlet, d = doublet, t = triplet, dd = doublet of doublets, ddd = doublet of doublets of doublets, td = triplet of doublets, br = broad, m= multiplet. The coupling constants were given in Hertz (Hz) and, wherever possible, assignment of protons was made. The carbons in the molecular skeletons were not necessarily numbered following the IUPAC nomenclature rules; it was exclusively done for assigning NMR signals. All electrospray ionization (ESI-MS) spectra were recorded on a Thermo-Quest LCQ deca and the theoretical isotopic distributions of the mass signals were calculated using IsoPro 3.0 software. Melting points of compounds were measured on a BÜCHI 510 instrument and were not corrected. Infrared spectra were recorded on a Perkin Elmer FT-IR instrument. Elemental analysis was performed using the EA-3000 CHNS analyzer. UV-vis spectra were recorded on a Cary Win 50 (298 K) spectrometer. Binding constants were determined through UV-vis titrations assuming a 1:1 binding scheme or with SPECFIT/32TM global analysis system by Spectrum Software Associates (Marlborough, MA). Column chromatography was performed either on silica gel (60-400 mesh) or neutral alumina (Fluka, 0.05-0.15 mm, Brockmann Activity 1). Merck silica gel (60 F254) or neutral alumina (150 F254) sheets were used for thin layer chromatography (TLC). All complex preparations were performed directly in the NMR tube using CD_2Cl_2 and CD_3CN as solvent. Compounds (**1**,[1] **3**,[2] **6**,[3] **9**,[4] **10**,[5] and **11**[6]) were synthesized according to literature known procedures.

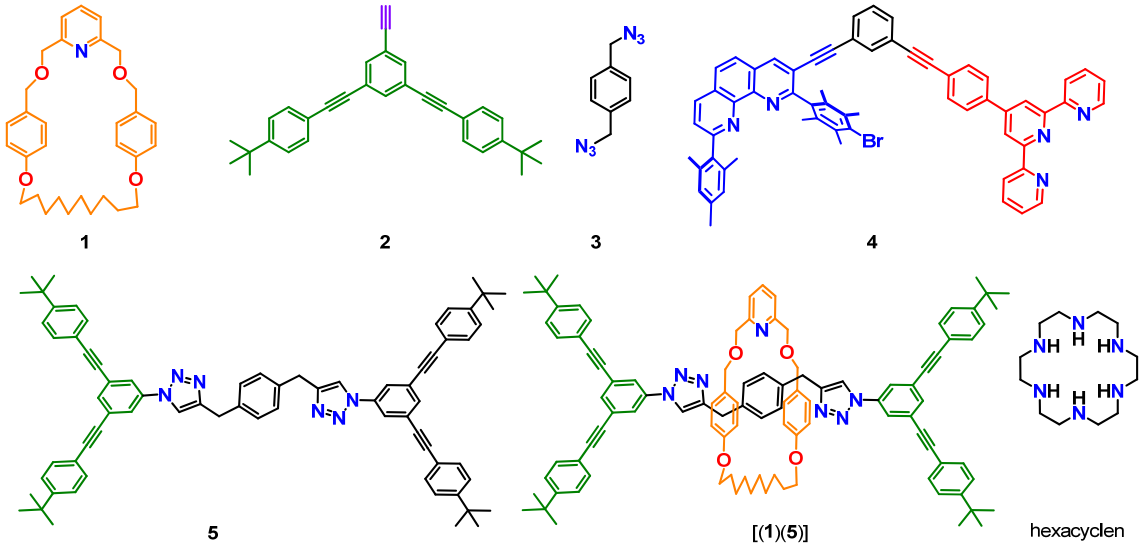
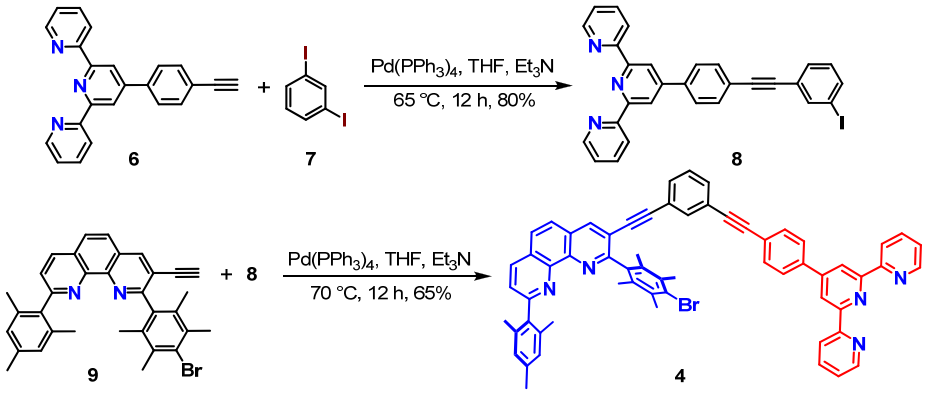
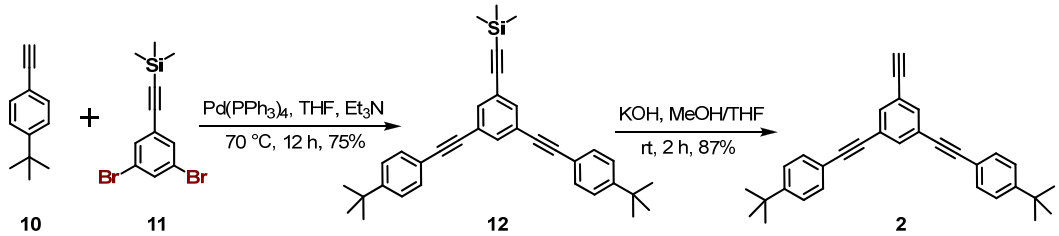


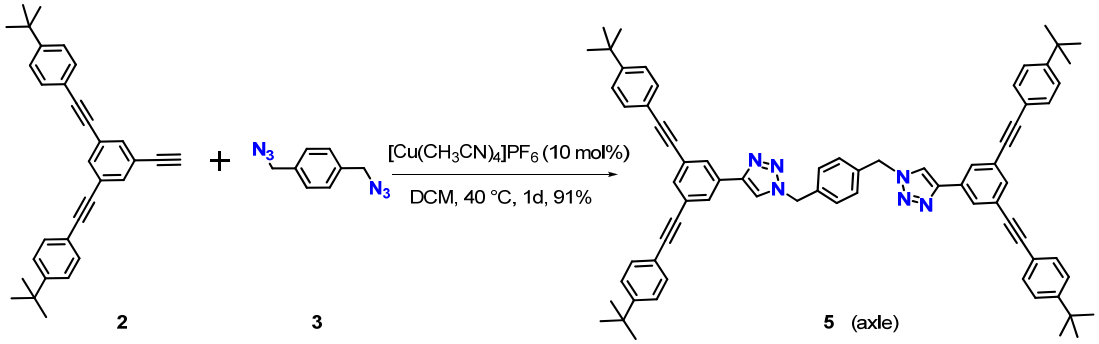
Chart 1. Ligands used in the present study.



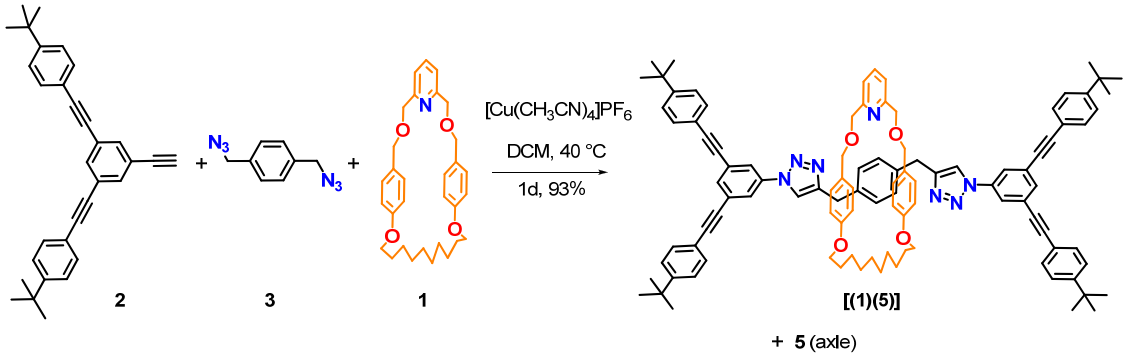
Scheme S1. Synthetic scheme used in the preparation of ligand **4.**



Scheme S2. Synthetic scheme used in the preparation stopper **2**



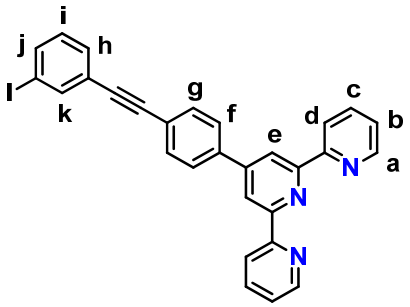
Scheme S3. Synthetic scheme used in preparation of axle **5**



Scheme S4. Synthetic scheme used in preparation of rotaxane [(**1**)(**5**)].

1.2 Synthesis of ligands 1-5 and rotaxane [(1)(5)]

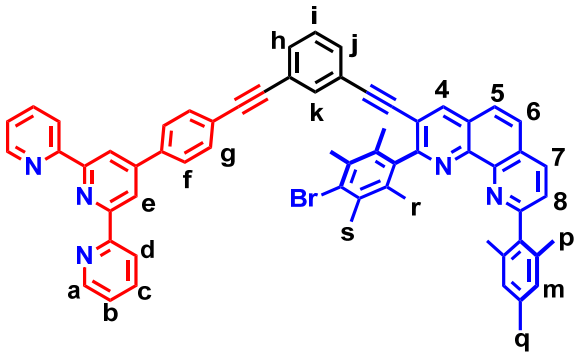
4'-(4-((3-Iodophenyl)ethynyl)phenyl)-2,2':6',2''-terpyridine (8)



In an oven-dried 100-mL sealed tube, a mixture of **6** (400 mg, 1.19 mmol) and **7** (3.95 g, 11.9 mmol) was dissolved in dry THF (15 mL) and Et_3N (20 mL). After thorough deaeration, $Pd(PPh_3)_4$ (137 mg, 119 μmol) was added and the mixture was refluxed at 65 °C for 12 h. The reaction mixture was cooled down to room temperature and the solvents were removed in *vacuo*.

The column chromatographic purification (silica, DCM, R_f = 0.4) of the crude product on silica gel using DCM as eluent provided compound **8** as yellowish solid (509 mg, 952 µmol, 80%) in pure form. **Mp**: 210 °C. **IR** (KBr): $\tilde{\nu}$ = 531, 621, 638, 660, 674, 792, 849, 893, 914, 989, 1038, 1142, 1165, 1385, 1413, 1441, 1566, 1604, 2190, 2919, 3012 cm^{-1}. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 7.10 (t, ^3J = 8.0 Hz, 1H, i-H), 7.37 (ddd, ^3J = 7.6 Hz, ^3J = 4.8 Hz, ^4J = 1.2 Hz, 2H, b-H), 7.52 (dt, ^3J = 8.0 Hz, ^4J = 0.8 Hz, 1H, h-H), 7.67 (d, ^3J = 8.0 Hz, 2H, g-H), 7.69 (td, ^3J = 8.0 Hz, ^4J = 0.8 Hz, 1H, j-H), 7.88 (ddd, ^3J = 8.0 Hz, ^3J = 7.6 Hz, ^4J = 1.2 Hz, 2H, c-H), 7.90 (d, ^3J = 8.0 Hz, 2H, f-H), 7.93 (t, ^4J = 0.8 Hz, 1H, k-H), 8.68 (ddd, ^3J = 8.0 Hz, ^4J = 1.2 Hz, ^5J = 0.8 Hz, 2H, d-H), 8.73 (ddd, ^3J = 4.8 Hz, ^4J = 1.2 Hz, ^5J = 0.8 Hz, 2H, a-H), 8.75 (s, 2H, e-H) ppm. **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 156.1, 156.0, 149.2, 149.0, 140.2, 138.5, 137.4, 136.9, 132.2, 130.7, 129.9, 127.3, 125.2, 123.9, 129.4, 121.3, 118.6, 93.7, 90.4, 89.0 ppm. **ESI-MS**: *m/z* (%) = 536.4 (100) [(**8** + H)$^+$]. **Elemental analysis** ($C_{29}H_{18}IN_3$•0.4H_2O): Calcd. C, 64.19; H, 3.49; N, 7.74. Found, C, 64.38; H, 3.39; N, 7.38.

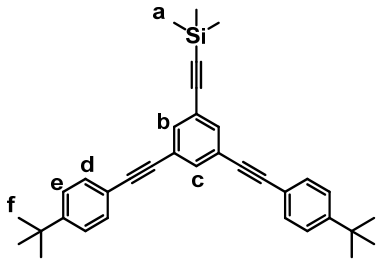
3-((3-((4-([2,2':6',2''-Terpyridin]-4'-yl)phenyl)ethynyl)phenyl)ethynyl)-2-(4-bromo-2,3,5,6-tetramethylphenyl)-9-mesityl-1,10-phenanthroline (4)



Compound **8** (210 mg, 392 µmol) and phenanthroline **9** (209 mg, 392 µmol) were loaded into an oven-dried 100-mL tube under nitrogen atmosphere. After addition of dry diisopropyl amine (10 mL) and dry DMF (15 mL), the mixture was deaerated by bubbling nitrogen through it for 30 min. Solid $Pd(PPh_3)_4$ (45.2 mg, 39.2 µmol) was added under a steady flow of nitrogen and the mixture stirred at 70 °C for 12 h. After completion, the solvents were evaporated under reduced pressure. The residue was dissolved in DCM (200 mL) and washed with water (200 mL). After drying over Na_2SO_4, the solvent was removed and the crude product was purified by column chromatography (SiO_2,) using DCM as eluent to afford 397 mg (254 mmol, 65%) of product **4** as

a colorless solid (silica gel, DCM, R_f = 0.5). **Mp:** >250 °C. **IR (KBr):** $\tilde{\nu}$ = 522, 621, 630, 641, 691, 730, 790, 845, 989, 890, 1030, 1141, 1160, 1380, 1419, 1448, 1461, 1510, 1535, 1567, 1600, 2190, 2927, 3222 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 2.01 (s, 6H, r-H), 2.10 (s, 6H, p-H), 2.26 (s, 3H, q-H), 2.50 (s, 6H, s-H), 6.94 (s, 2H, m-H), 7.09 (dt, ^3J = 8.0 Hz, ^4J = 0.8 Hz, 1H, j-H), 7.25 (t, ^4J = 0.8 Hz, 1H, k-H), 7.29 (t, ^3J = 8.0 Hz, 1H, i-H), 7.39 (ddd, ^3J = 7.6 Hz, ^3J = 4.8 Hz, ^4J = 1.2 Hz, 2H, b-H), 7.49 (dt, ^3J = 8.0 Hz, ^4J = 0.8 Hz, 1H, h-H), 7.59 (d, ^3J = 7.6 Hz, 1H, 8-H), 7.73 (d, ^3J = 8.0 Hz, 2H, f/g), 7.86 (d, ^3J = 8.0 Hz, 5/6-H), 7.90 (d, ^3J = 8.0 Hz, 6/5-H), 7.91(ddd, ^3J = 8.0 Hz, ^3J = 7.6 Hz, ^4J = 1.2 Hz, 2H, c-H), 7.95 (d, ^3J = 8.0 Hz, 2H, f/g), 8.30 (d, ^3J = 7.6 Hz, 1H, 7-H), 8.49 (s, 1H, 4-H), 8.70 (ddd, ^3J = 8.0 Hz, ^4J = 1.2 Hz, ^5J = 0.8 Hz, 2H, d-H), 8.76 (ddd, ^3J = 4.8 Hz, ^4J = 1.2 Hz, ^5J = 0.8 Hz, 2H, a-H), 8.80 (s, 2H, e-H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 18.6, 20.5, 21.0, 21.1, 87.5, 89.7, 89.8, 94.6, 118.6, 119.8, 121.3, 123.1, 123.5, 123.7, 123.8, 125.2, 125.6, 126.8, 127.1, 127.3, 127.6, 128.4, 128.5, 129.2, 131.0, 131.6, 132.2, 133.8, 134.2, 134.6, 135.8, 136.1, 136.8, 137.5, 138.0, 138.3, 138.4, 139.1, 144.8, 145.9, 149.1, 149.3, 156.0, 156.1, 160.6, 162.6 ppm. **ESI-MS**: *m/z* (%) = 942.6 (100) [(**4**+ H)$^+$]. **Elemental analysis:** Calcd. for $C_{62}H_{46}BrN_5$•0.5H_2O: C, 78.39; H, 4.99; N, 7.37; Found: C, 78.14; H, 4.97; N, 7.26.

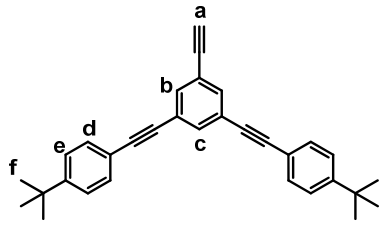
((3,5-Bis((4-*tert.*-butylphenyl)ethynyl)phenyl)ethynyl)trimethylsilane (12)



Compounds **10** (1.30 g, 8.21 mmol) and **11** (1.10 g, 3.31 mmol) were loaded into an oven-dried 100 mL tube under nitrogen atmosphere. Dry diisopropyl amine (30 mL) was added to the mixture and deaerated by bubbling nitrogen through it for 30 min. Solid $Pd(PPh_3)_4$ (300 mg, 259 μmol) was added under a steady flow of nitrogen and the mixture stirred at 75 °C for 24 h. After completion, the solvents were evaporated under reduced pressure. The residue was dissolved in DCM (200 mL) and washed with water (200 mL). After drying over Na_2SO_4, the solvent was removed and the crude product was purified by column chromatography (SiO_2,) using hexane as

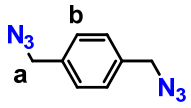
eluent to afford 1.40 g (2.87 mmol, 86%) of product **12** as a colorless solid (silica gel, hexane, R_f = 0.4). **Mp:** 75 °C. **IR (KBr):** $\tilde{\nu}$ = 662, 678, 737, 790, 852, 881, 980, 1030, 1141, 1167, 1380, 1422, 1440, 1490, 1510, 1535, 1566, 1604, 2161, 2911 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 0.26 (s, 9H, a-H), 1.34 (s, 18H, f-H), 7.38 (d, ^3J = 8.0 Hz , 4H, e/d-H), 7.46 (d, ^3J = 8.0 Hz , 4H, d/e-H), 7.57 (d, ^4J = 1.6 Hz , 2H, b-H), 7.62 (t, ^4J = 1.6 Hz, 1H, c-H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 0.13, 31.1, 34.8, 87.1, 90.5, 95.4, 103.4, 119.7, 123.7, 124.1, 125.4, 131.4, 134.1(2C), 151.8 ppm. **Elemental analysis:** Calcd. for $C_{35}H_{38}Si$: C, 86.36; H, 7.87; Found: C, 86.32; H, 7.97.

4,4'-((5-Ethynyl-1,3-phenylene)bis(ethyne-2,1-diyl))bis(4-*tert*.-butylbenzene) (2)



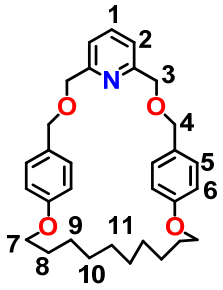
Compound **12** (500 mg, 1.02 mmol) was first dissolved in a mixture of methanol (20 mL) and THF (20 mL) in a 100 mL flask, then 15 mL of 1 N aqueous KOH was slowly added. After stirring for 2 h at room temperature, the solution was extracted with DCM (3 × 50 mL). After the organic layer had been dried over Na_2SO_4, the solvent was removed under reduced pressure to afford 360 mg (1.01 mmol, 87%) of the pure product **2** as a yellowish solid. **MP:** 55 °C. **IR (KBr)**: $\tilde{\nu}$ = 485, 512, 560, 598, 680, 736, 833, 878, 946, 1016, 1104, 1201, 1266, 1363, 1393, 1407, 1464, 1504, 1580, 2209, 2867, 2962, 3038 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 1.33 (s, 18H, f-H), 3.10 (s, 1H, a-H), 7.38 (d, ^3J = 8.0 Hz, 2H, e/d-H), 7.45 (d, ^3J = 8.0 Hz, 2H, d/e-H), 7.59 (d, ^4J = 1.6 Hz , 2H, b-H), 7.66 (t, ^4J = 1.6 Hz, 1H, c-H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)**: δ = 31.1, 34.8, 78.1, 82.1, 87.0, 91.5, 119.6, 122.7, 124.2, 125.4, 131.4, 134.3, 134.6, 151.9 ppm. **Elemental analysis**: Calcd. for $C_{32}H_{30}$: C, 92.71; H, 7.29. Found C, 92.79; H, 7.49.

1,4-Bis(azidomethyl)benzene (3)[2]



α,α′-Dibromo-p-xylene (1.25 g, 4.73 mmol) and NaN_3 (614 mg, 9.46 mmol) in a 100 mL of DMF were refluxed for 24 h. DCM was added to the mixture and the organic layer was separated. The aqueous layer was extracted with DCM and the combined organic layers were dried over $MgSO_4$. Solvent was removed under reduced pressure and the azide **3** (783 mg, 4.16 mmol, 88%) was isolated as pure colorless liquid. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 4.36 (s, 4H, a-H), 7.34 (s, 4H, b-H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)**: 54.4, 128.5, 135.5 ppm.

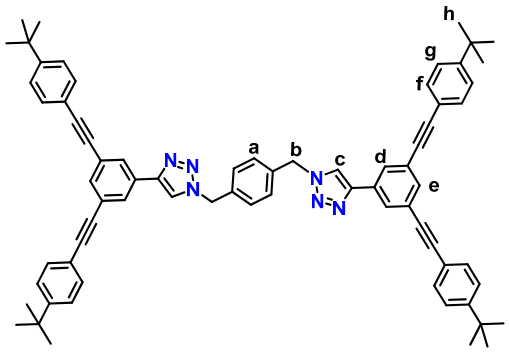
Characterization of macrocycle 1[1]



Prepared according to reference 1.

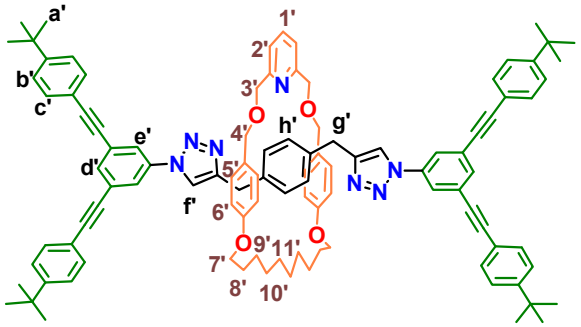
^{1}H NMR (500 MHz, CD_2Cl_2): δ = 1.15-1.35 (m, 8H, 10-, 11-H), 1.42 (m, 4H, 9-H), 1.73 (m, 4H, 8-H), 3.96 (t, ^3J = 6.5 Hz, 4H, 7-H), 4.39 (s, 4H, 3-H), 4.55 (s, 4H, 4-H), 6.82 (d, ^3J = 8.5 Hz, 4H, 6-H), 7.22 (d, ^3J = 8.5 Hz, 4H, 5-H), 7.32 (d, ^3J = 7.5 Hz, 2H, 2-H), 7.69 (t, ^3J = 7.5 Hz, 1H, 1-H) ppm. **^{13}C NMR (125 MHz, CD_2Cl_2):** δ = 25.9, 28.8, 28.9, 29.5, 67.8, 71.8, 72.4, 114.8, 120.6, 159.2, 130.1, 130.2, 137.3, 158.2 ppm. **Elemental analysis**: Calcd. for [$C_{31}H_{39}NO_4$•0.5H_2O]: C, 74.67; H, 8.09; N, 2.81; Found C, 74.97; H, 8.15; N, 2.73.

Axle 5



Compound **2** (100 mg, 240 µmol), diazide **3** (23.0 mg, 120 µmol) and $[Cu(CH_3CN)_4]PF_6$ (8.90 mg, 24.0 µmol) in 25 mL of DCM were stirred at 40 °C for 24 h. Solvent was removed under reduced pressure and the crude product was purified by column chromatography (silica gel, DCM/hexane = 1:4, R_f = 0.4), afforded 111 mg (109 µmol, 91%) of product **5** as a colorless solid. **Mp**: 136 °C. IR (KBr): $\tilde{\nu}$ = 485, 516, 560, 685, 736, 777, 833, 877, 959, 1051, 1085, 1104, 1201, 1266, 1318, 1363, 1393, 1408, 1464, 1504, 1514, 1585, 2212, 2866, 2959, 3083 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 1.31 (s, 36H, h-H), 5.59 (s, 4H, b-H), 7.33 (s, 4H, a-H), 7.36 (d, ^3J = 8.4 Hz, g/f-H), 4.75 (d, ^3J = 8.4 Hz, f/g-H), 7.62 (t, ^3J = 1.2 Hz, 2H, e-H), 7.74 (s, 2H, c-H), 7.92 (d, ^3J = 1.2 Hz, 4H, d-H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 31.1, 34.7, 53.8, 87.6, 90.5, 119.8, 119.9, 124.4, 125.4, 128.1, 128.8, 130.8, 131.3, 133.9, 135.3, 147.0, 151.8 ppm. **Elemental analysis**: Calcd. for $C_{72}H_{68}N_6$: C, 85.00; H, 6.74; N, 8.26; Found C, 85.16; H, 6.73; N, 8.32.

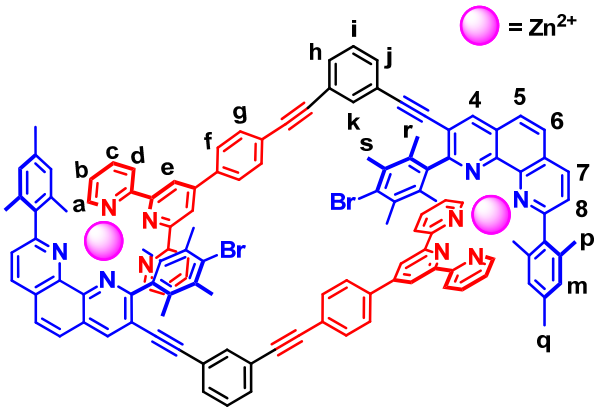
[2]Rotaxane [(1)(5)]



Macrocycle **1** (50.0 mg, 102 µmol), compound **2** (212 mg, 510 µmol), diazide **3** (48.0 mg, 255 µmol) and $[Cu(CH_3CN)_4]PF_6$ (38.0 mg, 102 µmol) were stirred in 15 mL of DCM at 40 °C for 24 h. Thereafter, cyclam (20.4 mg, 102 µmol) was added and the solvent removed under reduced pressure. The crude material was purified by column chromatography (silica gel, DCM, $R_f = 0.3$) affording 148 mg (142 mg, 94.8 µmol, 93%) of product [(**1**)(**5**)] as a colorless solid. **Mp**: 115 °C. **IR (KBr):** $\tilde{\nu}$ = 589, 637, 719, 795, 826, 955, 1040, 11, 1175, 1208, 1302, 1389, 1455, 1470, 1512, 1583, 1611, 1594, 1721, 1888, 2216, 2860, 2951, 3080 cm^{-1}. **^{1}H NMR (600 MHz, CD_2Cl_2):** δ = 1.23-1.32 (m, 8H, 10'-, 11'-H), 1.33 (s, 36H, a'-H), 1.36-1.42 (m, 4H, 9'-H), 1.64-1.70 (m, 4H, 8'-H), 3.84 (t, ^3J = 6.5 Hz, 4H, 7'-H), 4.22 (s, 4H, 3'-H), 4.44 (s, 4H, 4'-H), 5.03 (s, 4H, g'-H), 6.50 (d, ^3J = 8.5 Hz, 4H, 6'-H), 6.71 (s, 4H, h'-H), 6.89 (d, ^3J = 8.5 Hz, 4H, 5'-H), 7.29 (d, ^3J = 7.5 Hz, 2H, 2'-H), 7.39 (d, ^3J = 8.0 Hz, 8H, b'-/c'-H), 7.49 (d, ^3J = 8.0 Hz, 8H, c'-/b'-H), 7.60 (t, ^3J = 1.8 Hz, 2H, d'-H), 7.63 (t, ^3J = 7.5 Hz, 1H, 1'-H), 7.71 (s, 2H, f'-H), 7.89 (d, ^3J = 1.8 Hz, 4H, e'-H) ppm. **^{13}C NMR (100 MHz, CD_2Cl_2):** δ = 26.1, 29.0, 29.1, 30.1, 30.2, 35.1, 53.8, 67.5, 71.7, 73.1, 88.1, 90.6, 114.5, 120.2, 120.3, 121.3, 124.6, 125.9, 128.5, 128.7, 129.3, 130.4, 131.7, 131.9, 133.6, 135.2, 137.5, 146.5, 152.4, 158.1, 159.1 ppm. **ESI-MS**: *m/z* (%) = 1508.6 (100) [((**1**)(**5**) + H)$^+$]. **Elemental analysis:** Calcd.for $C_{103}H_{107}N_7O_4$: C, 82.09; H, 7.16; N, 6.51; Found C, 81.78; H, 7.07; N, 6.43.

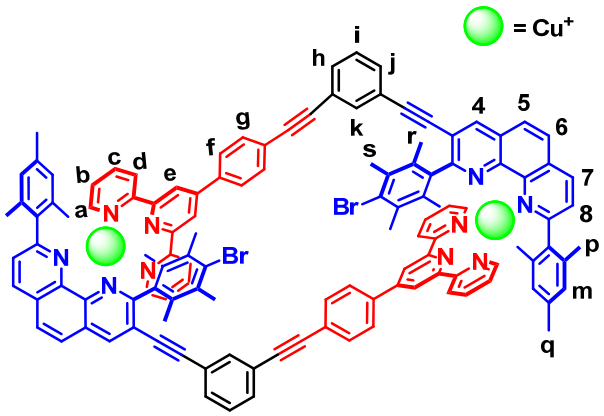
2. Synthesis and characterization of complexes

Complex $[Zn_2(4)_2]^{4+}$



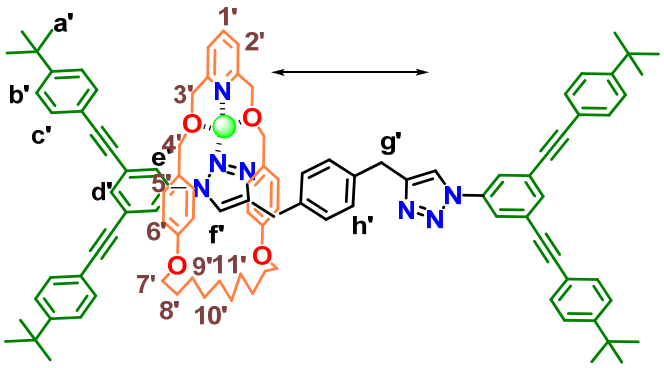
Ligand **1** (440 µg, 0.467 µmol) was placed in an NMR tube and $Zn(OTf)_2$ (170 µg, 0.467 µmol) in CD_3CN was added. To this mixture, 500 µL of CD_2Cl_2 was added and subsequently the NMR was recorded. **Yield**: Quantitative. **Mp:** >250 °C. **^{1}H NMR (400 MHz, CD_2Cl_2):** δ = 1.00 (s, 12H, r-H), 1.29 (s, 12H, p-H), 1.77 (s, 6H, q-H), 1.97 (s, 12H, s-H), 6.11 (t, ^4J = 0.8 Hz, 2H, k-H), 6.26 (s, 4H, m-H), 7.32 (t, ^3J = 8.0 Hz, 2H, i-H), 7.39 (dt, ^3J = 8.0 Hz, ^4J = 0.8 Hz, 2H, j-H), 7.45 (dt, ^3J = 8.0 Hz, ^4J = 0.8 Hz, 2H, h-H), 7.57 (ddd, ^3J = 8.0, ^3J = 7.6 Hz, ^4J = 1.2 Hz, 4H, c-H), 7.78 (d, ^3J = 8.0 Hz, 4H, f/g), 7.81 (ddd, ^3J = 4.8 Hz, ^4J = 1.2 Hz, ^5J = 0.8 Hz, 4H, a-H), 8.14 (d, ^3J = 8.0 Hz, 4H, g/f), 8.15 (d, ^3J = 8.4 Hz, 2H, 8-H), 8.35 (ddd, ^3J = 7.6 Hz, ^3J = 4.8 Hz, ^4J = 1.2 Hz, 4H, b-H), 8.50 (d, ^3J = 8.0 Hz, 2H, 5/6-H), 8.56 (d, ^3J = 8.0 Hz, 2H, 6/5-H), 8.70 (s, 4H, e-H), 8.80 (d, ^3J = 8.0 Hz, 4H, d-H), 9.04 (s, 2H, 4-H), 9.12 (d, ^3J = 8.4 Hz, 2H, 7-H). **ESI-MS:** *m/z* (%) = 503.6 (17) $[Zn_2(\mathbf{4})_2]^{4+}$, 720.6 (30) $[Zn_2(\mathbf{4})_2(OTf)]^{3+}$, 1156.3 (100) $[Zn_2(\mathbf{4})_2(OTf)_2]^{3+}$. **Elemental analysis:** Calcd. for $C_{126}H_{92}Br_2F_6N_{10}O_6S_2Zn_2 \cdot H_2O$: C, 58.52; H, 3.61; N, 5.33; Found C, 58.38; H, 3.81; N, 5.12.

Complex $[Cu_2(4)_2]^{2+}$



Ligand **1** (413 µg, 0.439 µmol) and $[Cu(CH_3CN)_4]PF_6$ (163 µg, 0.439 µmol) were placed in an NMR tube in 500 µL of CD_2Cl_2. Subsequently the NMR was recorded. **Yield**: Quantitative. **Mp:** >250 °C. **^{1}H NMR (400 MHz, CD_2Cl_2):** δ = 1.48 (s, 12H, r-H), 1.59 (s, 12H, p-H), 1.90 (s, 6H, q-H), 1.92 (s, 12H, s-H), 6.41 (s, 4H, m-H), 6.44 (t, ^4J = 0.8 Hz, 2H, k-H), 7.15 (ddd, ^3J = 8.0, ^3J = 7.6 Hz, ^4J = 1.2 Hz, 4H, c-H), 7.32 (t, ^3J = 8.0 Hz, 2H, i-H), 7.38 (td, ^3J = 8.0 Hz, ^4J = 0.8 Hz, 2H, j-H), 7.44(td, ^3J = 8.0 Hz, ^4J = 0.8 Hz, 2H, h-H), 7.62 (ddd, ^3J = 4.8 Hz, ^4J = 1.2 Hz, ^5J = 0.8 Hz, 4H, a-H), 7.69 (ddd, ^3J = 7.6 Hz, ^3J = 4.8 Hz, ^4J = 1.2 Hz, 4H, b-H), 7.80 (d, ^3J = 8.0 Hz, 4H, g/f), 7.87 (d, ^3J = 8.4 Hz, 2H, 8-H), 8.01 (d, ^3J = 8.0 Hz, 4H, f/g), 8.02 (d, ^3J = 8.0 Hz, 4H, d-H), 8.21 (d, ^3J = 8.0 Hz, 2H, 5/6-H), 8.27 (s, 4H, e-H), 8.29 (d, ^3J = 8.0 Hz, 2H, 6/5-H), 8.71 (s, 2H, 4-H), 8.72 (d, ^3J = 8.4 Hz, 2H, 7-H). **ESI-MS:** *m/z* (%) = 1004.7 (100) $[Cu_2(\mathbf{4})_2]^{2+}$. **Elemental analysis:** Calcd. for $C_{124}H_{92}Br_2Cu_2F_{12}N_{10}P_2$•$2H_2O$: C, 63.78; H, 4.14; N, 6.00; Found C, 63.39; H, 4.32; N, 5.92.

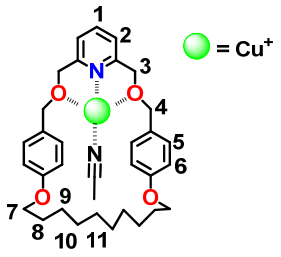
Complex [Cu(1)(5)]$^{+}$



Rotaxane [(**1**)(**5**)] (897 µg, 0.595 µmol), $[Cu(CH_3CN)_4]PF_6$ (221 µg, 0.595 µmol) were dissolved in 500 µL of CD_2Cl_2. Subsequently the NMR was recorded. **Yield**: Quantitative. **Mp**: 146 °C. **^{1}H NMR (400 MHz, CD_2Cl_2):** δ = 1.30-1.38 (m, 44H, 10'-, 11'-, a'-H), 1.39-1.45 (m, 4H, 9'-H), 1.59-1.65 (m, 4H, 8'-H), 3.61(t, ^3J = 6.5 Hz, 4H, 7'-H), 4.50 (s, 4H, 3'-H), 4.69 (s, 4H, 4'-H), 5.64 (s, 4H, g'-H), 6.06 (d, ^3J = 8.5 Hz, 4H, 6'-H), 6.79 (d, ^3J = 8.5 Hz, 4H, 5'-H), 7.36-7.44 (m, 20H, b'-, c'-, h'-H), 7.45 (d, ^3J = 7.5 Hz, 2H, 2'-H), 7.58 (t, ^3J = 1.8 Hz, 2H, d'-H), 7.59-7.66 (m, 6H, f'- e'-H), 7.95 (t, ^3J = 7.5 Hz, 1H, 1'-H). **ESI-MS:** *m/z* (%) = 1570.9 (100) [Cu(**1**)(**5**)]$^+$. **Elemental analysis:** Calcd. for $C_{103}H_{107}CuF_6N_7O_4P$: C, 72.11; H, 6.29; N, 5.72; Found C, 72.32; H, 6.15; N, 5.98.

2.1 Synthesis and characterization of model complex

Model complex $[Cu(1)]^+$



Macrocycle **1** (390 µg, 0.796 µmol) and $[Cu(CH_3CN)_4]PF_6$ (296 µg, 0.796 µmol) were mixed in 500 µL of CD_2Cl_2 at 25 °C in an NMR tube. Subsequently the NMR was recorded. **Yield**: quantitative. **^{1}H NMR (500 MHz, CD_2Cl_2):** δ = 1.25-1.35 (m, 8H, 10-, 11-H), 1.43 (m, 4H, 9-H), 1.74 (m, 4H, 8-H), 3.94 (t, ^3J = 6.5 Hz, 4H, 7-H), 4.90 (s, 4H, 3-H), 5.11 (s, 4H, 4-H), 6.84 (d, ^3J = 8.5 Hz, 4H, 6-H), 7.36 (d, ^3J = 7.5 Hz, 2H, 2-H), 7.42 (d, ^3J = 8.5 Hz, 4H, 5-H), 8.02 (t, ^3J = 7.5 Hz, 1H, 1-H) ppm. **ESI-MS**: *m/z* (%) = 552.6 (100) $[Cu(\mathbf{1})]^+$.

3. Model study

Self-sorting was tested by mixing ligand **4**, macrocycle **1** and $[Cu(CH_3CN)_4]PF_6$ (0.808 µmol) in a molar ratio of 1:1:1 in CD_2Cl_2 at 25 °C. The ^{1}H NMR spectrum was measured subsequently. Complex $[Cu_2(\mathbf{4})_2]^{2+}$ formed quantitatively while the macrocycle **1** was left uncoordinated in the solution. Furthermore $Zn(OTf)_2$ (0.808 µmol) was added to the mixture. According to the ^{1}H NMR spectrum, both $[Zn_2(\mathbf{4})_2]^{4+}$ and $[Cu(\mathbf{1})]^+$ formed quantitatively

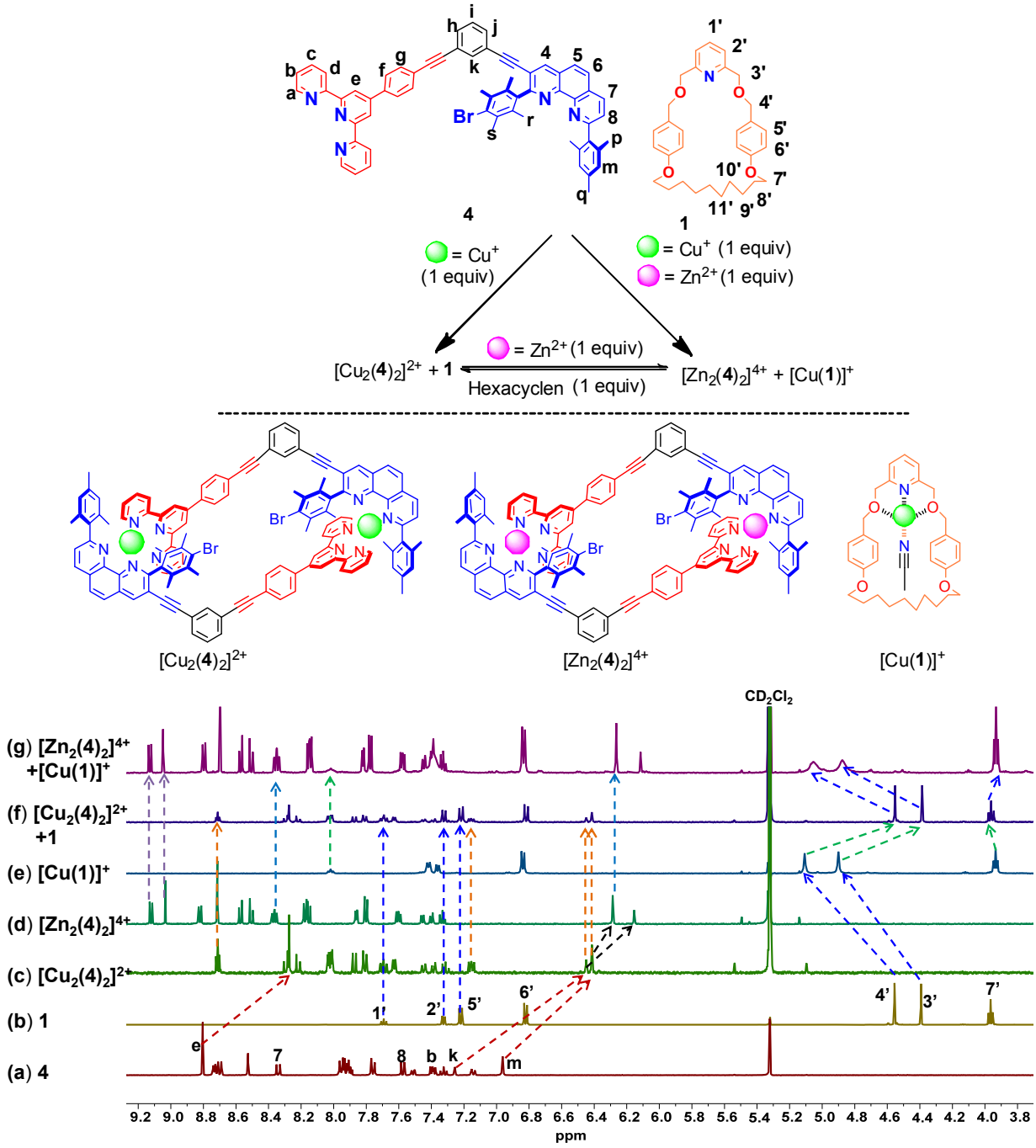
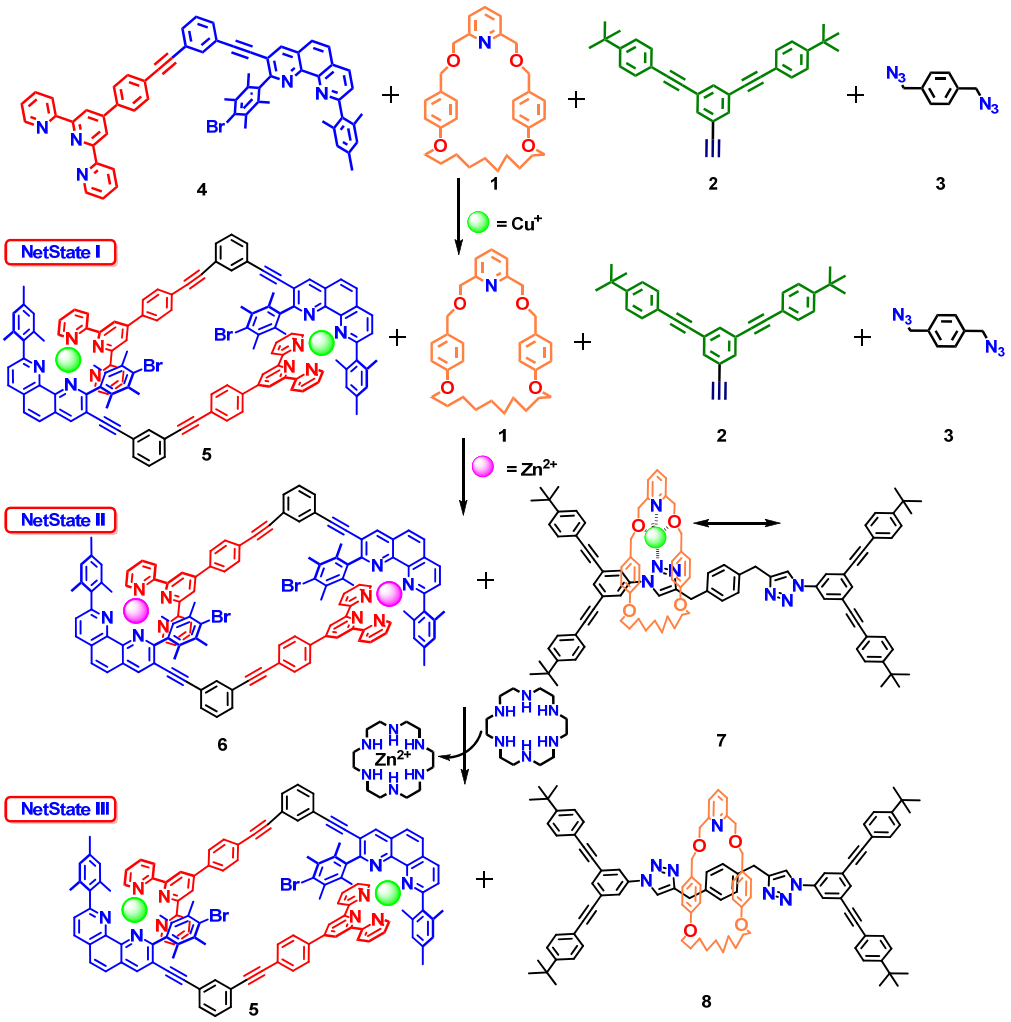


Figure S1. ^{1}H NMR (400 MHz, 298 K) of (a) ligand **4**; (b) macrocycle **1**; (c) $[Cu_2(\mathbf{4})_2]^{2+}$; (d) $[Zn_2(\mathbf{4})_2]^{4+}$; (e) $[Cu(\mathbf{4})]^{2+}$; (f) solution after mixing of **1**, **4**, $[Cu(CH_3CN)_4]PF_6$ in a ratio of 1:1:1 to generate $[Cu_2(\mathbf{4})_2]^{2+}$ + **1**; (g) after addition of an equimolar amount of $Zn(OTf)_2$ which reshuffled the metal ions to form $[Zn_2(\mathbf{4})_2]^{4+}$ and $[Cu(\mathbf{1})]^{+}$.

4. Network states (remote control of synthesis and shuttling of rotaxane)



Preparation of NetState I

Macrocycle **1** (560 µg, 1.14 µmol), compound **2** (2.37 mg, 5.70 µmol)**,** diazide **3** (536 µg, 2.85 µmol), ligand **4** (1.07 mg, 1.14 µmol), $[Cu(CH_3CN)_4]PF_6$ (424 µg,1.14 µmol) and the external standard 1,3,5-trimethoxybenzene (TMB) (192 µg,1.14 µmol) were mixed in CD_2Cl_2 in an NMR tube. The mixture was heated at 40 °C for 24 h and subjected to ^{1}H NMR analysis. ^{1}H NMR clearly showed binding of Cu^+ to ligand **4** thus generating $[Cu_2(\mathbf{4})_2]^{2+}$. All remaining components remained free in solution The red color of the solution also indicated formation of $[Cu_2(\mathbf{4})_2]^{2+}$.

Preparation of NetState II

$Zn(OTf)_2$ (414 μg, 1.14 μmol) in CD_3CN was added to the solution of Netstate I. Immediately the solution turned colorless exhibiting a bright skyblue fluorescence, indicative of formation of $[Zn_2(\mathbf{4})_2]^{4+}$ and $[Cu(\mathbf{1})]^{+}$. The mixture was furthermore heated for 24 h and subjected to ^{1}H NMR measurement without any further purification. Analysis of the ^{1}H NMR confirmed the formation of NetState II, i.e., $\{[Zn_2(\mathbf{4})_2]^{4+} + [Cu(\mathbf{1})(\mathbf{5})]^{+}\}$.

Preparation of NetState III

Hexacyclen (294 μg,1.14 μmol) was added to Netstate II. The mixture immediately turned red which indicated regeneration of $[Cu_2(\mathbf{4})_2]^{2+}$ and metal-free [2]rotaxane. Analysis of the ^{1}H NMR confirmed the formation of NetState III, i.e., $\{[Cu_2(\mathbf{4})_2]^{2+} + [(\mathbf{1})(\mathbf{5})]\}$.

5. NMR spectra: ^{1}H, ^{13}C, ^{1}H-^{1}H COSY, ^{1}H-^{1}H NOESY

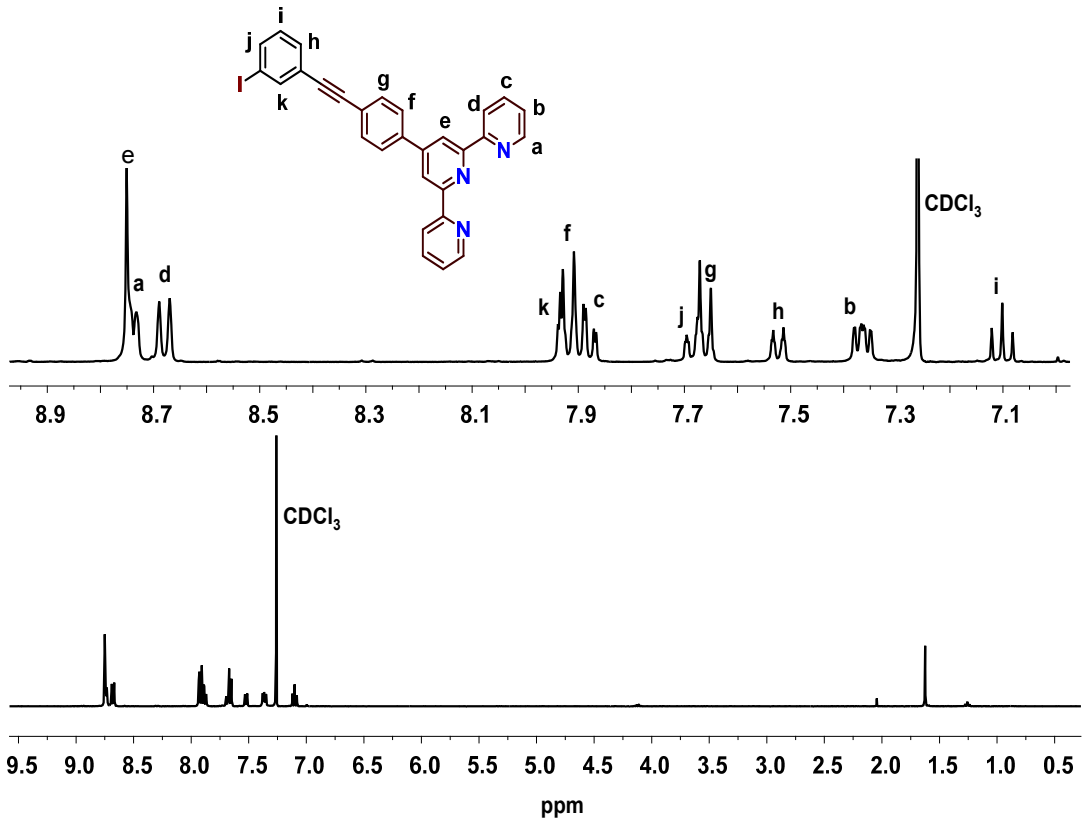


Figure S2. ^{1}H NMR spectrum of **8** in $CDCl_3$ (400 MHz, 298 K).

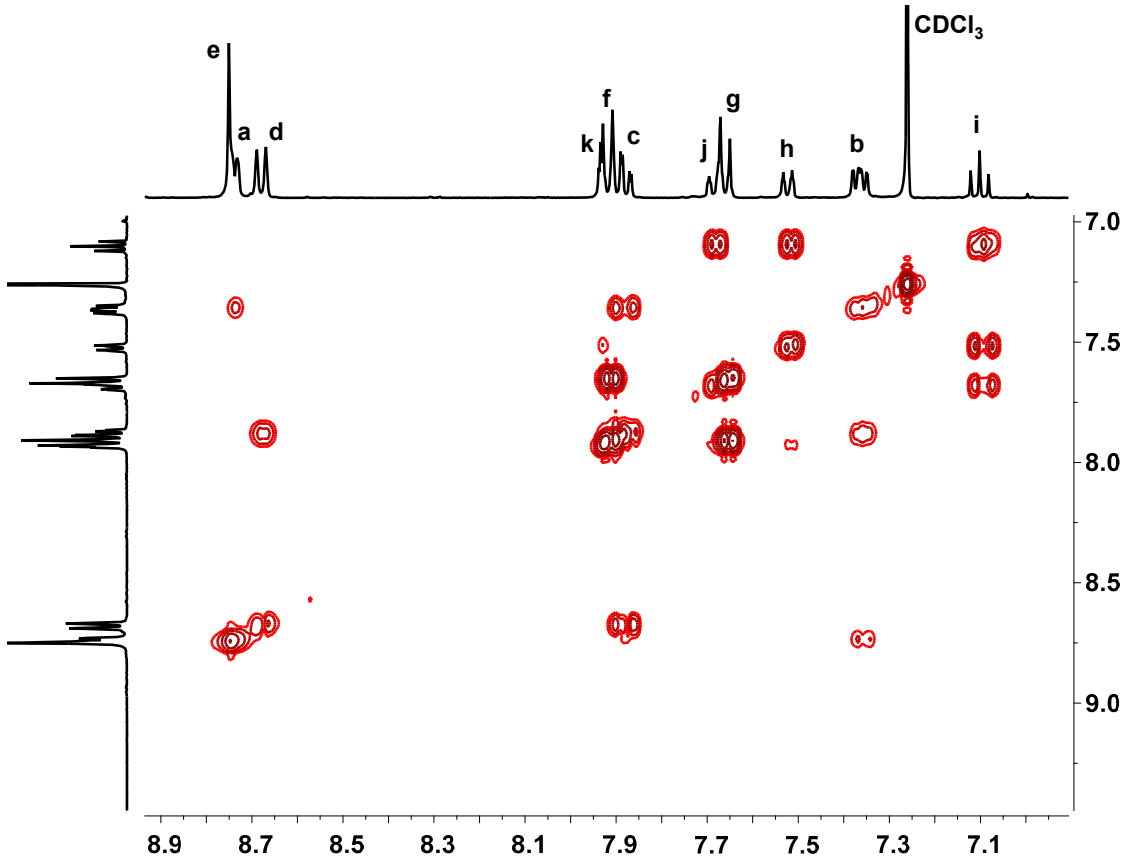


Figure S3. ^{1}H ^{1}H COSY NMR spectrum of **8** in $CDCl_3$ (400 MHz, 298 K).

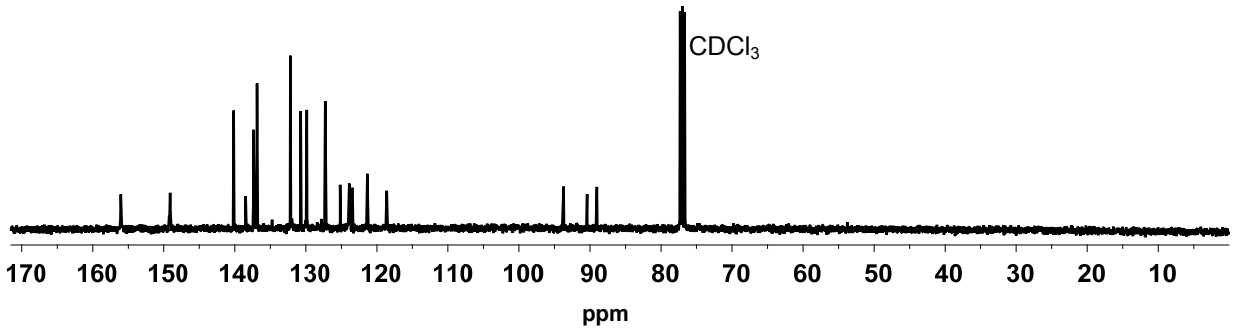


Figure S4. ^{13}C NMR spectrum of **8** in $CDCl_3$ (400 MHz, 298 K).

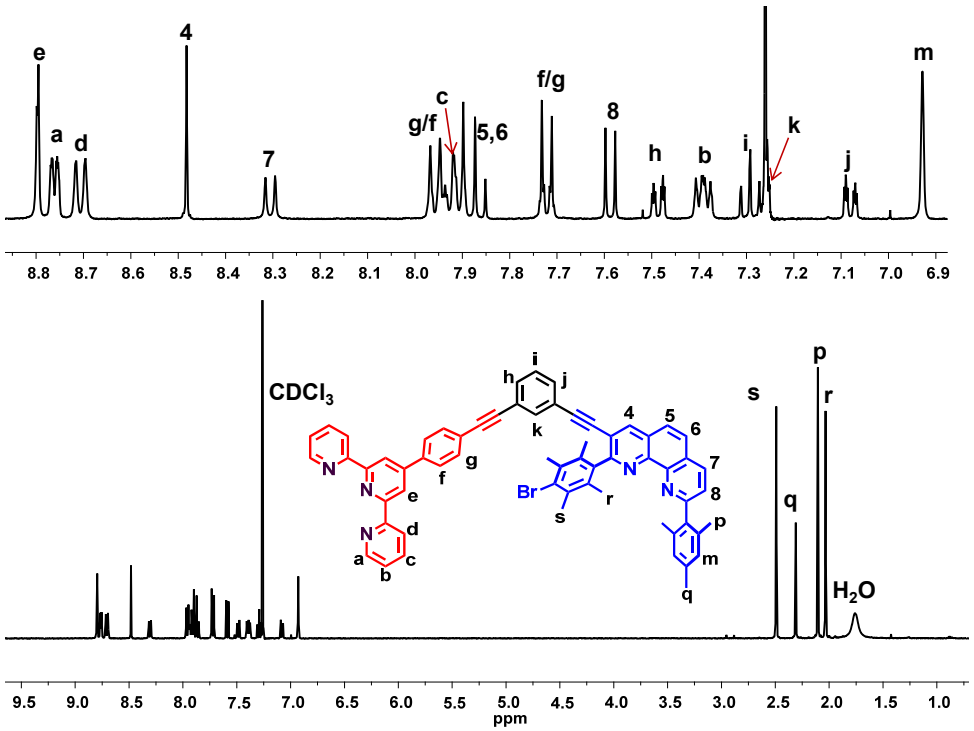


Figure S5. ^{1}H NMR spectrum of **4** in $CDCl_3$ (400 MHz, 298 K).

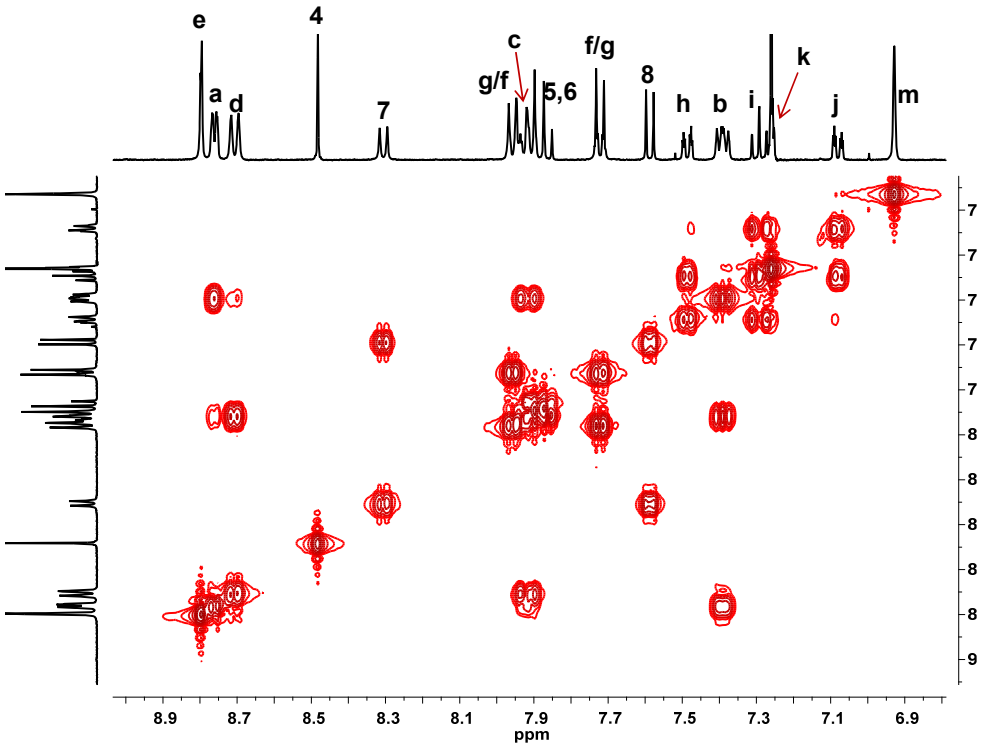


Figure S6. ^{1}H ^{1}H COSY NMR spectrum of **4** in $CDCl_3$ (400 MHz, 298 K).

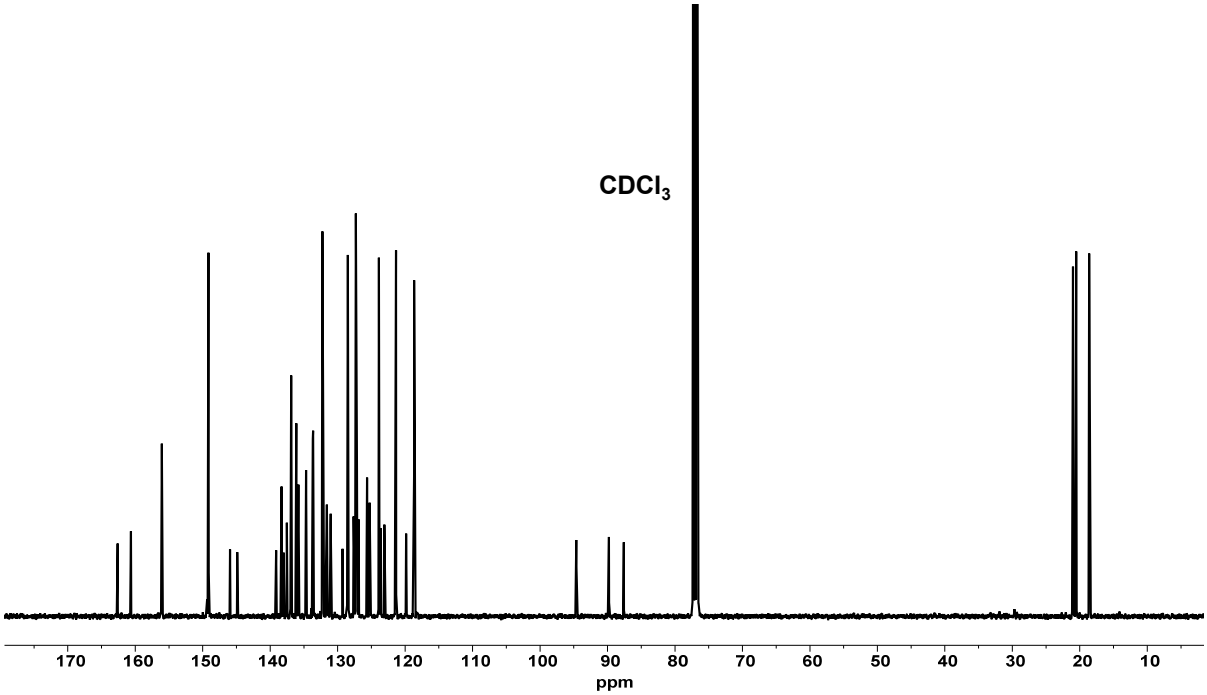


Figure S7. ^{13}C NMR spectrum of **4** in $CDCl_3$ (400 MHz, 298 K).

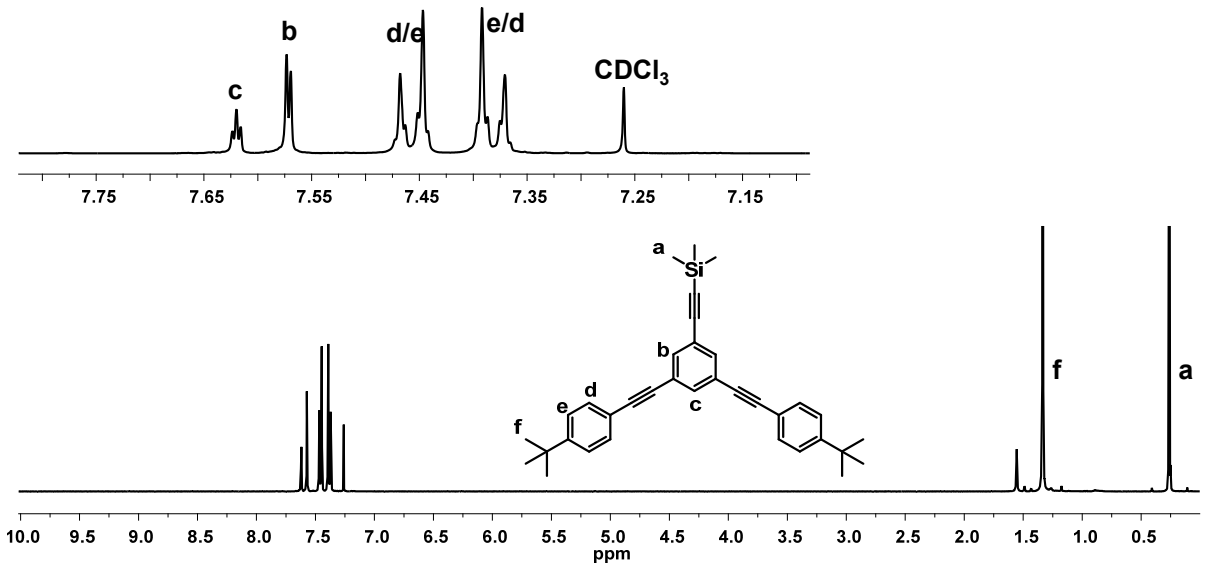


Figure S8. ^{1}H NMR spectrum of **12** in $CDCl_3$ (400 MHz, 298 K).

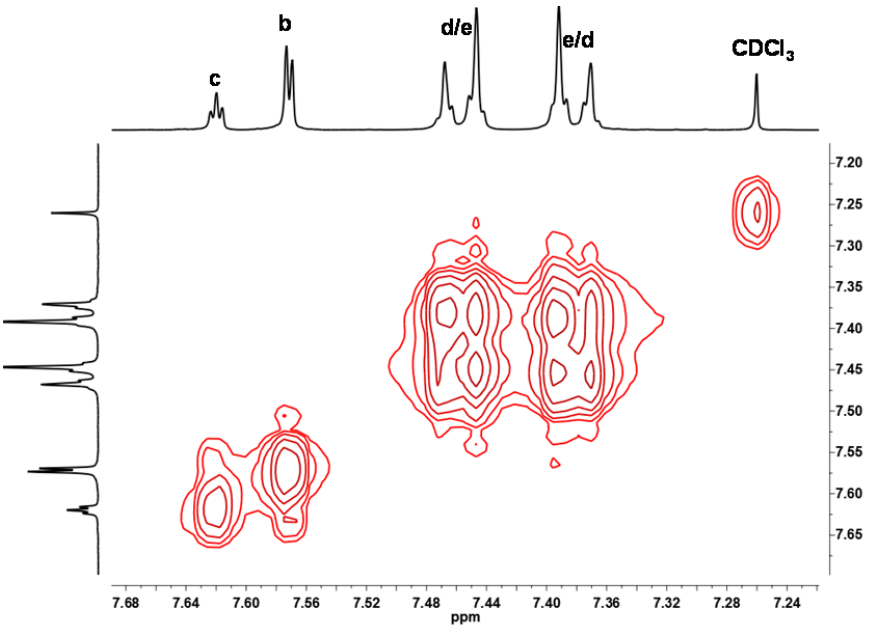


Figure S9. ^{1}H ^{1}H COSY NMR spectrum of **12** in $CDCl_3$ (400 MHz, 298 K).

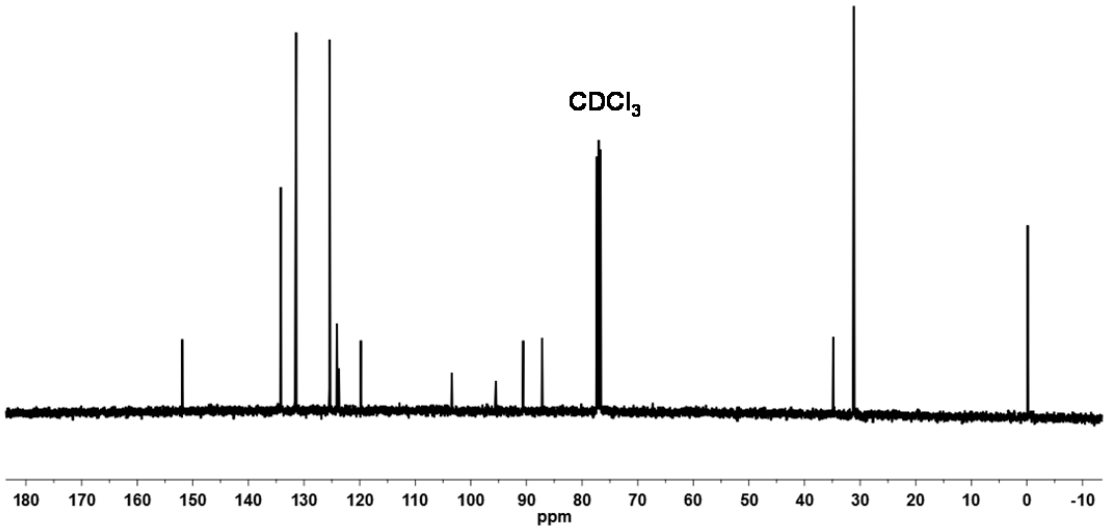


Figure S10. ^{13}C NMR spectrum of **12** in $CDCl_3$ (400 MHz, 298 K).

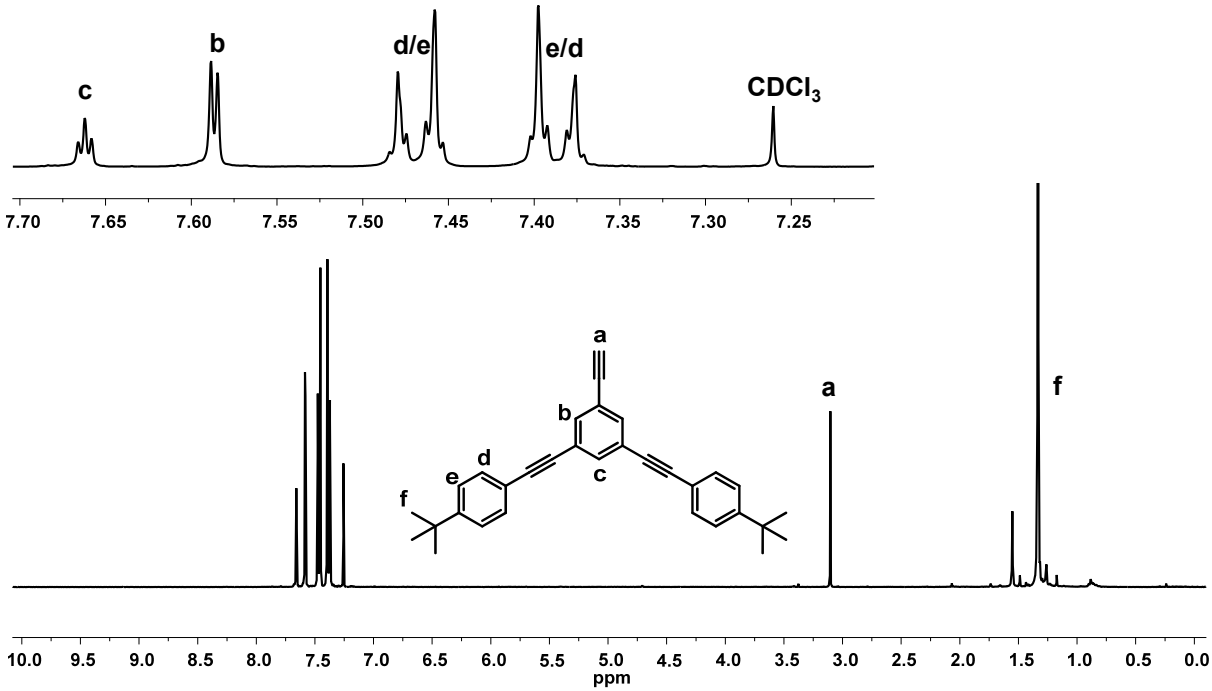


Figure S11. ^{1}H NMR spectrum of **2** in $CDCl_3$ (400 MHz, 298 K).

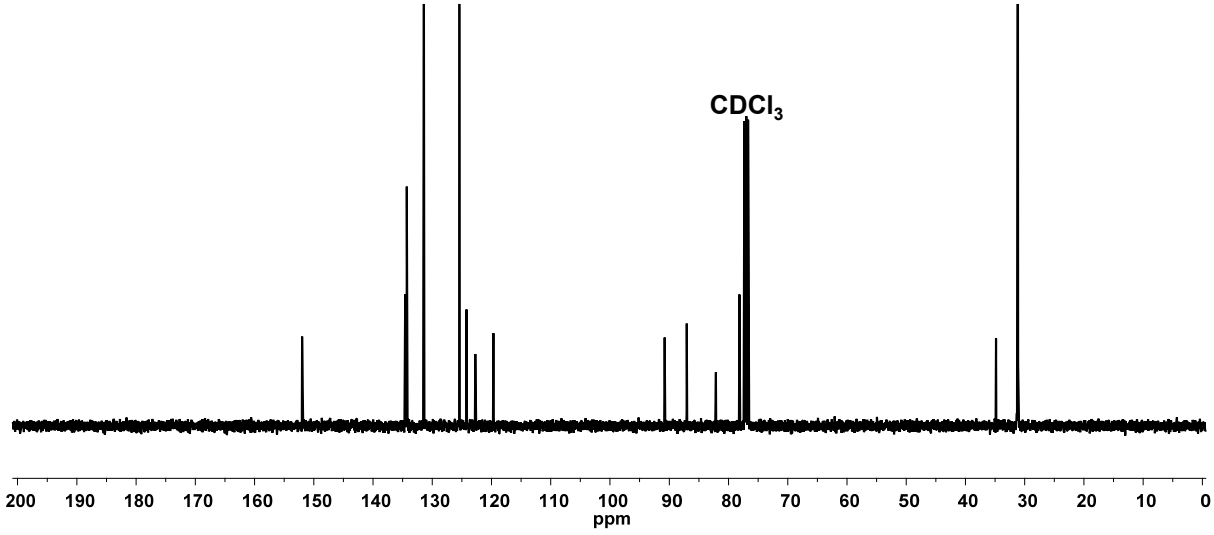


Figure S12. ^{13}C NMR spectrum of **2** in $CDCl_3$ (400 MHz, 298 K).

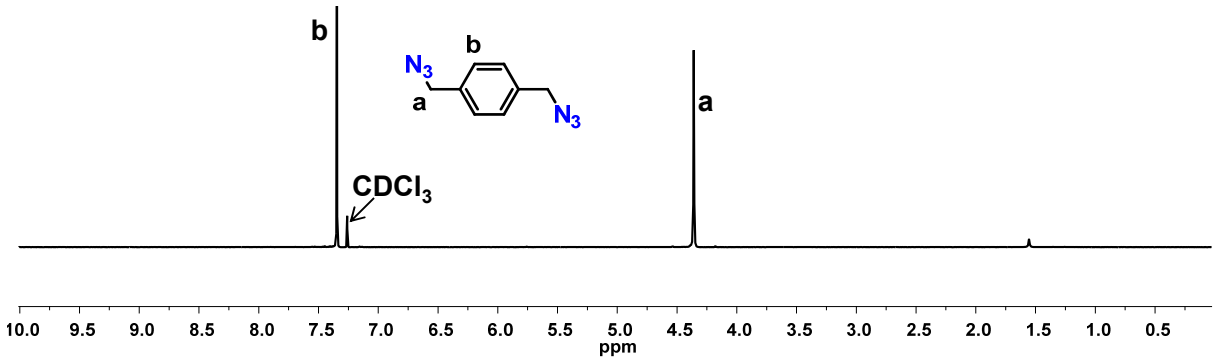


Figure S13. ^{1}H NMR spectrum of **3** in $CDCl_3$ (400 MHz, 298 K).

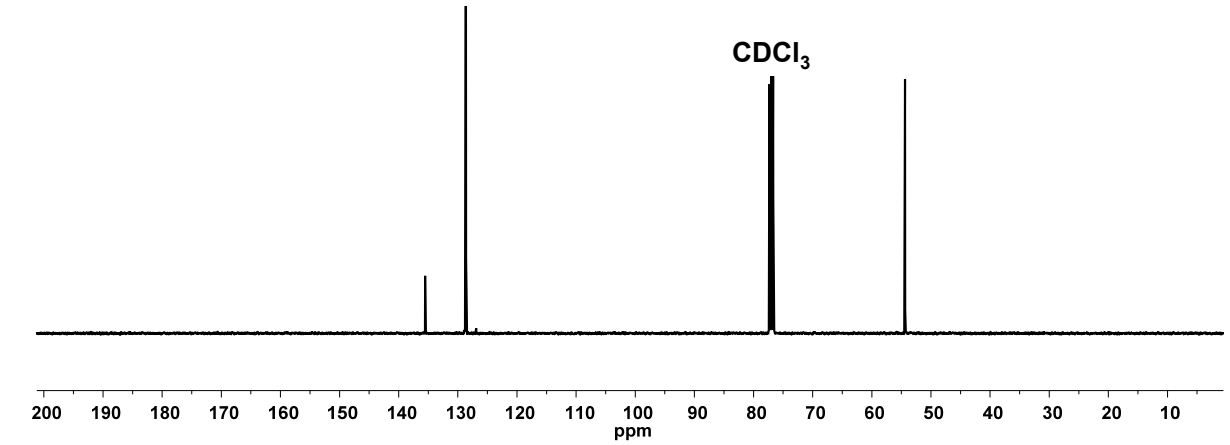


Figure S14. ^{13}C NMR spectrum of **3** in $CDCl_3$ (400 MHz, 298 K).

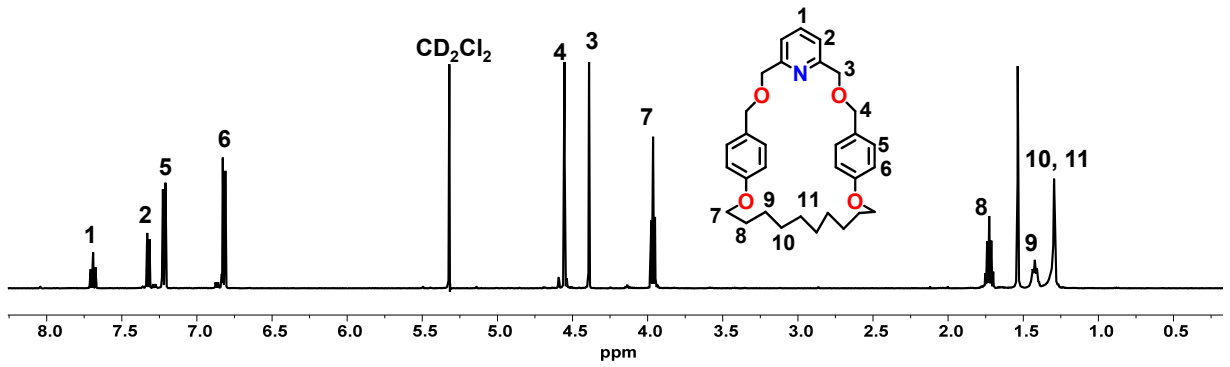


Figure S15. ^{1}H NMR spectrum of **1** in CD_2Cl_2 (500 MHz, 298 K).

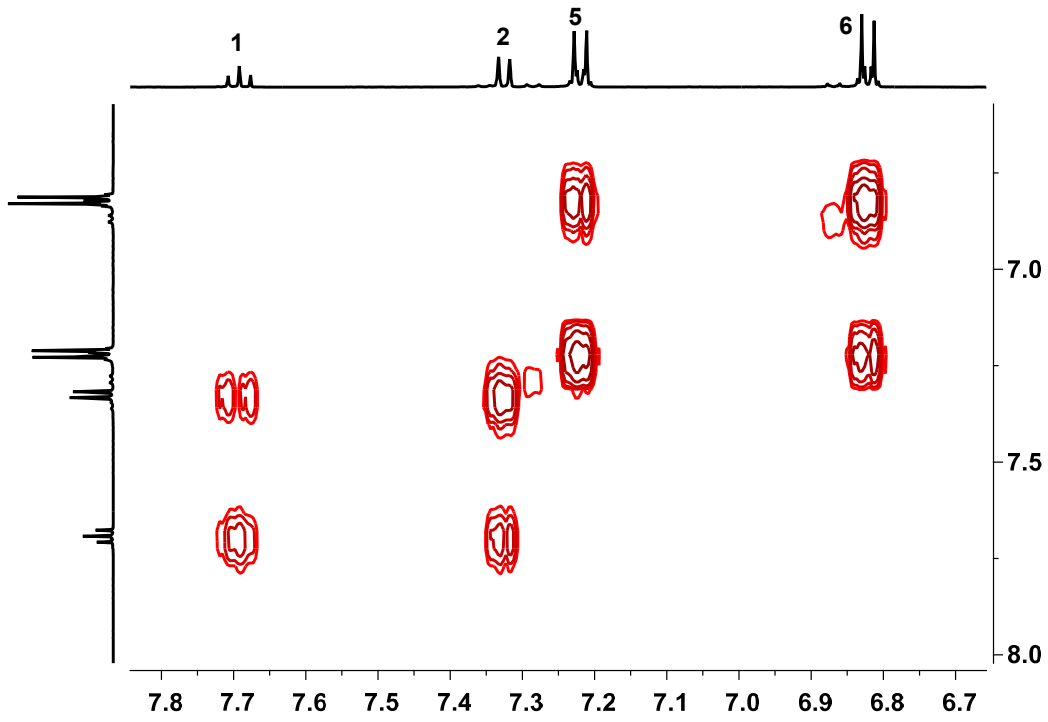


Figure S16. ^{1}H ^{1}H COSY NMR spectrum of **1** in CD_2Cl_2 (500 MHz, 298 K).

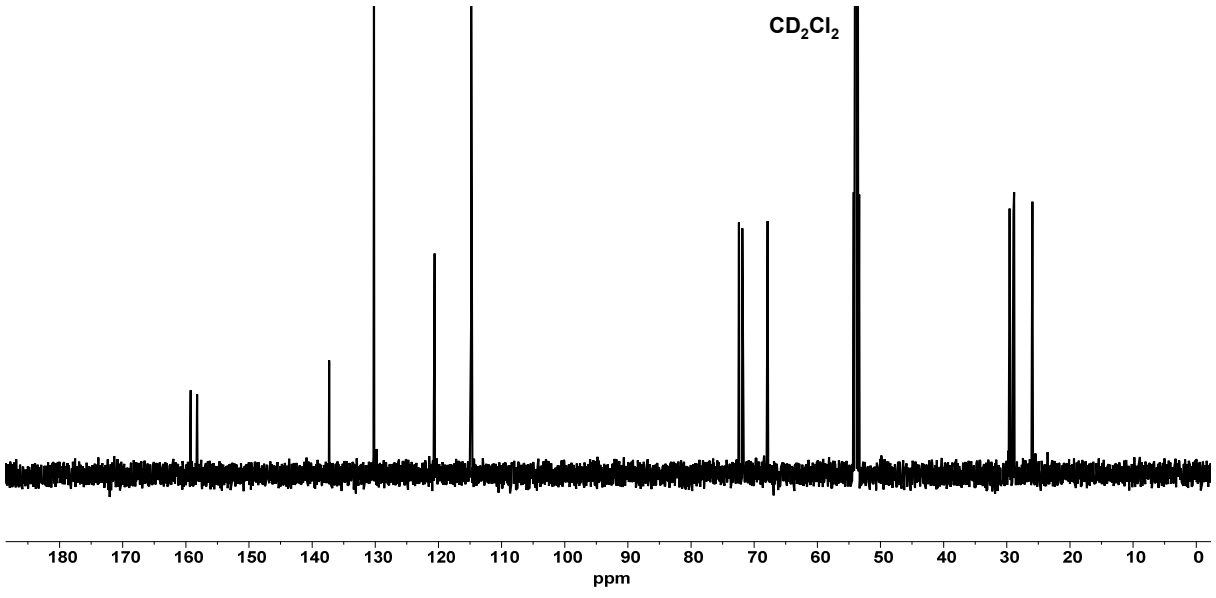


Figure S17. ^{13}C NMR spectrum of **1** in CD_2Cl_2 (500 MHz, 298 K).

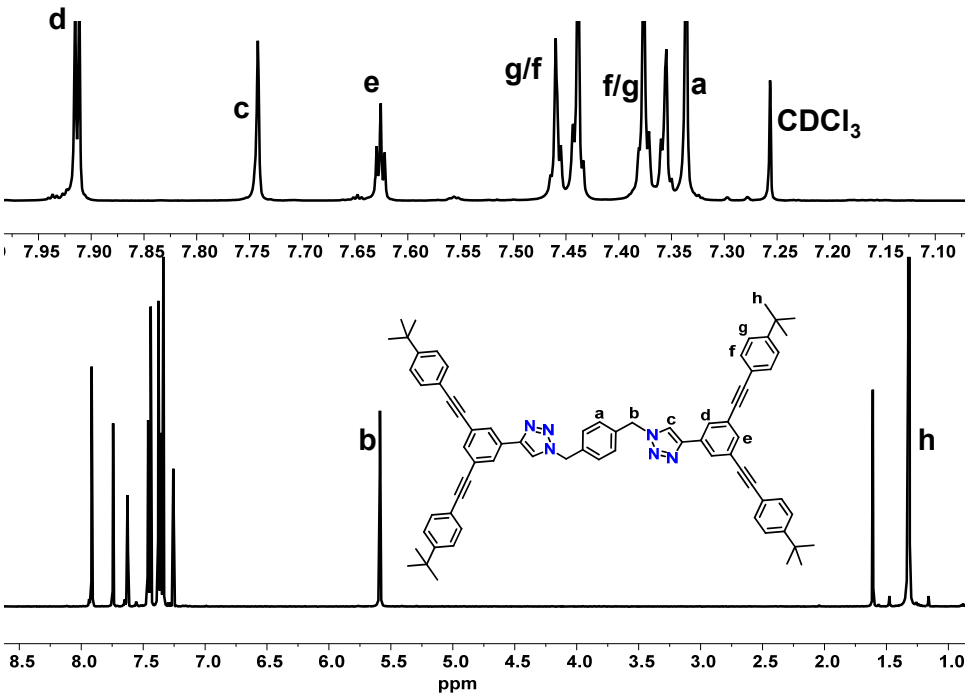


Figure S18. ^{1}H NMR spectrum of **5** in $CDCl_3$ (400 MHz, 298 K).

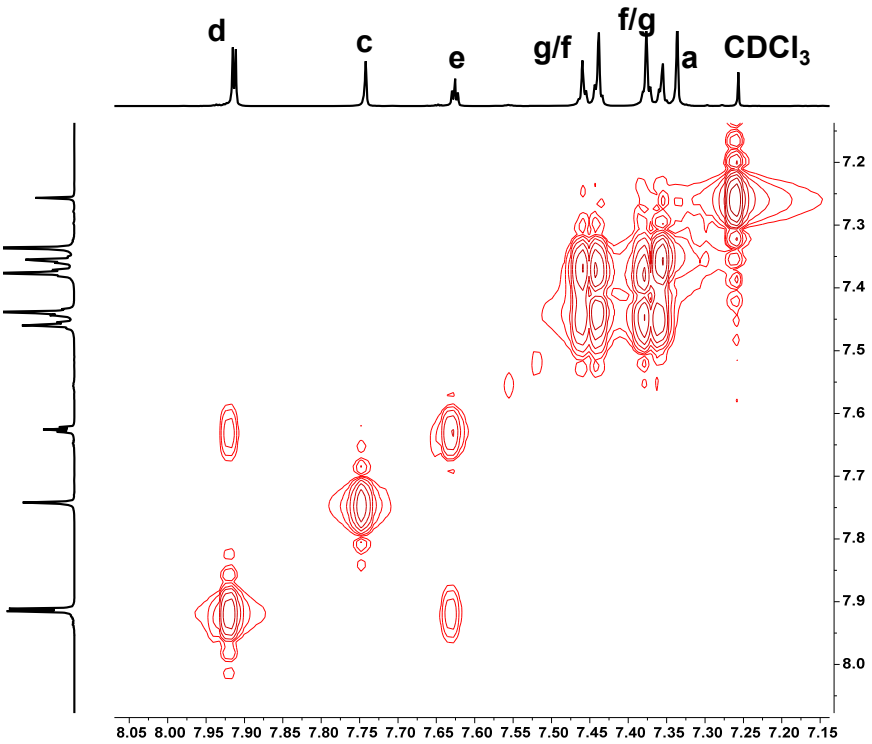


Figure S19. ^{1}H ^{1}H COSY NMR spectrum of **5** in $CDCl_3$ (400 MHz, 298 K).

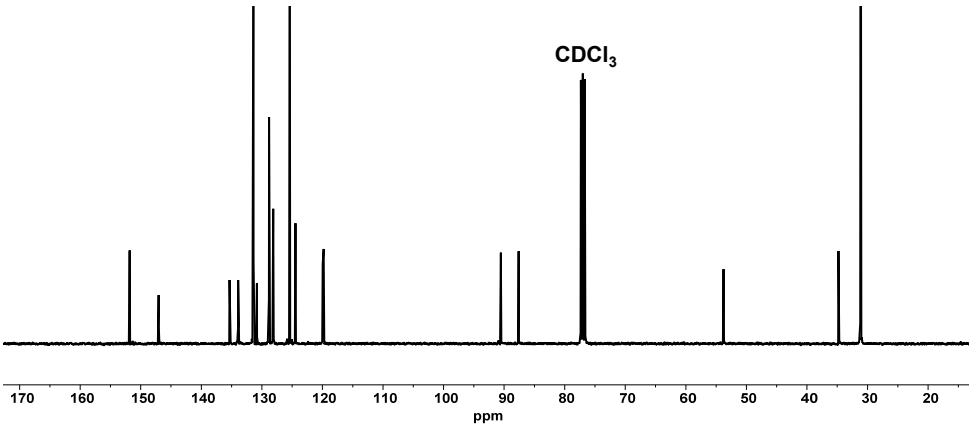


Figure S20. ^{13}C NMR spectrum of **5** in $CDCl_3$ (400 MHz, 298 K).

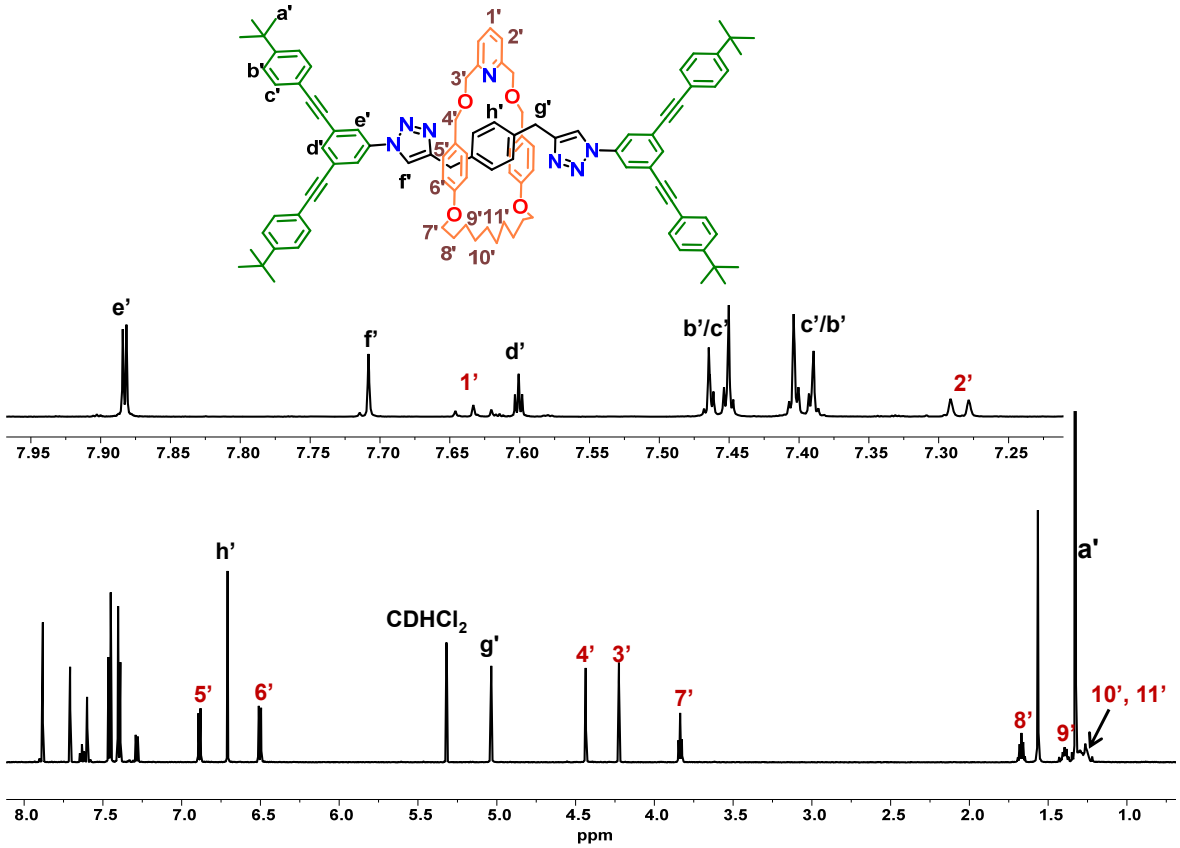


Figure S21. ^{1}H NMR spectrum of [(**1**)(**5**)] in CD_2Cl_2 (600 MHz, 298 K).

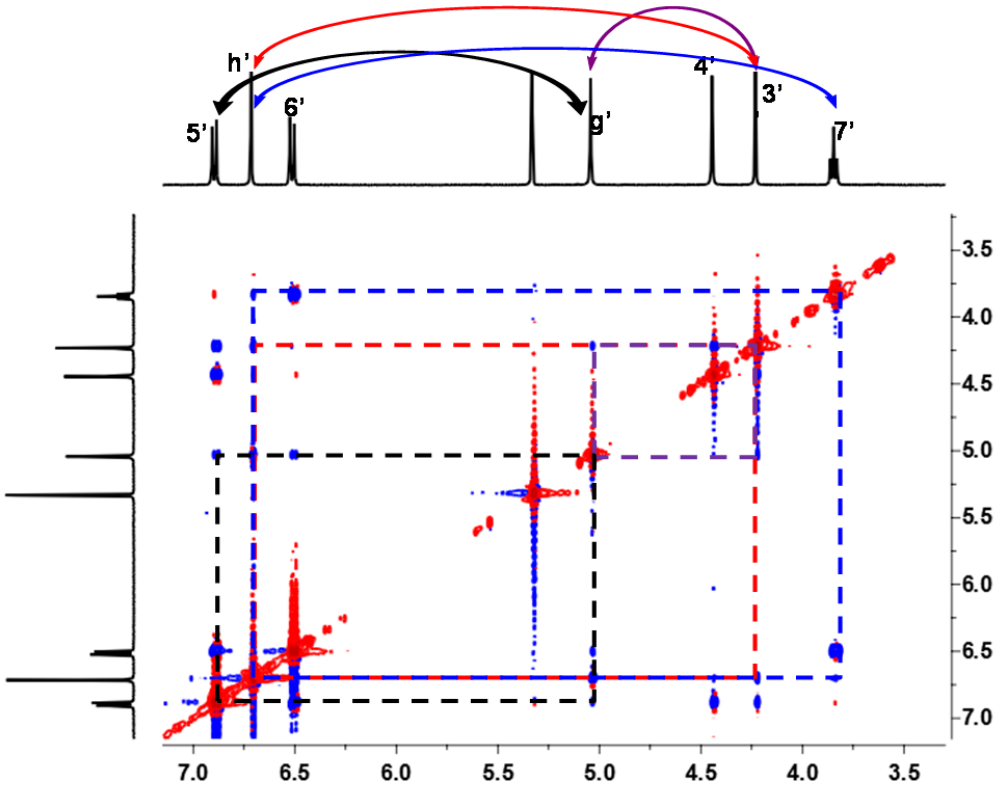


Figure S22. ^{1}H- ^{1}H NOESY NMR spectrum of [(**1**)(**5**)] in CD_2Cl_2 (600 MHz, 298 K).

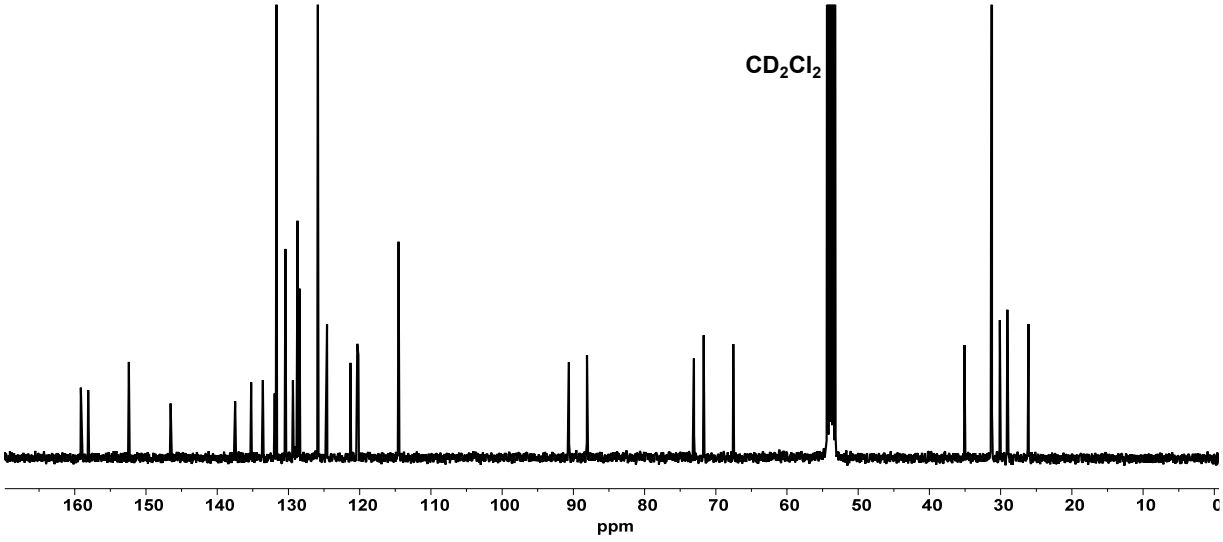


Figure S23. ^{13}C NMR spectrum of [(**1**)(**5**)] in CD_2Cl_2 (400 MHz, 298 K).

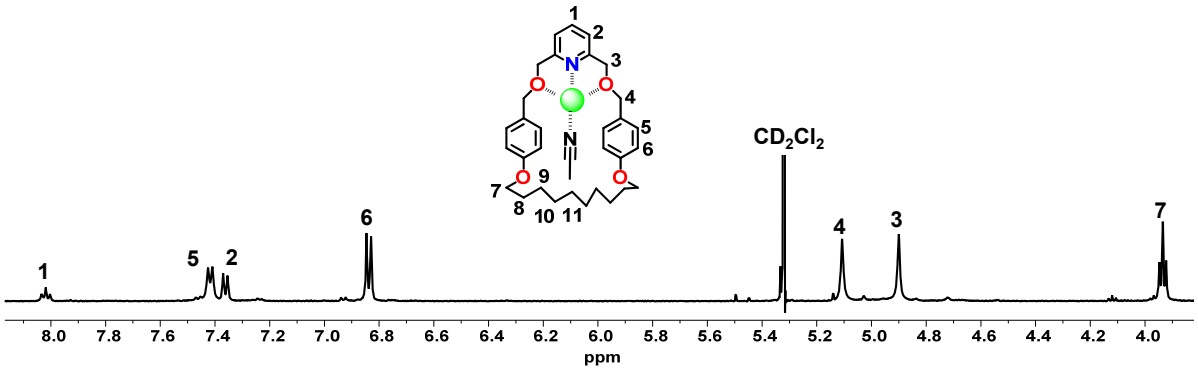


Figure S24. ^{1}H NMR spectrum of $[Cu(\mathbf{1})]^{+}$ in CD_2Cl_2 (500 MHz, 298 K).

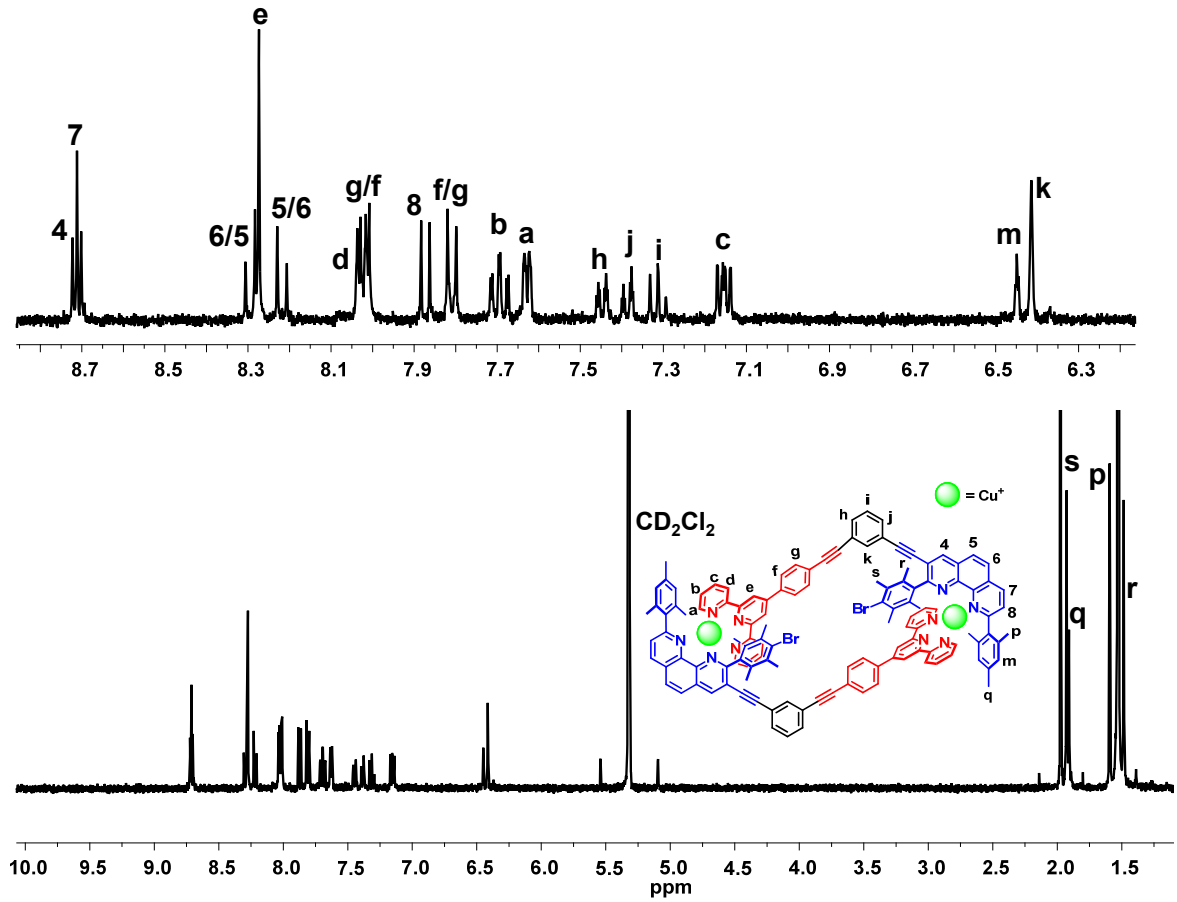


Figure S25. ^{1}H NMR spectrum of $[Cu_2(\mathbf{4})_2]^{2+}$ in CD_2Cl_2 (400 MHz, 298 K).

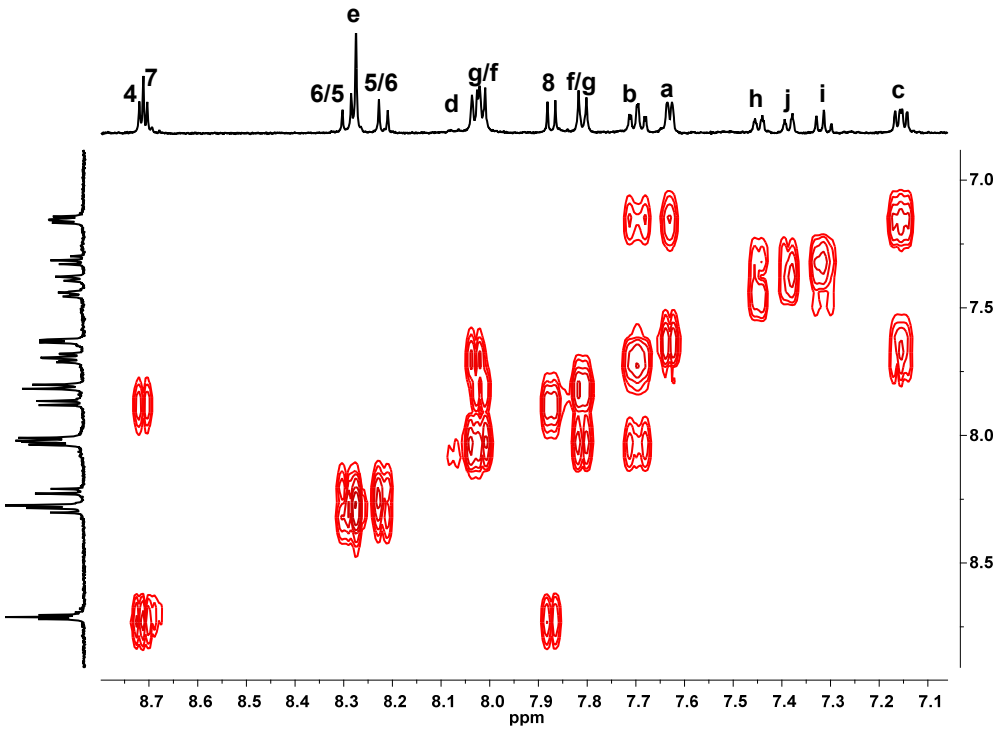


Figure S26. ^{1}H ^{1}H COSY NMR spectrum of $[Cu_2(\mathbf{4})_2]^{2+}$ in CD_2Cl_2 (400 MHz, 298 K).

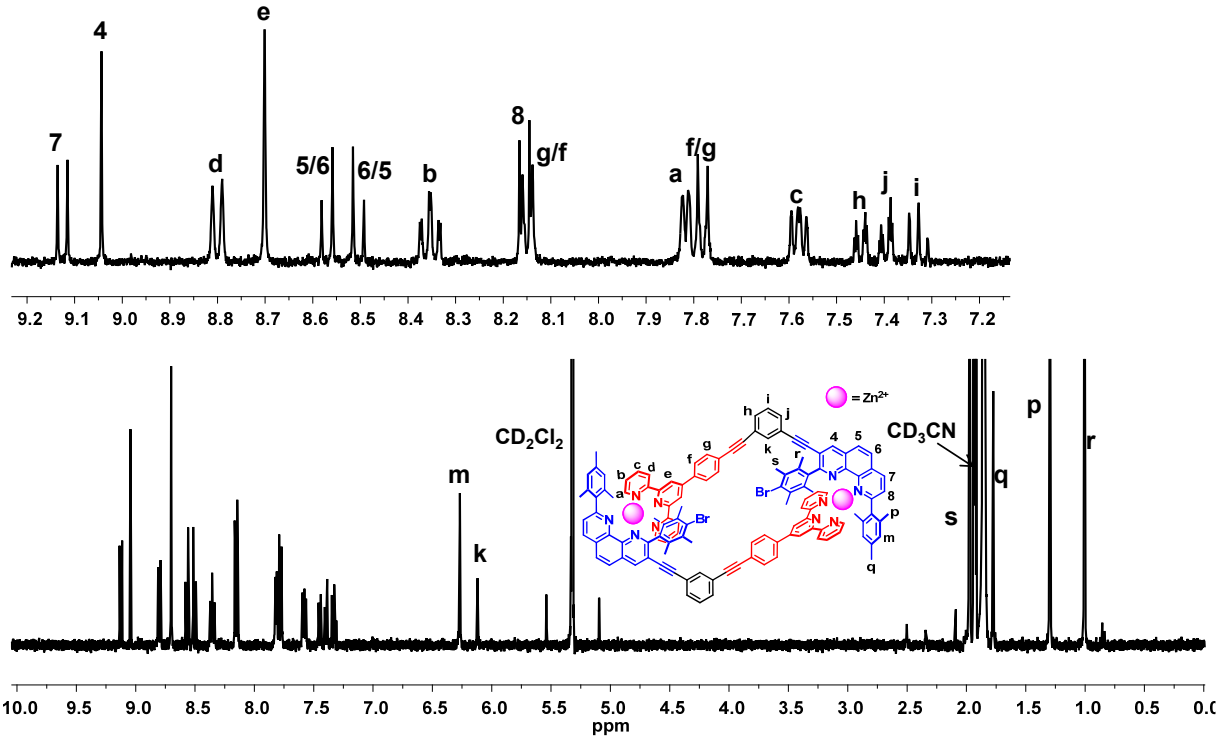


Figure S27. ^{1}H NMR spectrum of $[Zn_2(\mathbf{4})_2]^{4+}$ in CD_2Cl_2 (400 MHz, 298 K).

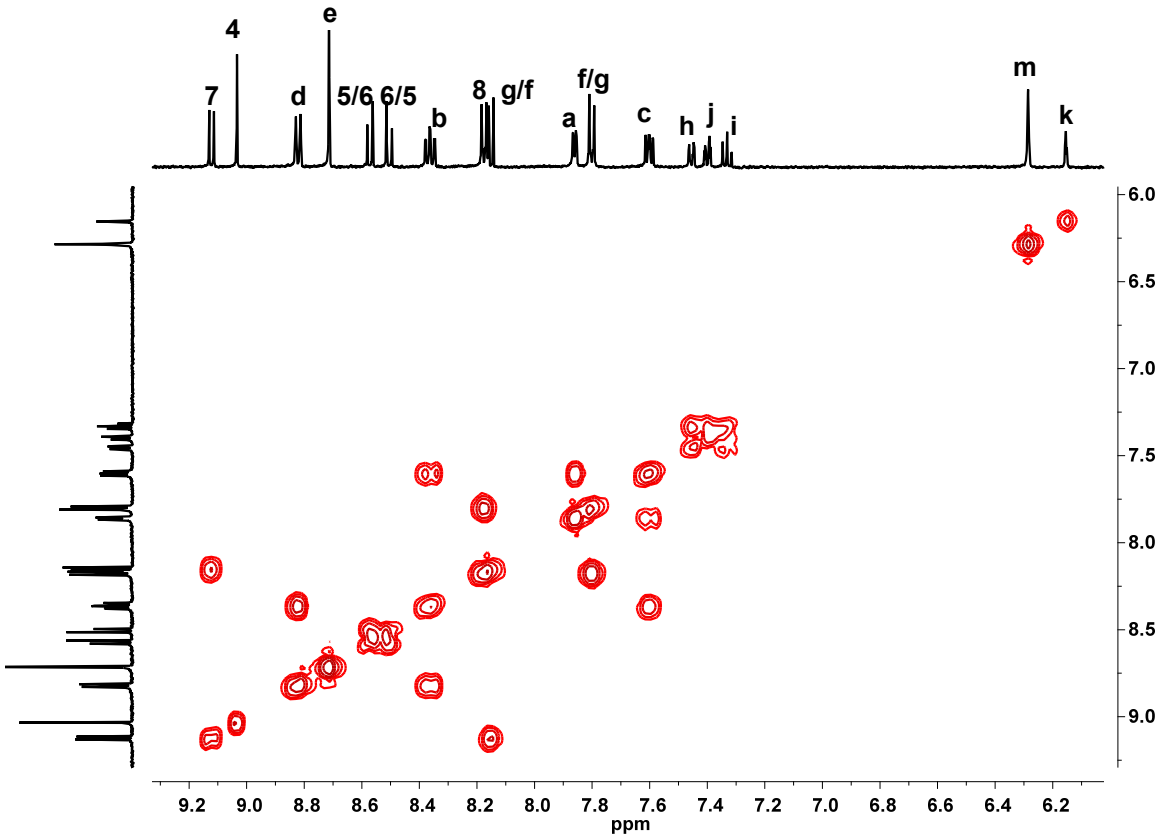


Figure S28. ^{1}H ^{1}H COSY NMR spectrum of $[Zn_2(\mathbf{4})_2]^{4+}$ in CD_2Cl_2 (400 MHz, 298 K).

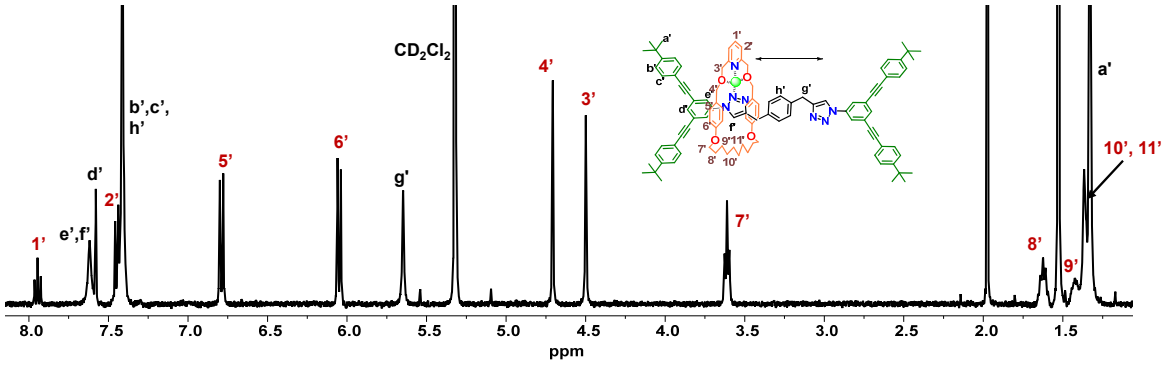


Figure S29. ^{1}H NMR spectrum of $[Cu(\mathbf{1})(\mathbf{5})]^{+}$ in CD_2Cl_2 (400 MHz, 298 K).

6. Comparison of NMR spectra

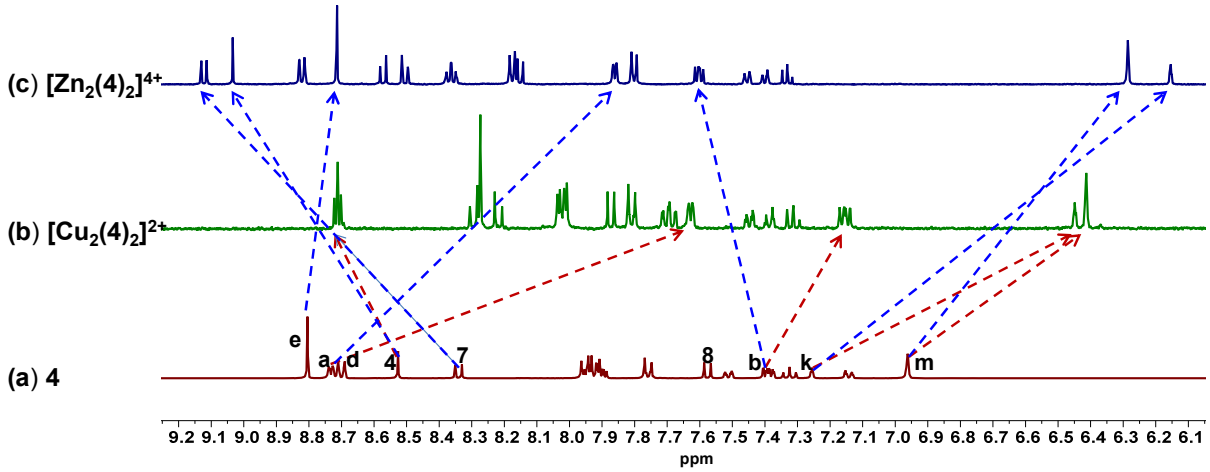


Figure S30. Comparison of partial ^{1}H NMR spectra (400 MHz, CD_2Cl_2, 298 K) of (a) **4**, (b) complex $[Cu_2(\mathbf{4})_2]^{2+}$ and (c) complex $[Zn_2(\mathbf{4})_2]^{4+}$.

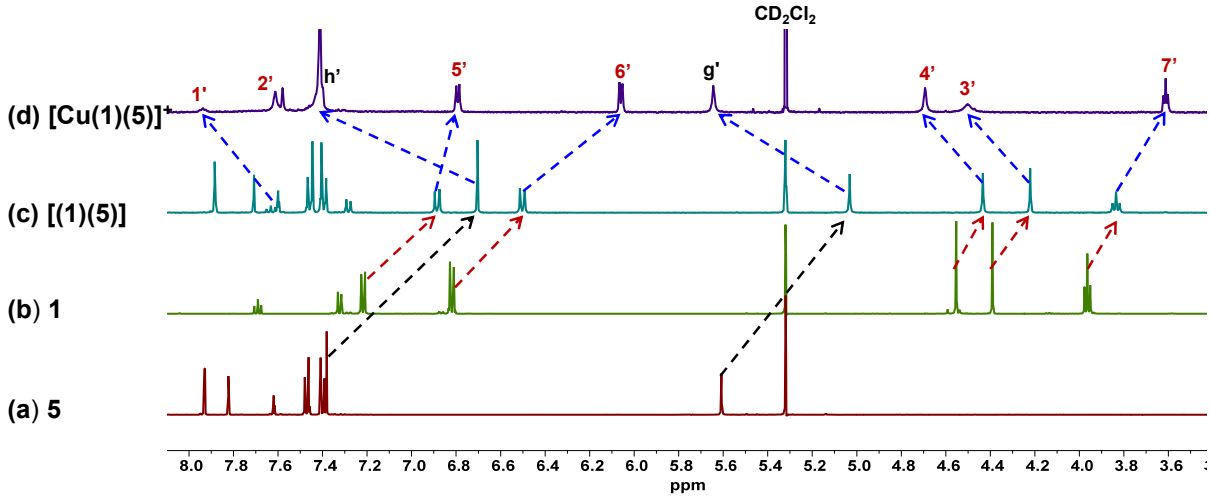


Figure S31. Comparison of partial ^{1}H NMR spectra (400 MHz, CD_2Cl_2, 298 K) of (a) axle **5**, (b) ligand **1**, (c) [2]rotaxane [(**1**)(**5**)], and (d) complex $[Cu(\mathbf{1})(\mathbf{5})]^{+}$.

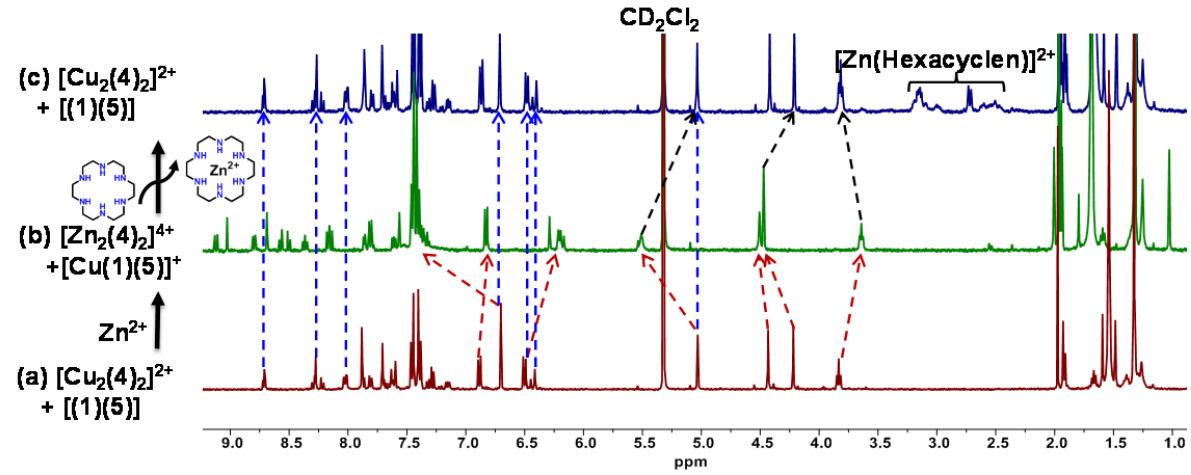


Figure S32. Comparison of partial ^{1}H NMR spectra (400 MHz, CD_2Cl_2, 298 K) of (a) complex mixture $[Cu_2(\mathbf{4})_2]^{2+}$ + [(**1**)(**5**)]; (b) addition of equimolar mixture of $Zn(OTf)_2$ to generate complexes $[Zn_2(\mathbf{4})_2]^{4+}$ + $[Cu(\mathbf{1})(\mathbf{5})]^{+}$; (c) after addition of equimolar amount of hexacyclen to form complex $[Cu_2(\mathbf{4})_2]^{2+}$ and [(**1**)(**5**)].

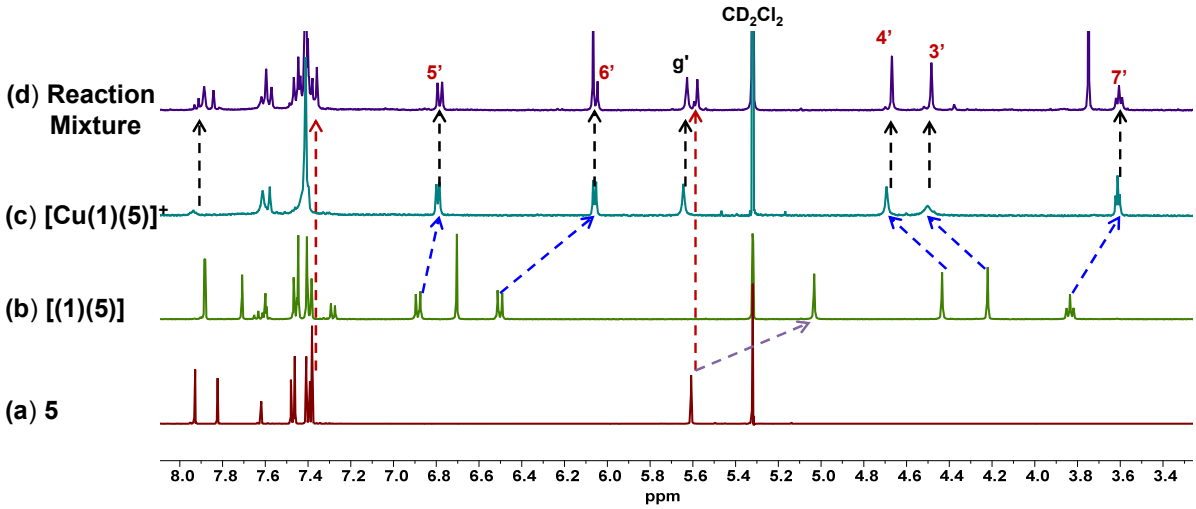


Figure S33. Comparison of partial ^{1}H NMR spectra (400 MHz, CD_2Cl_2, 298 K) of (a) axle **14**; (b) rotaxane [(**1**)(**5**)]; (c) complexed rotaxane $[Cu(\mathbf{1})(\mathbf{5})]^{+}$; (d) reaction mixture of substrates **1**, **2**, **3** and $[Cu(CH_3CN)_4]PF_6$ (ratio 1:5:2.5:1) after heating at 40 °C for 24 h.

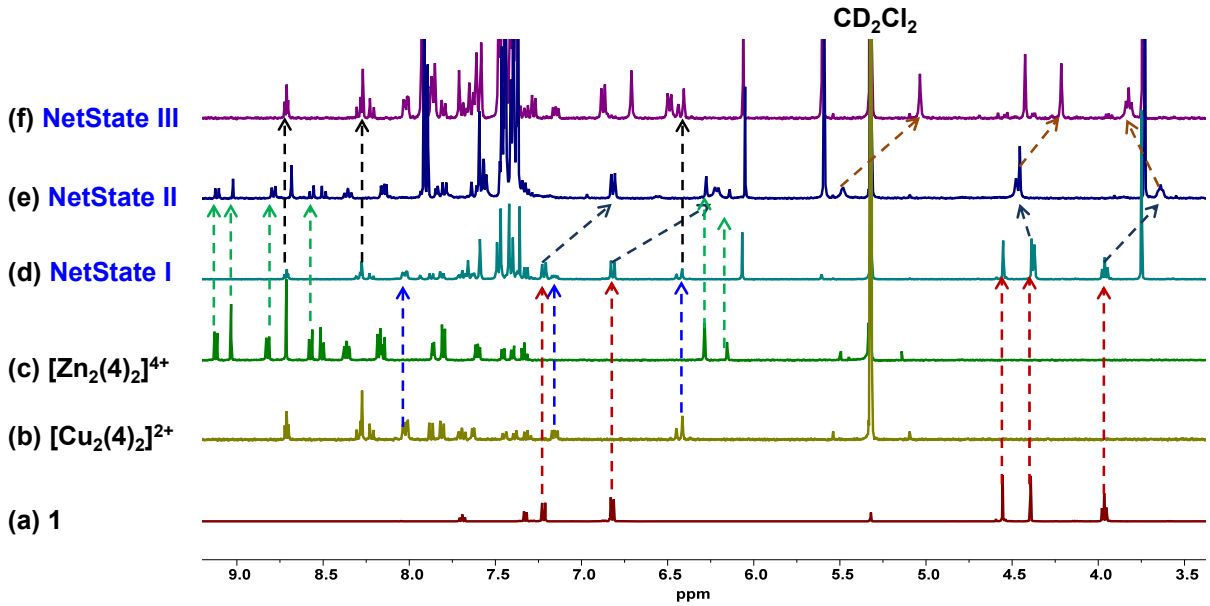


Figure S34. Comparison of partial ^{1}H NMR spectra (400 MHz, CD_2Cl_2, 298 K) of (a) macrocycle **1**; (b) complex **5**; (c) complex **6**; (d) Netstate I; (e) Netstate II; (f) Netstate III.

7. ESI-MS spectra

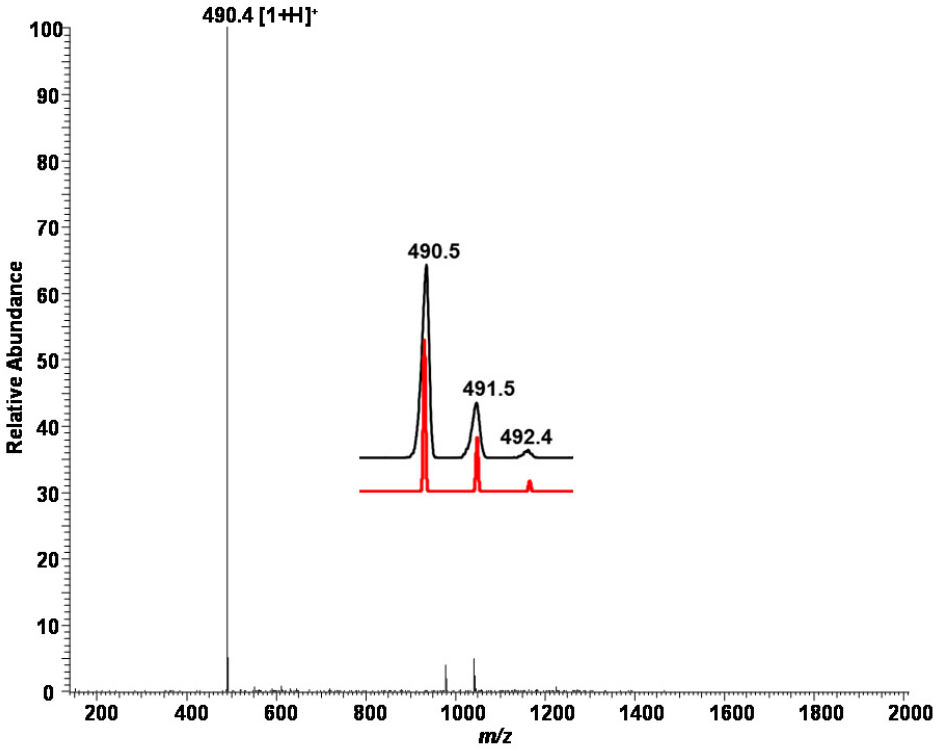


Figure S35. ESI-MS of **1** after protonation.

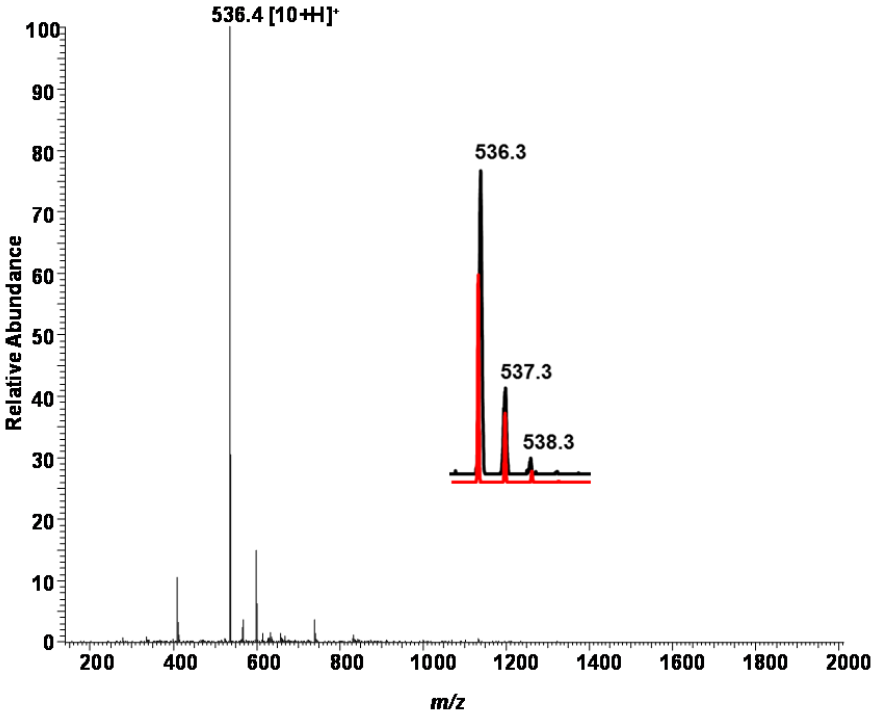


Figure S36. ESI-MS of **10** after protonation.

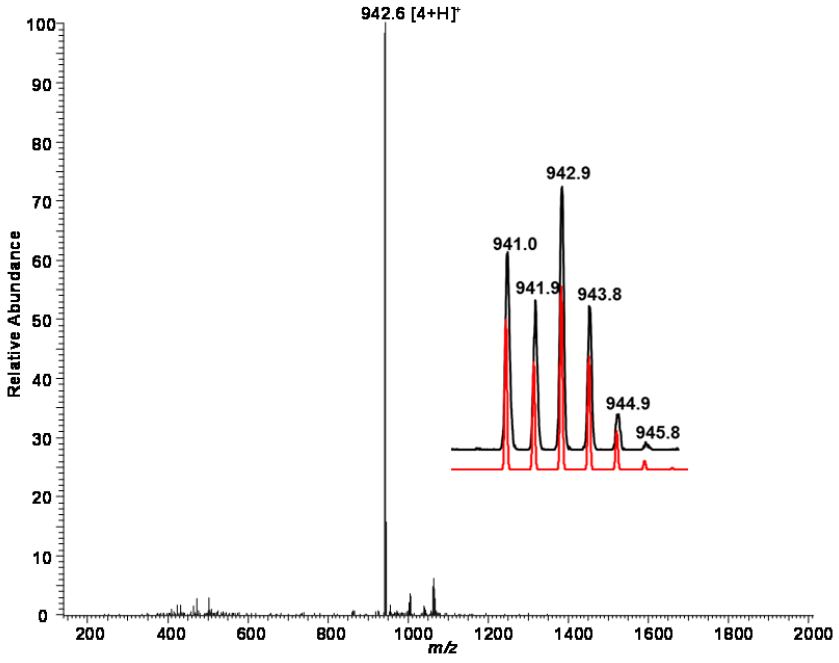


Figure S37. ESI-MS of **4** after protonation.

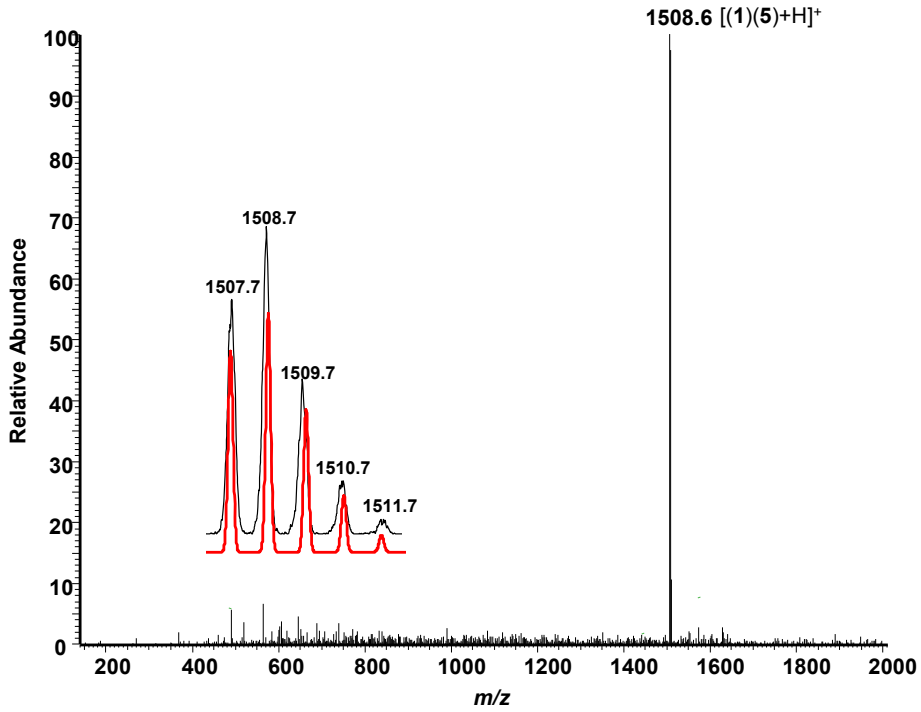


Figure S38. ESI-MS of [(**1**)(**5**)] after protonation.

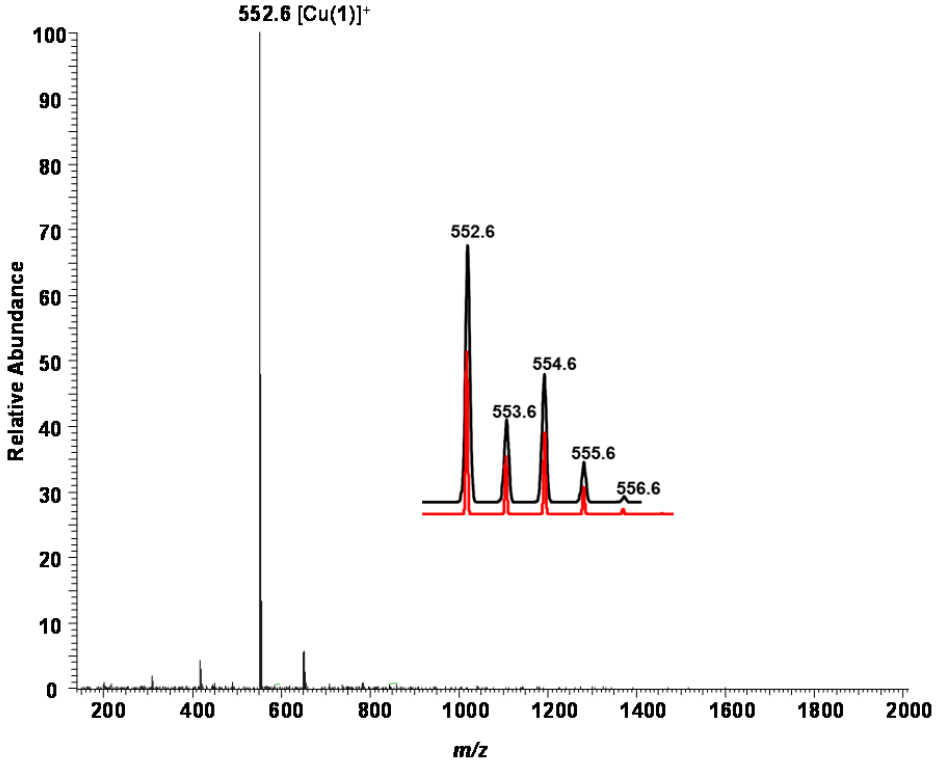


Figure S39. ESI-MS of complex [Cu(**1**)]$^{+}$.

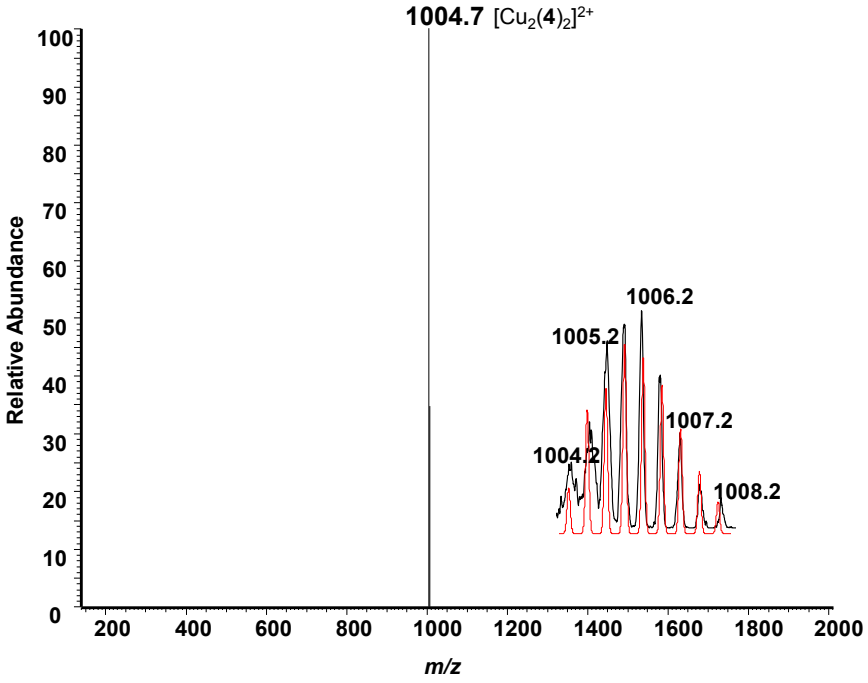


Figure S40. ESI-MS of complex $[Cu_2(\mathbf{4})_2]^{2+}$.

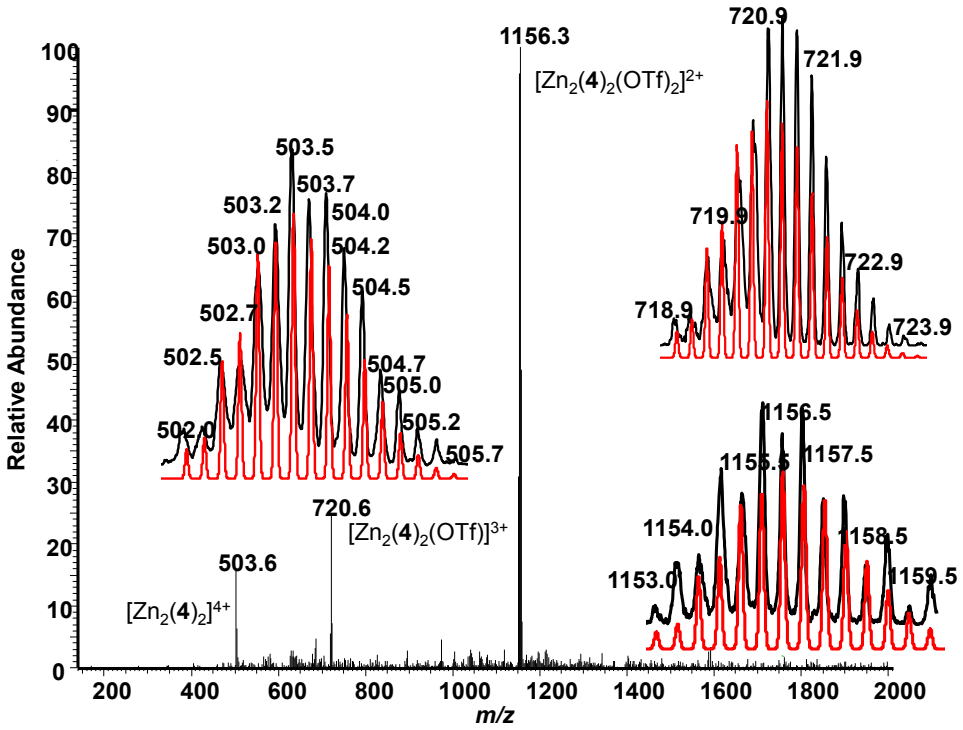


Figure S41. ESI-MS of complex $[Zn_2(\mathbf{4})_2]^{4+}$.

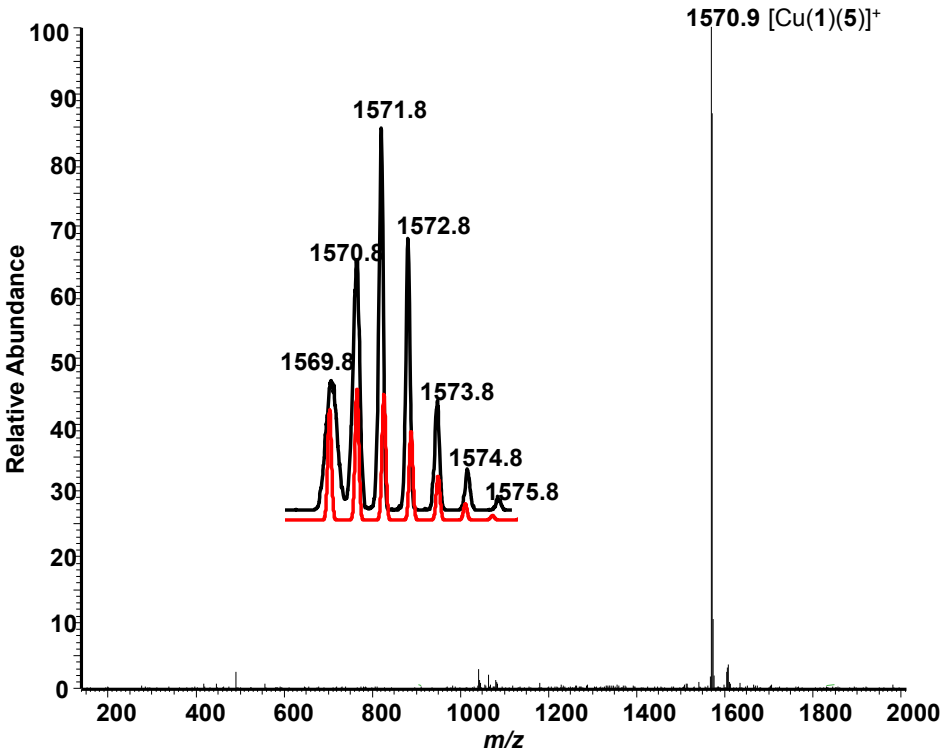


Figure S42. ESI-MS of complex $[Cu(\mathbf{1})(\mathbf{5})]^{+}$.

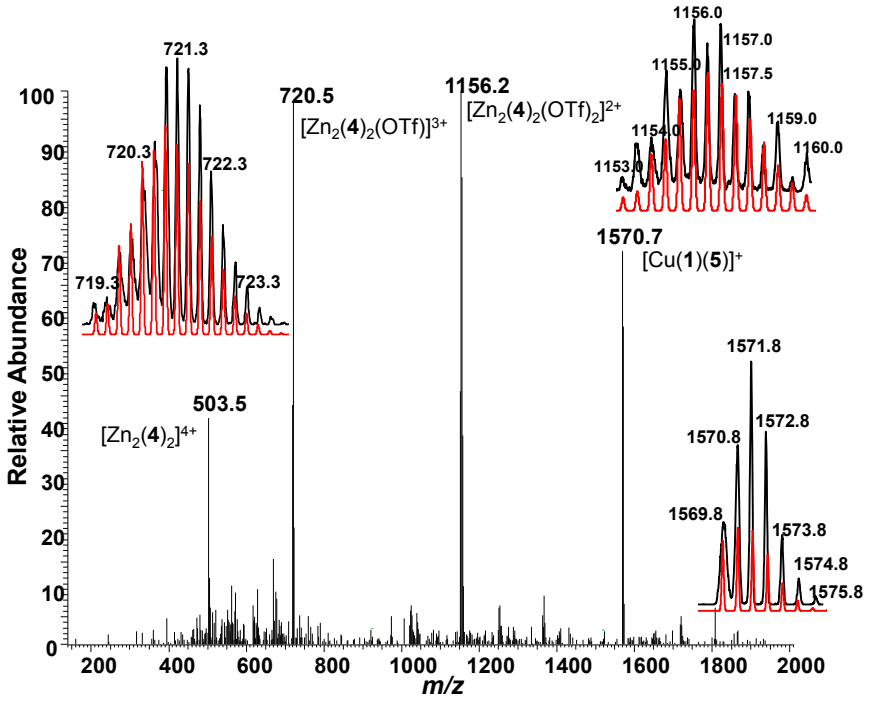


Figure S43. Complex mixture of $\{[Zn_2(\mathbf{4})_2]^{4+} + [Cu(\mathbf{1})(\mathbf{5})]^{+}\}$

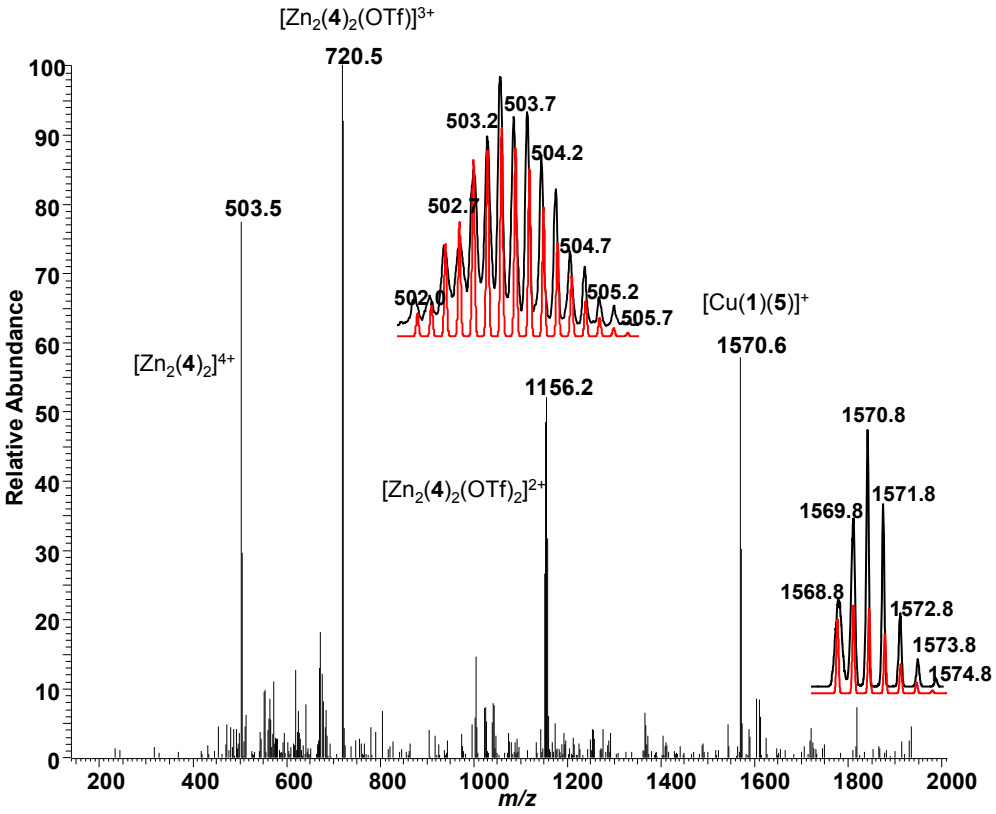


Figure S44. ESI-MS of Netstate II = $[Zn_2(\mathbf{4})_2]^{4+}$ + $[Cu(\mathbf{1})(\mathbf{5})]^{+}$.

8. Variable temperature studies and determination of kinetic parameters

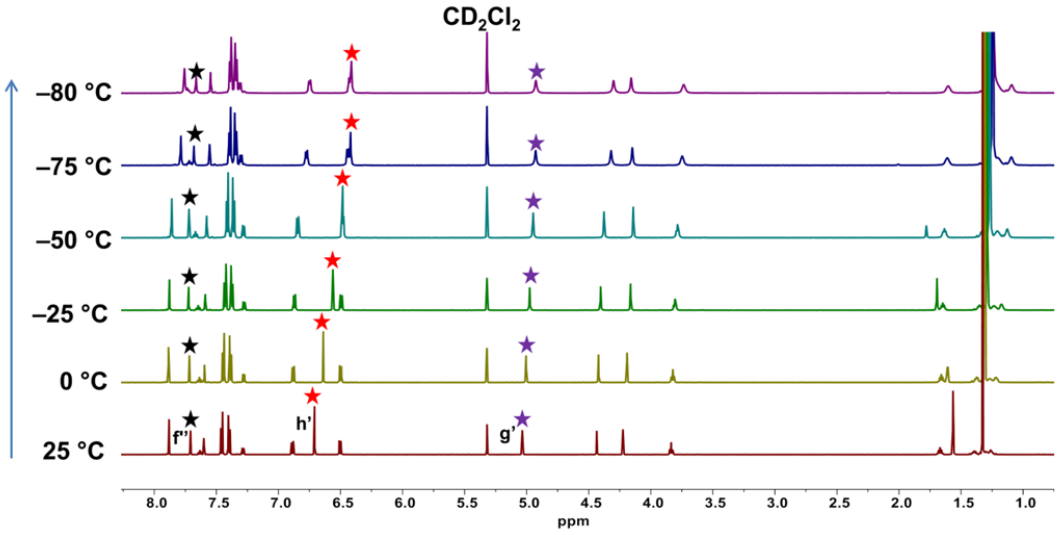


Figure S45. Partial VT-^{1}H NMR (CD_2Cl_2, 600 MHz) of [(**1**)(**5**)].

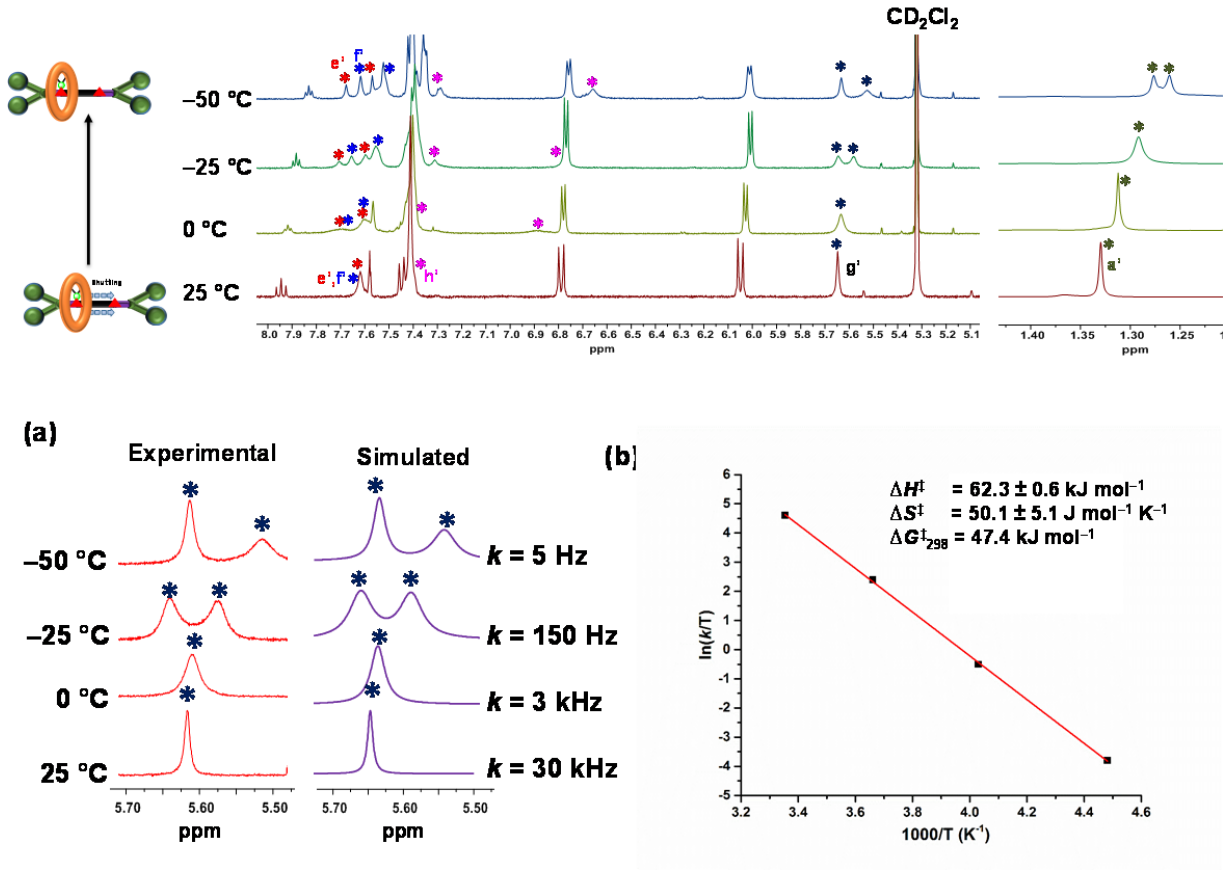


Figure S46. Top: Partial VT-^{1}H NMR (CD_2Cl_2, 600 MHz) of $[Cu(\mathbf{1})(\mathbf{5})]^+$ showing the splitting of protons. (a) Simulated and experimental VT-^{1}H NMR (CD_2Cl_2, 600 MHz) of $[Cu(\mathbf{1})(\mathbf{5})]^+$ showing the splitting of g'-H (black asterisk marked) and (b) Eyring plot for the shuttling exchange in $[Cu(\mathbf{1})(\mathbf{5})]^+$.

9. UV-vis spectra and measurement of binding constants.

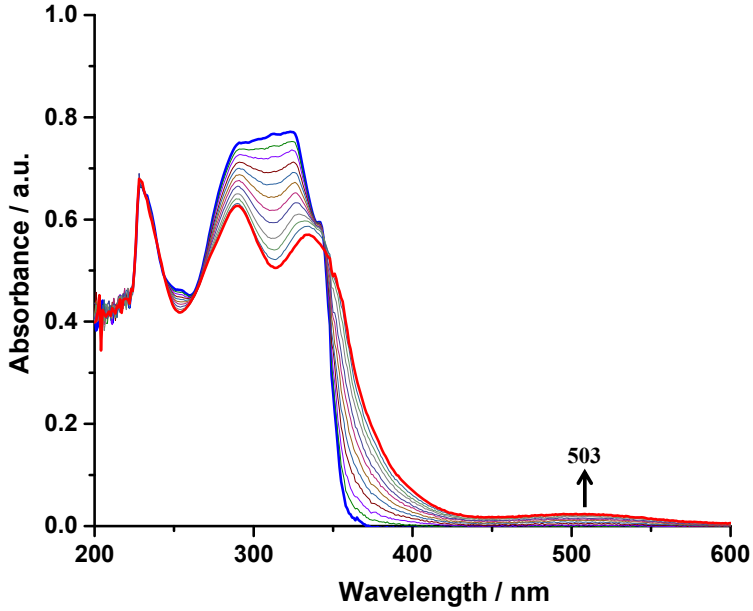


Figure S47. UV-vis spectra of **4** (4.5×10^{-6} M) in CH_2Cl_2 (2 mL) upon addition of $[Cu(CH_3CN)_4]PF_6$ (5.8×10^{-4} M) at 298 K to afford the complex $[Cu_2(\mathbf{4})_2]^{2+}$. The wavelength region 600-200 nm was analyzed.

Result: $\log \beta_{[Cu_2(\mathbf{4})_2]^{2+}} = 22.18 \pm 0.42$.

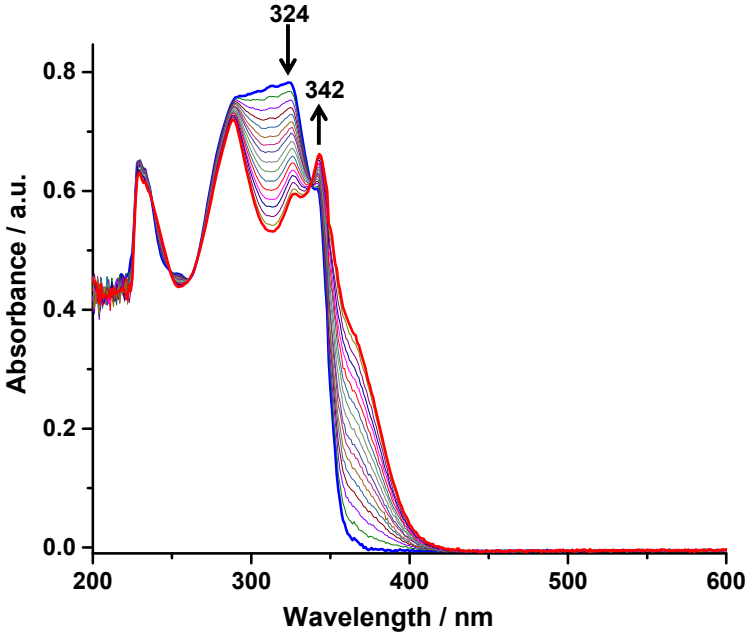


Figure S48. UV-vis spectra of **4** (4.5×10^{-6} M) in CH_2Cl_2 (2 mL) upon addition of $[Zn(OTf)_2]$ (5.2×10^{-4} M) at 298 K to afford the complex $[Zn_2(\mathbf{4})_2]^{4+}$.

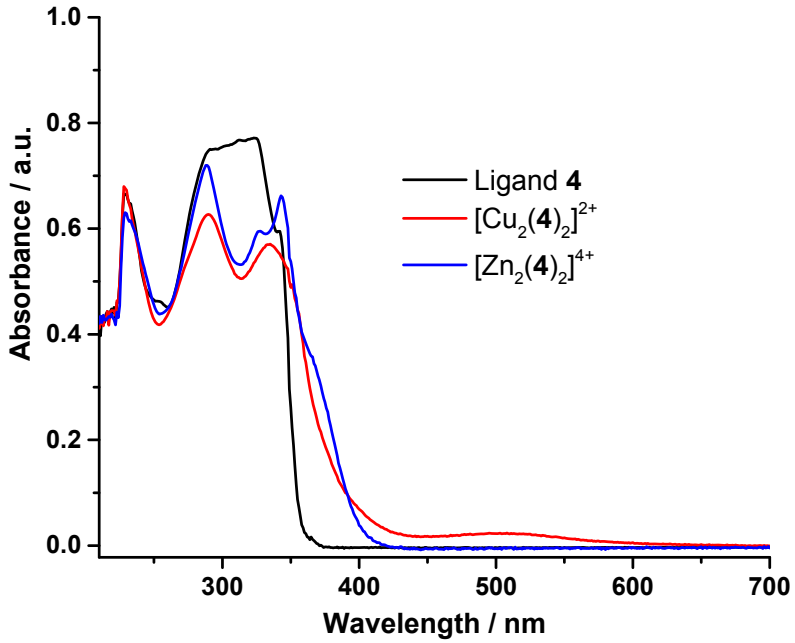


Figure S49. Comparison of UV-vis spectra of ligand **4**, $[Cu_2(\mathbf{4})_2]^{2+}$ and $[Zn_2(\mathbf{4})_2]^{4+}$ (4.5×10^{-6} M)

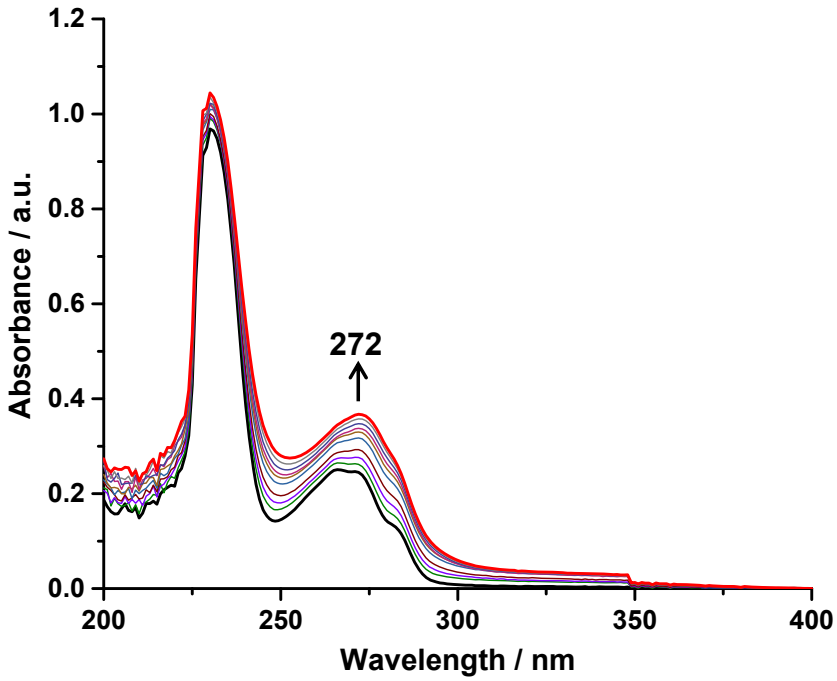


Figure S50. UV-vis spectra of **1** (4.1×10^{-5} M) in CH_2Cl_2 (2 mL) upon addition of $[Cu(CH_3CN)_4]PF_6$ (9.8×10^{-3} M) at 298 K to afford the complex $[Cu(\mathbf{1})]^+$. The wavelength region 400-200 nm was analyzed. Result: log $K_{[Cu(\mathbf{1})]^+}$ = 4.48 ± 0.23.

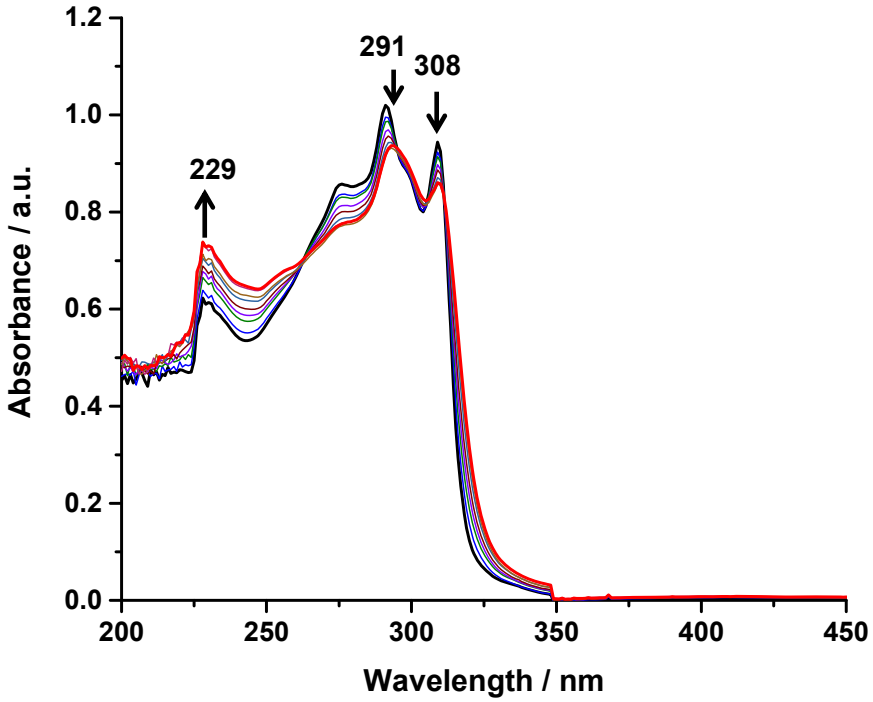


Figure S51. UV-vis spectra of [(**1**)(**5**)] (7.4×10^{-6} M) in CH_2Cl_2 (2 mL) upon addition of $[Cu(CH_3CN)_4]PF_6$ (9.8×10^{-3} M) at 298 K to afford the complex $[Cu(\mathbf{1})(\mathbf{5})]^+$. The wavelength region 450-200 nm was analyzed. Result: log $K_{[Cu(\mathbf{1})(\mathbf{5})]^+} = 7.40 \pm 0.31$.

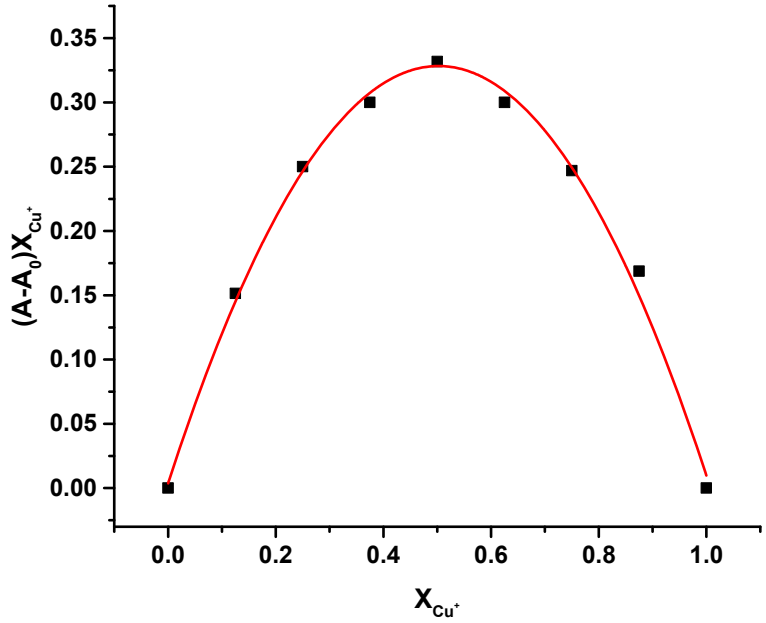


Figure S52. Job plot analysis of complex $[Cu_2(\mathbf{4})_2]^{2+}$ (2:2) using UV-vis absorption data at λ = 290 nm**.**

10. Fluorescence spectra

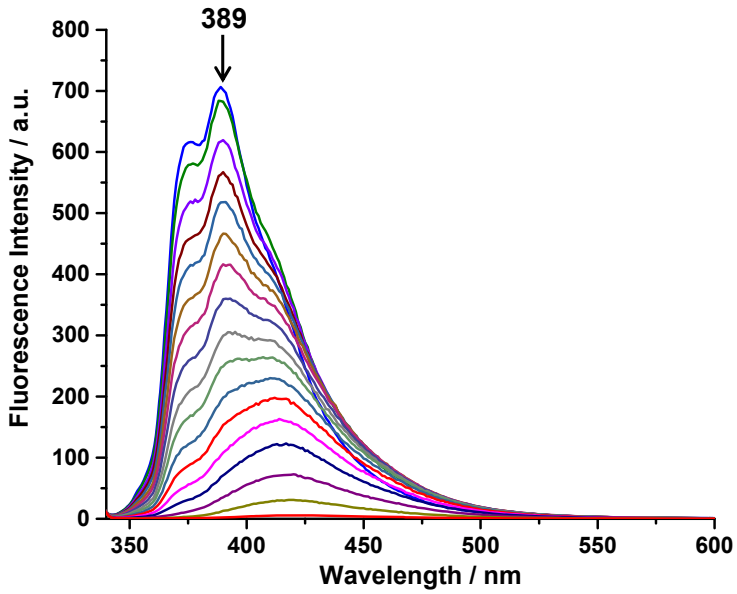


Figure S53. Fluorescence spectra (λ_{exc} = 337 nm) of **4** (7.1 × 10^{-6} M) in CH_2Cl_2 (2 mL) upon addition of $[Cu(CH_3CN)_4]PF_6$ (6.8 ×10^{-4} M) at 298 K to afford the complex $[Cu_2(\mathbf{4})_2]^{2+}$.

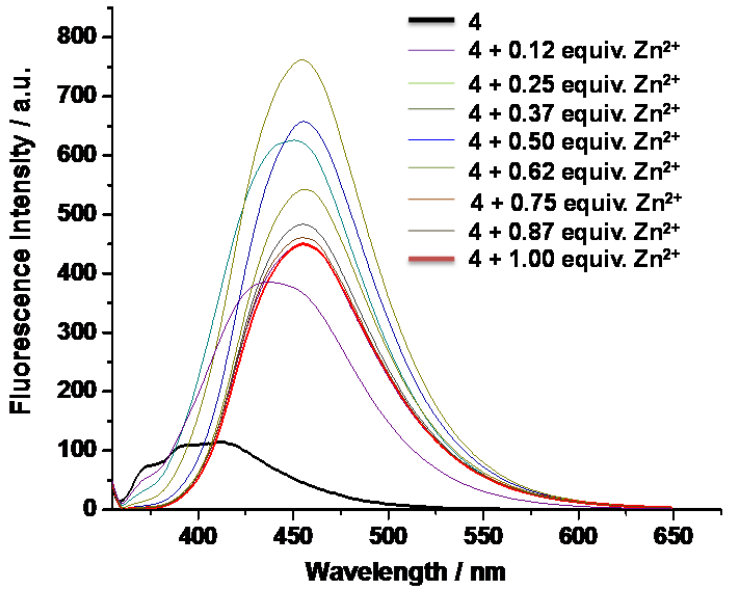


Figure S54. Fluorescence spectra (λ_{exc} = 337 nm) of **4** (1.0 × 10^{-6} M) in CH_2Cl_2 (2 mL) upon addition of $Zn(OTf)_2$ (1.0 ×10^{-4} M) at 298 K to afford the complex $[Zn_2(\mathbf{4})_2]^{4+}$. The spectrum remains constant with more than one equiv. of zinc(II) ions.

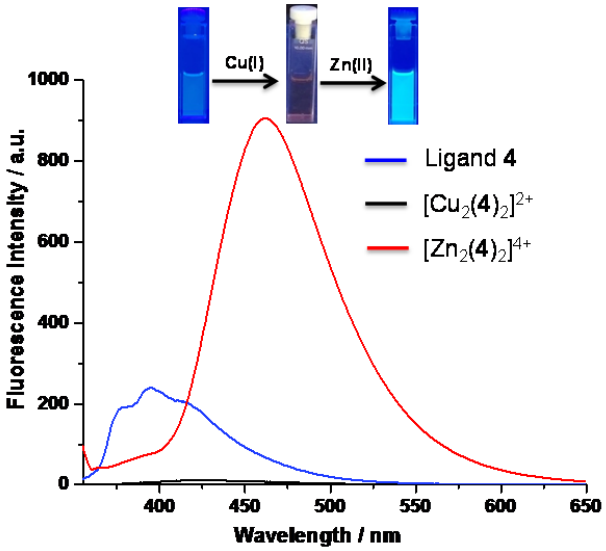


Figure S55. Comparison of fluorescence spectra of ligand **4**, $[Cu_2(\mathbf{4})_2]^{2+}$ and $[Zn_2(\mathbf{4})_2]^{4+}$ (2.0×10^{-6} M) (λ_{exc} = 337 nm).

11. X-ray crystallography (CCDC-1955166)

We were successful in growing single crystals by diffusing hexane into the dichloromethane solution of $[Cu_2(\mathbf{4})_2](PF_6)_2$.

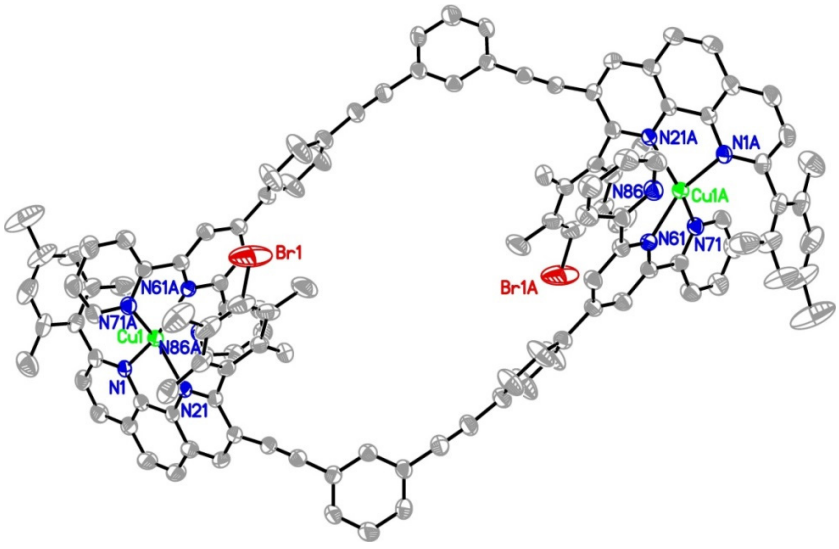


Figure S56. Perspective view of complex $[Cu_2(\mathbf{4})_2]^{2+}$ (X-ray structure) with thermal ellipsoids drawn at 50% probability. Color code: C, gray; N, blue; Br, red; Cu, green.

Crystal structure determination. Data were collected at 173 K on a STOE IPDS two-circle diffractometer with a GENIX microfocus tube with mirror optics using MoK_α radiation (λ = 0.71073 Å) and were scaled using the frame scaling procedure in the *X-AREA* program system[7] (Stoe & Cie, 2002). The structure was solved by direct methods using the program *SHELXS*[8] (Sheldrick, 2008) and refined against F^2 with full-matrix least-squares techniques using the program *SHELXL* (Sheldrick, 2008). One phenyl ring is disordered over two positions with a site occupation factor of 0.512(19) for the major occupied site. The displacement ellipsoids of the disordered atoms were restrained to an isotropic behaviour. The contribution of the severely disordered solvent was suppressed using the *SQUEEZE* routine in the *PLATON* program (Spek, 2009).

Table 1. Crystal data and structure refinement for complex $[Cu_2(\mathbf{4})_2](PF_6)_2$

Identification code	$[Cu_2(\mathbf{4})_2](PF_6)_2$	
Empirical formula	$C_{124}\ H_{92}\ Br_2\ Cu_2\ F_{12}\ N_{10}\ P_2$	
Formula weight	2298.91	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.3313(7) Å	α = 102.772(4)°.
	b = 13.2935(7) Å	β = 95.686(4)°.
	c = 22.2033(10) Å	γ = 105.641(4)°.
Volume	3369.1(3) Å^3	
Z	1	
Density (calculated)	1.133 Mg/m^3	
Absorption coefficient	0.994 mm^{-1}	
F(000)	1172	
Crystal size	0.180 x 0.140 x 0.130 mm^3	
Theta range for data collection	3.231 to 25.701°.	
Index ranges	-14<=h<=14, -16<=k<=16, -26<=l<=26	
Reflections collected	36153	
Independent reflections	12604 [R(int) = 0.0490]	
Completeness to theta = 25.000°	99.7 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	1.000 and 0.566
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12604 / 48 / 729
Goodness-of-fit on F^2	1.032
Final R indices [I>2sigma(I)]	R1 = 0.0692, wR2 = 0.1756
R indices (all data)	R1 = 0.1031, wR2 = 0.1941
Extinction coefficient	n/a
Largest diff. peak and hole	1.200 and -0.637 e.$Å^{-3}$

12. Computational Results

Energy minimized structures

Full geometry optimizations were performed with the Gaussian 09 Rev D.018 suite of programs. The DFT level of theory B3LYP/6-31G(d) and separately Lanl2dz basis set for metals were chosen for structure optimization.

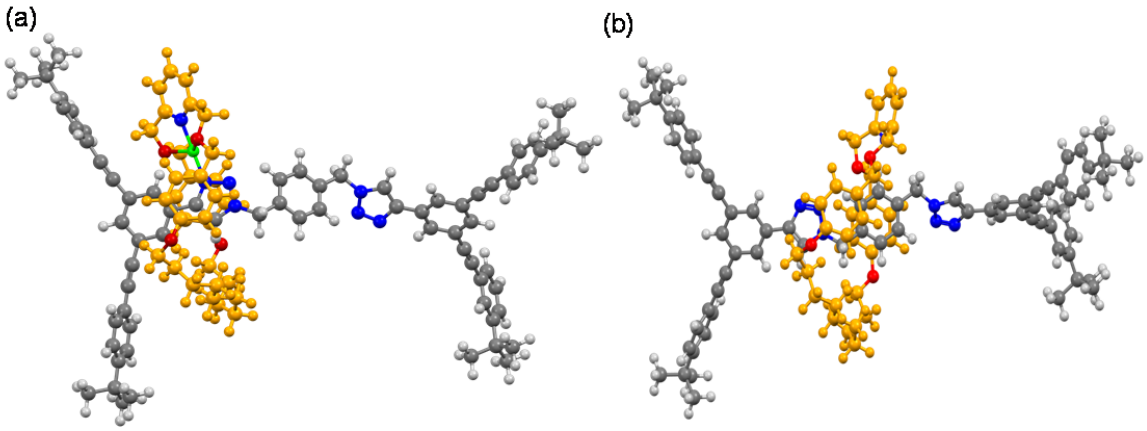


Figure S57. (a) Energy-optimized structure of $[Cu(\mathbf{1})(\mathbf{5})]^+$. (b) Energy-optimized structure of [2]rotaxane [(**1**)(**5**)].

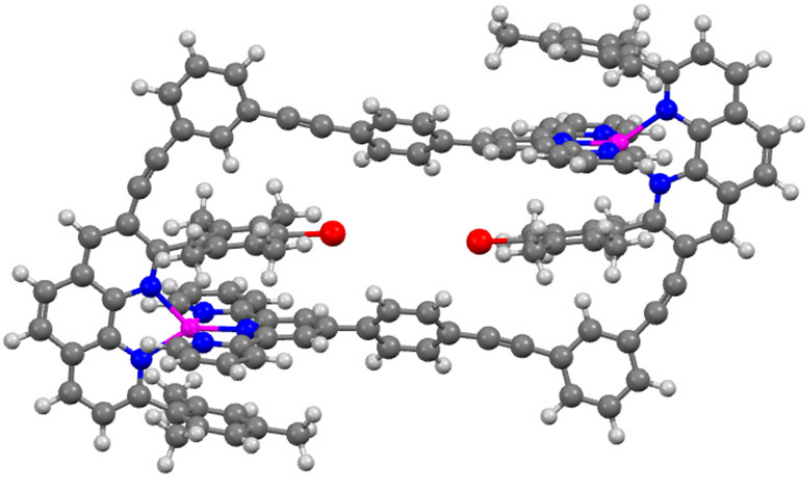


Figure S58. Energy-optimized structure of $[Zn_2(\mathbf{4})_2]^{4+}$.

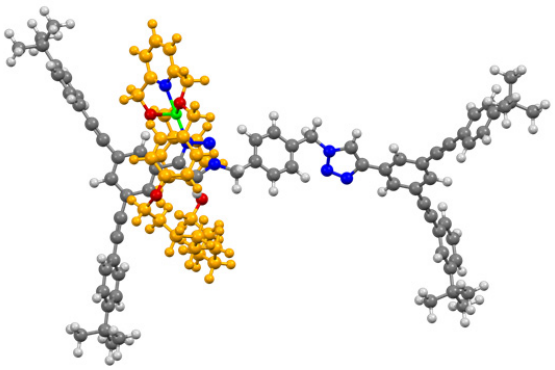


Figure S59. Energy-optimized structure of $[Cu(\mathbf{1})(\mathbf{5})]^{+}$, calculated using Gaussian 09 at B3LYP/6-31G(d) and separately Lanl2dz basis set for copper(I)

C	0.310000000	-3.983400000	1.099200000
C	0.630500000	-4.796800000	0.000400000
C	-0.885100000	-3.259000000	1.093400000
C	-0.228500000	-4.859600000	-1.095500000
C	-1.739100000	-3.309200000	-0.012700000
C	-1.411500000	-4.101000000	-1.118400000
C	1.318000000	-3.793800000	2.205900000
H	0.860200000	-3.354500000	3.095700000
H	1.818800000	-4.720500000	2.487000000
C	2.350000000	-1.505700000	1.733400000
C	3.516900000	-1.130400000	1.099400000
C	4.090200000	0.162500000	0.763400000
C	5.463700000	0.228500000	0.518300000
C	3.309700000	1.306700000	0.582200000
C	6.063500000	1.388500000	0.005200000
H	6.103300000	-0.599700000	0.802200000
C	3.895100000	2.499300000	0.109500000
H	2.241700000	1.277800000	0.753800000
C	5.270700000	2.529900000	-0.200600000
N	7.518200000	-2.703700000	-0.936400000
C	8.407000000	-3.399300000	-0.173500000
C	7.899300000	-2.268400000	-2.161900000
C	9.678400000	-3.717500000	-0.640000000
C	7.934200000	-3.758600000	1.201600000
C	9.145500000	-2.591600000	-2.696200000
C	6.988000000	-1.287200000	-2.852600000
C	10.043900000	-3.332100000	-1.932600000
H	10.374900000	-4.242200000	0.002000000
H	7.181400000	-4.560800000	1.165200000
H	8.770000000	-4.092400000	1.827200000
O	7.328100000	-2.555100000	1.755500000
H	9.416000000	-2.237100000	-3.682900000
H	7.378100000	-0.280600000	-2.664900000
H	6.966500000	-1.455700000	-3.935100000
O	5.653600000	-1.297600000	-2.296900000
H	11.023700000	-3.573200000	-2.322500000
C	6.830000000	-2.693700000	3.130800000
C	4.592700000	-1.960200000	-3.096700000
H	7.673300000	-2.999300000	3.766300000
H	6.060900000	-3.475400000	3.167300000
C	6.268900000	-1.363200000	3.539000000
H	4.784000000	-1.708900000	-4.147300000
H	4.662900000	-3.047100000	-2.974900000
C	3.276900000	-1.430000000	-2.622100000
C	5.011800000	-1.274300000	4.149400000
C	7.005500000	-0.186300000	3.318700000
C	3.009800000	-0.055800000	-2.701000000
C	2.315100000	-2.273600000	-2.044300000
C	4.493300000	-0.036000000	4.539800000
H	4.434800000	-2.178200000	4.320700000
C	6.494100000	1.053000000	3.699600000
H	7.971400000	-0.248700000	2.830200000
C	1.834000000	0.483900000	-2.178800000
H	3.747500000	0.607400000	-3.140000000
C	1.139300000	-1.750800000	-1.518200000
H	2.500700000	-3.340400000	-1.978700000
C	5.237000000	1.126900000	4.315600000
H	3.529600000	0.042100000	5.028600000
H	7.058700000	1.963800000	3.539600000
C	0.916800000	-0.366700000	-1.547500000
H	1.662500000	1.551300000	-2.230700000
H	0.392000000	-2.378500000	-1.059500000
O	4.751700000	2.358600000	4.761300000
O	-0.208200000	0.067100000	-0.875100000
C	4.187000000	3.267900000	3.737300000
C	-0.523400000	1.496800000	-0.809800000
C	2.719700000	2.963000000	3.469100000
H	4.316700000	4.265600000	4.163200000
H	4.782300000	3.188300000	2.819900000
H	-0.942800000	1.820100000	-1.769900000

H	0.390000000	2.072100000	-0.611200000
C	-1.504600000	1.649200000	0.340400000
C	1.815600000	3.184600000	4.690600000
H	2.634100000	1.919500000	3.132500000
H	2.396800000	3.585500000	2.625800000
H	-2.410400000	1.066900000	0.133000000
H	-1.033700000	1.194500000	1.221700000
C	-1.850500000	3.116900000	0.632800000
C	0.382400000	2.653700000	4.501800000
H	2.276600000	2.693900000	5.556700000
H	1.779700000	4.259500000	4.923000000
H	-0.932800000	3.713600000	0.643000000
H	-2.465200000	3.525500000	-0.180400000
C	-2.582600000	3.308800000	1.973300000
C	-0.378600000	3.280800000	3.321200000
H	-0.186700000	2.822800000	5.426200000
H	0.418300000	1.560800000	4.361300000
H	-3.572000000	2.832900000	1.927300000
H	-2.758800000	4.382900000	2.114900000
C	-1.818800000	2.755600000	3.193200000
H	0.166400000	3.082200000	2.389700000
H	-0.395500000	4.375200000	3.433900000
H	-2.378000000	3.010000000	4.104200000
H	-1.798500000	1.656500000	3.152200000
H	5.710900000	3.435000000	-0.599700000
C	3.045000000	3.629600000	-0.078500000
C	2.174400000	4.477700000	-0.178700000
C	7.446400000	1.279600000	-0.339100000
C	8.573600000	0.896800000	-0.609100000
C	9.890600000	0.417300000	-0.871100000
C	10.477300000	0.526800000	-2.147700000
C	10.622700000	-0.235400000	0.144300000
C	11.753400000	0.012400000	-2.392700000
H	9.935300000	1.036900000	-2.938300000
C	11.894100000	-0.737000000	-0.111700000
H	10.188900000	-0.321300000	1.134200000
C	12.493600000	-0.625400000	-1.382200000
H	12.178800000	0.137300000	-3.379900000
H	12.440200000	-1.207800000	0.698200000
C	1.045100000	5.346100000	-0.241600000
C	0.670100000	6.120700000	0.877300000
C	0.231500000	5.386500000	-1.388700000
C	-0.495300000	6.880200000	0.847300000
H	1.292400000	6.107300000	1.764900000
C	-0.934700000	6.152900000	-1.404200000
H	0.512200000	4.806100000	-2.260700000
C	-1.332300000	6.905800000	-0.287000000
H	-0.762400000	7.459100000	1.724000000
H	-1.538500000	6.155700000	-2.301700000
H	-1.135700000	-2.617300000	1.932200000
H	-2.634700000	-2.701800000	-0.026400000
H	0.033800000	-5.474100000	-1.948800000
H	1.566800000	-5.346600000	-0.003700000
C	-2.279300000	-4.130900000	-2.364700000
H	-2.971900000	-3.284500000	-2.355800000
H	-1.668300000	-4.053300000	-3.269900000
C	-4.419500000	-5.471300000	-2.753100000
C	-4.627800000	-6.841300000	-2.837200000
H	-5.081400000	-4.630900000	-2.863600000
C	-5.844700000	-7.604100000	-3.104700000
C	-5.789800000	-9.005500000	-3.116400000
C	-7.065300000	-6.957800000	-3.345500000
C	-6.948100000	-9.764200000	-3.364400000
H	-4.846800000	-9.500900000	-2.925500000
C	-8.235900000	-7.699400000	-3.593200000
H	-7.130200000	-5.875800000	-3.338300000
C	-8.168700000	-9.104700000	-3.601300000
C	-6.885700000	-11.191200000	-3.375400000
C	-9.476200000	-7.030100000	-3.825500000
H	-9.064800000	-9.683000000	-3.787800000
C	-6.835400000	-12.408500000	-3.367200000
C	-10.537800000	-6.461500000	-4.011900000
C	-6.806600000	-13.833400000	-3.268200000
C	-11.782500000	-5.790100000	-4.206600000
C	-6.829500000	-14.465000000	-2.007000000
C	-6.757100000	-14.624900000	-4.431100000
C	-12.206000000	-5.405200000	-5.494400000
C	-12.621800000	-5.493800000	-3.114600000
C	-6.803900000	-15.854800000	-1.935300000
H	-6.869000000	-13.860600000	-1.108300000
C	-6.733000000	-16.027200000	-4.369400000
H	-6.743500000	-14.121400000	-5.390900000
C	-13.421200000	-4.747500000	-5.674800000
H	-11.575400000	-5.628600000	-6.347800000

C	-13.834800000	-4.834400000	-3.308600000
H	-12.314100000	-5.785200000	-2.116600000
C	-6.756600000	-16.629500000	-3.101100000
H	-6.823900000	-16.344700000	-0.967400000
C	-14.263800000	-4.441800000	-4.589700000
H	-13.714000000	-4.471900000	-6.680500000
H	-14.450200000	-4.625100000	-2.443200000
H	-6.741900000	-17.707600000	-3.010300000
H	1.543800000	-0.925600000	2.144600000
N	4.174300000	-2.295600000	0.738700000
N	3.491100000	-3.373500000	1.146200000
N	2.377200000	-2.869000000	1.759300000
N	-3.091800000	-5.331000000	-2.461700000
N	-2.473800000	-6.572600000	-2.374800000
N	-3.414000000	-7.475000000	-2.602000000
C	13.920200000	-1.162800000	-1.594600000
C	14.896600000	-0.375900000	-0.682500000
H	14.634200000	-0.480400000	0.375000000
H	15.918900000	-0.747200000	-0.816000000
H	14.882000000	0.690200000	-0.931600000
C	13.980000000	-2.665500000	-1.212600000
H	13.687900000	-2.829900000	-0.170300000
H	13.316700000	-3.257800000	-1.850900000
H	14.999200000	-3.045600000	-1.340900000
C	14.391500000	-1.013500000	-3.055800000
H	13.749600000	-1.571000000	-3.748300000
H	14.410000000	0.035500000	-3.369700000
H	15.408000000	-1.407500000	-3.154500000
C	-2.631500000	7.727700000	-0.260000000
C	-2.298200000	9.214800000	0.025500000
H	-3.220000000	9.806700000	0.050300000
H	-1.792100000	9.340100000	0.987900000
H	-1.648000000	9.622700000	-0.756000000
C	-3.552500000	7.179600000	0.861900000
H	-3.800300000	6.128300000	0.679400000
H	-3.076800000	7.251700000	1.845300000
H	-4.486100000	7.752500000	0.895100000
C	-3.397900000	7.649500000	-1.596200000
H	-2.801400000	8.041500000	-2.427500000
H	-3.693900000	6.621600000	-1.833400000
H	-4.310600000	8.250400000	-1.528400000
C	-15.628800000	-3.768400000	-4.814800000
C	-6.689000000	-16.840500000	-5.676300000
C	-15.559000000	-2.738600000	-5.968400000
H	-15.346000000	-3.211900000	-6.931900000
H	-16.522500000	-2.225800000	-6.063500000
H	-14.786600000	-1.985700000	-5.776600000
C	-16.118800000	-3.029800000	-3.548000000
H	-16.325000000	-3.719300000	-2.723400000
H	-15.381400000	-2.294100000	-3.208200000
H	-17.052200000	-2.501700000	-3.770500000
C	-16.658300000	-4.870900000	-5.181900000
H	-17.647100000	-4.428200000	-5.351800000
H	-16.354800000	-5.399600000	-6.092100000
H	-16.742300000	-5.606200000	-4.374300000
C	-5.407500000	-16.471000000	-6.467400000
H	-5.365700000	-17.038500000	-7.404600000
H	-5.382000000	-15.404900000	-6.715100000
H	-4.511800000	-16.704700000	-5.880900000
C	-7.937100000	-16.504700000	-6.532400000
H	-7.917500000	-17.075800000	-7.468100000
H	-8.855300000	-16.759200000	-5.991900000
H	-7.977700000	-15.440500000	-6.785700000
C	-6.675800000	-18.360900000	-5.415500000
H	-5.796600000	-18.663000000	-4.835500000
H	-7.573800000	-18.685100000	-4.878300000
H	-6.646800000	-18.896200000	-6.370600000
Cu	5.819700000	-2.239700000	-0.171100000

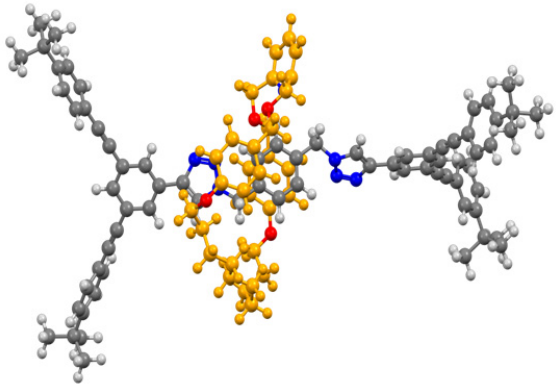


Figure S60. Energy-optimized structure of [(**1**)(**5**)], calculated using Gaussian 09 at B3LYP/6-31G(d) level of theory.

C	-8.479800000	2.496000000	-0.382600000
C	-8.603000000	3.876100000	-0.631000000
C	-8.032400000	2.076100000	0.885200000
C	-8.338500000	4.812800000	0.383300000
C	-7.760000000	3.012000000	1.897900000
C	-7.920400000	4.389200000	1.659200000
C	-8.711900000	1.476900000	-1.480400000
H	-8.011300000	0.651700000	-1.331100000
H	-9.727100000	1.080700000	-1.401200000
C	-8.336600000	1.207200000	-3.974200000
C	-8.442300000	2.033200000	-5.024000000
C	-8.270700000	1.717500000	-6.461300000
C	-8.801700000	2.586000000	-7.432800000
C	-7.524800000	0.609800000	-6.915500000
C	-8.618200000	2.375600000	-8.807200000
H	-9.366500000	3.413400000	-7.140200000
C	-7.273600000	0.431800000	-8.291500000
H	-7.095400000	-0.052000000	-6.219900000
C	-7.837600000	1.297900000	-9.242000000
N	-9.200300000	7.615500000	0.490200000
C	-10.361300000	8.115100000	0.844100000
C	-8.427700000	8.333100000	-0.302300000
C	-10.546600000	9.505400000	0.945300000
C	-11.484000000	7.127000000	0.655300000
C	-8.492400000	9.737200000	-0.290700000
C	-7.931200000	7.538900000	-1.496200000
C	-9.531900000	10.339300000	0.440800000
H	-11.469000000	9.912000000	1.240300000
H	-11.699300000	6.703300000	1.639300000
H	-12.372100000	7.647500000	0.288700000
O	-11.110100000	6.085800000	-0.339200000
H	-7.878200000	10.314500000	-0.917700000
H	-8.675100000	7.627000000	-2.292500000
H	-6.989900000	7.943000000	-1.871900000
O	-7.827100000	6.125700000	-1.149600000
H	-9.659900000	11.381900000	0.420900000
C	-11.902800000	4.933800000	0.074700000
C	-6.627900000	6.051500000	-0.302000000
H	-12.942100000	5.254400000	0.212800000
H	-11.538600000	4.577700000	1.040700000
C	-11.981800000	3.763600000	-0.876700000
H	-5.828000000	6.668000000	-0.725000000
H	-6.867700000	6.459300000	0.683500000
C	-6.004000000	4.688700000	-0.109600000
C	-11.908500000	2.455000000	-0.360300000
C	-12.276000000	3.942300000	-2.241500000
C	-5.475000000	3.969400000	-1.196900000
C	-5.810900000	4.187200000	1.192000000
C	-12.044600000	1.342600000	-1.205500000
H	-11.748100000	2.299400000	0.667300000
C	-12.399800000	2.828500000	-3.091100000
H	-12.387800000	4.910600000	-2.635400000
C	-4.853700000	2.724200000	-0.991200000
H	-5.556700000	4.353200000	-2.172300000
C	-5.215800000	2.932300000	1.396000000
H	-6.143400000	4.735900000	2.024200000
C	-12.262500000	1.524900000	-2.581400000
H	-11.977000000	0.373200000	-0.805400000
H	-12.598700000	2.972300000	-4.112800000
C	-4.764300000	2.174200000	0.302600000
H	-4.488500000	2.192100000	-1.820500000
H	-5.139500000	2.545700000	2.370900000
O	-12.377800000	0.441200000	-3.393500000
O	-4.313700000	0.914400000	0.558100000
C	-11.363500000	0.008000000	-4.257400000
C	-4.354400000	-0.156500000	-0.339000000
C	-10.176400000	-0.621400000	-3.478500000
H	-11.781000000	-0.735400000	-4.939900000
H	-11.004000000	0.853100000	-4.848600000
H	-3.376100000	-0.293900000	-0.800400000
H	-5.090600000	0.052100000	-1.112000000
C	-4.793100000	-1.445400000	0.401200000
C	-10.550000000	-1.976900000	-2.817400000
H	-9.857700000	0.084800000	-2.712500000
H	-9.344900000	-0.781800000	-4.168600000
H	-3.973600000	-1.800100000	1.030500000
H	-5.636400000	-1.196000000	1.047500000
C	-5.204800000	-2.569200000	-0.593400000
C	-9.863700000	-2.201800000	-1.441400000
H	-11.629900000	-2.004400000	-2.649300000
H	-10.294900000	-2.793900000	-3.496400000
H	-5.502300000	-2.139400000	-1.547300000
H	-4.334900000	-3.207200000	-0.771400000
C	-6.371900000	-3.451600000	-0.073800000

C	-8.354400000	-2.561200000	-1.526700000
H	-10.382200000	-3.027500000	-0.945900000
H	-9.989300000	-1.306900000	-0.827200000
H	-6.150600000	-3.753200000	0.953500000
H	-6.423500000	-4.357400000	-0.683500000
C	-7.765500000	-2.758100000	-0.099400000
H	-7.817900000	-1.759800000	-2.032600000
H	-8.239500000	-3.483000000	-2.100800000
H	-8.451300000	-3.390200000	0.471700000
H	-7.709500000	-1.788300000	0.399100000
H	-7.669600000	1.144000000	-10.268100000
C	-6.399100000	-0.586000000	-8.764500000
C	-5.659100000	-1.447200000	-9.164300000
C	-9.271000000	3.228600000	-9.741100000
C	-9.822500000	3.954600000	-10.527300000
C	-10.499600000	4.779300000	-11.471200000
C	-9.943000000	5.994100000	-11.901500000
C	-11.757000000	4.388800000	-11.958400000
C	-10.636700000	6.804400000	-12.817000000
H	-9.005100000	6.303300000	-11.540100000
C	-12.445600000	5.204500000	-12.870500000
H	-12.191500000	3.485600000	-11.640800000
C	-11.901100000	6.427000000	-13.319800000
H	-10.184700000	7.703700000	-13.115200000
H	-13.385300000	4.882900000	-13.214400000
C	-4.752100000	-2.443600000	-9.623600000
C	-5.227900000	-3.629100000	-10.205300000
C	-3.372900000	-2.278400000	-9.423200000
C	-4.325600000	-4.640600000	-10.573700000
H	-6.259200000	-3.770300000	-10.353600000
C	-2.477200000	-3.296500000	-9.788800000
H	-3.004000000	-1.397500000	-8.982400000
C	-2.936300000	-4.502700000	-10.360400000
H	-4.711600000	-5.518200000	-11.004100000
H	-1.455000000	-3.136200000	-9.612700000
H	-7.897300000	1.052500000	1.084700000
H	-7.437800000	2.674700000	2.840400000
H	-8.458500000	5.837300000	0.179500000
H	-8.899600000	4.217100000	-1.579600000
C	-7.673700000	5.392700000	2.765300000
H	-6.878000000	6.080800000	2.470800000
H	-8.584600000	5.976100000	2.917800000
C	-7.724300000	5.180900000	5.281000000
C	-6.766500000	4.826800000	6.149700000
H	-8.589700000	5.729300000	5.489100000
C	-6.697200000	5.123400000	7.588700000
C	-5.439600000	5.177400000	8.222100000
C	-7.858100000	5.371500000	8.349100000
C	-5.338700000	5.481600000	9.591200000
H	-4.563300000	5.006900000	7.665300000
C	-7.762400000	5.667600000	9.721300000
H	-8.805600000	5.330800000	7.894600000
C	-6.501900000	5.725300000	10.340000000
C	-4.062900000	5.584300000	10.220400000
C	-8.928100000	5.923600000	10.504100000
H	-6.428400000	5.958900000	11.363400000
C	-2.991200000	5.667700000	10.764000000
C	-9.889700000	6.141700000	11.196700000
C	-1.719300000	5.775600000	11.400100000
C	-11.028200000	6.393300000	12.018100000
C	-1.030700000	6.999000000	11.377800000
C	-1.161700000	4.669900000	12.066400000
C	-11.677400000	5.336500000	12.675900000
C	-11.484100000	7.705900000	12.219900000
C	0.212800000	7.104500000	12.018400000
H	-1.440000000	7.834200000	10.887600000
C	0.086800000	4.757300000	12.721700000
H	-1.694000000	3.763100000	12.069100000
C	-12.778600000	5.591200000	13.510800000
H	-11.333900000	4.349600000	12.557400000
C	-12.585800000	7.952600000	13.056700000
H	-10.994000000	8.512900000	11.756700000
C	0.764500000	5.994900000	12.680100000
H	0.733300000	8.017500000	12.003800000
C	-13.276600000	6.899600000	13.695500000
H	-13.220200000	4.776100000	14.003500000
H	-12.879400000	8.950300000	13.200600000
H	1.698100000	6.116000000	13.144400000
H	-8.133200000	0.182100000	-3.996600000
N	-8.720900000	3.316000000	-4.467400000
N	-8.795600000	3.282700000	-3.232400000
N	-8.543500000	2.000600000	-2.824500000
N	-7.290100000	4.749100000	4.010500000
N	-6.067500000	4.166100000	4.195500000

N	-5.751100000	4.187200000	5.394700000
C	-12.688200000	7.285700000	-14.322400000
C	-12.922100000	6.469200000	-15.632400000
H	-13.524100000	5.581500000	-15.433400000
H	-13.445600000	7.080500000	-16.370100000
H	-11.964000000	6.156100000	-16.052200000
C	-14.063300000	7.685800000	-13.700500000
H	-14.669000000	6.801700000	-13.497000000
H	-13.906100000	8.226200000	-12.764800000
H	-14.615800000	8.328900000	-14.388500000
C	-11.950000000	8.604700000	-14.716200000
H	-11.784500000	9.226000000	-13.834100000
H	-10.989300000	8.378400000	-15.182700000
H	-12.551300000	9.173900000	-15.428600000
C	-1.986800000	-5.647500000	-10.745800000
C	-2.062500000	-5.887400000	-12.285700000
H	-1.372500000	-6.681500000	-12.578000000
H	-3.070500000	-6.180800000	-12.582100000
H	-1.792100000	-4.973700000	-12.818800000
C	-2.405400000	-6.946300000	-9.986700000
H	-2.401200000	-6.765600000	-8.909800000
H	-3.405100000	-7.265000000	-10.284600000
H	-1.707400000	-7.755700000	-10.209500000
C	-0.494300000	-5.359400000	-10.384100000
H	-0.134500000	-4.479700000	-10.921000000
H	-0.388600000	-5.193700000	-9.310200000
H	0.131400000	-6.209900000	-10.663300000
C	-14.444600000	7.178200000	14.657300000
C	0.669500000	3.521300000	13.426300000
C	-15.465100000	5.994400000	14.689900000
H	-15.018000000	5.106800000	15.139100000
H	-16.339600000	6.265500000	15.285400000
H	-15.793600000	5.755200000	13.676600000
C	-15.252600000	8.450100000	14.240800000
H	-14.649800000	9.351100000	14.361600000
H	-15.569000000	8.368500000	13.199200000
H	-16.140500000	8.555800000	14.867900000
C	-13.867500000	7.390900000	16.089400000
H	-14.675000000	7.590900000	16.796500000
H	-13.329200000	6.498700000	16.415200000
H	-13.178100000	8.237300000	16.095900000
C	0.935700000	2.405700000	12.368200000
H	1.379200000	1.529900000	12.846200000
H	0.005700000	2.101000000	11.885900000
H	1.622700000	2.773700000	11.603500000
C	-0.338800000	3.000600000	14.498900000
H	0.088700000	2.152600000	15.038000000
H	-0.563700000	3.793700000	15.214800000
H	-1.269100000	2.674500000	14.032400000
C	2.018700000	3.808800000	14.160300000
H	2.780000000	4.131500000	13.447600000
H	1.882100000	4.584200000	14.916600000
H	2.377500000	2.904500000	14.656600000

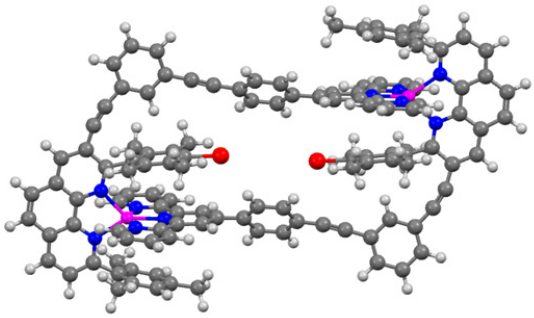


Figure S61. Energy-optimized structure of $[Zn_2(\mathbf{4})]^{4+}$, calculated using Gaussian 09 at B3LYP/6-31G(d) and separately Lanl2dz basis set for Zn(II).

C	-8.479800000	2.496000000	-0.382600000
C	-8.603000000	3.876100000	-0.631000000
C	-8.032400000	2.076100000	0.885200000
C	-8.338500000	4.812800000	0.383300000
C	-7.760000000	3.012000000	1.897900000
C	-7.920400000	4.389200000	1.659200000
C	-8.711900000	1.476900000	-1.480400000
H	-8.011300000	0.651700000	-1.331100000
H	-9.727100000	1.080700000	-1.401200000
C	-8.336600000	1.207200000	-3.974200000
C	-8.442300000	2.033200000	-5.024000000
C	-8.270700000	1.717500000	-6.461300000
C	-8.801700000	2.586000000	-7.432800000
C	-7.524800000	0.609800000	-6.915500000
C	-8.618200000	2.375600000	-8.807200000
H	-9.366500000	3.413400000	-7.140200000

C	-7.273600000	0.431800000	-8.291500000
H	-7.095400000	-0.052000000	-6.219900000
C	-7.837600000	1.297900000	-9.242000000
N	-9.200300000	7.615500000	0.490200000
C	-10.361300000	8.115100000	0.844100000
C	-8.427700000	8.333100000	-0.302300000
C	-10.546600000	9.505400000	0.945300000
C	-11.484000000	7.127000000	0.655300000
C	-8.492400000	9.737200000	-0.290700000
C	-7.931200000	7.538900000	-1.496200000
C	-9.531900000	10.339300000	0.440800000
H	-11.469000000	9.912000000	1.240300000
H	-11.699300000	6.703300000	1.639300000
H	-12.372100000	7.647500000	0.288700000
O	-11.110100000	6.085800000	-0.339200000
H	-7.878200000	10.314500000	-0.917700000
H	-8.675100000	7.627000000	-2.292500000
H	-6.989900000	7.943000000	-1.871900000
O	-7.827100000	6.125700000	-1.149600000
H	-9.659900000	11.381900000	0.420900000
C	-11.902800000	4.933800000	0.074700000
C	-6.627900000	6.051500000	-0.302000000
H	-12.942100000	5.254400000	0.212800000
H	-11.538600000	4.577700000	1.040700000
C	-11.981800000	3.763600000	-0.876700000
H	-5.828000000	6.668000000	-0.725000000
H	-6.867700000	6.459300000	0.683500000
C	-6.004000000	4.688700000	-0.109600000
C	-11.908500000	2.455000000	-0.360300000
C	-12.276000000	3.942300000	-2.241500000
C	-5.475000000	3.969400000	-1.196900000
C	-5.810900000	4.187200000	1.192000000
C	-12.044600000	1.342600000	-1.205500000
H	-11.748100000	2.299400000	0.667300000
C	-12.399800000	2.828500000	-3.091100000
H	-12.387800000	4.910600000	-2.635400000
C	-4.853700000	2.724200000	-0.991200000
H	-5.556700000	4.353200000	-2.172300000
C	-5.215800000	2.932300000	1.396000000
H	-6.143400000	4.735900000	2.024200000
C	-12.262500000	1.524900000	-2.581400000
H	-11.977000000	0.373200000	-0.805400000
H	-12.598700000	2.972300000	-4.112800000
C	-4.764300000	2.174200000	0.302600000
H	-4.488500000	2.192100000	-1.820500000
H	-5.139500000	2.545700000	2.370900000
O	-12.377800000	0.441200000	-3.393500000
O	-4.313700000	0.914400000	0.558100000
C	-11.363500000	0.008000000	-4.257400000
C	-4.354400000	-0.156500000	-0.339000000
C	-10.176400000	-0.621400000	-3.478500000
H	-11.781000000	-0.735400000	-4.939900000
H	-11.004000000	0.853100000	-4.848600000
H	-3.376100000	-0.293900000	-0.800400000
H	-5.090600000	0.052100000	-1.112000000
C	-4.793100000	-1.445400000	0.401200000
C	-10.550000000	-1.976900000	-2.817400000
H	-9.857700000	0.084800000	-2.712500000
H	-9.344900000	-0.781800000	-4.168600000
H	-3.973600000	-1.800100000	1.030500000
H	-5.636400000	-1.196000000	1.047500000
C	-5.204800000	-2.569200000	-0.593400000
C	-9.863700000	-2.201800000	-1.441400000
H	-11.629900000	-2.004400000	-2.649300000
H	-10.294900000	-2.793900000	-3.496400000
H	-5.502300000	-2.139400000	-1.547300000
H	-4.334900000	-3.207200000	-0.771400000
C	-6.371900000	-3.451600000	-0.073800000
C	-8.354400000	-2.561200000	-1.526700000
H	-10.382200000	-3.027500000	-0.945900000
H	-9.989300000	-1.306900000	-0.827200000
H	-6.150600000	-3.753200000	0.953500000
H	-6.423500000	-4.357400000	-0.683500000
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H	-7.817900000	-1.759800000	-2.032600000
H	-8.239500000	-3.483000000	-2.100800000
H	-8.451300000	-3.390200000	0.471700000
H	-7.709500000	-1.788300000	0.399100000
H	-7.669600000	1.144000000	-10.268100000
C	-6.399100000	-0.586000000	-8.764500000
C	-5.659100000	-1.447200000	-9.164300000
C	-9.271000000	3.228600000	-9.741100000
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C	-10.636700000	6.804400000	-12.817000000
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C	-11.901100000	6.427000000	-13.319800000
H	-10.184700000	7.703700000	-13.115200000
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C	-4.752100000	-2.443600000	-9.623600000
C	-5.227900000	-3.629100000	-10.205300000
C	-3.372900000	-2.278400000	-9.423200000
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C	-2.477200000	-3.296500000	-9.788800000
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H	-7.437800000	2.674700000	2.840400000
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H	-8.899600000	4.217100000	-1.579600000
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C	-1.719300000	5.775600000	11.400100000
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C	-1.030700000	6.999000000	11.377800000
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H	-10.989300000	8.378400000	-15.182700000
H	-12.551300000	9.173900000	-15.428600000
C	-1.986800000	-5.647500000	-10.745800000
C	-2.062500000	-5.887400000	-12.285700000

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H	-0.388600000	-5.193700000	-9.310200000
H	0.131400000	-6.209900000	-10.663300000
C	-14.444600000	7.178200000	14.657300000
C	0.669500000	3.521300000	13.426300000
C	-15.465100000	5.994400000	14.689900000
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C	-15.252600000	8.450100000	14.240800000
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C	-13.867500000	7.390900000	16.089400000
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C	0.935700000	2.405700000	12.368200000
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H	1.622700000	2.773700000	11.603500000
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H	0.088700000	2.152600000	15.038000000
H	-0.563700000	3.793700000	15.214800000
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H	2.377500000	2.904500000	14.656600000

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