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Electronic Supporting Information (ESI)

Reversible switching from a three- to a nine-fold degenerate dynamic slider-on-deck through catenation

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1. Synthesis

1.1 General Information

All commercial reagents were used without further purification. Solvents were dried with the appropriate desiccants and distilled prior to use. Bruker Avance (400 MHz), Jeol ECZ (500MHz) and Varian (600 MHz) spectrometers were used to measure ^{1}H and ^{13}C NMR spectra employing 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-d8: δ_H 1.72 ppm, 3.58 ppm, δ_C 25.3 ppm, 67.2 ppm). The following abbreviations were used to describe NMR peak pattern: s = singlet, d = doublet, t = triplet, dd = doublet of doublets, ddd = doublet of doublets of doublets, td = triplet of doublets, brs = broad singlet, brd = broad doublet, m = multiplet. The coupling constant values are given in Hertz (Hz) and, wherever possible, assignment of protons is provided. The numbering of different carbons in different molecular skeletons does not necessarily follow IUPAC nomenclature rules; it was exclusively implemented 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 are not corrected. Infrared spectra were recorded on a Perkin Elmer Spectrum-Two FT-IR spectrometer. Elemental analysis was performed using the EA-3000 CHNS analyzer. UV-vis spectra were recorded on a Cary Win 50 (298 K) spectrometer. 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). The multi-component assembly of rotors was performed directly in the NMR tube with CD_2Cl_2 as solvent. Compounds **3**,[1] **5**,[2] **7**,[3] **6**,[4] **8**,[5] **9**,[2] **10**,[6] **13**[7] and complexes [**4**•**5**] [2] and ([Cu(**3**)$_2$]$^+$) [1] were prepared according to reported procedures available in literature.

1.2 Ligands used in this study

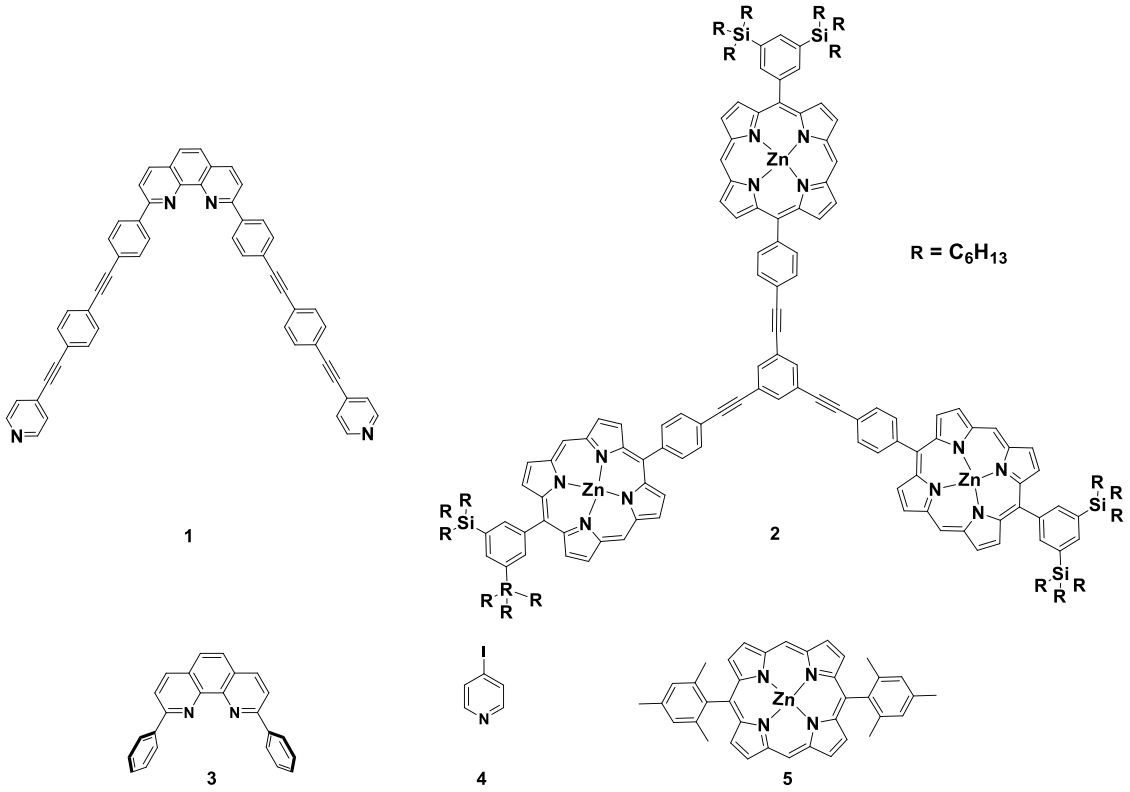
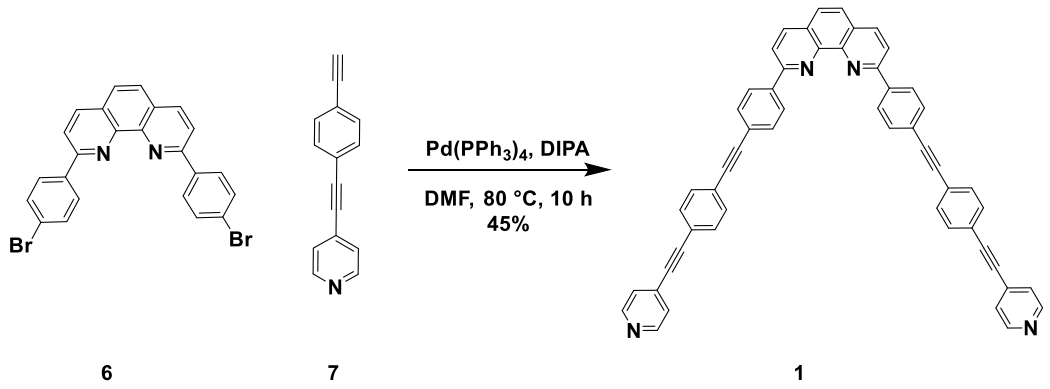


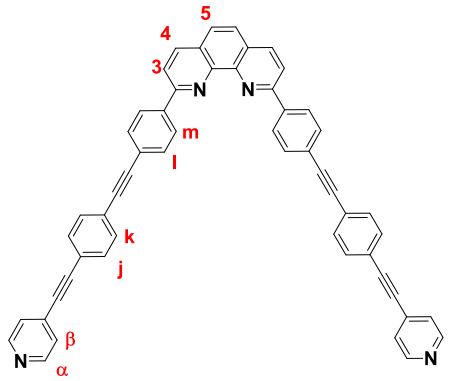
Figure S1: Ligands used in this study.

1.3. Synthesis of 1



Scheme S1: Synthetic route to Ligand **1.**

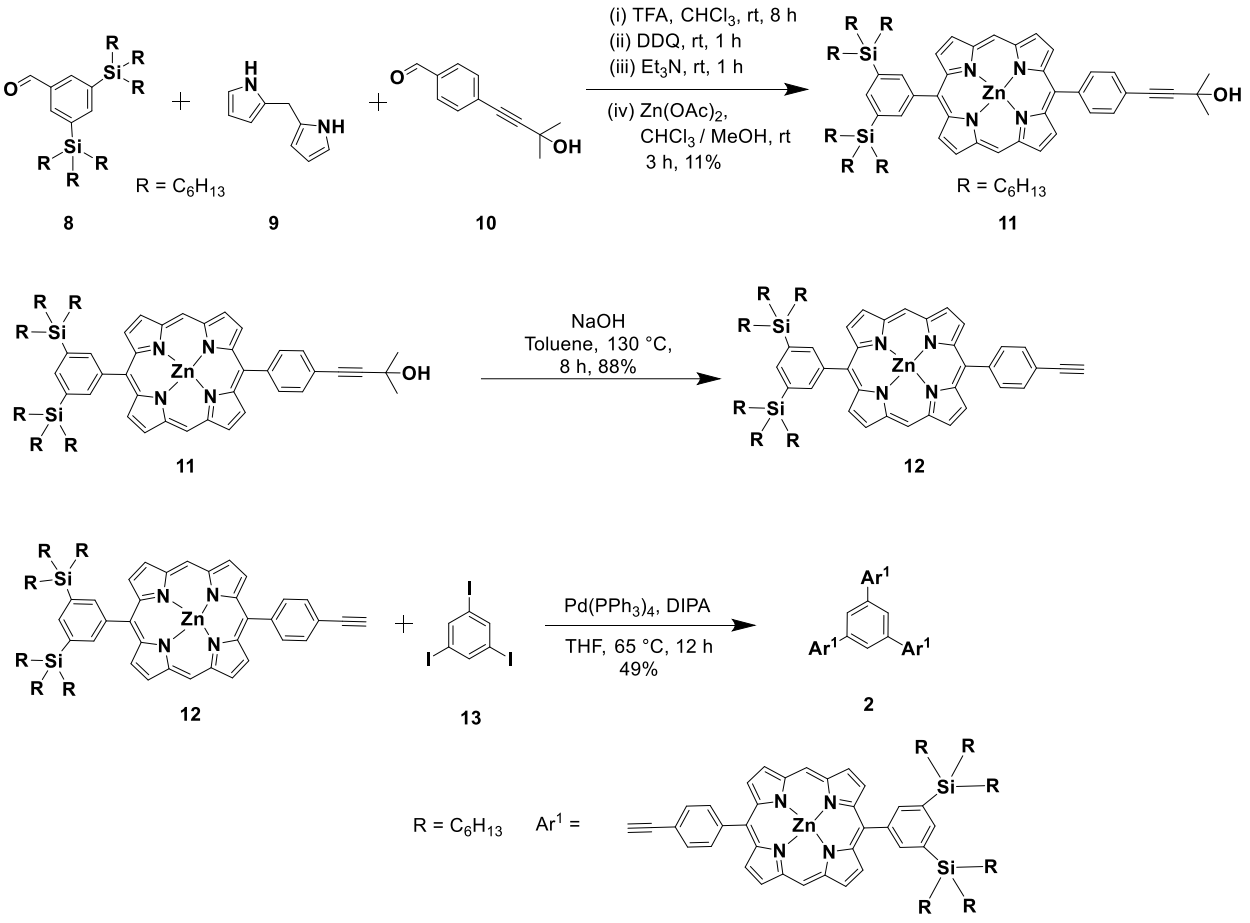
Synthesis of compound 1



1

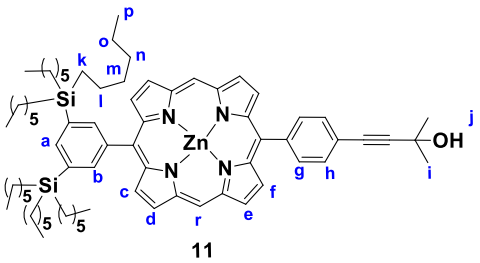
In a reaction tube, compound **7**[3] (50.0 mg, 160 µmol) and **6** (50.0 mg, 130 µmol) were dissolved in DMF and diisopropylamine (30 mL, 1:4, *v*/*v*) mixture. The solution was subjected to 15 min of sparging with N_2. $Pd(PPh_3)_4$ (15.1 mg, 13.0 µmol) was added under an inert N_2 atmosphere. The tube was sealed with a screw cap and stirred at 65 °C for 12 h (TLC). After cooling to room temp. and evaporation of the solvents, a crude brown residue was obtained. Purification of the residue by column chromatography using gradients of DCM-MeOH eluent (R_f = 0.2 in 2.5% MeOH in DCM on SiO_2) yielded the desired compound **1** as a pale-yellow solid (45.1 mg, 60.0 µmol, 45%). **Mp** > 250 °C. **IR (KBr):** $\tilde{\nu}$ = 524, 545, 599, 630, 664, 723, 745, 795, 821, 839, 893, 990, 1015, 1093, 1111, 1182, 1214, 1266, 1288, 1311, 1403, 1488, 1502, 1589, 1929, 2215, 3037, 3132 cm^{-1}. **^{1}H NMR (500 MHz, CD_2Cl_2):** δ = 8.60 (d, ^3J = 6.0 Hz, 4H, α-H), 8.51 (d, ^3J = 8.6 Hz, 4H, m-H), 8.40 (d, ^3J = 8.4 Hz, 2H, 4-H), 8.22 (d, ^3J = 8.4 Hz, 2H, 3-H), 7.87 (s, 2H, 5-H), 7.81 (d, ^3J = 8.6 Hz, 4H, l-H), 7.62 (m, 8H, j, k-H), 7.42 (d, ^3J = 6.0 Hz, 4H, β-H) ppm. **^{13}C NMR (125 MHz, CD_2Cl_2):** δ 155.9, 150.3, 146.7, 140.0, 137.5, 132.7, 132.3, 132.1, 131.4, 128.7, 127.9, 126.8, 125.8, 124.5, 124.3, 122.5, 120.4, 93.6, 92.1, 90.7, 88.8. **ESI-MS:** *m/z (%)* = 735.9 (100) [**1**+H]$^+$. **Elemental analysis** ($C_{54}H_{30}N_4 \cdot 0.2H_2O$): Calcd. C, 87.83; H, 4.15; N, 7.59. Found, C, 87.39; H, 3.71; N, 7.39.

1.4. Synthesis of Deck 2



Scheme S2: Synthetic route to Ligand **2**

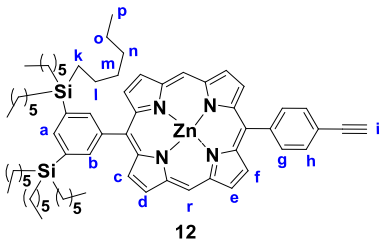
Synthesis of compound 11



In a 1 L flask, compounds **8** (1.33 g, 191 µmol), **9** (560 mg, 383 µmol), and **10** (361 mg, 191 µmol) were dissolved in a mixture of $CHCl_3$ (750 ml) and sparged with N_2 for 15 min. TFA (0.5 mL) was then slowly added dropwise over 10 min and the mixture was allowed to stir for 6 h

(TLC). DDQ (650 mg, 287 μmol) was then added and stirring continued for 1 h, followed by addition of triethylamine (500 μL) to quench the acid. The solvent was then reduced to a 150 mL. A solution of $Zn(OAc)_2$•$2H_2O$ (1.00 g, 456 μmol) in MeOH was added slowly into the crude mixture and stirred at room temperature for 4 h till completion (monitored by TLC). The solvent was then evaporated affording a dark red residue. The purification of the crude residue by chromatography running elution gradients of DCM-hexane (R_f = 0.4 in 80% DCM in hexane on SiO_2) yielded the desired product **11** (225 mg, 190 μmol, 11%) as a pink, glassy solid. **IR (KBr):** $\tilde{\nu}$ = 566, 699, 719, 729, 736, 781, 808, 849, 903, 960, 993, 1059, 1101, 1148, 1285, 1314, 1397, 1465, 1522, 1627, 2854, 2871, 2921, 2956, 3026, 3118, 3430 cm^{-1}. **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 10.30 (s, 2H, r-H), 9.44 (d, ^3J = 4.6 Hz, 2H, e-H), 9.40 (d, ^3J = 4.6 Hz, 2H, d-H), 9.16 (d, ^3J = 4.6 Hz, 2H, f-H), 9.08 (d, ^3J = 4.6 Hz, 2H, c-H), 8.37 (s, 2H, b-H), 8.20 (d, ^3J = 7.9 Hz, 2H, g-H), 8.05 (s, 1H, a-H), 7.86 (d, ^3J = 7.9 Hz, 2H, h-H), 2.10 (brs, 1H, j-H), 1.75 (s, 6H, i-H), 0.88-1.53 (m, 78H, k-, l-, m-, n-, o-, p-H) ppm. **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 150.6, 149.9, 149.7, 149.5, 143.0, 140.9, 140.8, 139.2, 135.1, 134.7, 133.0, 132.2, 132.0, 131.8, 130.1, 122.1, 121.9, 119.0, 106.4, 94.9, 82.5, 66.0, 33.7, 31.8, 31.7, 24.2, 22.8, 14.3, 12.9. **Elemental analysis** ($C_{73}H_{102}N_4OSi_2Zn$): Calcd. C, 74.74; H, 8.76; N, 4.78. Found, C, 74.41; H, 8.59; N, 4.47.

Synthesis of compound 12

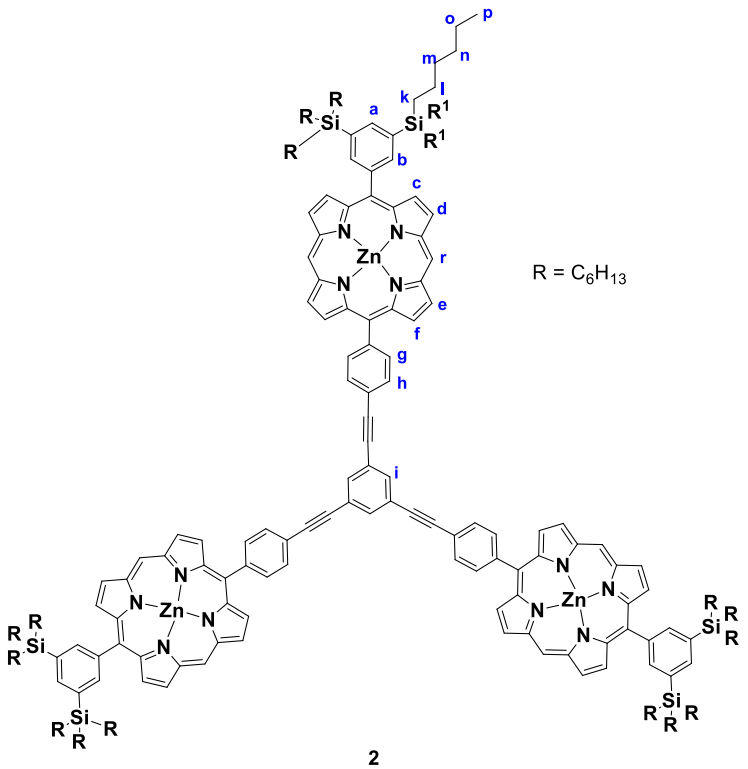


12

In a 250 mL flask, compound **11** (223 mg, 190 μmol) was dissolved in 80 mL of toluene, treated with NaOH granules (76.0 mg, 1.90 mmol) and refluxed at 125 °C for 4 h (TLC). Upon completion, the solvent was evaporated furnishing a dark pink residue which was dissolved in DCM, washed with H_2O, brine and subsequently dried over anhydrous $MgSO_4$. The solvent was evaporated affording a pink solid that was further purified by column chromatography running DCM-hexane eluent gradients (R_f = 0.85 in 80% DCM in hexane on SiO_2) to obtain the desired compound **12** (186 mg, 0.160 mmol, 88%) as a bright pink glassy solid. **IR (KBr):** $\tilde{\nu}$ = 603, 639,

696, 717, 776, 814, 845, 960, 994, 1007, 1059, 1101, 1145, 1180, 1287, 1312, 1375, 1396, 1456, 1496, 1522, 1553, 1627, 2583, 2921, 2956, 3279, 3318 cm^{-1}. **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 10.34 (s, 2H, r-H), 9.45 (m, 4H, e-, d-H), 9.16 (d, ^3J = 4.6 Hz, 2H, f-H), 9.12 (d, ^3J = 4.6 Hz, 2H, c-H), 8.34 (s, 2H, b-H), 8.24 (d, ^3J = 7.9 Hz, 2H, g-H), 8.02 (s, 1H, a-H), 7.94 (d, ^3J = 7.9 Hz, 2H, h-H), 3.35 (s, 1H, i-H), 0.86-1.54 (m, 78H, k-, l-, m-, n-, o-, p-H) ppm. **^{13}C NMR (125 MHz, $CDCl_3$):** δ 150.7, 149.9, 149.7, 149.6, 143.5, 140.9, 140.7, 139.2, 135.1, 134.7, 133.0, 132.3, 132.1, 131.9, 130.6, 121.9, 121.5, 118.9, 106.5, 84.0, 78.3, 33.7, 31.8, 24.2, 22.8, 14.3, 12.9. **Elemental analysis** ($C_{70}H_{96}N_4Si_2Zn•H_2O$): Calcd. C, 74.20; H, 8.72; N, 4.94. Found, C, 74.14; H, 8.73; N, 4.70.

Synthesis of compound 2



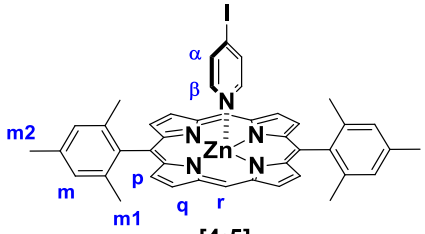
2

In a reaction tube, compounds **12**(186 mg, 160 µmol) and **13** (17.0 mg, 40.0 µmol)) were dissolved in THF and diisopropylamine (30 mL, 1:4, v/v). The solution was subjected to 15 min of sparging with N_2. Then, $Pd(PPh_3)_4$ (5.00 mg, 4.00 µmol) was added under an inert N_2 atmosphere. The tube was sealed with a screw cap and stirred at 65 °C for 12 h (TLC). After cooling to room temp. and evaporation of the solvents, the crude pink residue was dissolved in

DCM, washed with H_2O, brine and subsequently dried over anhydrous $MgSO_4$. The solvent was evaporated to obtain a pink solid which was further purified by size-exclusion column chromatography (R_f = 0.45 in 50% DCM in hexane on SiO_2) on Biobeads®-SX3 using distilled THF as the eluent to obtain the desired compound **2** as a bright-pink crystalline solid (60.5 mg, 177 μmol, 49%). **Mp** = 179-180 °C. **IR (KBr):** $\tilde{\nu}$ **=** 699, 718, 781, 808, 850, 962, 993, 1059, 1100, 1147, 1179, 1287, 1315, 1375, 1395, 1464, 1521, 1578, 2852, 2870.7, 2919, 2954 cm^{-1}. **^{1}H NMR (500 MHz, $CDCl_3$):** δ 10.43 (s, 6H, r-H), 9.57 (d, ^3J = 4.6 Hz, 6H, e-H), 9.50 (d, ^3J = 4.6 Hz, 6H, d-H), 9.25 (d, ^3J = 4.6 Hz, 6H, f-H), 9.18 (d, ^3J = 4.6 Hz, 6H, c-H), 8.40 (d, ^3J = 7.9 Hz, 6H, g-H), 8.38 (s, 6H, b-H), 8.16 (d, ^3J = 7.9 Hz, 6H, h-H), 8.15 (s, 3H, i-H), 8.08 (s, 3H, a-H), 0.86-1.53 (m, 234H, k-, l-, m-, n-, o-, p-H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$):** δ 150.9, 150.2, 150.0, 149.8, 143.8, 141.3, 141.1, 139.7, 135.5, 135.3, 134.9, 133.2, 132.5, 132.3, 132.1, 130.6, 125.0, 122.5, 122.2, 119.2, 106.6, 91.4, 89.2, 34.0, 32.1, 24.5, 23.1, 14.4, 13.1 ppm. **Elemental analysis** ($C_{216}H_{288}N_{12}Si_6Zn_3$): Calcd. C, 75.92; H, 8.49; N, 4.92. Found, C, 75.99; H, 8.30; N, 4.74.

2. Synthesis and characterization of complexes

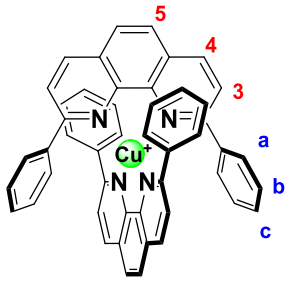
Complex C1



[4•5]

In an NMR tube, compound **4** (430 µg, 209 µmol) and **5** (1.30mg, 213 µmol) were dissolved in 560 µL of CD_2Cl_2 to obtain a clear pink solution. The sample was submitted for NMR measurement. Data were in full agreement with those reported.[1] **Yield:** Quantitative (by NMR). **^{1}H NMR (400 MHz, $CDCl_3$):** δ= 10.14 (s, 2H, r-H), 9.34 (d, ^3J = 4.4 Hz, 4H, q-H), 8.87 (d, ^3J = 4.4 Hz, 4H, p-H), 7.33 (s, 4H, m-H), 6.42 (d, ^3J = 5.4 Hz, 2H, β-H), 4.10 (brs, 2H, α-H), 2.66 (s, 6H, m2-H), 1.80 (s, 12H, m1-H) ppm.

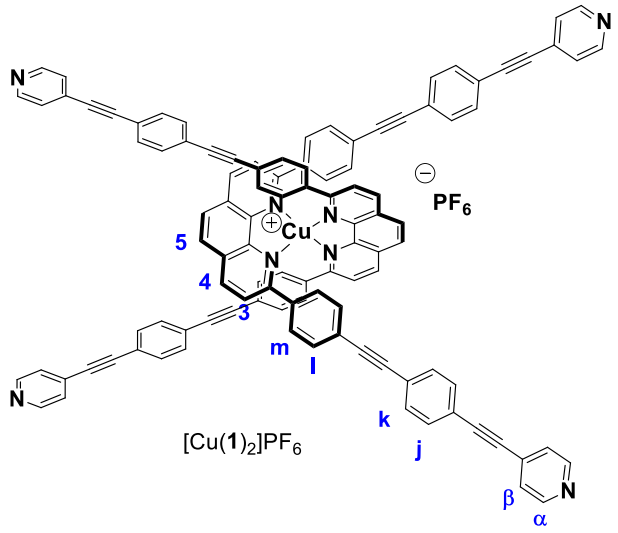
Complex C2



$[Cu(\mathbf{3})_2]^+$

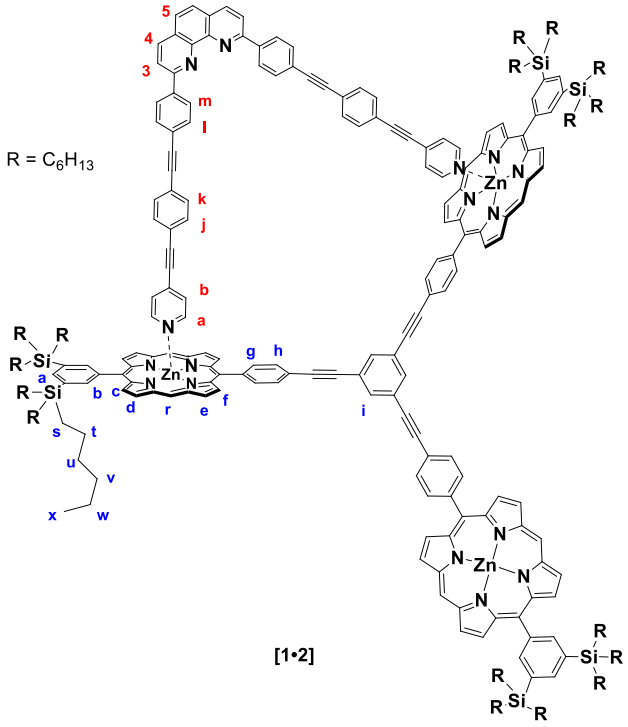
In an NMR tube, compound **3** (1.02 mg, 306 µmol) and $[Cu(CH_3CN)_4]PF_6$ (570 µg, 153 µmol) were dissolved in 560 µL of CD_2Cl_2 to obtain a clear orange solution. The sample was submitted for NMR measurement. **Yield:** Quantitative (by NMR). **^{1}H NMR (400 MHz, CD_2Cl_2):** δ = 8.48 (d, ^3J = 8.3 Hz, 4H, 4-H), 8.01 (s, 4H, 5-H), 7.88 (d, ^3J = 8.3 Hz, 4H, 3-H), 7.42 (m, 8H, a-H), 6.80 (m, 4H, c-H), 6.54 (m, 8H, b-H) ppm. Data agree with those reported in the literature. [1]

Complex $[Cu(\mathbf{1})_2]PF_6$



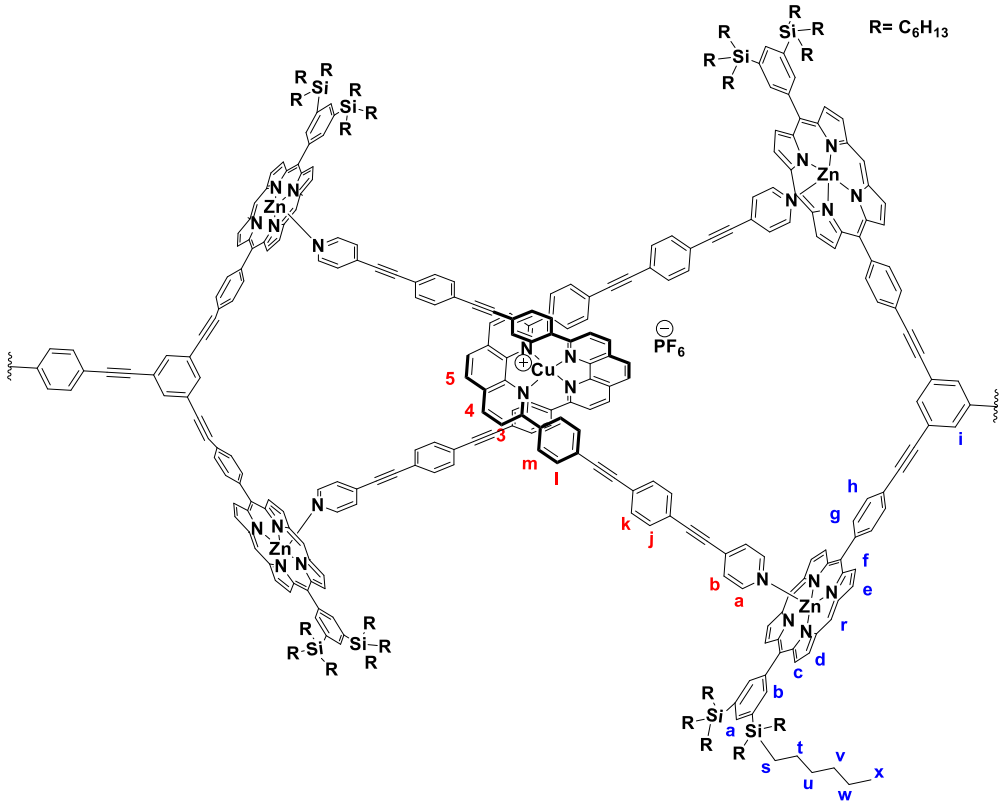
In an NMR tube, compound **1** (417 µg, 0.568 µmol) and $[Cu(CH_3CN)_4]PF_6$ (105 µg, 0.284 µmol) were dissolved in 560 µL of CD_2Cl_2 to obtain a light orange solution. The sample was submitted for NMR measurement. **Yield:** Quantitative (by NMR). **Mp**> 250 °C. **IR (KBr):** $\tilde{\nu}$ = 523, 557, 601, 666, 749, 801, 839, 988, 1015, 1116, 1149, 1181, 1263, 1288, 1313, 1356, 1403, 1488, 1503, 1541, 1590, 2218, 3129 cm^{-1}. **^{1}H NMR (400 MHz, CD_2Cl_2):** δ= 8.60-8.63 (m, 12H, α-, 4-H), 8.08 (s, 4H, 5-H), 7.99 (d, ^3J = 8.4 Hz, 4H, 3-H), 7.62 (d, ^3J =8.6 Hz, 8H, k-H), 7.55 (d, ^3J = 8.6 Hz, 8H, j-H), 7.46 (d, ^3J = 8.6 Hz, 8H, m-H), 7.42 (d, ^3J = 6.0 Hz, 8H, β-H), 6.77 (d, ^3J = 8.6 Hz, 8H, l-H) ppm. **ESI-MS:** *m/z (%)* = 1533.4 (100) $[Cu(\mathbf{1})_2]^+$. **Elemental analysis** ($C_{108}H_{60}CuF_6N_8P\cdot0.9CH_2Cl_2$): Calcd. C, 74.54; H, 3.55; N, 6.39. Found, C, 74.92; H, 3.15; N, 6.26.

Complex DS1 = [1•2]



In an NMR tube, compound **1** (561 µg, 0.764 µmol) and **2** (2.61mg, 0.764 µmol) were dissolved in 560 µL of CD_2Cl_2 to obtain a clear red solution. The sample was submitted for NMR measurement. **Yield:** Quantitative (by NMR). **Mp**> 250 °C. **IR (KBr):** $\tilde{\nu}$ = 539, 601, 665, 686, 699, 718, 802, 1016, 1057, 1097, 1180, 1213, 1261, 1311, 1400, 1456, 1502, 1519, 1542, 1584, 1601, 1629, 2213, 2851, 2867, 2918, 2960, 3121 cm^{-1}. **^{1}H NMR (500 MHz, CD_2Cl_2):** δ= 10.31 (s, 6H, r-H), 9.48 (d, ^3J = 4.6 Hz, 6H, e-H), 9.44 (d, ^3J = 4.6 Hz, 6H, d-H), 9.18 (d, ^3J = 4.6 Hz, 6H, f-H), 9.14 (d, ^3J = 4.6 Hz, 6H, c-H), 8.40 (s, 6H, b-H), 8.38 (d, ^3J = 7.9 Hz, 6H, g-H), 8.35 (d, ^3J = 8.6 Hz, 4H, m-H), 8.20 (d, ^3J = 8.4 Hz, 2H, 4-H), 8.15 (s, 3H, i-H), 8.14 (d, ^3J = 7.9 Hz, 6H, h-H), 8.08 (s, 3H, a-H), 8.04 (d, ^3J = 8.4 Hz, 2H, 3-H), 7.68 (s, 2H, 5-H), 7.63 (d, ^3J = 8.6 Hz, 4H, l-H), 7.28 (brs, 4H, k-H), 7.00 (brs, 4H, j-H), 5.44 (brs, 4H, β-H), 2.19 (brs, 4H, α-H), 0.81-1.58 (m, 234H, s-, t-, u-, v-, w-, x-H), ppm. **Elemental analysis** ($C_{270}H_{318}N_{16}Si_6Zn_3$): Calcd. C, 78.10; H, 7.72; N, 5.40. Found, C, 77.83; H, 7.64; N, 5.24.

Complex DS2 = ([Cu (**1**)$_2$] PF_6•(**2**)$_2$)

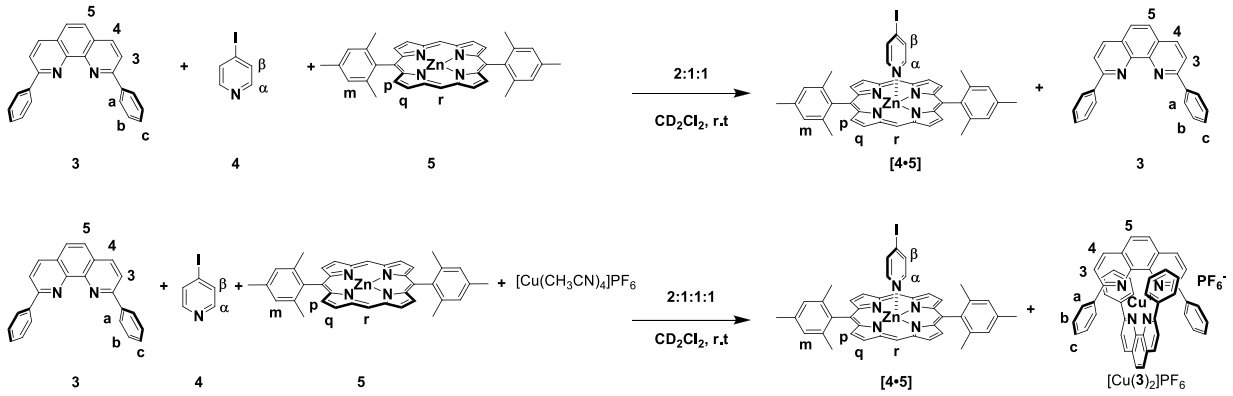


In an NMR tube, compound **1** (561 µg, 0.764 µmol) and **2** (2.61 mg, 0.764 µmol) and $[Cu(CH_3CN)_4]PF_6$ (0.143 mg, 0.384 µmol) were dissolved in 560 µL of CD_2Cl_2 furnishing a dark pink solution. The sample was submitted for NMR measurement. **Mp**> 250 °C. **Yield:** Quantitative (by NMR). **IR (KBr):** $\tilde{\nu}$ = 560, 698, 833, 1018, 1060, 1098, 1262, 1400, 1462, 1581, 1628, 2852, 2921, 2960, 3125 cm^{-1}. **^{1}H NMR (500 MHz, CD_2Cl_2):** δ= 10.33 (s, 12H, r-H), 9.50 (d, ^3J = 4.6 Hz, 12H, e-H), 9.44 (d, ^3J = 4.6 Hz, 12H, d-H), 9.20 (d, ^3J = 4.6 Hz, 12H, f-H), 9.14 (d, ^3J = 4.6 Hz, 12H, c-H), 8.39 (d, ^3J = 7.9 Hz, 12H, g-H), 8.37 (brs, 16H, b-, 4-H), 8.13-8.15 (m, 22H, i-, h-, 5-H), 8.07 (s, 6H, a-H), 7.75 (brd, 4H, 3-H), 7.18 (brs, 16H, j-, k-H), 7.04 (brs, 8H, m-H), 6.48 (brs, 8H, l-H), 5.46 (brs, 8H, β-H), 2.19 (brs, 8H, α-H), 0.86-1.53 (m, 468H, s-, t-, u-, v-, w-, x-H) ppm. **Elemental analysis** ($C_{540}H_{636}CuF_6N_{32}PSi_{12}Zn_6$): Calcd. C, 76.19; H, 7.53; N, 5.27. Found, C, 75.87; H, 7.18; N, 5.20.

3. Model studies

Firstly, self-sorting was tested by mixing ligands **3, 4, 5** in a 2:1:1 molar ratio in CD_2Cl_2 at 298 K. The ^{1}H-NMR measured subsequently was compared with those of ligand **3** (Fig. S2a), [Cu(**3**)$_2$]PF_6 (Fig. S2b), and [**4•5**] (Fig. S2c) which indicated quantitative formation of [**4•5**] and free ligand **3** (Fig. S2d).

Secondly, ligands **3, 4, 5** and $[Cu(CH_3CN)_4]PF_6$ were mixed in a 2:1:1:1 molar ratio in CD_2Cl_2 at 298 K. The ^{1}H-NMR spectrum when compared with those of the free ligands **3, 4, 5** and of complex [**4•5**] indicated the formation of a quantitative, non-interacting mixture of two complexes [**4•5**] and [Cu(**3**)$_2$]PF_6 (Fig. S2e).



Scheme S3: Self-sorting of ligands **3**, **4**, **5** with and without $[Cu(CH_3CN)_4]PF_6$.

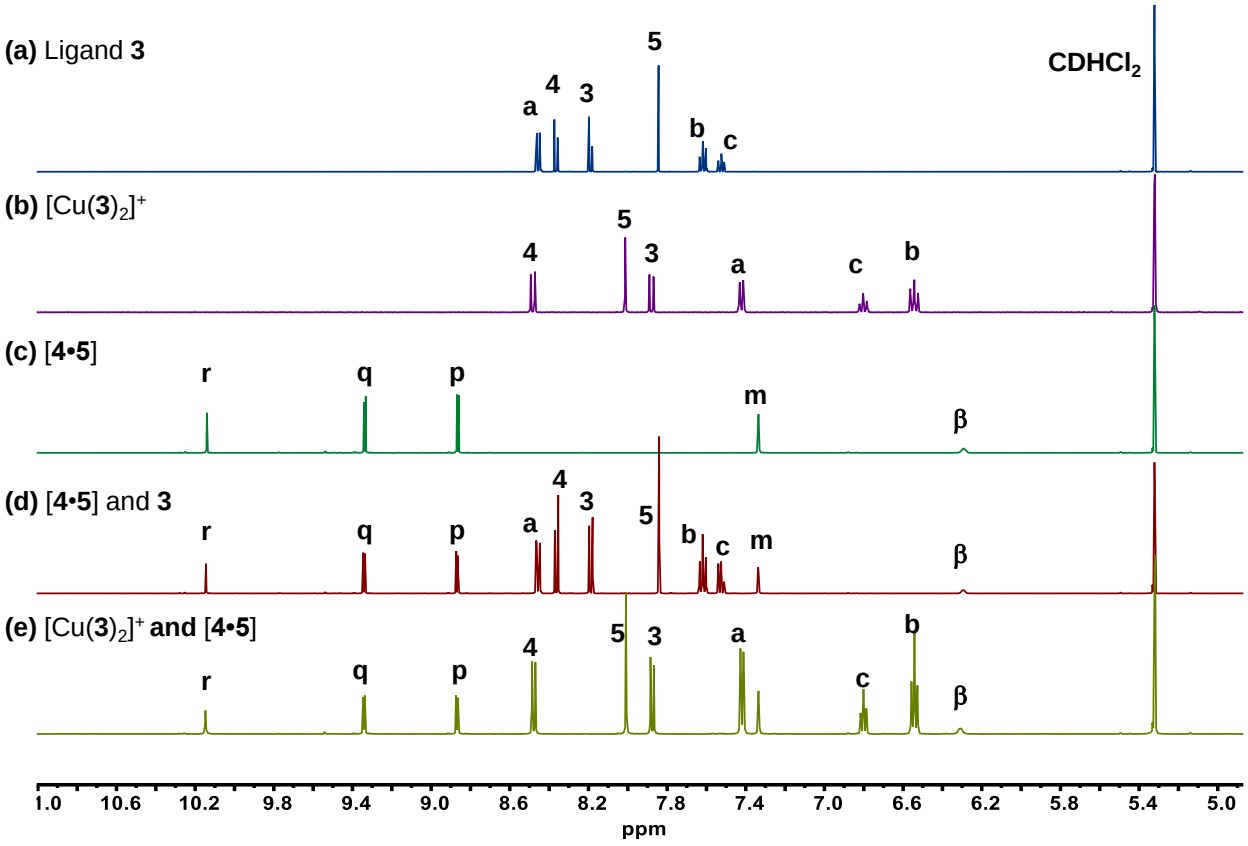


Figure S2: Comparison of ^{1}H-NMR spectra (CD_2Cl_2, 500MHz) of individual complexes [**4•5**] and [Cu(**3**)$_2$]$^{+}$ with ligands **3**, **4**, **5**.

4. NMR Spectra: ^{1}H, ^{13}C, ^{1}H-^{1}H COSY, ^{1}H-^{1}H NOESY

Compound 1

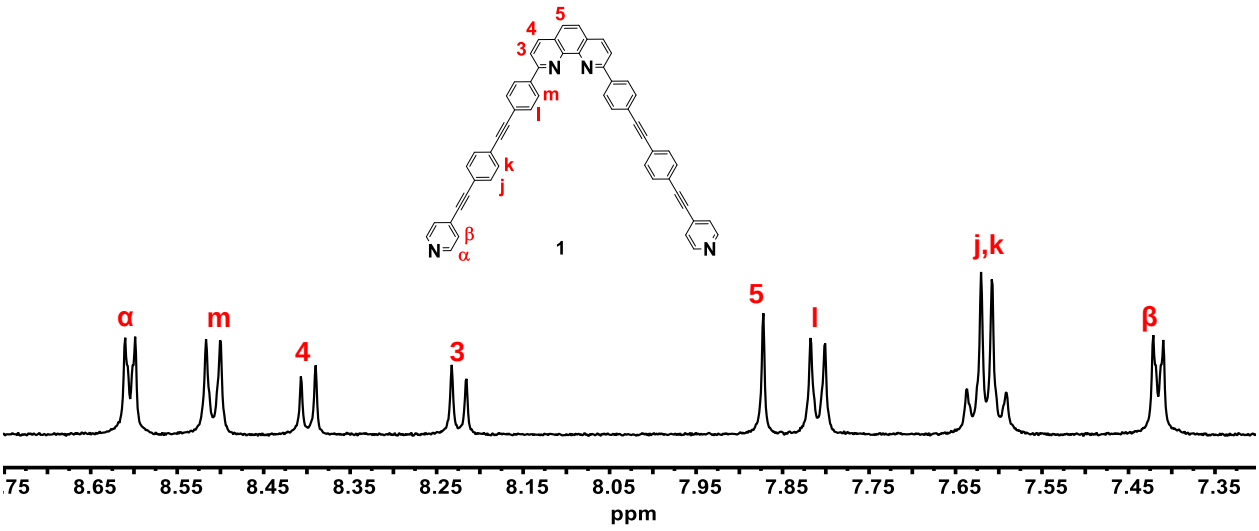


Figure S3 : ^{1}H-NMR spectrum of compound **1** (CD_2Cl_2, 500 MHz, 298 K)

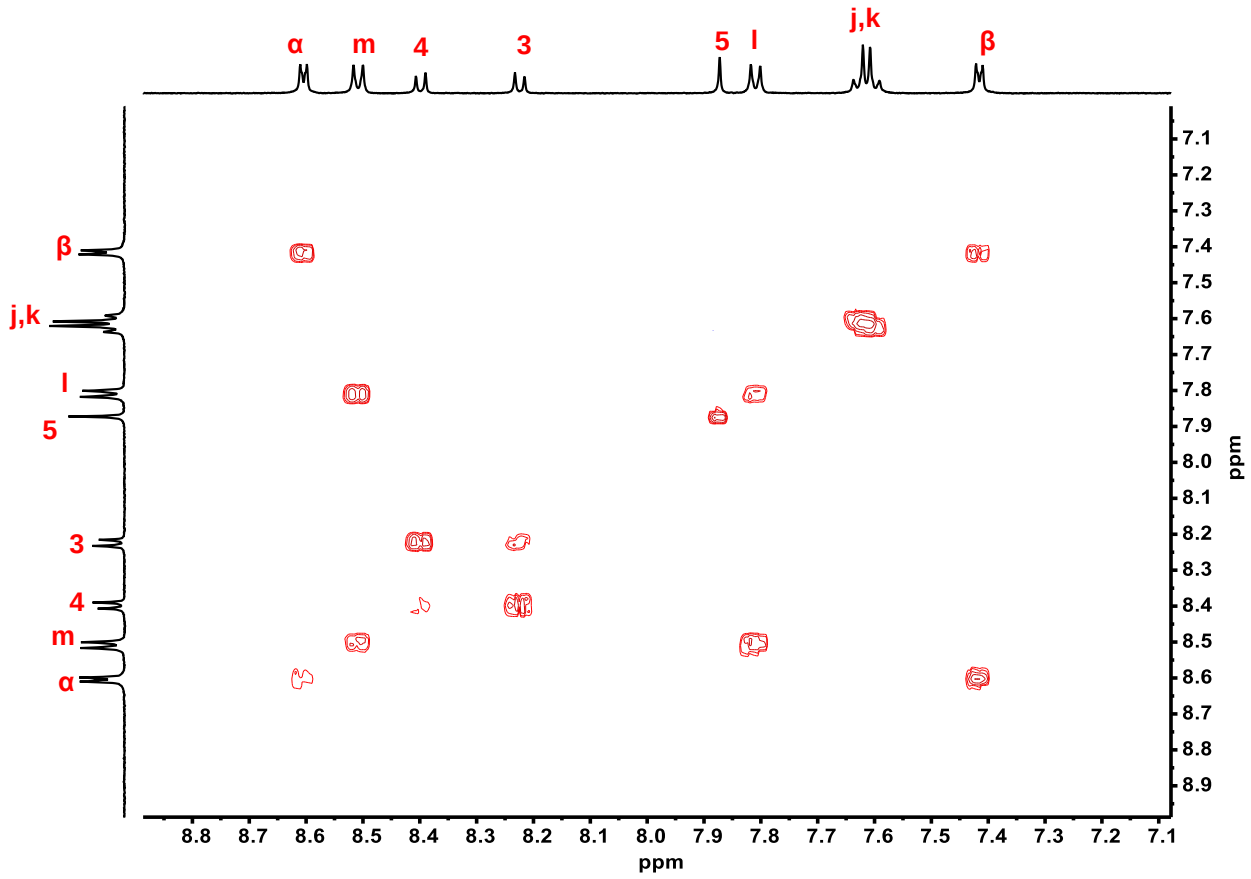


Figure S4: ^{1}H-^{1}H COSY spectrum of compound **1** (CD_2Cl_2, 500 MHz, 298 K)

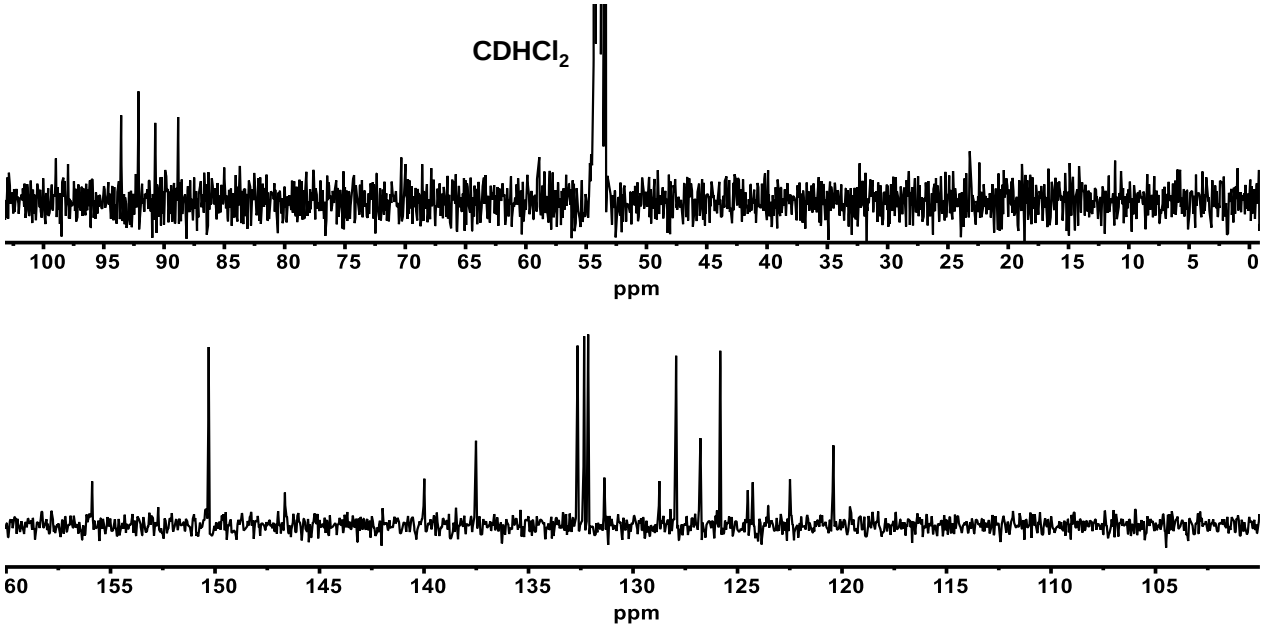


Figure S5: ^{13}C spectrum of compound **1** (CD_2Cl_2, 125 MHz, 298 K)

Compound 11

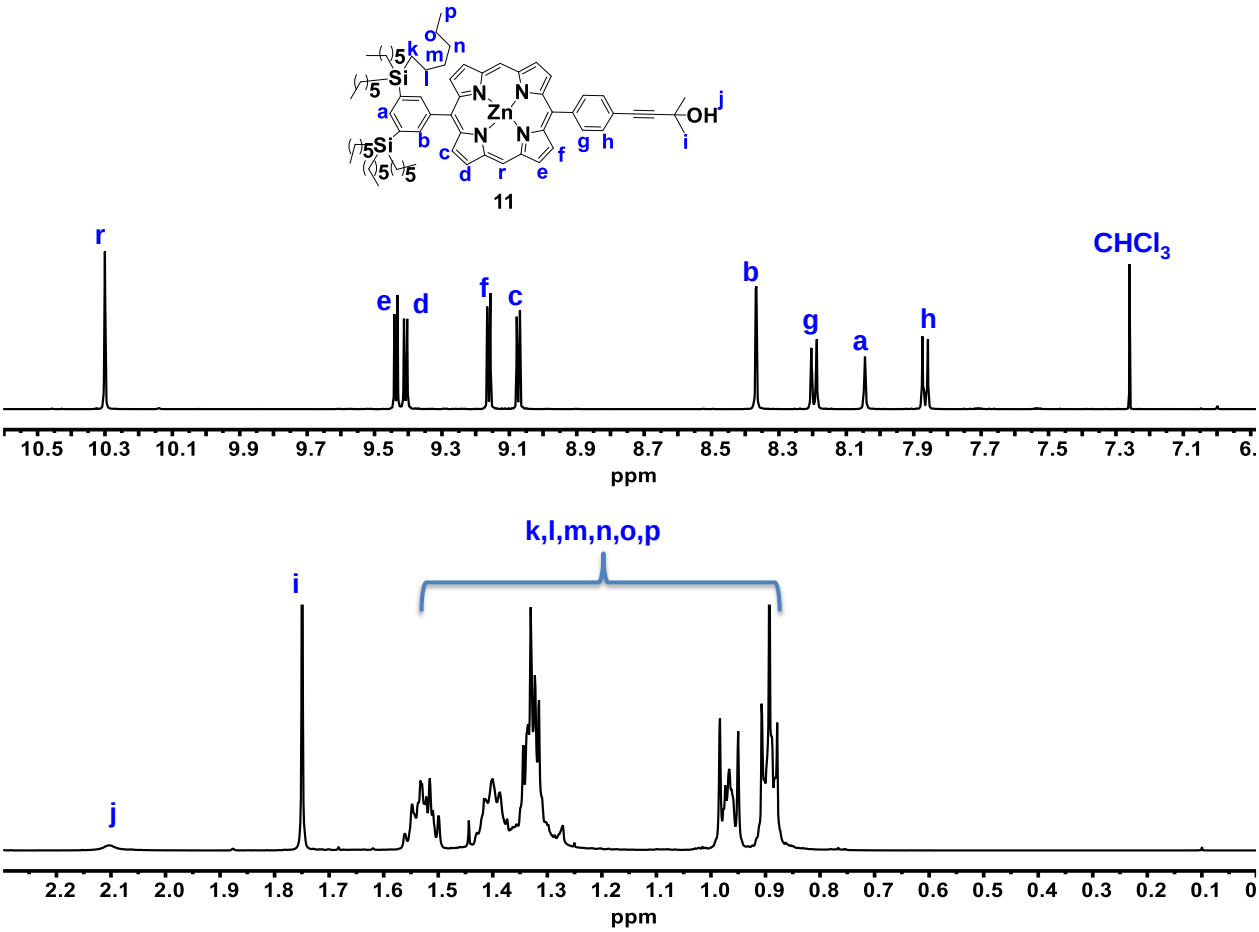


Figure S6: ^{1}H-NMR spectrum of compound **11** ($CDCl_3$, 500 MHz, 298 K)

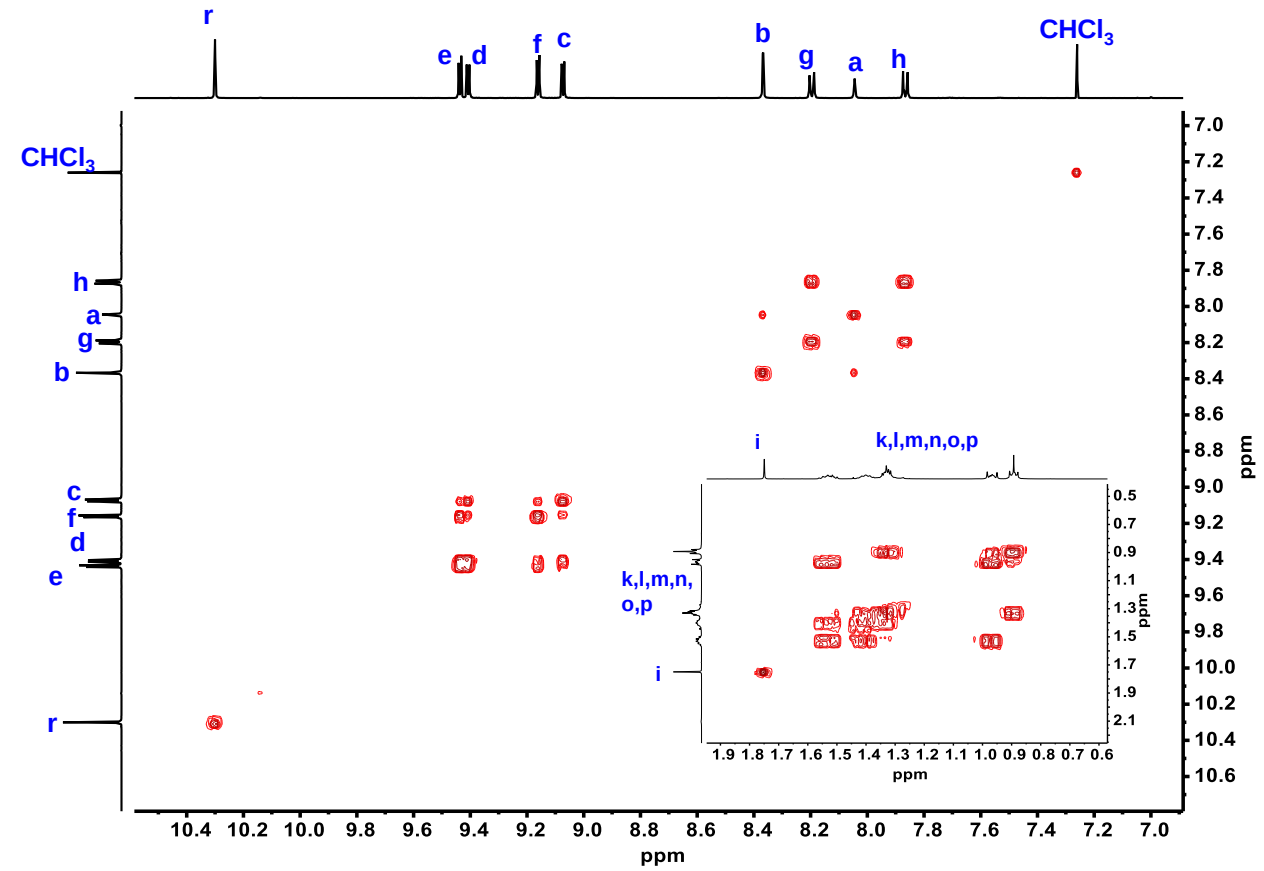


Figure S7: ^{1}H-^{1}H COSY spectrum of compound **11** ($CDCl_3$, 500 MHz, 298 K)

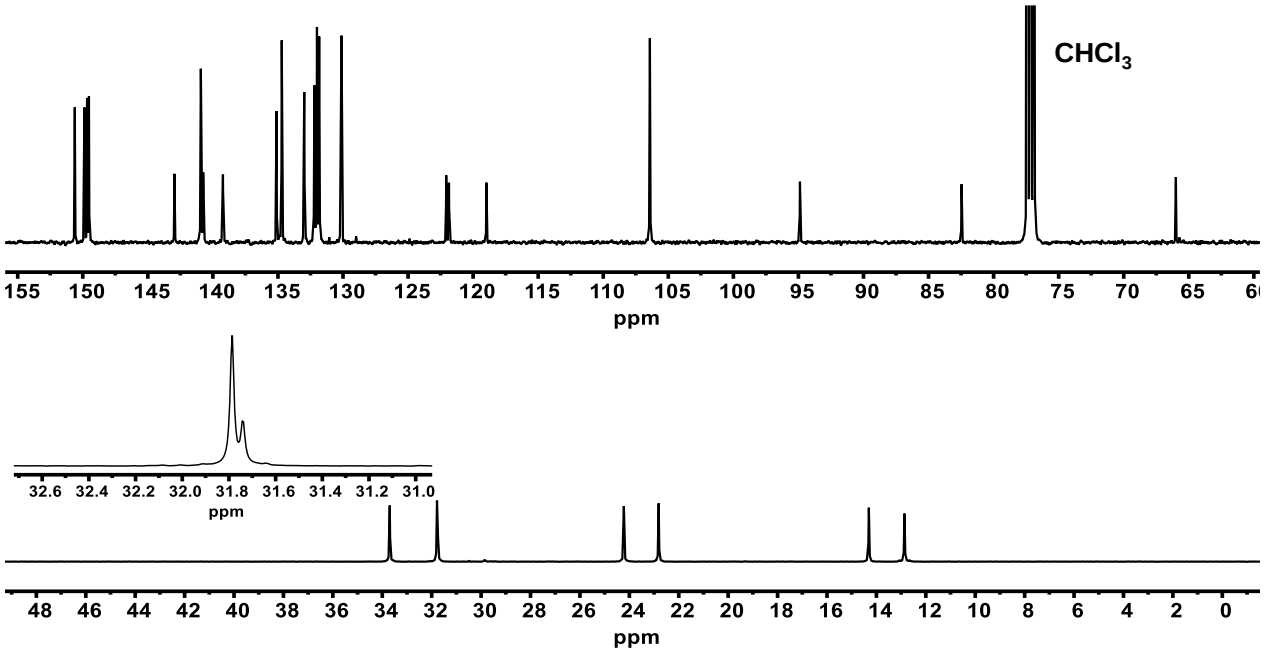


Figure S8: ^{13}C spectrum of compound **11** ($CDCl_3$, 125 MHz, 298 K)

Compound 12

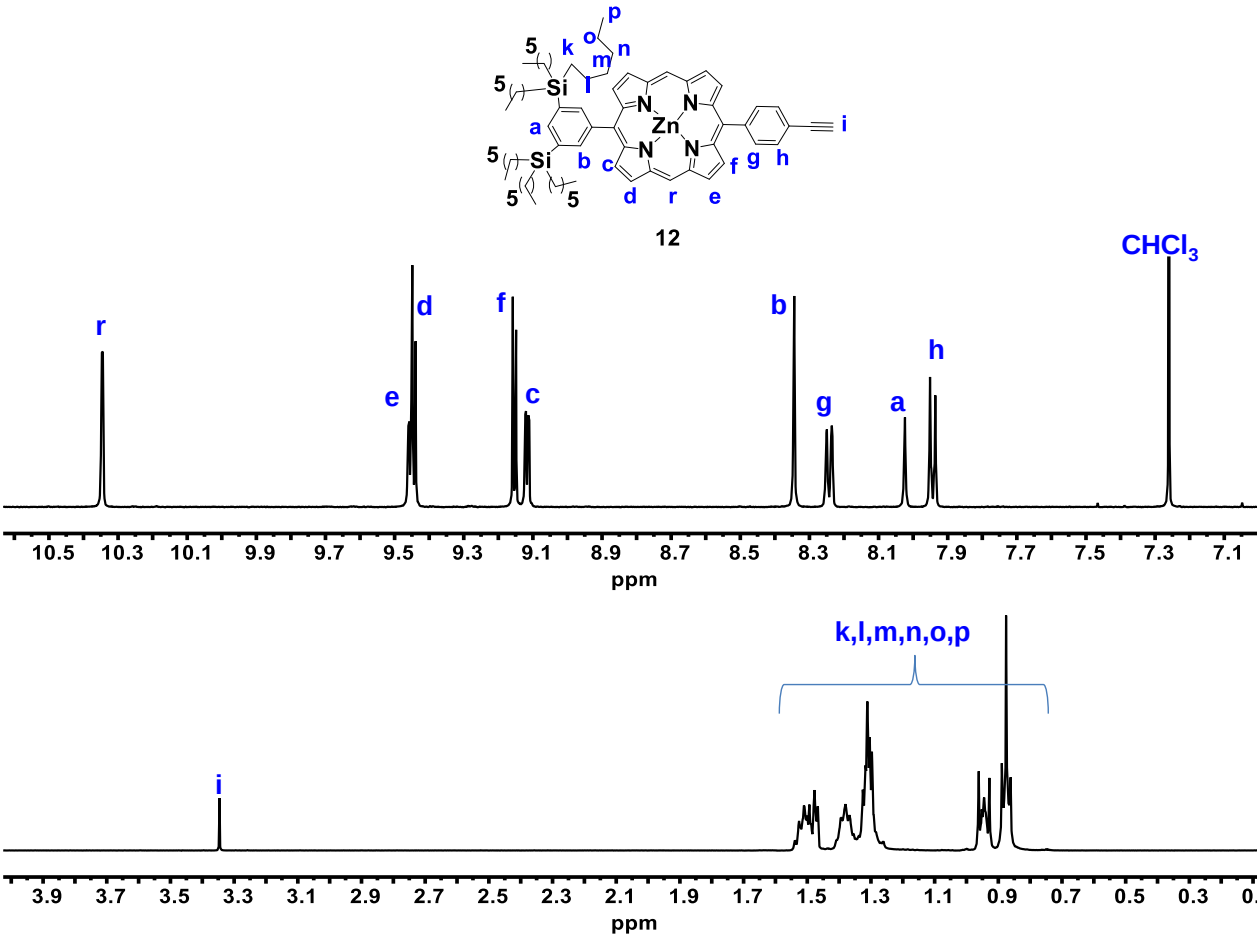


Figure S9: ^{1}H-NMR spectrum of compound **12** ($CDCl_3$, 500 MHz, 298 K)

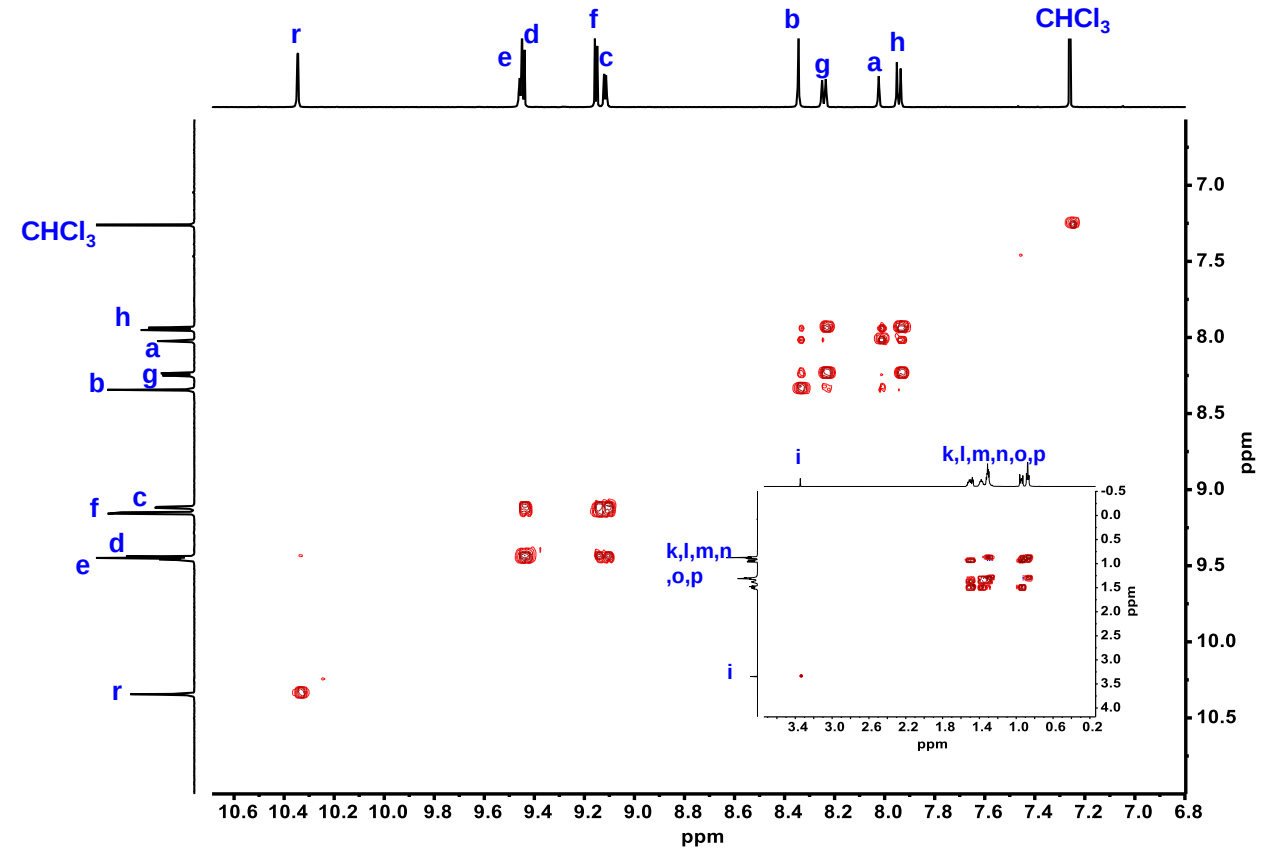


Figure S10: ^{1}H-^{1}H COSY spectrum of compound **12** ($CDCl_3$, 500 MHz, 298 K)

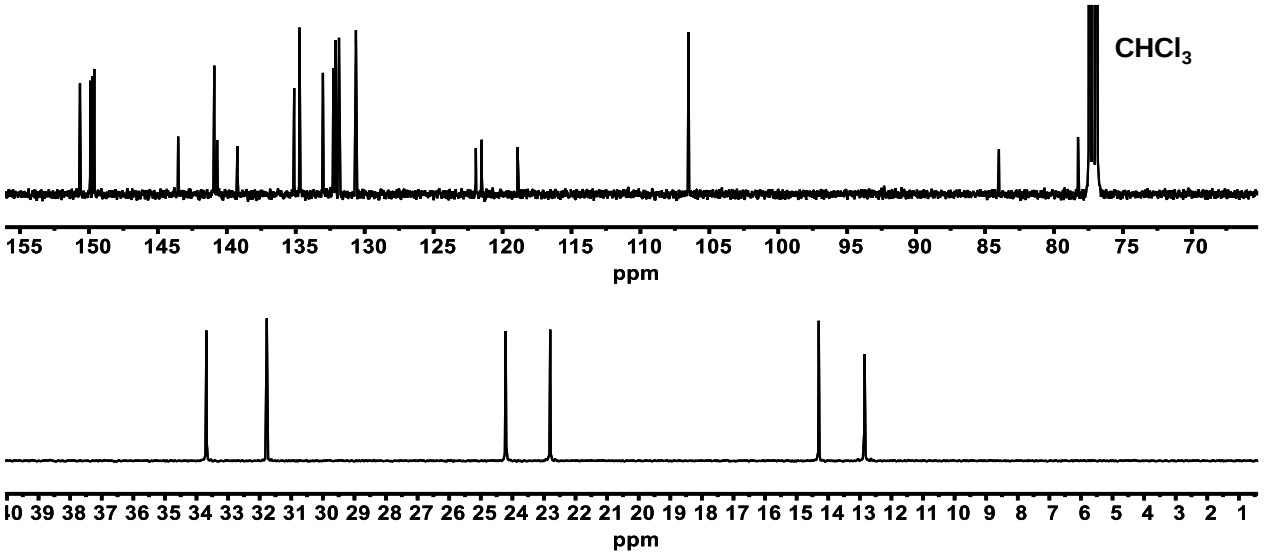


Figure S11: ^{13}C spectrum of compound **12** ($CDCl_3$, 125 MHz, 298 K)

Compound 2

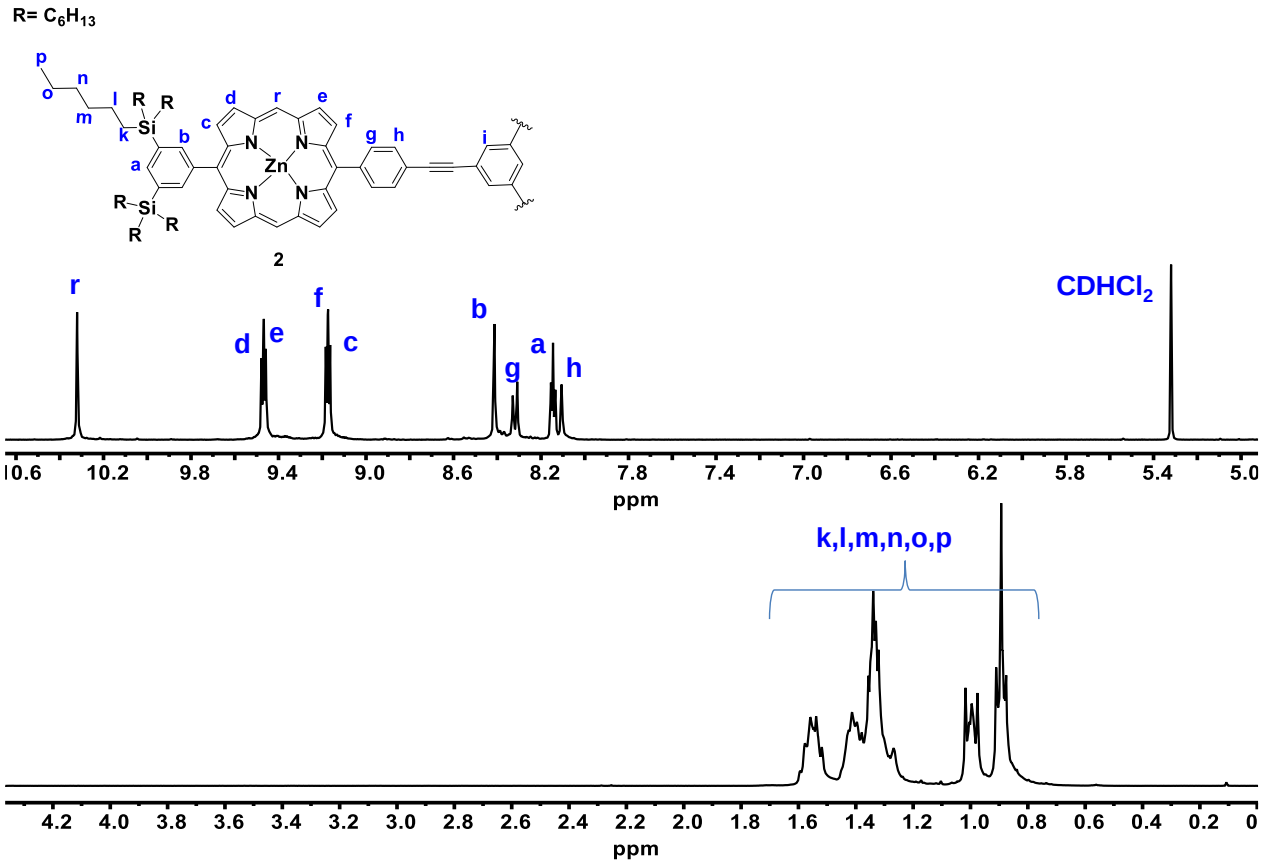


Figure S12: ^{1}H-NMR spectrum of compound **2** (CD_2Cl_2, 400 MHz, 298 K)

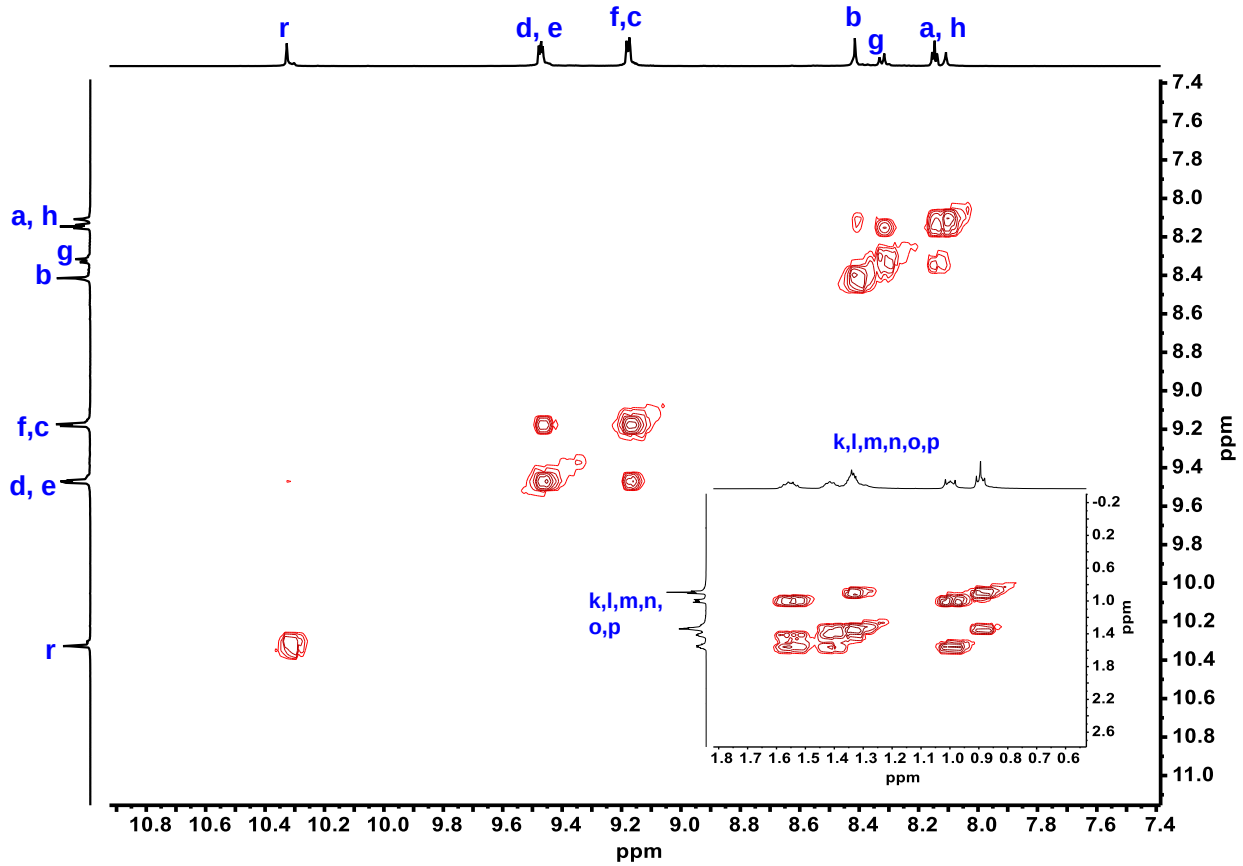


Figure S13: ^{1}H-^{1}H COSY spectrum of compound **2** (CD_2Cl_2, 500 MHz, 298 K)

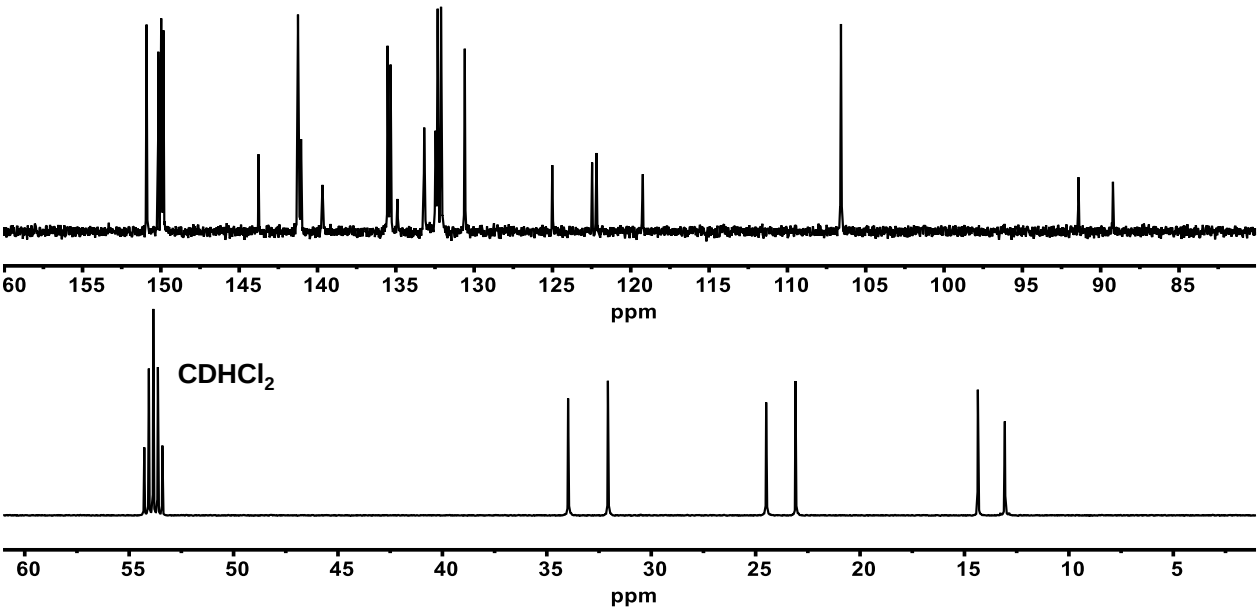


Figure S14: ^{13}C spectrum of compound **2** (CD_2Cl_2, 125 MHz, 298 K)

Complex $[Cu(1)_2]PF_6$

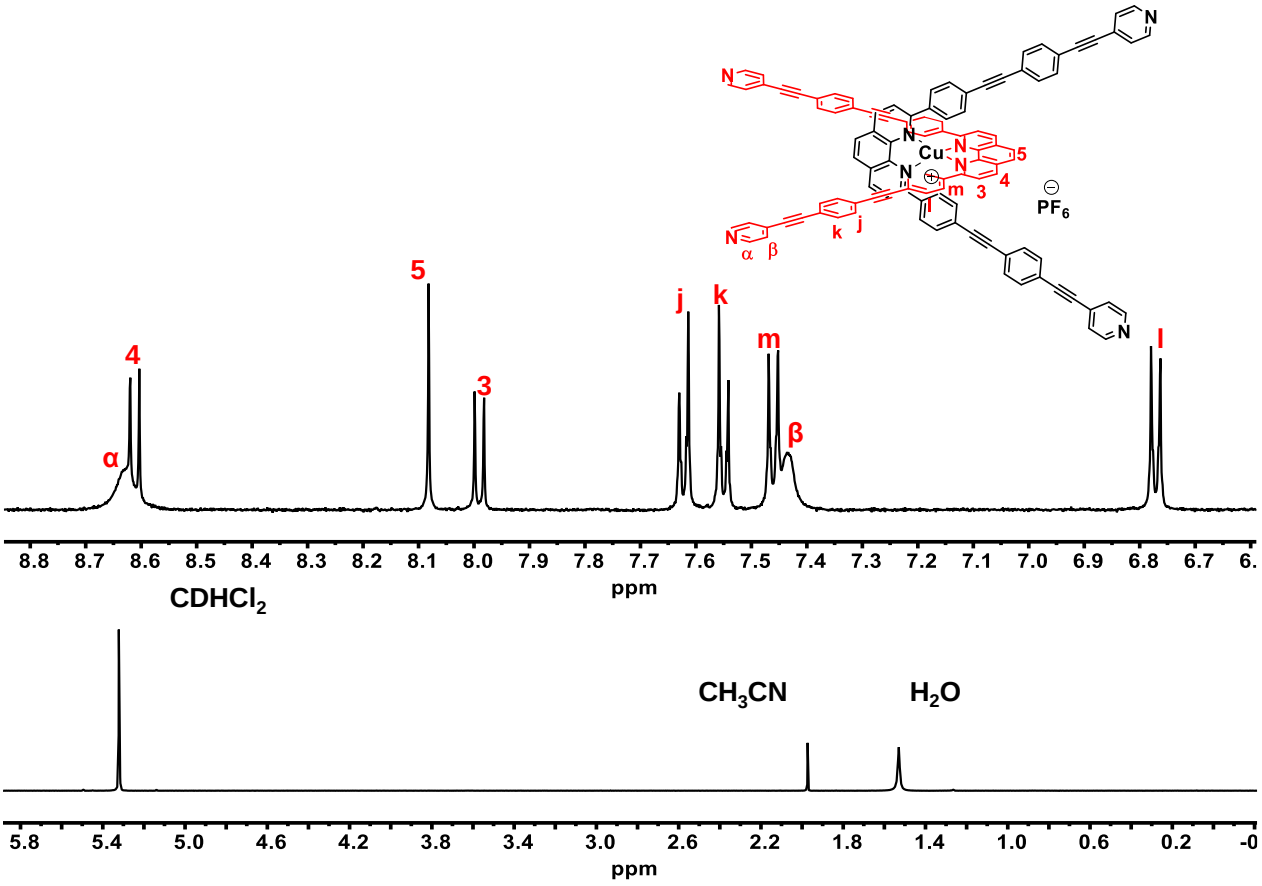


Figure S15: ^{1}H-NMR spectrum of compound $[Cu(\mathbf{1})_2]PF_6$ (CD_2Cl_2, 400 MHz, 298 K)

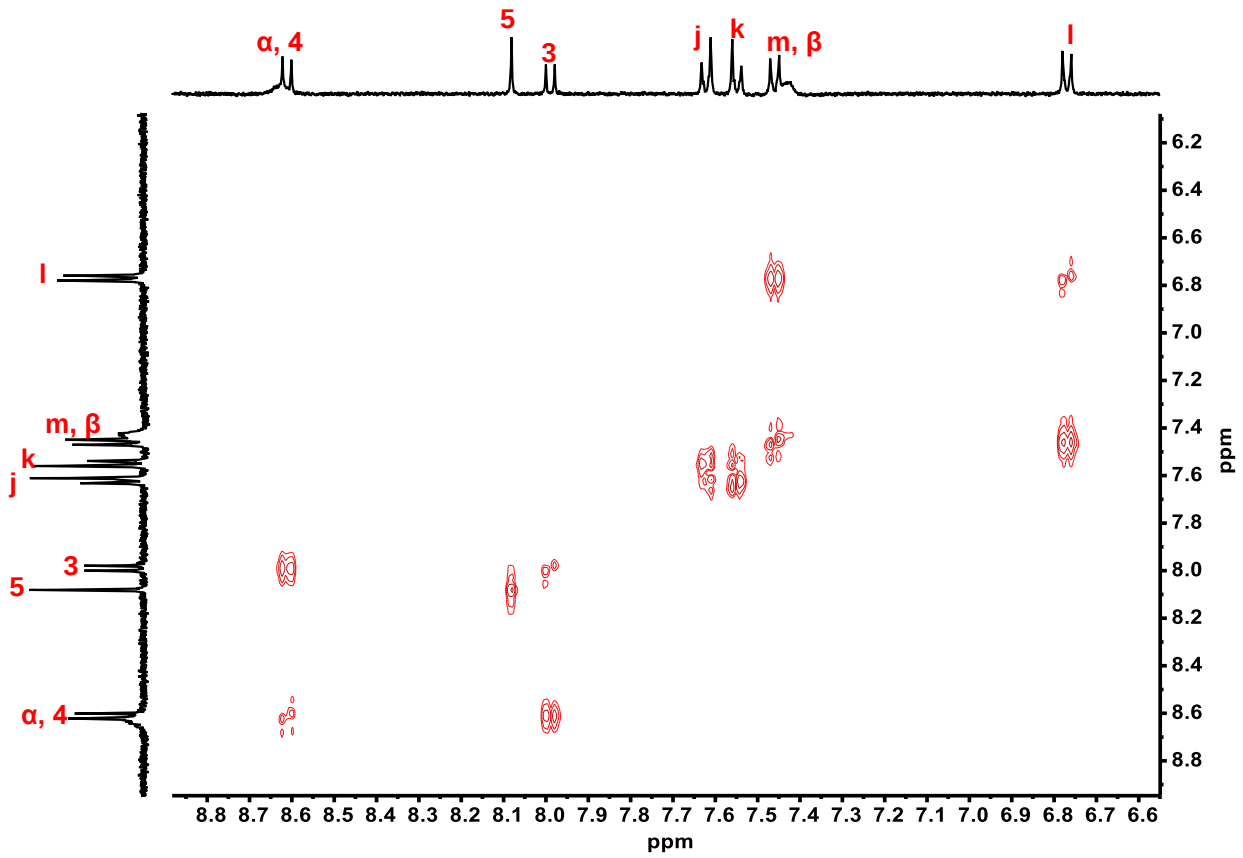


Figure S16: ^{1}H-^{1}H COSY spectrum of complex $[Cu(\mathbf{1})_2]PF_6$ (CD_2Cl_2, 400 MHz, 298 K)

Complex DS1

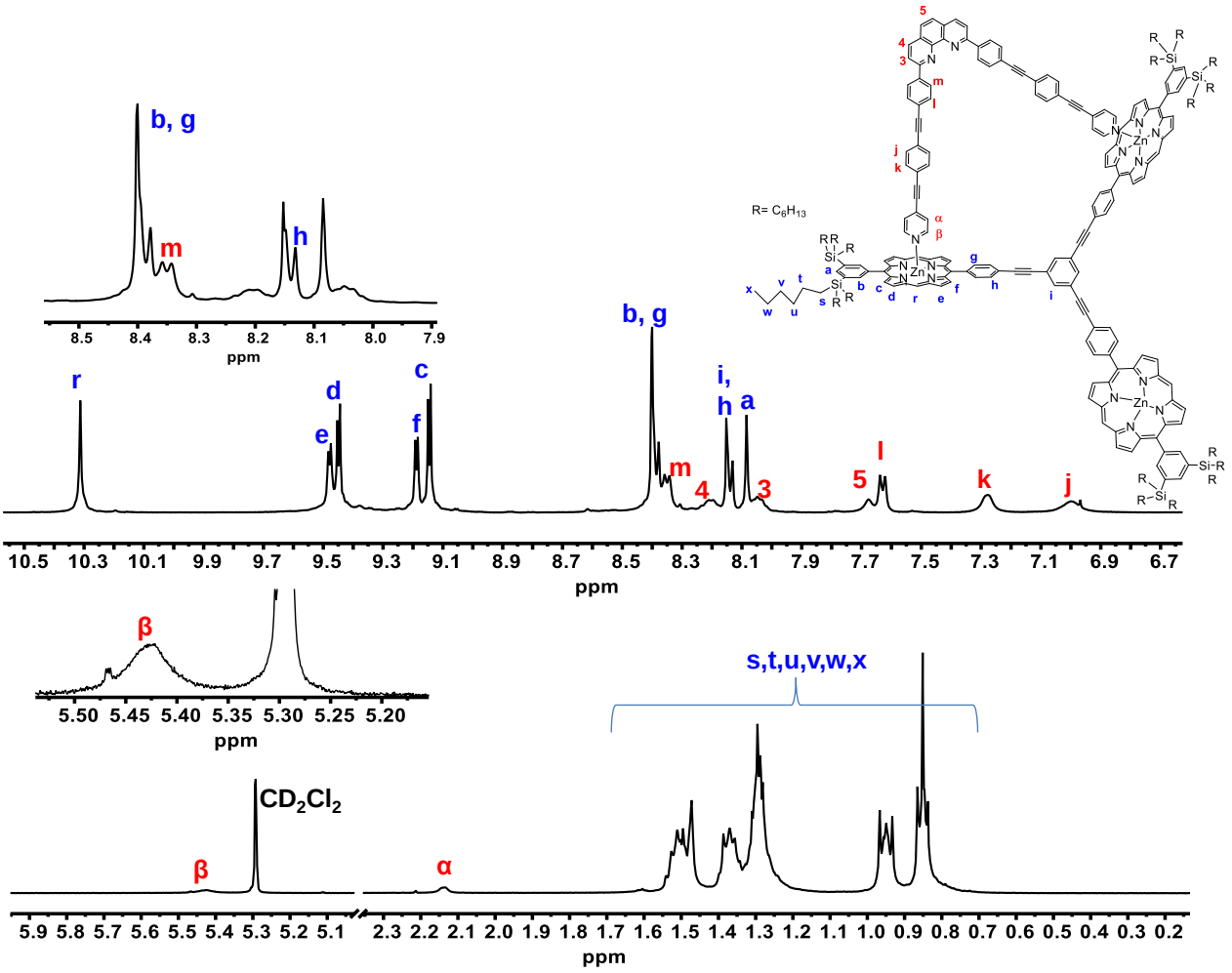


Figure S17: ^{1}H-NMR spectrum of complex [**1•2**] = **DS1** (CD_2Cl_2, 500 MHz, 298 K)

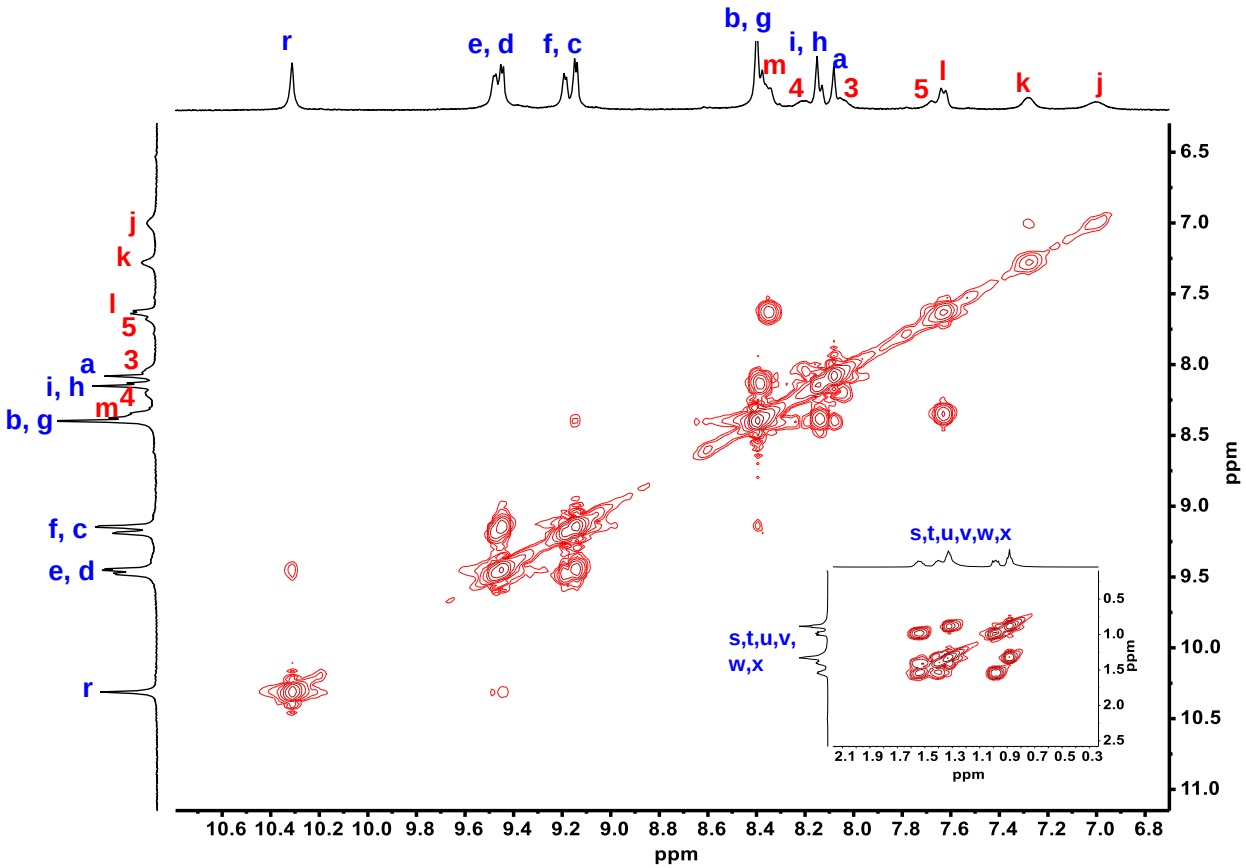


Figure S18: ^{1}H-^{1}H COSY spectrum of complex [**1•2**] = **DS1** (CD_2Cl_2, 400 MHz, 298 K)

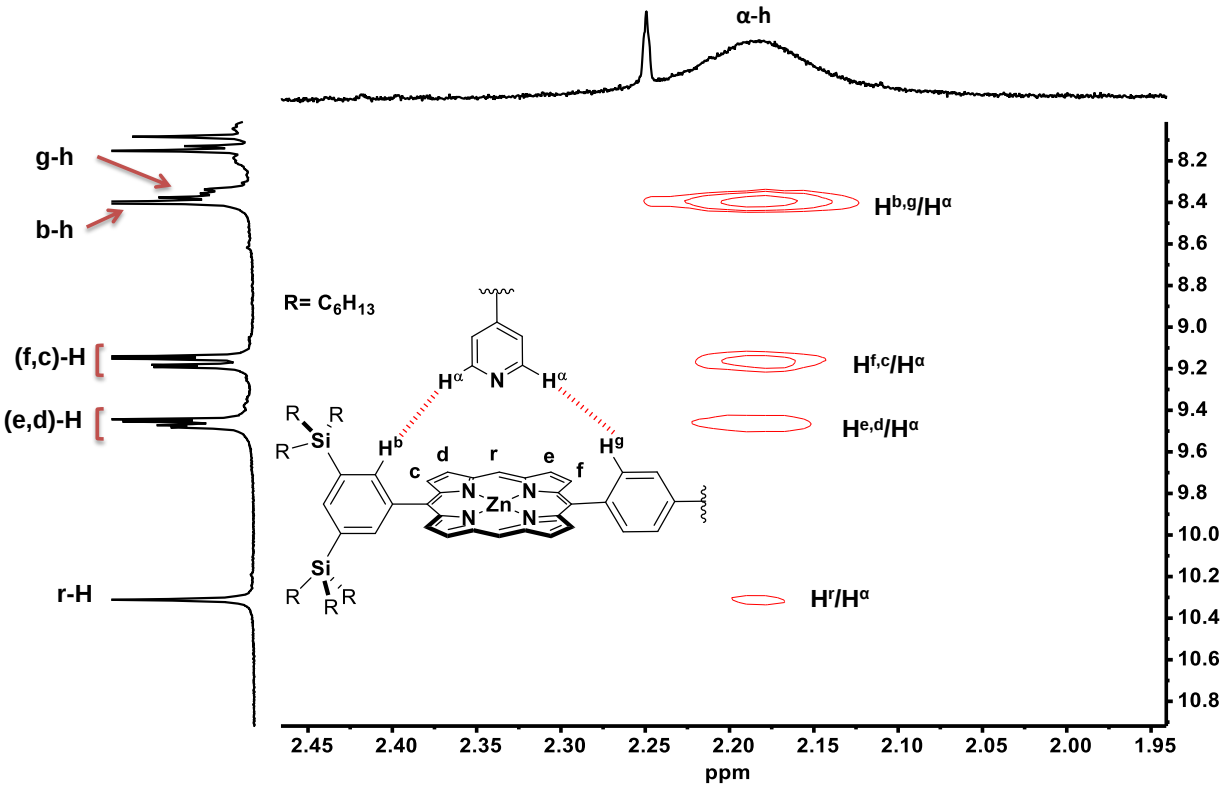


Figure S19: Partial ^{1}H-^{1}H NOESY spectrum of complex [**1•2**] = **DS1** showing correlations of pyridine H^{α} protons with protons (H^{b}, H^{c}, H^{d}, H^{e}, H^{f}, H^{g}, H^{r}, on the porphyrin core of **2**. (CD_2Cl_2, 400 MHz, 298 K)

Complex DS2

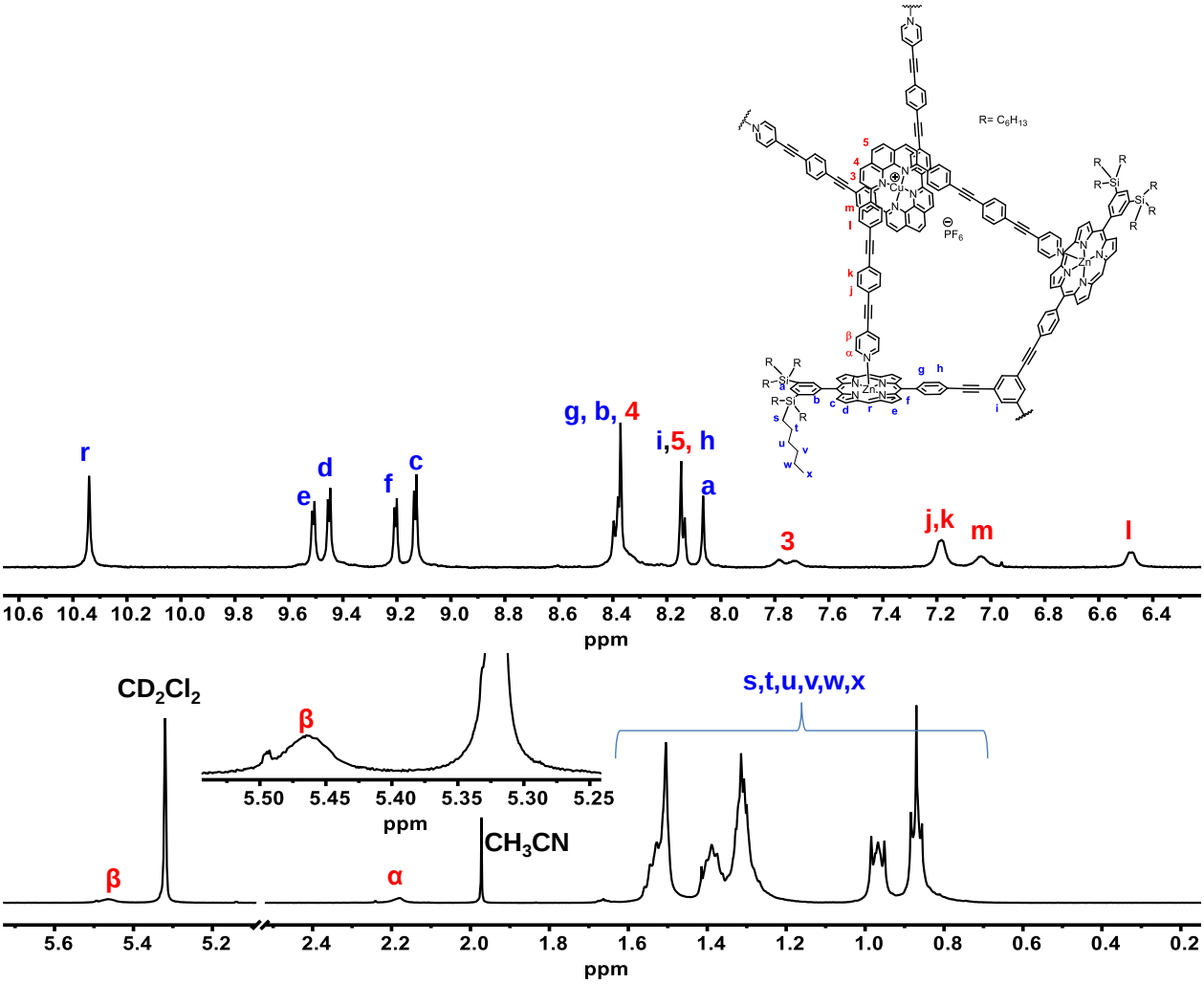


Figure S20: ^{1}H-NMR spectrum of complex [Cu(**1**)$_2$•(**2**)$_2$]PF_6 = **DS2** (CD_2Cl_2, 500 MHz, 298 K)

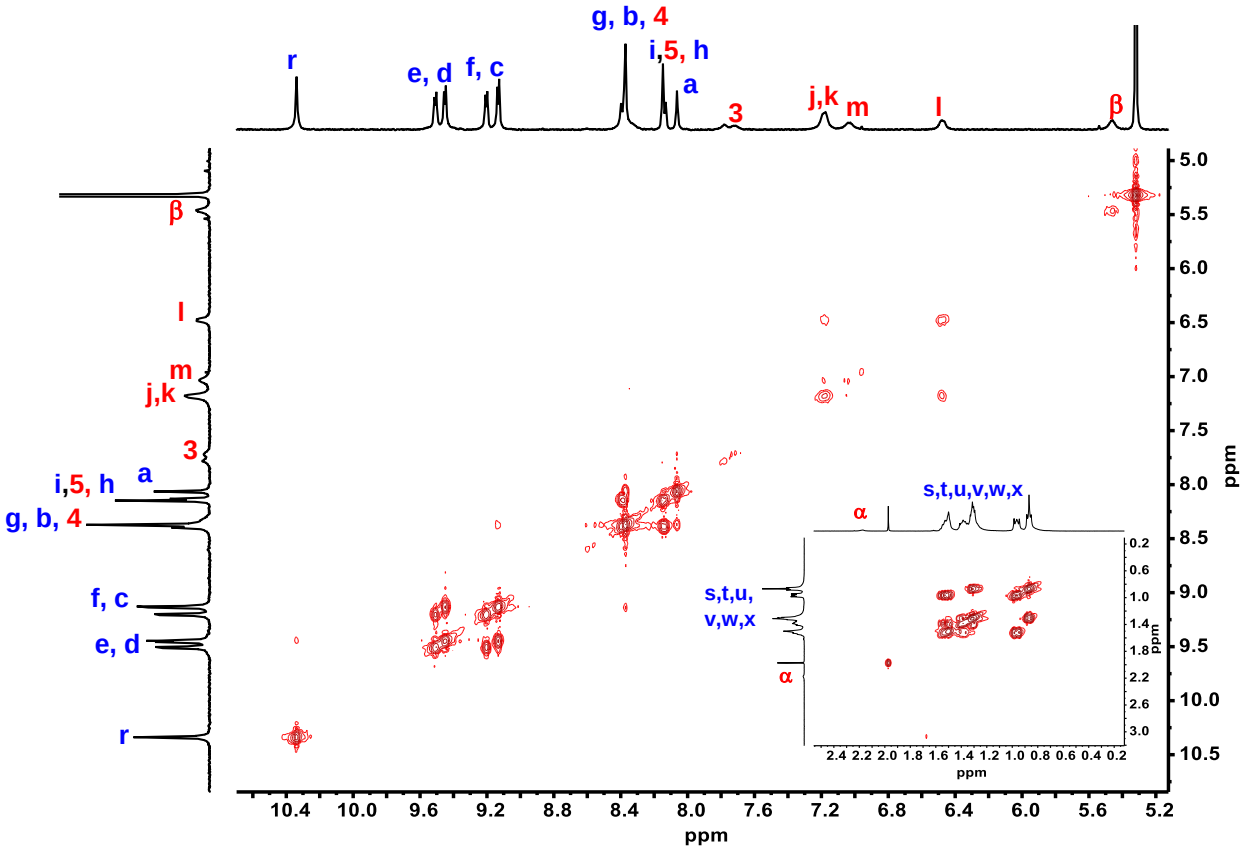


Figure S21: ^{1}H-^{1}H COSY spectrum of complex **DS2** = [Cu(**1**)$_2$•(**2**)$_2$]PF_6 (CD_2Cl_2, 400 MHz, 298 K)

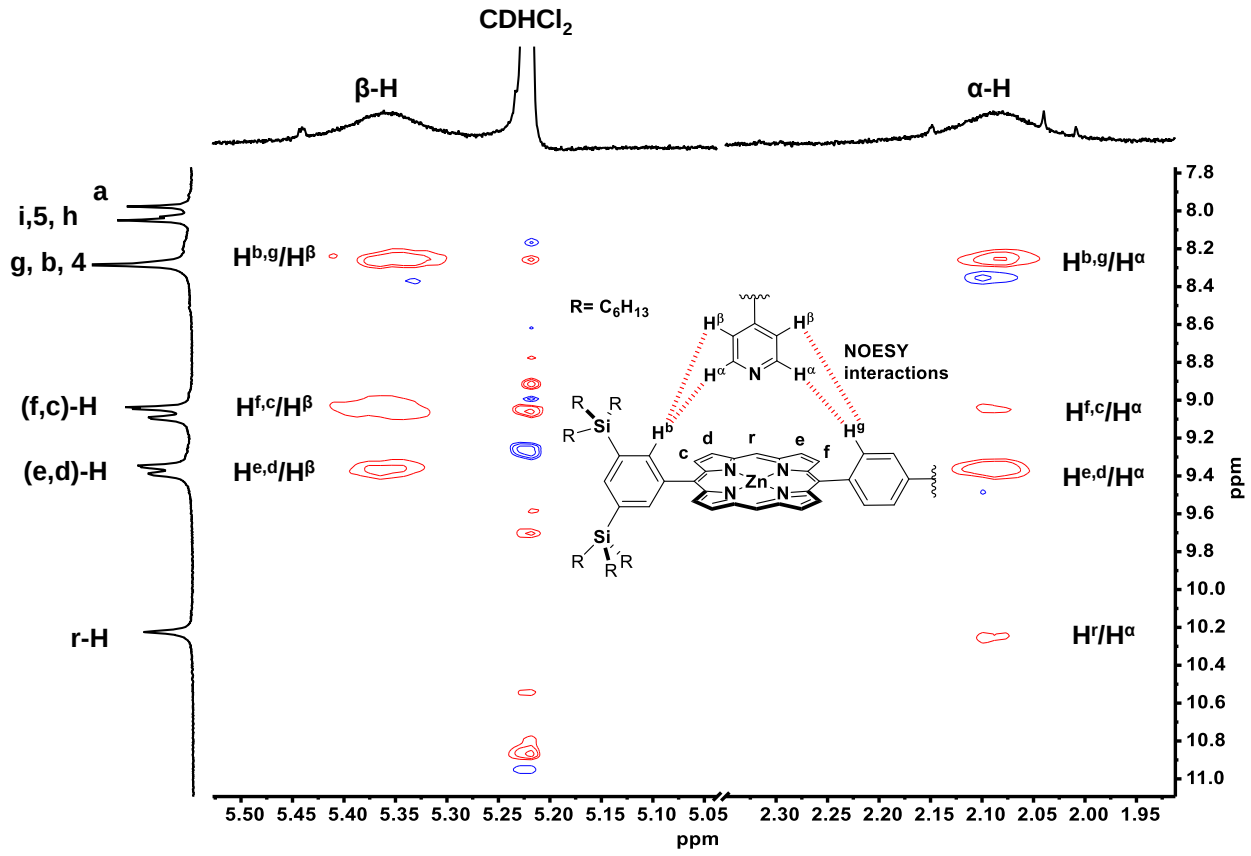


Figure 22: Partial ^{1}H-^{1}H NOESY spectrum of complex $[Cu(\mathbf{1})_2\bullet(\mathbf{2})_2]PF_6$ = **DS2** showing correlations of pyridine H^{α} and H^{β} protons with protons (H^{b}, H^{c}, H^{d}, H^{e}, H^{f}, H^{g}, H^{r}, on the porphyrin core of **2**. (CD_2Cl_2, 400 MHz, 298 K)

5. ^{1}H-NMR of reversible interconversion of monomer to catenate slider

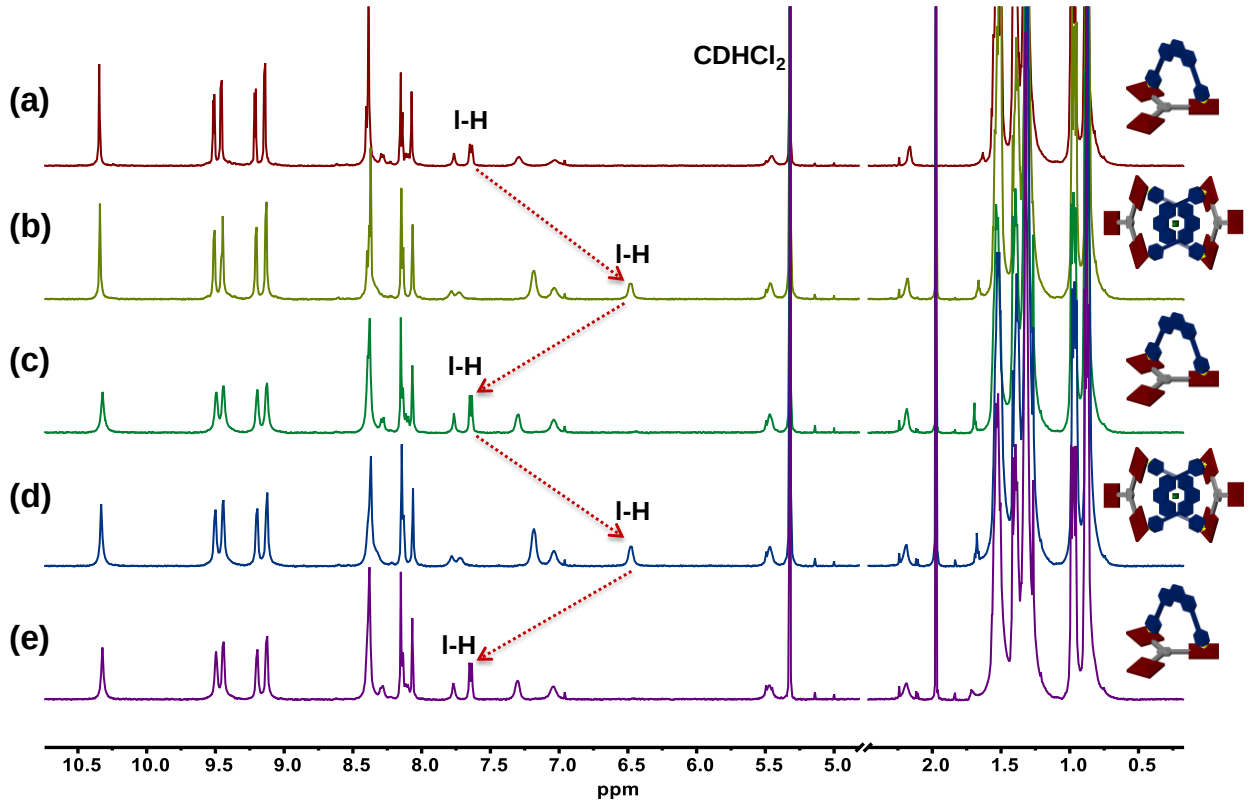


Figure S23: ^{1}H-NMR of interconversion cycles of the slider-on-deck to catenate sliders by addition of $[Cu(CH_3CN)_4]PF_6$ and cyclam sequentially over 2 cycles. (a) Complex [**1**•**2**] readily self-assembled by addition of 1:1 addition of **1** and **2**. (b) Quantitative conversion of complex [**1**•**2**] into **[**$Cu(\mathbf{1})_2$•$(\mathbf{2})_2]PF_6$ by addition of 0.5 equiv. of $[Cu(CH_3CN)_4]PF_6$. (c) Quantitative conversion of $[Cu\mathbf{(1)}_2$•$(\mathbf{2})_2]PF_6$ into complex [**1**•**2**] by addition of 0.5 equiv. of cyclam followed by sonication at 50 °C for 30 min (1. cycle). (d) Quantitative conversion of complex [**1**•**2**] into **[**$Cu(\mathbf{1})_2$•$(\mathbf{2})_2]PF_6$ by addition of 0.5 equiv. of $[Cu(CH_3CN)_4]PF_6$ yet again. Quantitative conversion of **[**$Cu(\mathbf{1})_2$•$(\mathbf{2})_2]PF_6$ into complex [**1**•**2**] by addition of 0.5 equiv. of cyclam followed by sonication at 50 °C for 30 min. (2. cycle) (CD_2Cl_2, 500 MHz, 298 K)

6. ^{1}H-^{1}H DOSY NMR

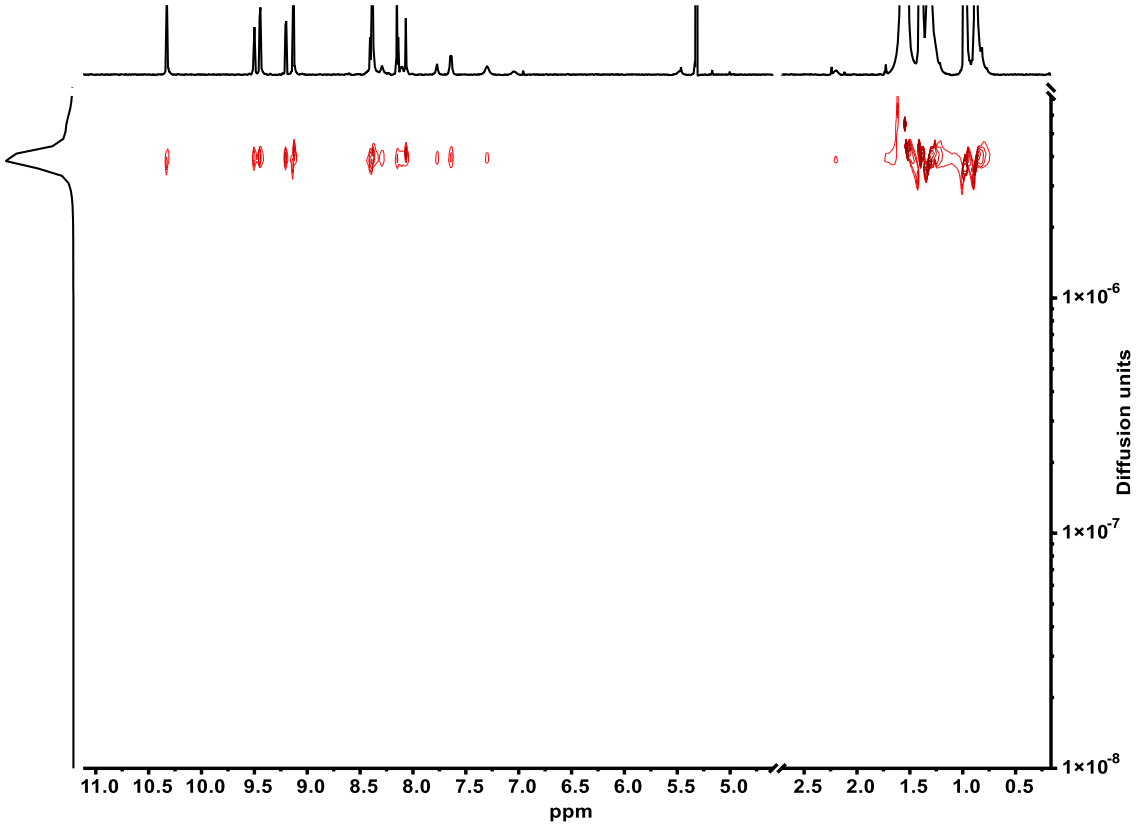


Figure S24: ^{1}H-DOSY NMR of **DS2** = [Cu(**1**)$_2$•(**2**)$_2$]PF_6 in CD_2Cl_2 (600 MHz, 298 K). Diffusion coefficient D = 3.30×10^{-10} m^2 s^{-1}, Experimental hydrodynamic radius r = 16.1 Å.

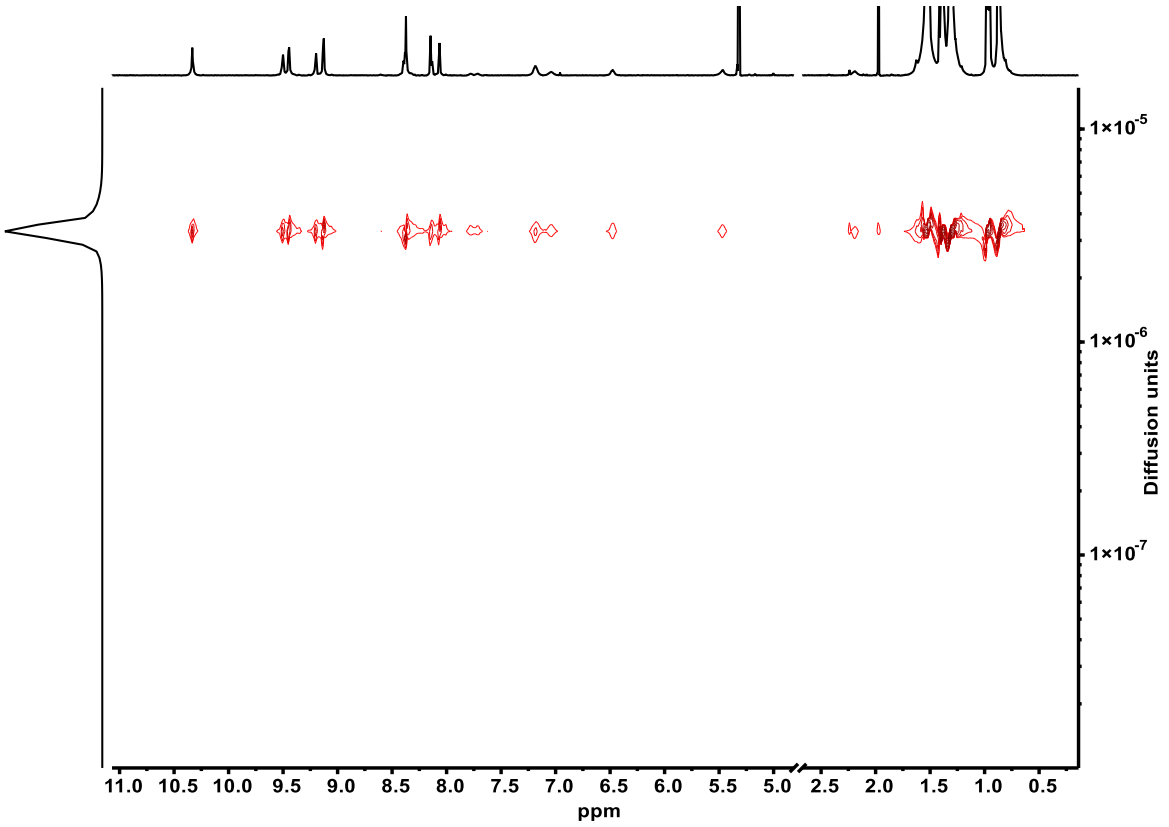


Figure S25: ^{1}H-DOSY NMR of **DS1** = [**1**•**2**] in CD_2Cl_2 (600 MHz, 298 K). Diffusion coefficient $D = 3.82 \times 10^{-10}$ m^2 s^{-1}, Experimental hydrodynamic radius $r = 13.9$ Å.

7. Variable Temperature Studies

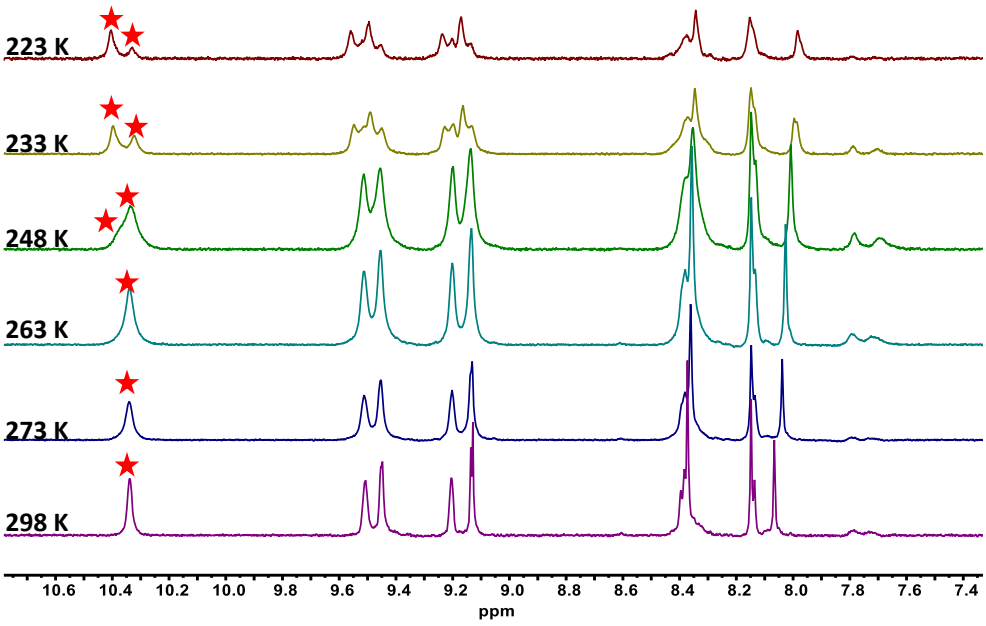


Figure S26: Partial ^{1}H VT-NMR (CD_2Cl_2, 600 MHz) of [Cu(**1**)$_2$]•(**2**)$_2$ = **DS2** shows the splitting of r-H (red star marked) in the aromatic region. Upon lowering the temperature r-H splits into two sets in 2:1 ratio. Signal at 10.41 ppm corresponds to pyridine-coordinated zinc porphyrins: [Cu(**1**)$_2$•(**2**)$_2$]PF_6, whereas the uncoordinated zinc porphyrin **2** shows a singlet at 10.33 ppm. Broadening and splitting of other aromatic protons is also observed.

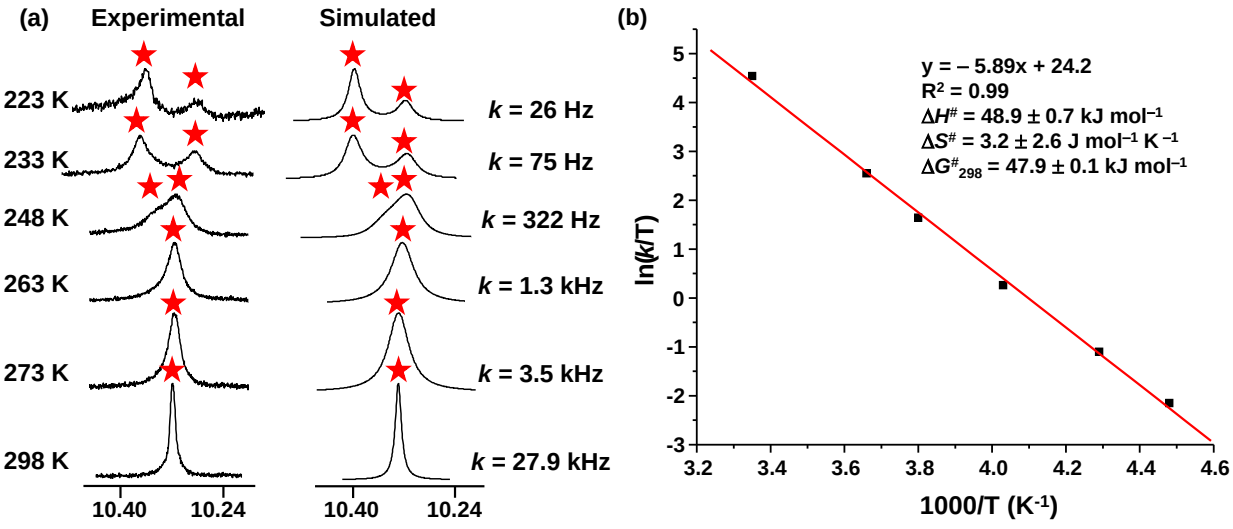


Figure S27: (a) Partial ^{1}H VT-NMR of [Cu(**1**)$_2$•(**2**)$_2$]PF_6 = **DS2** (CD_2Cl_2, 600 MHz) at different temperatures showing experimental and theoretical splitting of r-H with corresponding rate constants. (b) Eyring plot for sliding dynamics in [Cu(**1**)$_2$•(**2**)$_2$]PF_6.

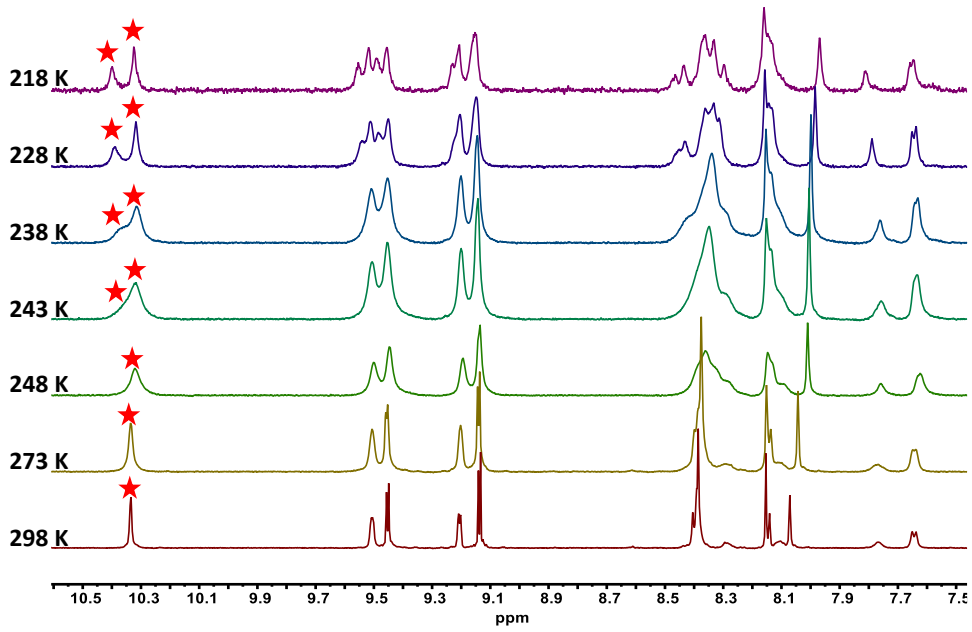


Figure S28: Partial ^{1}H VT-NMR (CD_2Cl_2, 600 MHz) of [**1•2**] (1:1) = **DS1** shows the splitting of r-H (red star marked) in the aromatic region. Upon lowering the temperature r-H splits into two sets in 2:1 ratio. Signal at 10.40 ppm corresponds to pyridine-coordinated zinc porphyrins **1•2** (1:1) and the uncoordinated zinc porphyrin of **2** shows a singlet at 10.32 ppm. Broadening and splitting of other aromatic protons is also observed.

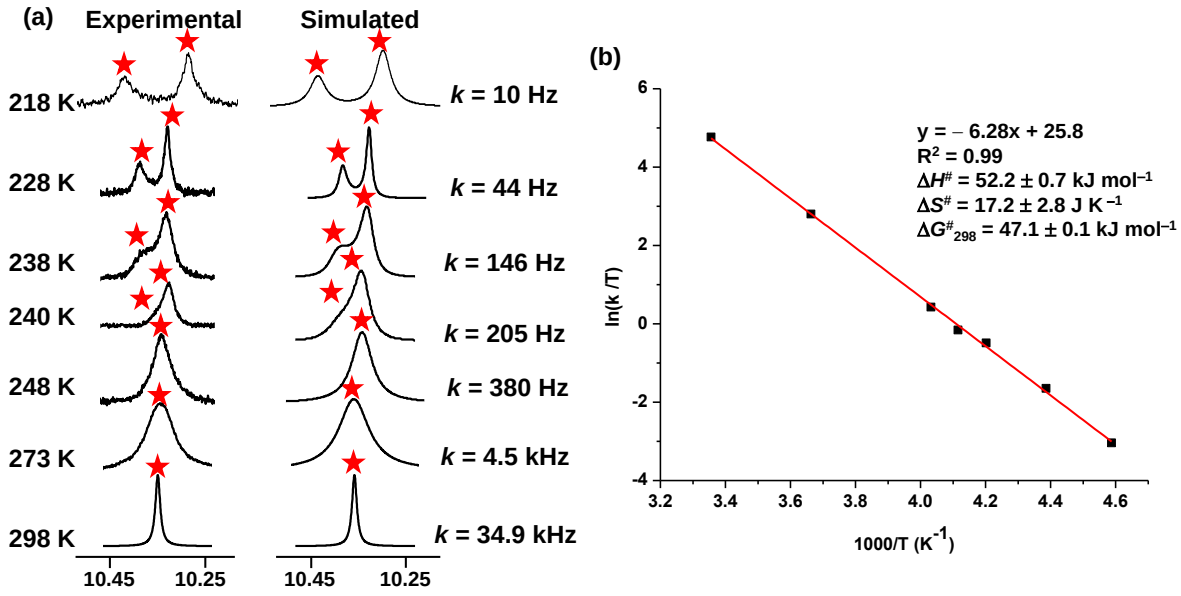


Figure S29: Partial ^{1}H VT-NMR of [**1•2**] (1:1) = **DS1** (CD_2Cl_2, 600 MHz) at different temperatures showing experimental and theoretical splitting of r-H with corresponding rate constants. (b) Eyring plot for sliding dynamics in [**1•2**] (1:1).

8. ESI-MS Spectra

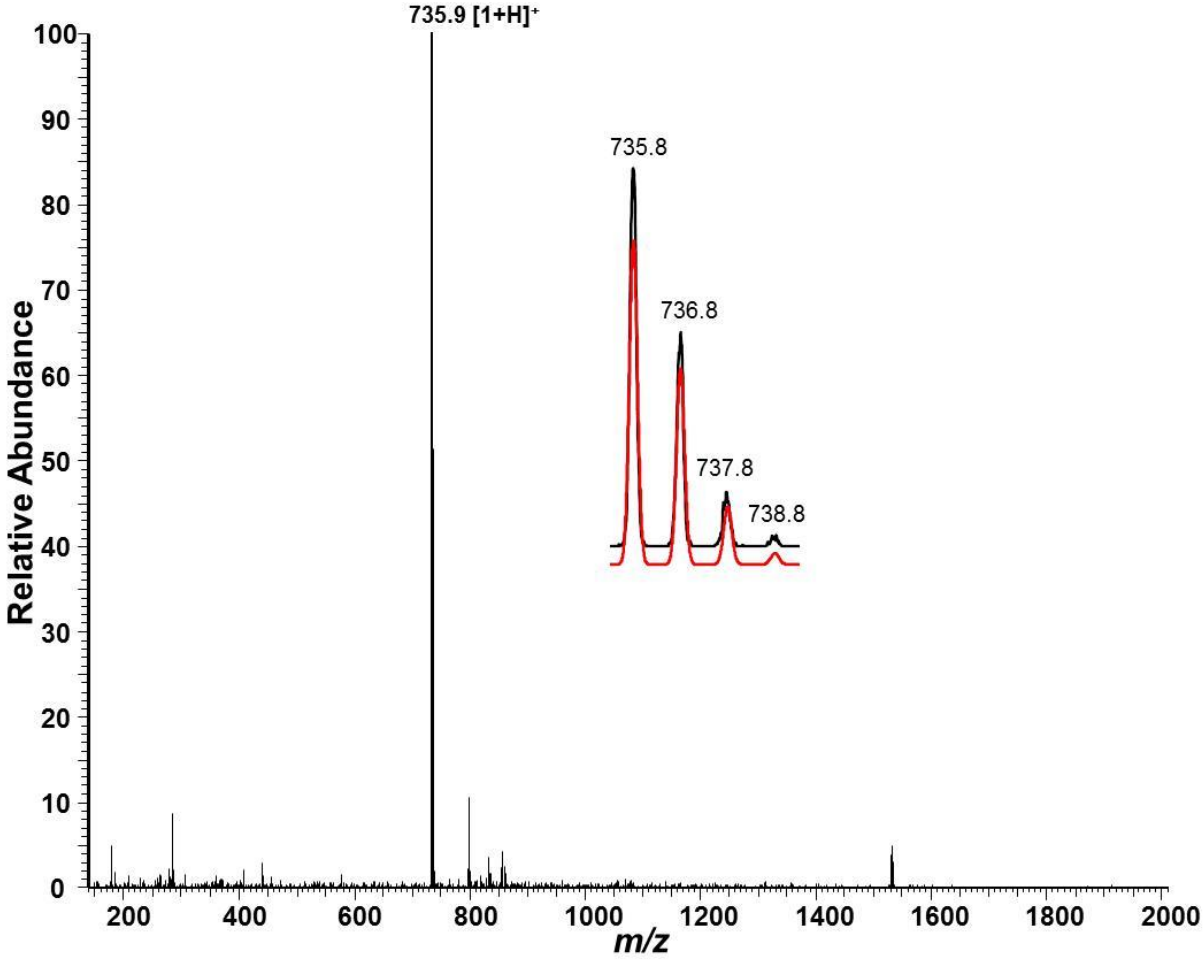


Figure S30 : ESI-MS of **1** after protonation. Inset: The experimental and theoretical isotopic distributions of ligand **1** are in good agreement.

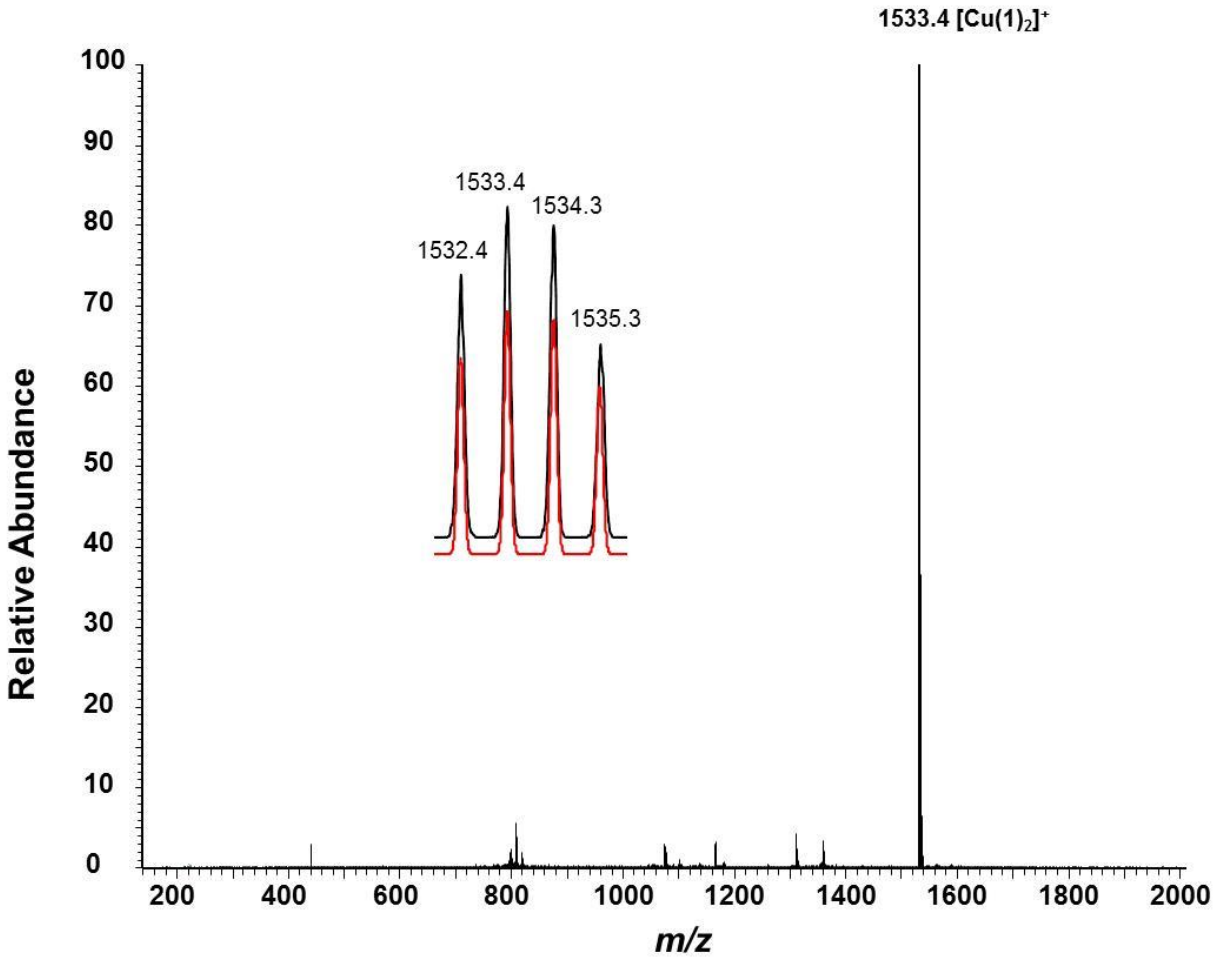


Figure S31: ESI-MS of complex **[**Cu(**1**)$_2$]$^+$. Inset: The experimental and theoretical isotopic distributions of complex **[**Cu(**1**)$_2$]$^+$ correlate well.

9. UV-Vis Studies

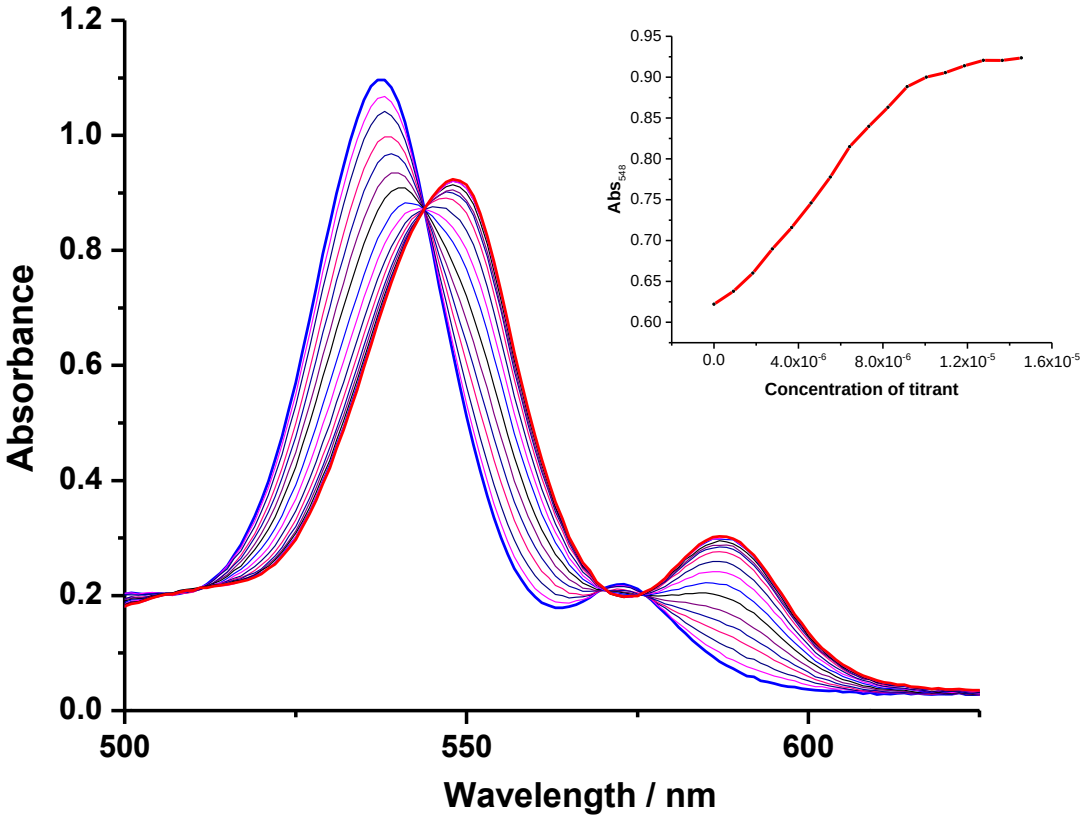


Figure S32: UV-vis spectra of **2** (1.02×10^{-4} M) in CH_2Cl_2 (2 mL) upon addition of **1** (9.24×10^{-4} M) in CH_2Cl_2 at 298 K to afford the complex [**1•2**]. The wavelength region 500-630 nm was analyzed.

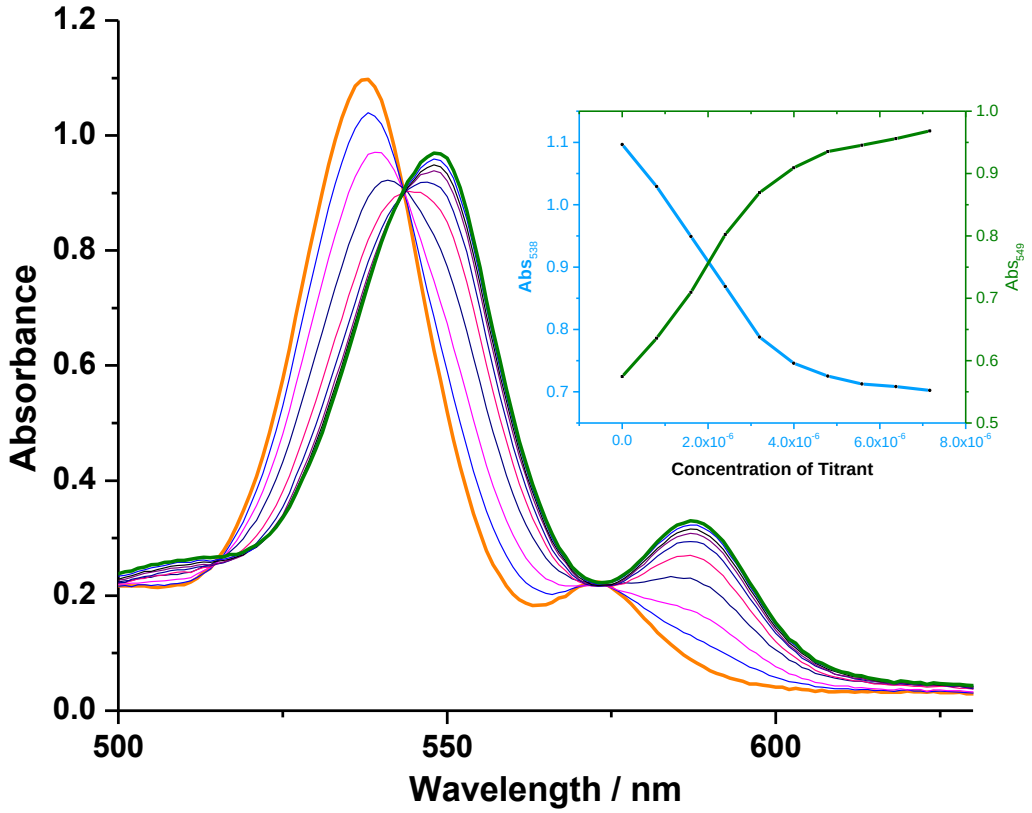


Figure S33: UV-vis spectra of **2** (1.02×10^{-4} M) in CH_2Cl_2 (2 mL) upon addition of $[Cu(\mathbf{1})_2]PF_6$ (8.03×10^{-4} M) in CH_2Cl_2 at 298 K to afford the complex $[(Cu\ (\mathbf{1})_2)\bullet(\mathbf{2})_2]\ ]PF_6$.

10. Computational studies

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.

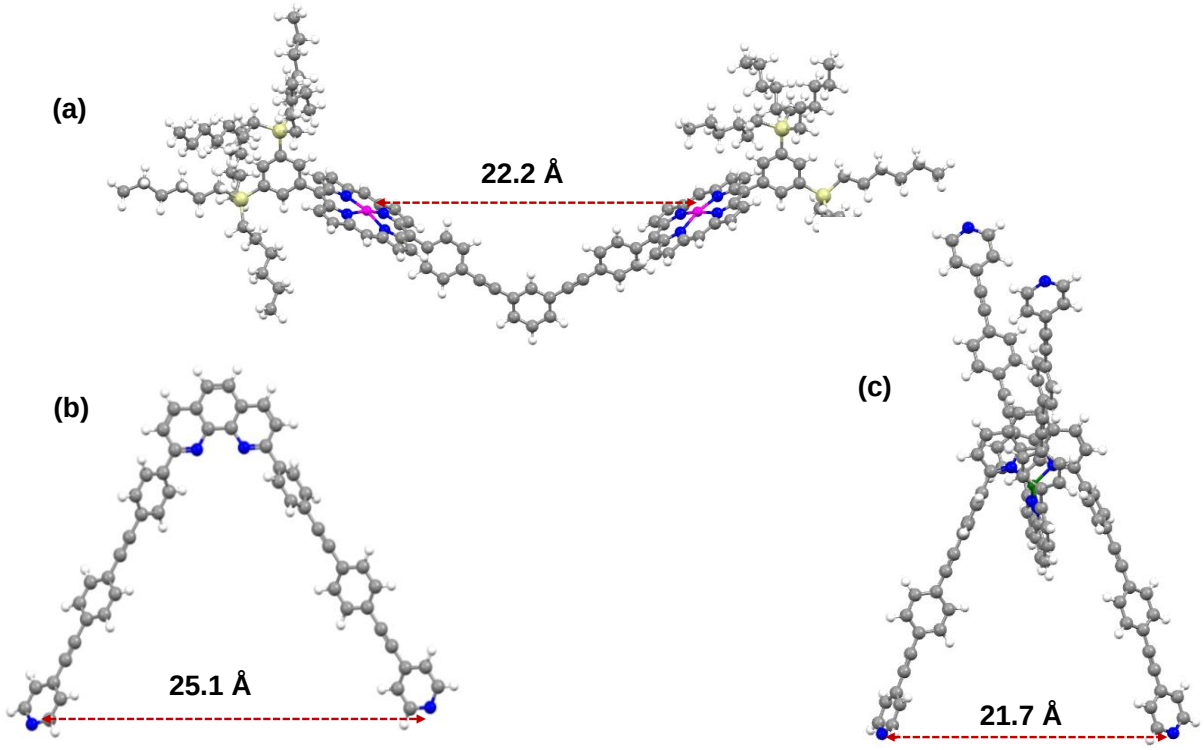


Figure S34. Energy optimized (a) Partial structure of deck **2**. (b) Structure of arm **1**. (c) Structure of catenate arm $[Cu(\mathbf{1})_2]^+$.

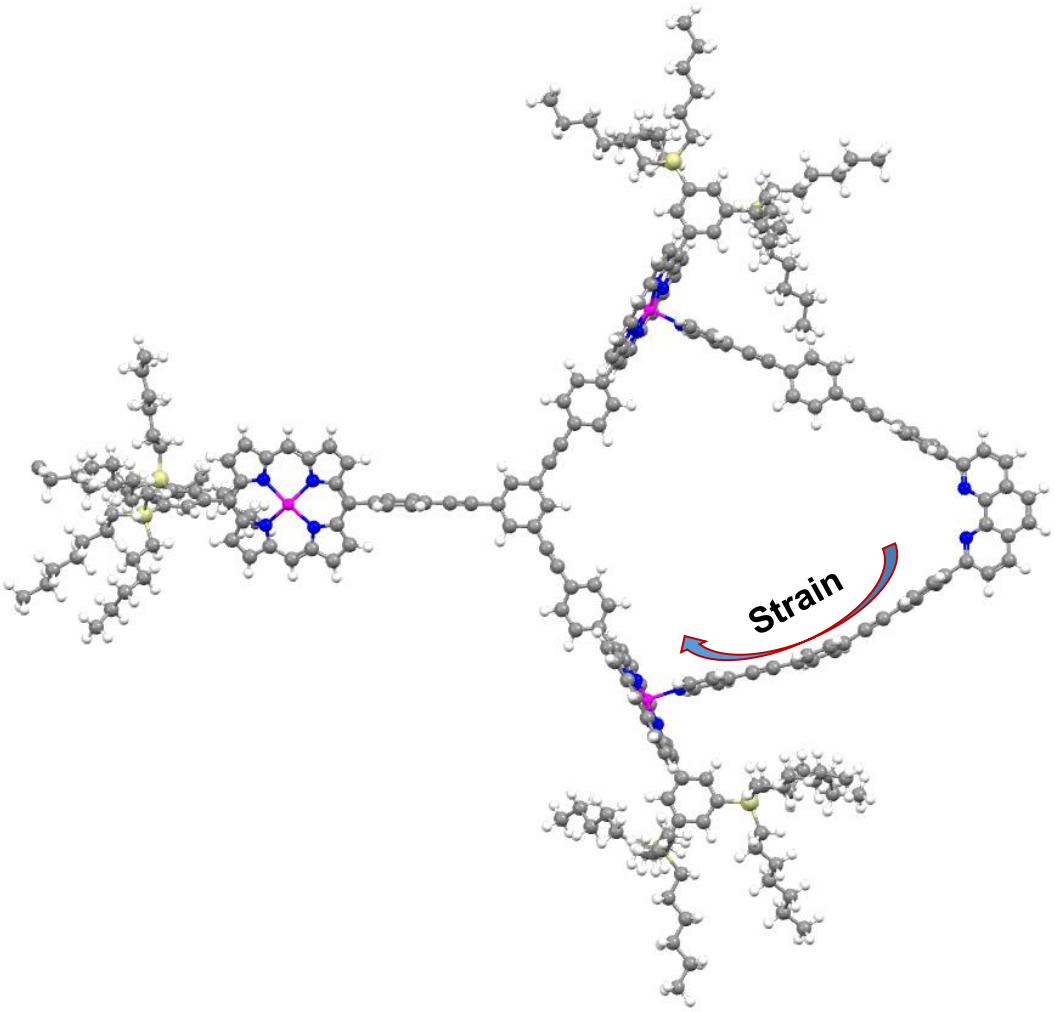


Figure S35. Energy-optimized structure of [**1**•**2**].

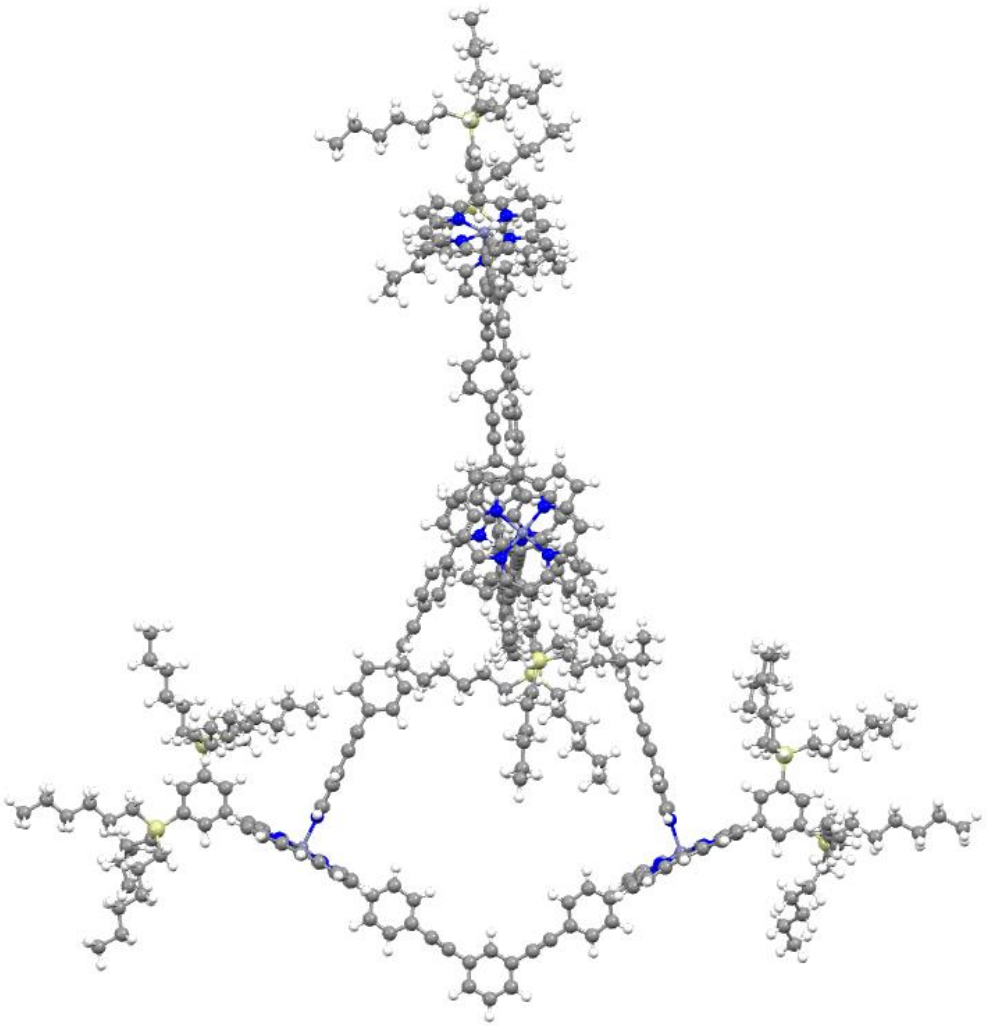


Figure S36. Energy-optimized partial structure of $[Cu(\mathbf{1})_2 \bullet (\mathbf{2})_2]^+$.

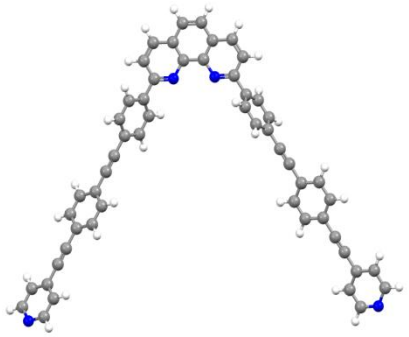


Figure S37. Energy-optimized structure of arm **1** calculated using Gaussian 09 at B3LYP/6-31G(d)

C	-5.454500000	-11.310100000	8.957600000
C	-4.074600000	-11.310100000	8.957600000
C	-3.355300000	-10.093400000	8.957600000
C	-4.052900000	-8.861500000	8.959600000
C	-6.153300000	-10.090000000	8.958600000
C	-1.920200000	-10.101900000	8.955900000
C	-3.303500000	-7.624900000	8.961100000
C	-1.888600000	-7.673100000	8.959300000
C	-1.216900000	-8.941300000	8.956200000
C	-1.142900000	-6.472400000	8.961000000
H	-0.043800000	-6.529100000	8.959600000
C	-1.781500000	-5.249200000	8.964700000
C	-3.186500000	-5.194400000	8.966600000
H	-1.410700000	-11.077700000	8.954100000
H	-6.013700000	-12.257000000	8.956700000
H	-3.515600000	-12.258000000	8.956900000
H	-0.116100000	-8.941800000	8.954600000
H	-1.200900000	-4.315300000	8.966200000
C	-7.693300000	-10.099700000	8.958200000
C	-8.394400000	-9.513100000	10.012100000
C	-8.386900000	-10.693200000	7.903700000
C	-9.789300000	-9.520800000	10.011600000
H	-7.847400000	-9.044800000	10.843100000
C	-9.782300000	-10.701400000	7.903500000
H	-7.834300000	-11.155000000	7.072600000
C	-10.483200000	-10.115300000	8.957400000
H	-10.342000000	-9.058700000	10.842300000
H	-10.329000000	-11.169500000	7.072000000
C	-3.890200000	-3.824600000	8.970800000
C	-4.958500000	-3.587000000	8.105400000
C	-3.460900000	-2.822500000	9.840600000
C	-5.596800000	-2.346800000	8.109600000
H	-5.297100000	-4.377400000	7.420100000
C	-4.099100000	-1.581500000	9.844400000
H	-2.619300000	-3.009900000	10.523200000
C	-5.166800000	-1.343900000	8.978900000
H	-6.438600000	-2.159300000	7.427500000
H	-3.760400000	-0.791500000	10.530300000
C	-12.023200000	-10.124100000	8.957600000
C	-13.224400000	-10.131000000	8.957700000
C	-5.871400000	0.025500000	8.982700000
C	-6.421000000	1.093500000	8.985800000
C	-14.764300000	-10.139800000	8.957900000
C	-15.467600000	-9.091000000	8.364700000
C	-15.455800000	-11.196800000	9.549300000
C	-16.862400000	-9.099000000	8.363800000
H	-14.922200000	-8.257900000	7.898100000
C	-16.851200000	-11.204700000	9.548900000
H	-14.901600000	-12.023900000	10.016300000
C	-17.554200000	-10.155800000	8.956300000
H	-17.416800000	-8.272400000	7.896500000
H	-17.396200000	-12.038200000	10.015300000
C	-7.125700000	2.462900000	8.989600000
C	-8.213200000	2.685000000	9.834900000
C	-6.675800000	3.481300000	8.149600000
C	-8.851000000	3.925400000	9.839400000
H	-8.567400000	1.882000000	10.497500000
C	-7.314200000	4.722100000	8.153700000
H	-5.818200000	3.306500000	7.483700000
C	-8.401700000	4.943900000	8.998500000
H	-9.708300000	4.100500000	10.505500000
H	-6.959400000	5.524900000	7.491200000
C	-19.094200000	-10.164100000	8.955500000
C	-20.295400000	-10.170500000	8.955000000
C	-9.106600000	6.313100000	9.003300000
C	-9.656500000	7.381000000	9.007100000
C	-21.835400000	-10.178800000	8.954200000
C	-22.537800000	-9.145600000	8.333300000
C	-22.527700000	-11.219700000	9.572700000
C	-23.932600000	-9.153200000	8.331600000
H	-21.991800000	-8.325300000	7.845300000
C	-23.923100000	-11.227000000	9.571400000
H	-21.974100000	-12.034400000	10.061600000
H	-24.486400000	-8.338900000	7.842400000
H	-24.468700000	-12.047800000	10.059200000
C	-10.361300000	8.750200000	9.012000000
C	-11.444800000	8.973600000	9.862100000
C	-9.915700000	9.767300000	8.168100000
C	-12.082900000	10.213900000	9.867500000
H	-11.795800000	8.171700000	10.527700000
C	-10.554400000	11.008000000	8.173100000
H	-9.061300000	9.591500000	7.498500000
H	-12.937000000	10.390000000	10.537300000
H	-10.202800000	11.809700000	7.507500000
N	-5.466900000	-8.891400000	8.960000000
N	-3.931400000	-6.357600000	8.964700000
N	-24.625300000	-10.193800000	8.951000000
N	-11.637900000	11.231000000	9.022600000

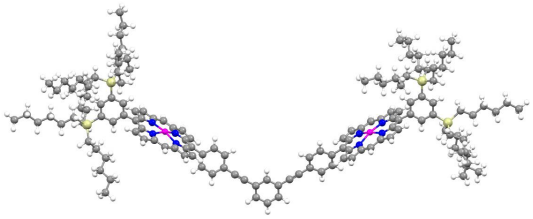


Figure S38. Energy-optimized partial structure of deck **2** calculated using Gaussian 09 at B3LYP/6-31G(d).

C	3.796100000	7.845500000	0.576700000
C	4.650000000	6.997100000	0.641800000
C	5.632000000	5.966800000	0.759100000
C	6.810900000	5.992300000	-0.007000000
C	5.420800000	4.919800000	1.673600000
C	7.772500000	4.977500000	0.146300000
H	6.981400000	6.771800000	-0.692300000

C	6.385000000	3.910900000	1.832200000
H	4.541500000	4.890900000	2.249300000
C	7.567300000	3.934400000	1.070500000
H	8.652700000	5.007500000	-0.428800000
H	6.218100000	3.136800000	2.523600000
C	8.586700000	2.876500000	1.249700000
C	8.433500000	1.651800000	0.663900000
C	9.785500000	3.166800000	2.007000000
N	9.277400000	0.618900000	0.679400000
C	7.280500000	1.358600000	-0.083300000
N	10.846400000	2.383500000	2.177300000
C	9.962700000	4.417000000	2.619900000
Zn	11.043500000	0.489100000	1.600200000
C	8.698900000	-0.331700000	-0.051200000
C	7.443300000	0.056700000	-0.531700000
H	6.463300000	1.979400000	-0.280700000
C	11.740200000	3.122700000	2.828900000
C	11.237600000	4.385000000	3.166400000
H	9.303400000	5.227500000	2.632000000
N	11.389600000	-1.255400000	0.702200000
N	12.969100000	0.565600000	2.087900000
C	9.183000000	-1.556900000	-0.389400000
H	6.789000000	-0.489300000	-1.136800000
C	13.028400000	2.811500000	3.134700000
H	11.731900000	5.162100000	3.660600000
C	10.511100000	-1.950500000	-0.010000000
C	12.480000000	-2.014200000	0.776500000
C	13.593600000	1.563500000	2.701200000
C	13.870400000	-0.400100000	1.956400000
H	8.602100000	-2.203600000	-0.983000000
H	13.631200000	3.507000000	3.645000000
C	11.011200000	-3.195200000	-0.406400000
C	12.295500000	-3.240700000	0.116500000
C	13.667000000	-1.706300000	1.374900000
C	14.939100000	1.272900000	2.952900000
C	15.120700000	-0.013300000	2.463400000
H	10.530200000	-3.930000000	-0.972400000
H	12.979100000	-4.023900000	0.007400000
C	14.772200000	-2.674600000	1.367200000
H	15.647700000	1.876500000	3.427400000
H	16.004200000	-0.570500000	2.490800000
C	14.883300000	-3.609700000	2.408000000
C	15.702700000	-2.673900000	0.314900000
C	15.909600000	-4.567900000	2.383200000
C	16.742800000	-3.618400000	0.285400000
C	16.810000000	-4.587900000	1.303400000
C	2.766400000	8.834400000	0.542900000
C	2.664700000	9.729700000	-0.536600000
C	1.842100000	8.909200000	1.601300000
C	1.642100000	10.693700000	-0.554700000
H	3.349600000	9.681900000	-1.333200000
C	0.817500000	9.873100000	1.585300000
H	1.916600000	8.238600000	2.408700000
C	0.719600000	10.766100000	0.503300000
H	-0.043200000	11.489600000	0.479800000
C	-0.119700000	9.935300000	2.661200000
C	-0.903400000	9.976500000	3.576200000
C	-1.821800000	10.014500000	4.669400000
C	-1.544100000	9.296700000	5.846400000
C	-3.013400000	10.755200000	4.575000000
C	-2.454500000	9.310600000	6.917200000
H	-0.655000000	8.741300000	5.929100000
C	-3.919900000	10.775500000	5.649500000
H	-3.233600000	11.294100000	3.699000000
H	-2.237400000	8.766300000	7.790100000
C	-3.649000000	10.049000000	6.825200000
H	-4.808600000	11.331700000	5.565800000
C	-4.612400000	10.057300000	7.950000000
C	-4.412300000	10.863300000	9.035400000
C	-5.824800000	9.270600000	7.856100000
C	-3.275100000	11.684100000	9.115800000
N	-5.196600000	11.018600000	10.103300000
N	-6.826500000	9.216000000	8.729500000
C	-6.090800000	8.491400000	6.719300000
C	-3.390300000	12.371300000	10.314900000
H	-2.498800000	11.781500000	8.422800000
C	-4.594100000	11.923800000	10.870800000
Zn	-6.897900000	10.066200000	10.527000000
C	-7.758600000	8.450100000	8.169000000
H	-5.491300000	8.360000000	5.873700000
C	-7.353600000	7.954200000	6.924000000
H	-2.725600000	13.077800000	10.704200000
C	-5.001500000	12.429800000	12.066100000
N	-7.136200000	11.165700000	12.170800000
N	-8.774100000	9.446500000	10.743000000
C	-8.992900000	8.136800000	8.647500000
H	-7.891800000	7.340400000	6.271100000
H	-4.405800000	13.143400000	12.560100000
C	-6.249400000	12.026700000	12.655000000
C	-8.145700000	11.151000000	13.040200000
C	-9.585100000	9.657600000	11.774500000
C	-9.446800000	8.668700000	9.903600000
H	-9.630800000	7.515900000	8.086100000
C	-6.650600000	12.569900000	13.880100000
C	-7.886100000	11.992000000	14.135100000
C	-9.321100000	10.462300000	12.946600000
C	-10.815000000	9.003000000	11.605200000
C	-10.724500000	8.355100000	10.380900000
H	-6.141700000	13.265100000	14.471300000
H	-8.495700000	12.178200000	14.963500000
C	-10.344800000	10.570100000	14.005100000
H	-11.633700000	8.994400000	12.254600000
H	-11.450200000	7.757400000	9.925000000
C	-11.325400000	11.579400000	13.969900000
C	-10.329500000	9.647300000	15.064000000
C	-12.300200000	11.663700000	14.982700000
C	-11.258700000	9.755900000	16.111800000
C	-12.244100000	10.759000000	16.060400000
H	14.187700000	-3.596500000	3.196600000
H	15.604300000	-1.963100000	-0.448700000
H	-11.331700000	12.264800000	13.173000000
H	-9.605800000	8.886500000	15.070900000
H	-12.948800000	10.824600000	16.836000000
H	17.546000000	-5.331000000	1.260400000
Si	-11.218900000	8.565000000	17.522100000
Si	-13.621900000	12.974700000	14.910300000
Si	16.016100000	-5.784100000	3.770900000
Si	17.966200000	-3.638200000	-1.106400000
C	17.555600000	-6.865400000	3.648800000
H	17.546800000	-7.555200000	4.494300000
H	17.505400000	-7.453200000	2.730000000
C	18.872700000	-6.045500000	3.663800000
H	19.192800000	-5.863300000	2.636200000
H	18.713800000	-5.083500000	4.154200000

C	19.999200000	-6.803000000	4.412300000
H	20.127200000	-7.793800000	3.970300000
H	19.714500000	-6.917100000	5.461200000
C	21.339000000	-6.027700000	4.326800000
H	21.653400000	-5.972900000	3.281700000
H	21.193800000	-5.013200000	4.705400000
C	22.444100000	-6.727400000	5.159900000
H	22.567000000	-7.753500000	4.805600000
H	22.140700000	-6.750300000	6.209400000
C	23.796300000	-5.978400000	5.035000000
H	24.104500000	-5.958600000	3.987100000
H	23.676600000	-4.950600000	5.385400000
C	24.902800000	-6.666400000	5.869200000
H	25.045500000	-7.692500000	5.526900000
H	25.839500000	-6.119500000	5.751900000
H	24.625400000	-6.673600000	6.924400000
C	16.011100000	-4.807700000	5.388000000
H	16.610300000	-3.904300000	5.253000000
H	14.980700000	-4.508200000	5.589800000
C	14.469400000	-6.865800000	3.685000000
H	13.587900000	-6.228900000	3.782800000
H	14.447400000	-7.348000000	2.705800000
C	16.579800000	-5.602900000	6.593400000
H	17.664800000	-5.483800000	6.609600000
H	16.349900000	-6.663400000	6.493400000
C	15.973300000	-5.091000000	7.927100000
H	16.168300000	-4.021500000	8.032800000
H	14.890300000	-5.240100000	7.892100000
C	16.515100000	-5.838700000	9.175000000
H	15.902500000	-5.545200000	10.031700000
H	16.408000000	-6.916500000	9.031100000
C	17.998300000	-5.500600000	9.483500000
H	18.642500000	-5.951300000	8.725800000
H	18.137900000	-4.417400000	9.465500000
C	14.450200000	-7.945000000	4.795400000
H	14.355300000	-7.462800000	5.770200000
H	15.387200000	-8.504000000	4.763800000
C	13.273700000	-8.939000000	4.617400000
H	12.329600000	-8.423100000	4.806300000
H	13.273100000	-9.315600000	3.592100000
C	13.420600000	-10.134100000	5.596600000
H	13.347100000	-9.770500000	6.624400000
H	14.403800000	-10.589800000	5.454900000
C	12.331000000	-11.209700000	5.351900000
H	11.347200000	-10.787600000	5.567800000
H	12.358000000	-11.522900000	4.305600000
C	12.558100000	-12.451800000	6.246800000
H	12.511800000	-12.168800000	7.299300000
H	11.784600000	-13.193800000	6.043100000
H	13.534300000	-12.891100000	6.034700000
C	18.447300000	-1.864400000	-1.554600000
H	18.593300000	-1.312200000	-0.624600000
H	19.395000000	-1.880100000	-2.095800000
C	17.213700000	-4.514000000	-2.599900000
H	16.562000000	-3.820900000	-3.133200000
H	18.016500000	-4.816500000	-3.272800000
C	19.500700000	-4.589700000	-0.543300000
H	19.909800000	-4.105500000	0.345500000
H	19.193500000	-5.604000000	-0.281300000
C	20.595000000	-4.669500000	-1.638000000
H	21.025900000	-3.679000000	-1.796500000
H	20.149400000	-5.014700000	-2.572100000
C	21.720400000	-5.660000000	-1.234400000
H	22.239300000	-5.279800000	-0.351700000
H	21.274800000	-6.628100000	-0.991900000
C	22.736100000	-5.851400000	-2.392000000
H	23.214100000	-4.894400000	-2.613500000
H	22.201700000	-6.192500000	-3.282200000
C	23.824100000	-6.895500000	-2.027200000
H	24.394900000	-6.540500000	-1.166300000
H	23.346900000	-7.842900000	-1.766100000
C	24.793400000	-7.137100000	-3.209500000
H	25.289800000	-6.205100000	-3.483600000
H	25.548200000	-7.869300000	-2.918200000
H	24.243600000	-7.519200000	-4.071300000
C	16.376300000	-5.749700000	-2.185100000
H	16.945000000	-6.372000000	-1.491100000
H	15.466400000	-5.405400000	-1.687600000
C	15.997900000	-6.598900000	-3.427100000
H	15.660800000	-5.939700000	-4.230800000
H	16.884800000	-7.139800000	-3.766000000
C	14.864600000	-7.607800000	-3.105600000
H	15.133200000	-8.191200000	-2.222000000
H	13.947300000	-7.051900000	-2.896200000
C	14.621800000	-8.571400000	-4.297200000
H	14.480900000	-7.993700000	-5.213500000
H	15.494600000	-9.217000000	-4.420700000
C	13.371500000	-9.454100000	-4.070300000
H	12.479400000	-8.828300000	-4.014800000
H	13.263400000	-10.151700000	-4.902500000
H	13.473800000	-10.019700000	-3.143200000
C	17.382900000	-1.162400000	-2.445100000
H	17.718200000	-1.180800000	-3.485000000
H	16.442500000	-1.712300000	-2.399500000
C	17.068100000	0.298300000	-2.022800000
H	16.087100000	0.555300000	-2.432700000
H	17.006800000	0.365600000	-0.934200000
C	18.101100000	1.325200000	-2.556700000
H	19.071500000	1.148600000	-2.088200000
H	18.201300000	1.200500000	-3.637500000
C	17.634500000	2.775700000	-2.256700000
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C	18.543300000	3.826600000	-2.937600000
H	18.531700000	3.685200000	-4.019500000
H	18.174100000	4.827900000	-2.708900000
H	19.566300000	3.732200000	-2.571600000
C	-11.417400000	9.504500000	19.149700000
H	-12.383100000	10.012800000	19.146800000
H	-10.625500000	10.251600000	19.223400000
C	-11.343200000	8.545200000	20.365400000
H	-10.383100000	8.025400000	20.357900000
H	-12.144600000	7.807100000	20.290200000
C	-11.484300000	9.299700000	21.712800000
H	-10.673100000	10.025400000	21.806000000
H	-12.439100000	9.829700000	21.732700000
C	-11.423600000	8.304500000	22.902700000
H	-10.474100000	7.764400000	22.870000000
H	-12.240300000	7.584500000	22.808200000
C	-11.545100000	9.033100000	24.266200000
H	-10.723100000	9.744600000	24.372700000
H	-12.490400000	9.578900000	24.304400000
C	-11.497000000	8.031600000	25.445500000
H	-10.552400000	7.485500000	25.434600000

H	-11.582000000	8.574300000	26.388200000
H	-12.323200000	7.323000000	25.368500000
C	-12.636700000	7.329000000	17.362000000
H	-13.586600000	7.864800000	17.406700000
H	-12.579400000	6.653200000	18.217500000
C	-9.600800000	7.591400000	17.572700000
H	-9.518800000	6.988800000	16.666400000
H	-9.658700000	6.907400000	18.420600000
C	-12.568900000	6.506400000	16.047600000
H	-13.113300000	7.036900000	15.263200000
H	-11.531700000	6.387800000	15.731000000
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H	-12.616200000	4.581000000	17.037000000
C	-13.120100000	4.242200000	14.957600000
H	-13.784200000	4.680900000	14.209500000
H	-12.099000000	4.244400000	14.568800000
C	-13.549600000	2.777200000	15.238100000
H	-12.860700000	2.330900000	15.959500000
H	-14.556100000	2.766700000	15.662500000
C	-13.541400000	1.921200000	13.949200000
H	-14.254300000	2.324300000	13.228600000
H	-12.543800000	1.918100000	13.507500000
H	-13.824400000	0.895700000	14.192700000
C	-8.338300000	8.489700000	17.683900000
H	-7.837200000	8.491200000	16.712600000
H	-8.618800000	9.519100000	17.915200000
C	-7.353100000	7.991300000	18.778600000
H	-7.452200000	8.635100000	19.656300000
H	-7.600800000	6.969200000	19.072800000
C	-5.881600000	8.006900000	18.287400000
H	-5.781700000	7.308700000	17.452300000
H	-5.620700000	9.010200000	17.943300000
C	-4.912200000	7.585600000	19.423200000
H	-4.928400000	8.342900000	20.210400000
H	-5.237100000	6.632500000	19.847100000
C	-3.463200000	7.427700000	18.904600000
H	-2.807300000	7.162600000	19.735300000
H	-3.420300000	6.637500000	18.153200000
H	-3.118400000	8.364100000	18.463900000
C	-15.006600000	12.474100000	16.101000000
H	-15.212800000	11.410700000	15.959200000
H	-14.641500000	12.623900000	17.119500000
C	-16.334200000	13.252400000	15.918300000
H	-16.132300000	14.320900000	15.891700000
H	-16.792500000	12.951600000	14.975800000
C	-17.362400000	12.995800000	17.050800000
H	-16.907000000	13.221100000	18.017400000
H	-17.667600000	11.947600000	17.034300000
C	-18.603200000	13.907900000	16.842800000
H	-18.286400000	14.953200000	16.890700000
H	-19.025900000	13.716600000	15.853200000
C	-19.698700000	13.665700000	17.912600000
H	-19.284000000	13.843700000	18.907100000
H	-20.042400000	12.630900000	17.853000000
C	-20.906800000	14.610000000	17.696000000
H	-21.667400000	14.409800000	18.452100000
H	-20.588400000	15.650400000	17.780500000
H	-21.338100000	14.446000000	16.707100000
C	-14.184000000	13.069900000	13.103100000
H	-13.347500000	13.467300000	12.524300000
H	-14.389500000	12.056700000	12.750700000
C	-15.438900000	13.946200000	12.851600000
H	-16.321300000	13.302600000	12.841200000
H	-15.550500000	14.672000000	13.651700000
C	-15.385300000	14.734100000	11.516700000
H	-14.463500000	15.319300000	11.479000000
H	-15.400000000	14.034900000	10.678400000
C	-16.600300000	15.697600000	11.421800000
H	-17.523800000	15.114200000	11.452000000
H	-16.585500000	16.373700000	12.280900000
C	-16.573900000	16.541600000	10.121700000
H	-15.642300000	17.110100000	10.074900000
H	-16.626200000	15.877900000	9.256000000
C	-17.764800000	17.529800000	10.072200000
H	-17.725700000	18.102400000	9.144300000
H	-18.707900000	16.982500000	10.112000000
H	-17.713900000	18.219600000	10.916400000
C	-12.810300000	14.612300000	15.411500000
H	-12.140000000	14.421800000	16.252400000
H	-12.214100000	14.962100000	14.566400000
C	-13.825600000	15.710200000	15.823900000
H	-14.196300000	15.498900000	16.829500000
H	-14.668500000	15.694300000	15.137000000
C	-13.278300000	17.160000000	15.772600000
H	-14.118300000	17.829400000	15.980400000
H	-12.918900000	17.369400000	14.762200000
C	-12.148000000	17.451100000	16.793700000
H	-12.384800000	16.961700000	17.741600000
H	-11.206600000	17.043200000	16.419300000
C	-11.980900000	18.972000000	17.070300000
H	-11.163900000	19.105700000	17.783700000
H	-12.896800000	19.356200000	17.526600000
C	-11.667400000	19.805700000	15.803000000
H	-10.777000000	19.416900000	15.307700000
H	-12.509400000	19.775200000	15.110100000
H	-11.490400000	20.844200000	16.088500000
C	18.420100000	-6.029000000	10.875800000
H	18.281400000	-7.109900000	10.925300000
H	19.471900000	-5.796700000	11.049800000
H	17.819800000	-5.552600000	11.652800000
H	1.565600000	11.374700000	-1.376500000

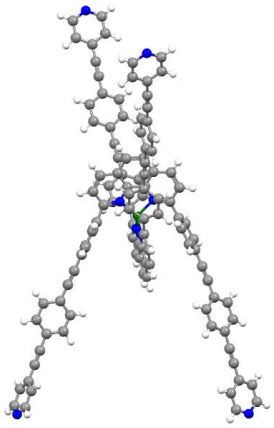

Figure S39. Energy-optimized structure of $[Cu(\mathbf{1})_2]^+$, calculated using Gaussian 09 at B3LYP/6-31G(d) and separately Lanl2dz basis set for copper(I)

N	-2.733900000	11.286700000	15.955900000
C	-2.990600000	10.205100000	15.180600000
C	-2.209600000	11.162900000	17.199500000
C	-2.713600000	8.911500000	15.655000000
H	-3.395800000	10.338600000	14.220200000
C	-1.915100000	9.891500000	17.721100000
H	-2.021100000	12.023500000	17.772200000
C	-2.168400000	8.749500000	16.941200000
H	-2.911000000	8.076800000	15.047300000
H	-1.504500000	9.801800000	18.684400000
C	-1.858900000	7.447900000	17.440400000
C	-1.600600000	6.343800000	17.850100000
C	-1.265700000	5.035000000	18.316500000
C	-0.021200000	4.473700000	17.980700000
C	-2.176900000	4.286300000	19.083600000
C	0.302400000	3.168600000	18.390400000
H	0.667400000	5.021400000	17.405000000
C	-1.853400000	2.978800000	19.491500000
H	-3.112200000	4.695100000	19.338700000
C	-0.615800000	2.409400000	19.139600000
H	1.227600000	2.753900000	18.113800000
H	-2.553900000	2.422800000	20.045500000
C	-0.308500000	1.049600000	19.465400000
C	-0.048300000	-0.096300000	19.740000000
C	0.225500000	-1.470500000	20.037800000
C	1.161500000	-1.835000000	21.021500000
C	-0.452100000	-2.484100000	19.338400000
C	1.414300000	-3.193000000	21.289500000
H	1.667200000	-1.094300000	21.571400000
C	-0.203100000	-3.838800000	19.621500000
H	-1.161000000	-2.231300000	18.604000000
C	0.746600000	-4.215400000	20.591100000
H	2.087000000	-3.438800000	22.047000000
H	-0.744200000	-4.572300000	19.100100000
C	0.952600000	-5.648200000	20.908300000
C	-0.030400000	-6.358800000	21.628300000
N	1.977600000	-6.341500000	20.440700000
C	0.078400000	-7.754600000	21.788600000
H	-0.864000000	-5.853600000	22.022600000
C	2.126200000	-7.653200000	20.549100000
C	1.165500000	-8.434100000	21.208400000
H	-0.673500000	-8.283500000	22.297800000
C	3.205000000	-8.259100000	19.862000000
C	1.300200000	-9.835500000	21.184300000
C	3.306100000	-9.656300000	19.790200000
N	4.033600000	-7.477700000	19.184600000
C	2.355200000	-10.441700000	20.470600000
H	0.585400000	-10.440800000	21.662100000
C	4.322600000	-10.179500000	18.970200000
C	5.006100000	-7.902500000	18.389700000
H	2.410500000	-11.490800000	20.425800000
C	5.170400000	-9.298800000	18.268600000
H	4.424400000	-11.217900000	18.842600000
C	5.764300000	-6.996400000	17.489100000
H	5.895200000	-9.689700000	17.614600000
C	5.261200000	-6.759800000	16.198500000
C	7.010600000	-6.424800000	17.813000000
C	5.894600000	-5.894200000	15.295100000
H	4.385800000	-7.233000000	15.899600000
C	7.677500000	-5.581900000	16.896700000
H	7.456500000	-6.634800000	18.741300000
C	7.107500000	-5.281200000	15.643800000
H	5.453900000	-5.707000000	14.358200000
H	8.608200000	-5.168100000	17.158100000
C	7.688700000	-4.359900000	14.708900000
C	8.113000000	-3.588900000	13.881200000
C	8.564700000	-2.659000000	12.885800000
C	9.939200000	-2.464000000	12.658500000
C	7.635400000	-1.892000000	12.157000000
C	10.378400000	-1.488100000	11.745600000
H	10.647700000	-3.031100000	13.189200000
C	8.074000000	-0.915500000	11.243400000
H	6.603600000	-2.028100000	12.309400000
C	9.449400000	-0.696400000	11.046500000
H	11.409600000	-1.335000000	11.606700000
H	7.367100000	-0.332100000	10.726800000
C	9.909700000	0.358700000	10.196900000
C	10.321300000	1.242400000	9.486700000
C	10.832100000	2.283400000	8.650700000
C	9.962900000	3.158200000	7.974800000
C	12.219800000	2.465600000	8.512500000
C	10.498200000	4.185800000	7.178800000
H	8.920900000	3.053000000	8.063400000
C	12.704100000	3.508500000	7.704500000
H	12.895100000	1.832600000	9.010700000
H	9.858300000	4.846400000	6.670300000
N	11.840500000	4.334000000	7.064700000
H	13.739200000	3.653900000	7.595700000
Cu	3.356800000	-5.794300000	19.383500000
N	2.981400000	-5.052400000	17.761400000
C	2.309600000	-5.565600000	16.740100000
C	3.675100000	-3.925500000	17.737800000
C	1.640900000	-6.894000000	16.801600000
C	2.336700000	-4.836000000	15.532500000
C	4.407900000	-3.566200000	18.893600000
C	3.723200000	-3.133600000	16.581800000
C	1.980100000	-7.925600000	15.902000000
C	0.615000000	-7.156600000	17.729000000
C	3.036800000	-3.615200000	15.452200000
H	1.843400000	-5.206200000	14.681200000
C	5.128800000	-2.363400000	18.930700000
N	4.395200000	-4.392900000	19.930200000
C	4.469400000	-1.939900000	16.610700000
C	1.406200000	-9.203900000	16.001200000
H	2.681500000	-7.760800000	15.140200000
C	-0.013300000	-8.414800000	17.793200000
H	0.279600000	-6.392000000	18.359500000
H	3.060000000	-3.083400000	14.546300000
C	5.787700000	-2.051900000	20.133400000
C	5.154100000	-1.550700000	17.780800000
C	4.999800000	-4.163400000	21.087600000
H	4.517900000	-1.328900000	15.756600000
C	0.394900000	-9.456100000	16.941800000
H	1.716200000	-9.964200000	15.343600000
H	-0.799600000	-8.568600000	18.474500000
C	5.713200000	-2.952200000	21.214300000
H	6.329000000	-1.156500000	20.231900000
H	5.698700000	-0.651300000	17.785100000
C	4.942300000	-5.082700000	22.250300000
C	-0.258800000	-10.728200000	16.937800000
H	6.200700000	-2.718600000	22.116500000
C	4.084200000	-4.812800000	23.334700000
C	5.850800000	-6.151200000	22.382200000
C	-0.788200000	-11.811400000	16.897800000

C	4.052500000	-5.641300000	24.469800000
H	3.463000000	-3.970600000	23.319400000
C	5.854900000	-6.957800000	23.538100000
H	6.559100000	-6.331900000	21.626500000
C	-1.419500000	-13.092100000	16.810100000
C	4.936700000	-6.727300000	24.580000000
H	3.372500000	-5.432400000	25.245000000
H	6.554100000	-7.739100000	23.621400000
C	-1.559000000	-13.895900000	17.955400000
C	-1.925200000	-13.549600000	15.578800000
C	4.874500000	-7.582700000	25.730100000
C	-2.210700000	-15.138600000	17.872200000
H	-1.183600000	-13.568200000	18.881100000
C	-2.577100000	-14.793200000	15.495100000
H	-1.825300000	-12.958900000	14.714200000
C	4.802300000	-8.290900000	26.705500000
C	-2.727900000	-15.589400000	16.644600000
H	-2.316600000	-15.727700000	18.736800000
H	-2.958200000	-15.119600000	14.570500000
C	4.720600000	-9.134300000	27.862400000
C	-3.409100000	-16.843700000	16.586300000
C	5.690400000	-10.130400000	28.079200000
C	3.634000000	-9.032300000	28.751800000
C	-3.981900000	-17.904100000	16.571100000
C	5.561800000	-11.030200000	29.152500000
H	6.505500000	-10.224300000	27.421700000
C	3.504500000	-9.932200000	29.826000000
H	2.896000000	-8.297800000	28.603300000
C	-4.668900000	-19.155000000	16.557300000
C	4.460900000	-10.944600000	30.023600000
H	6.282100000	-11.784900000	29.285600000
H	2.673900000	-9.859800000	30.467700000
C	-6.038500000	-19.222500000	16.868500000
C	-3.978700000	-20.343300000	16.260500000
C	4.291800000	-11.911700000	31.063400000
C	-6.683400000	-20.471200000	16.875700000
H	-6.579400000	-18.351400000	17.099900000
C	-4.670300000	-21.566500000	16.282300000
H	-2.953400000	-20.323900000	16.030400000
C	4.157900000	-12.732000000	31.936900000
N	-5.990600000	-21.599600000	16.586400000
H	-7.705800000	-20.534800000	17.109800000
H	-4.163700000	-22.461400000	16.066300000
C	4.008400000	-13.708400000	32.969400000
C	2.892700000	-13.679300000	33.825000000
C	4.963400000	-14.727600000	33.134100000
C	2.759600000	-14.662000000	34.821000000
H	2.159100000	-12.933400000	33.723400000
C	4.783500000	-15.686600000	34.145900000
H	5.805300000	-14.779400000	32.507100000
H	1.929200000	-14.650400000	35.465000000
N	3.697800000	-15.630600000	34.955200000
H	5.490200000	-16.453200000	34.277200000

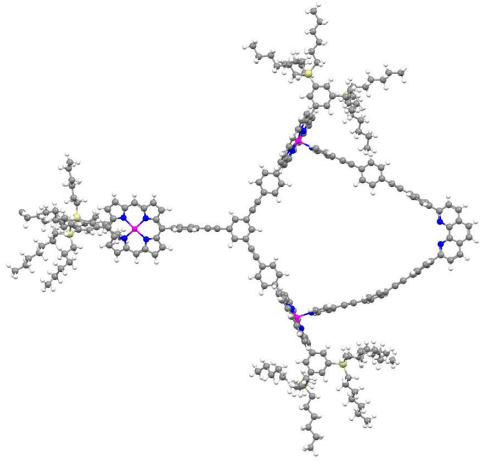

Figure S40. Energy-optimized structure of [**1•2**], calculated using Gaussian 09 at B3LYP/6-31G(d).

C	3.796100000	7.845500000	0.576700000
C	4.650000000	6.997100000	0.641800000
C	5.632000000	5.966800000	0.759100000
C	6.810900000	5.992300000	-0.007000000
C	5.420800000	4.919800000	1.673600000
C	7.772500000	4.977500000	0.146300000
H	6.981400000	6.771800000	-0.692300000
C	6.385000000	3.910900000	1.832200000
H	4.541500000	4.890900000	2.249300000
C	7.567300000	3.934400000	1.070500000
H	8.652700000	5.007500000	-0.428800000
H	6.218100000	3.136800000	2.523600000
C	8.586700000	2.876500000	1.249700000
C	8.433500000	1.651800000	0.663900000
C	9.785500000	3.166800000	2.007000000
N	9.277400000	0.618900000	0.679400000
C	7.280500000	1.358600000	-0.083300000
N	10.846400000	2.383500000	2.177300000
C	9.962700000	4.417000000	2.619900000
Zn	11.043500000	0.489100000	1.600200000
C	8.698900000	-0.331700000	-0.051200000
C	7.443300000	0.056700000	-0.531700000
H	6.463300000	1.979400000	-0.280700000
C	11.740200000	3.122700000	2.828900000
C	11.237600000	4.385000000	3.166400000
H	9.303400000	5.227500000	2.632000000
N	11.389600000	-1.255400000	0.702200000
N	12.969100000	0.565600000	2.087900000
C	9.183000000	-1.556900000	-0.389400000
H	6.789000000	-0.489300000	-1.136800000
C	13.028400000	2.811500000	3.134700000
H	11.731900000	5.162100000	3.660600000
C	10.511100000	-1.950500000	-0.010000000
C	12.480000000	-2.014200000	0.776500000
C	13.593600000	1.563500000	2.701200000
C	13.870400000	-0.400100000	1.956400000
H	8.602100000	-2.203600000	-0.983000000
H	13.631200000	3.507000000	3.645000000
C	11.011200000	-3.195200000	-0.406400000
C	12.295500000	-3.240700000	0.116500000
C	13.667000000	-1.706300000	1.374900000
C	14.939100000	1.272900000	2.952900000

C	15.120700000	-0.013300000	2.463400000
H	10.530200000	-3.930000000	-0.972400000
H	12.979100000	-4.023900000	0.007400000
C	14.772200000	-2.674600000	1.367200000
H	15.647700000	1.876500000	3.427400000
H	16.004200000	-0.570500000	2.490800000
C	14.883300000	-3.609700000	2.408000000
C	15.702700000	-2.673900000	0.314900000
C	15.909600000	-4.567900000	2.383200000
C	16.742800000	-3.618400000	0.285400000
C	16.810000000	-4.587900000	1.303400000
C	2.766400000	8.834400000	0.542900000
C	2.664700000	9.729700000	-0.536600000
C	1.842100000	8.909200000	1.601300000
C	1.642100000	10.693700000	-0.554700000
H	3.349600000	9.681900000	-1.333200000
C	0.817500000	9.873100000	1.585300000
H	1.916600000	8.238600000	2.408700000
C	0.719600000	10.766100000	0.503300000
H	-0.043200000	11.489600000	0.479800000
C	-0.119700000	9.935300000	2.661200000
C	-0.903400000	9.976500000	3.576200000
C	-1.821800000	10.014500000	4.669400000
C	-1.544100000	9.296700000	5.846400000
C	-3.013400000	10.755200000	4.575000000
C	-2.454500000	9.310600000	6.917200000
H	-0.655000000	8.741300000	5.929100000
C	-3.919900000	10.775500000	5.649500000
H	-3.233600000	11.294100000	3.699000000
H	-2.237400000	8.766300000	7.790100000
C	-3.649000000	10.049000000	6.825200000
H	-4.808600000	11.331700000	5.565800000
C	-4.612400000	10.057300000	7.950000000
C	-4.412300000	10.863300000	9.035400000
C	-5.824800000	9.270600000	7.856100000
C	-3.275100000	11.684100000	9.115800000
N	-5.196600000	11.018600000	10.103300000
N	-6.826500000	9.216000000	8.729500000
C	-6.090800000	8.491400000	6.719300000
C	-3.390300000	12.371300000	10.314900000
H	-2.498800000	11.781500000	8.422800000
C	-4.594100000	11.923800000	10.870800000
Zn	-6.897900000	10.066200000	10.527000000
C	-7.758600000	8.450100000	8.169000000
H	-5.491300000	8.360000000	5.873700000
C	-7.353600000	7.954200000	6.924000000
H	-2.725600000	13.077800000	10.704200000
C	-5.001500000	12.429800000	12.066100000
N	-7.136200000	11.165700000	12.170800000
N	-8.774100000	9.446500000	10.743000000
C	-8.992900000	8.136800000	8.647500000
H	-7.891800000	7.340400000	6.271100000
H	-4.405800000	13.143400000	12.560100000
C	-6.249400000	12.026700000	12.655000000
C	-8.145700000	11.151000000	13.040200000
C	-9.585100000	9.657600000	11.774500000
C	-9.446800000	8.668700000	9.903600000
H	-9.630800000	7.515900000	8.086100000
C	-6.650600000	12.569900000	13.880100000
C	-7.886100000	11.992000000	14.135100000
C	-9.321100000	10.462300000	12.946600000
C	-10.815000000	9.003000000	11.605200000
C	-10.724500000	8.355100000	10.380900000
H	-6.141700000	13.265100000	14.471300000
H	-8.495700000	12.178200000	14.963500000
C	-10.344800000	10.570100000	14.005100000
H	-11.633700000	8.994400000	12.254600000
H	-11.450200000	7.757400000	9.925000000
C	-11.325400000	11.579400000	13.969900000
C	-10.329500000	9.647300000	15.064000000
C	-12.300200000	11.663700000	14.982700000
C	-11.258700000	9.755900000	16.111800000
C	-12.244100000	10.759000000	16.060400000
H	14.187700000	-3.596500000	3.196600000
H	15.604300000	-1.963100000	-0.448700000
H	-11.331700000	12.264800000	13.173000000
H	-9.605800000	8.886500000	15.070900000
H	-12.948800000	10.824600000	16.836000000
H	17.546000000	-5.331000000	1.260400000
Si	-11.218900000	8.565000000	17.522100000
Si	-13.621900000	12.974700000	14.910300000
Si	16.016100000	-5.784100000	3.770900000
Si	17.966200000	-3.638200000	-1.106400000
C	17.555600000	-6.865400000	3.648800000
H	17.546800000	-7.555200000	4.494300000
H	17.505400000	-7.453200000	2.730000000
C	18.872700000	-6.045500000	3.663800000
H	19.192800000	-5.863300000	2.636200000
H	18.713800000	-5.083500000	4.154200000
C	19.999200000	-6.803000000	4.412300000
H	20.127200000	-7.793800000	3.970300000
H	19.714500000	-6.917100000	5.461200000
C	21.339000000	-6.027700000	4.326800000
H	21.653400000	-5.972900000	3.281700000
H	21.193800000	-5.013200000	4.705400000
C	22.444100000	-6.727400000	5.159900000
H	22.567000000	-7.753500000	4.805600000
H	22.140700000	-6.750300000	6.209400000
C	23.796300000	-5.978400000	5.035000000
H	24.104500000	-5.958600000	3.987100000
H	23.676600000	-4.950600000	5.385400000
C	24.902800000	-6.666400000	5.869200000
H	25.045500000	-7.692500000	5.526900000
H	25.839500000	-6.119500000	5.751900000
H	24.625400000	-6.673600000	6.924400000
C	16.011100000	-4.807700000	5.388000000
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H	14.980700000	-4.508200000	5.589800000
C	14.469400000	-6.865800000	3.685000000
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H	14.447400000	-7.348000000	2.705800000
C	16.579800000	-5.602900000	6.593400000
H	17.664800000	-5.483800000	6.609600000
H	16.349900000	-6.663400000	6.493400000
C	15.973300000	-5.091000000	7.927100000
H	16.168300000	-4.021500000	8.032800000
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C	16.515100000	-5.838700000	9.175000000
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C	17.998300000	-5.500600000	9.483500000
H	18.642500000	-5.951300000	8.725800000
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C	14.450200000	-7.945000000	4.795400000

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H	12.329600000	-8.423100000	4.806300000
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C	13.420600000	-10.134100000	5.596600000
H	13.347100000	-9.770500000	6.624400000
H	14.403800000	-10.589800000	5.454900000
C	12.331000000	-11.209700000	5.351900000
H	11.347200000	-10.787600000	5.567800000
H	12.358000000	-11.522900000	4.305600000
C	12.558100000	-12.451800000	6.246800000
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H	13.534300000	-12.891100000	6.034700000
C	18.447300000	-1.864400000	-1.554600000
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C	17.213700000	-4.514000000	-2.599900000
H	16.562000000	-3.820900000	-3.133200000
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H	19.193500000	-5.604000000	-0.281300000
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H	23.346900000	-7.842900000	-1.766100000
C	24.793400000	-7.137100000	-3.209500000
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C	15.997900000	-6.598900000	-3.427100000
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C	2.622600000	-6.954000000	20.858200000
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C	4.324700000	-8.693400000	21.036800000
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C	9.826500000	-3.411300000	7.777800000
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C	0.723400000	20.436200000	-12.314500000
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C	4.187800000	19.510100000	-11.962100000
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H	3.321400000	21.029200000	-13.261200000
H	5.210800000	19.532900000	-12.173200000
C	0.865800000	22.811200000	-13.051200000
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H	2.204400000	20.442800000	-17.446800000
H	0.912100000	19.233800000	-17.399900000
C	1.410600000	19.952400000	-19.399300000
H	-1.787200000	19.910800000	-16.750700000
H	-2.459800000	21.515700000	-17.101100000
C	-2.175500000	20.267100000	-18.856900000
H	1.846100000	26.387200000	-10.408900000
H	1.073700000	24.904400000	-10.949900000
C	3.037200000	24.578700000	-10.166100000
H	-1.705300000	25.825000000	-14.720800000
H	-1.948400000	24.681400000	-13.382100000
C	-3.097400000	26.521000000	-13.212800000
H	2.574200000	28.192700000	-14.439100000
H	0.815600000	28.440200000	-14.429600000
C	1.738800000	28.801300000	-16.350800000
H	1.416600000	24.494300000	-18.011600000
H	2.219900000	22.944700000	-18.320200000
C	1.821700000	24.102900000	-20.102200000
H	2.147600000	20.667700000	-19.769200000

H	0.468200000	20.127700000	-19.917800000
C	1.880000000	18.505400000	-19.706500000
H	-1.546800000	19.424900000	-19.152200000
H	-2.036100000	21.082900000	-19.568500000
C	-3.658800000	19.818000000	-18.902000000
H	2.500500000	24.104800000	-9.339200000
H	3.423200000	23.788700000	-10.814300000
C	4.215000000	25.396900000	-9.574400000
H	-3.094000000	26.658200000	-12.128700000
H	-3.080000000	27.503500000	-13.690700000
C	-4.394500000	25.770700000	-13.613100000
H	2.626600000	28.474600000	-16.896800000
H	0.853000000	28.573100000	-16.949000000
C	1.806200000	30.334300000	-16.119200000
H	1.025400000	24.739500000	-20.494900000
H	1.929300000	23.229700000	-20.750400000
C	3.152600000	24.897900000	-20.088800000
H	2.810100000	18.299600000	-19.172000000
H	1.115900000	17.811700000	-19.344200000
C	2.086300000	18.235200000	-21.221200000
H	-3.779900000	18.902600000	-18.318500000
H	-4.284900000	20.600800000	-18.467800000
C	-4.104900000	19.566100000	-20.367000000
H	4.824000000	25.803800000	-10.384300000
H	3.813000000	26.223400000	-8.983500000
C	5.095600000	24.503200000	-8.659300000
H	-4.356100000	25.512900000	-14.673900000
H	-4.463500000	24.850100000	-13.028300000
C	-5.648500000	26.644800000	-13.346900000
H	2.710400000	30.573800000	-15.554800000
H	0.935100000	30.645300000	-15.537100000
C	1.818500000	31.112300000	-17.461400000
H	3.020700000	25.804300000	-19.492800000
H	3.934100000	24.285900000	-19.632500000
C	3.586200000	25.286500000	-21.526100000
H	2.229600000	17.159200000	-21.351600000
H	1.189300000	18.530000000	-21.771100000
C	3.319500000	18.976500000	-21.803300000
H	-3.531500000	18.733400000	-20.781400000
H	-3.900600000	20.461900000	-20.958800000
C	-5.618800000	19.243100000	-20.455100000
H	4.462900000	24.004700000	-7.920600000
H	5.591700000	23.741300000	-9.264800000
C	6.166600000	25.327400000	-7.905800000
H	-5.626400000	27.015000000	-12.319500000
H	-5.641700000	27.499500000	-14.027600000
C	-6.955800000	25.844500000	-13.557600000
H	2.711300000	30.842800000	-18.029900000
H	0.935400000	30.844400000	-18.045900000
C	1.813300000	32.642300000	-17.226900000
H	2.791400000	25.869600000	-21.997000000
H	3.749300000	24.376800000	-22.109100000
C	4.891800000	26.123200000	-21.508600000
H	3.114600000	20.048000000	-21.850900000
H	4.184200000	18.811700000	-21.156500000
C	3.663500000	18.470300000	-23.224900000
H	-5.822400000	18.305600000	-19.933300000
H	-6.189500000	20.043100000	-19.977800000
C	-6.080300000	19.115500000	-21.926900000
H	5.685700000	26.080900000	-7.280000000
H	6.753900000	24.663100000	-7.269500000
H	6.831500000	25.818900000	-8.617000000
H	-7.011800000	25.027000000	-12.837200000
H	-7.813000000	26.504100000	-13.412100000
H	-6.988400000	25.437100000	-14.569000000
H	4.729900000	27.036000000	-20.930600000
H	5.688500000	25.544500000	-21.035400000
C	5.335200000	26.509100000	-22.939700000
H	2.811900000	18.614100000	-23.891200000
H	4.517300000	19.028000000	-23.613000000
H	3.919800000	17.410100000	-23.191100000
H	-5.540900000	18.305600000	-22.419800000
H	-7.149600000	18.900900000	-21.956000000
H	-5.892400000	20.049500000	-22.459200000
H	4.556300000	27.098000000	-23.426400000
H	6.249500000	27.102300000	-22.889500000
H	5.527100000	25.609700000	-23.526900000

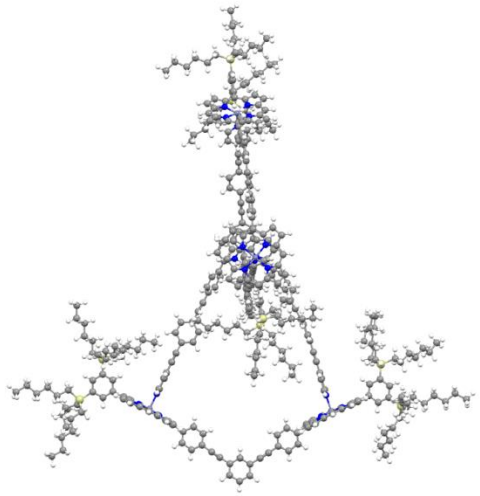

Figure 41. Energy-optimized structure of $[Cu(\mathbf{1})_2\bullet(\mathbf{2})_2]^+$, calculated using Gaussian 09 at B3LYP/6-31G(d) and separately Lanl2dz basis set for copper(I)

C	-0.235100000	2.156200000	-2.030600000
C	0.710700000	1.431900000	-1.848600000
C	1.811800000	0.563200000	-1.586000000
C	2.845000000	0.402900000	-2.525800000
C	1.869800000	-0.127200000	-0.362300000
C	3.930600000	-0.442800000	-2.239100000
H	2.812900000	0.916800000	-3.442900000
C	2.957500000	-0.968000000	-0.073700000
H	1.100700000	-0.013300000	0.345700000
C	3.993800000	-1.129200000	-1.011100000
H	4.700500000	-0.555100000	-2.947000000
H	2.992900000	-1.476500000	0.845600000
C	5.144900000	-2.006800000	-0.709900000
C	5.063600000	-3.355500000	-0.910100000
C	6.393300000	-1.414400000	-0.281800000
N	6.024700000	-4.268800000	-0.766400000
C	3.860300000	-3.940900000	-1.337600000
N	7.561100000	-2.025200000	-0.107600000
C	6.495400000	-0.031300000	-0.066300000
Zn	7.911300000	-3.983200000	-0.178700000
C	5.469300000	-5.432200000	-1.097900000
C	4.119100000	-5.299100000	-1.440900000
H	2.950700000	-3.470000000	-1.545300000
C	8.439300000	-1.058500000	0.145300000
C	7.832500000	0.200900000	0.222200000

H	5.744200000	0.690300000	-0.149300000
N	8.336600000	-5.878900000	-0.616800000
N	9.862000000	-3.610000000	-0.104600000
C	6.047800000	-6.661000000	-1.165600000
H	3.457600000	-6.046200000	-1.752000000
C	9.788900000	-1.161600000	0.277200000
H	8.290300000	1.125300000	0.390500000
C	7.456200000	-6.820100000	-0.934500000
C	9.518900000	-6.487500000	-0.572700000
C	10.437800000	-2.430400000	0.092600000
C	10.852900000	-4.491700000	-0.162300000
H	5.473600000	-7.495000000	-1.452800000
H	10.367600000	-0.301800000	0.459600000
C	8.049000000	-8.078500000	-1.081000000
C	9.397000000	-7.862700000	-0.833700000
C	10.737800000	-5.920000000	-0.340200000
C	11.833400000	-2.521700000	0.139700000
C	12.105300000	-3.872500000	-0.028200000
H	7.587700000	-8.980000000	-1.338200000
H	10.155100000	-8.581100000	-0.876100000
C	11.947800000	-6.753700000	-0.308400000
H	12.522200000	-1.750000000	0.287500000
H	13.049100000	-4.321000000	-0.036500000
C	12.340800000	-7.339800000	0.904000000
C	12.695300000	-6.979500000	-1.476200000
C	13.468600000	-8.174400000	0.948400000
C	13.831600000	-7.807100000	-1.444100000
C	14.184600000	-8.433600000	-0.233400000
C	-1.367200000	3.010100000	-2.190800000
C	-1.709600000	3.534300000	-3.449700000
C	-2.149500000	3.327200000	-1.066100000
C	-2.831300000	4.371800000	-3.578700000
H	-1.131300000	3.303000000	-4.297000000
C	-3.271900000	4.164400000	-1.193400000
H	-1.894000000	2.934500000	-0.123700000
C	-3.612600000	4.687300000	-2.453400000
H	-3.087300000	4.763000000	-4.520200000
H	-4.450600000	5.313600000	-2.559600000
C	-4.052100000	4.467000000	-0.037500000
C	-4.689000000	4.701600000	0.958200000
C	-5.417000000	4.964800000	2.156900000
C	-4.879600000	4.579200000	3.397900000
C	-6.673500000	5.593500000	2.107700000
C	-5.595900000	4.814000000	4.583600000
H	-3.940200000	4.108800000	3.444100000
C	-7.387300000	5.833500000	3.294500000
H	-7.085800000	5.883200000	1.184600000
H	-5.186600000	4.518700000	5.505900000
C	-6.853700000	5.442200000	4.537500000
H	-8.327400000	6.302500000	3.247500000
C	-7.614600000	5.685400000	5.781900000
C	-7.361300000	6.786900000	6.548900000
C	-8.701300000	4.797000000	6.133400000
C	-6.340400000	7.683800000	6.193400000
N	-7.992200000	7.182900000	7.655100000
N	-9.548500000	4.916300000	7.151100000
C	-9.010700000	3.688600000	5.329900000
C	-6.362600000	8.680000000	7.157700000
H	-5.695200000	7.635500000	5.372600000
C	-7.406500000	8.321700000	8.018200000
Zn	-9.479200000	6.261600000	8.617500000
C	-10.432700000	3.933500000	7.002600000
H	-8.526600000	3.367300000	4.461400000
C	-10.140500000	3.120800000	5.900800000
H	-5.749400000	9.524900000	7.207300000
C	-7.707000000	9.133300000	9.067400000
N	-9.656200000	7.813300000	9.854300000
N	-11.235300000	5.605100000	9.278400000
C	-11.539900000	3.676700000	7.749200000
H	-10.677600000	2.295300000	5.550800000
H	-7.147500000	10.010700000	9.226200000
C	-8.821200000	8.842800000	9.926900000
C	-10.564800000	8.014300000	10.807200000
C	-11.960200000	6.094900000	10.278300000
C	-11.904000000	4.549500000	8.830700000
H	-12.162100000	2.863800000	7.504600000
C	-9.149700000	9.724400000	10.962000000
C	-10.284400000	9.177400000	11.543500000
C	-11.666000000	7.256900000	11.084800000
C	-13.129900000	5.347200000	10.484700000
C	-13.093300000	4.334600000	9.536200000
H	-8.665400000	10.611100000	11.228100000
H	-10.826200000	9.582400000	12.340300000
C	-12.558200000	7.611000000	12.203600000
H	-13.881100000	5.509800000	11.192700000
H	-13.803200000	3.583300000	9.383400000
C	-13.651100000	8.481300000	12.032700000
C	-12.290900000	7.059200000	13.466300000
C	-14.487000000	8.794600000	13.121900000
C	-13.077900000	7.412500000	14.573100000
C	-14.177000000	8.272200000	14.392900000
H	11.777900000	-7.160500000	1.774000000
H	12.388400000	-6.527000000	-2.370200000
H	-13.845800000	8.886700000	11.082700000
H	-11.486500000	6.393300000	13.575500000
H	-14.775000000	8.517200000	15.220300000
H	14.996200000	-9.095400000	-0.208300000
Si	-12.702700000	6.707000000	16.236000000
Si	-15.958200000	9.914400000	12.891200000
Si	13.924100000	-8.929800000	2.572100000
Si	14.814500000	-8.126700000	-2.983400000
C	15.593700000	-9.800500000	2.517900000
H	15.783700000	-10.212600000	3.510700000
H	15.541100000	-10.628800000	1.808500000
C	16.759100000	-8.856700000	2.121400000
H	16.845800000	-8.824800000	1.034200000
H	16.566000000	-7.846200000	2.485600000
C	18.098200000	-9.353900000	2.724900000
H	18.261400000	-10.396100000	2.440600000
H	18.037400000	-9.290700000	3.814300000
C	19.293100000	-8.499100000	2.229400000
H	19.428900000	-8.662400000	1.157700000
H	19.078400000	-7.441800000	2.401500000
C	20.596000000	-8.879900000	2.980400000
H	20.790800000	-9.946800000	2.847900000
H	20.465100000	-8.675400000	4.045900000
C	21.808700000	-8.070800000	2.451700000
H	21.969000000	-8.305900000	1.397000000
H	21.603300000	-7.002200000	2.546500000
C	23.096600000	-8.404000000	3.242100000
H	23.323200000	-9.467900000	3.157600000
H	23.931100000	-7.829800000	2.836700000
H	22.966300000	-8.145900000	4.294200000
C	13.929900000	-7.540000000	3.852000000

H	14.342800000	-6.641700000	3.387100000
H	12.893300000	-7.338400000	4.129400000
C	12.568200000	-10.177300000	2.990700000
H	11.608100000	-9.657600000	3.010200000
H	12.543500000	-10.929900000	2.200100000
C	14.760800000	-7.866000000	5.120200000
H	15.820400000	-7.746000000	4.888700000
H	14.587000000	-8.895900000	5.430800000
C	14.370300000	-6.921600000	6.288400000
H	14.528200000	-5.882600000	5.990600000
H	13.306500000	-7.059000000	6.502100000
C	15.159300000	-7.211100000	7.593600000
H	14.668700000	-6.673000000	8.409200000
H	15.117800000	-8.280200000	7.814900000
C	16.639700000	-6.751600000	7.516300000
H	17.173400000	-7.347600000	6.773600000
H	16.679500000	-5.701000000	7.219700000
C	12.805900000	-10.867600000	4.355900000
H	12.740800000	-10.125100000	5.153300000
H	13.802500000	-11.313300000	4.362700000
C	11.758500000	-11.977500000	4.630300000
H	10.773100000	-11.522600000	4.754300000
H	11.728100000	-12.663400000	3.780600000
C	12.129900000	-12.771500000	5.910800000
H	12.142000000	-12.092300000	6.766600000
H	13.128500000	-13.197500000	5.786100000
C	11.122400000	-13.918500000	6.182800000
H	10.137400000	-13.495100000	6.391200000
H	11.051200000	-14.558100000	5.300200000
C	11.567200000	-14.782100000	7.387600000
H	11.634900000	-14.166400000	8.285700000
H	10.838600000	-15.576700000	7.555000000
H	12.540900000	-15.231500000	7.185100000
C	14.971000000	-6.526400000	-3.979500000
H	15.162800000	-5.713700000	-3.276600000
H	15.827200000	-6.608400000	-4.651300000
C	13.965400000	-9.458000000	-4.017200000
H	13.127200000	-9.013000000	-4.554800000
H	14.676300000	-9.844700000	-4.748100000
C	16.534100000	-8.729400000	-2.478000000
H	17.008000000	-7.961800000	-1.863000000
H	16.413800000	-9.634000000	-1.879000000
C	17.446700000	-9.056500000	-3.687600000
H	17.697900000	-8.135500000	-4.217100000
H	16.920200000	-9.725500000	-4.370000000
C	18.752600000	-9.754500000	-3.220200000
H	19.326700000	-9.067100000	-2.594700000
H	18.492500000	-10.635400000	-2.627700000
C	19.620100000	-10.201300000	-4.426800000
H	19.932700000	-9.320100000	-4.991700000
H	19.023100000	-10.844300000	-5.078100000
C	20.875500000	-10.984000000	-3.958400000
H	21.495000000	-10.337500000	-3.332900000
H	20.564800000	-11.849700000	-3.368700000
C	21.717400000	-11.478500000	-5.159200000
H	22.056300000	-10.629300000	-5.754200000
H	22.587700000	-12.025400000	-4.792800000
H	21.120300000	-12.142700000	-5.786300000
C	13.423500000	-10.614900000	-3.141200000
H	14.209800000	-10.982200000	-2.478500000
H	12.596300000	-10.238200000	-2.534900000
C	12.922200000	-11.785300000	-4.027700000
H	12.322300000	-11.387900000	-4.850100000
H	13.786900000	-12.307300000	-4.444700000
C	12.053600000	-12.782600000	-3.217600000
H	12.603100000	-13.110700000	-2.332300000
H	11.139800000	-12.275500000	-2.898100000
C	11.680500000	-14.021300000	-4.074200000
H	11.236600000	-13.694600000	-5.017400000
H	12.585200000	-14.593700000	-4.292200000
C	10.670600000	-14.936300000	-3.341500000
H	9.735700000	-14.399200000	-3.173600000
H	10.468000000	-15.817000000	-3.953100000
H	11.080300000	-15.255900000	-2.382400000
C	13.704700000	-6.222600000	-4.829800000
H	13.872200000	-6.559500000	-5.855700000
H	12.853400000	-6.781000000	-4.439200000
C	13.295500000	-4.725200000	-4.832300000
H	12.260800000	-4.664400000	-5.181800000
H	13.331900000	-4.332900000	-3.813300000
C	14.176300000	-3.851600000	-5.763500000
H	15.206900000	-3.852800000	-5.402600000
H	14.153300000	-4.270600000	-6.772200000
C	13.645000000	-2.393200000	-5.806600000
H	12.584800000	-2.400000000	-6.071700000
H	13.755300000	-1.938300000	-4.819500000
C	14.403800000	-1.534000000	-6.845600000
H	14.277800000	-1.957400000	-7.843400000
H	14.002400000	-0.519100000	-6.839400000
H	15.465700000	-1.498200000	-6.599600000
C	-12.799100000	8.073700000	17.536000000
H	-13.815600000	8.470000000	17.555700000
H	-12.113000000	8.874600000	17.255300000
C	-12.425400000	7.536600000	18.941000000
H	-11.412300000	7.130500000	18.915200000
H	-13.118600000	6.739300000	19.217300000
C	-12.482100000	8.647100000	20.021200000
H	-11.775200000	9.438500000	19.761800000
H	-13.489500000	9.067700000	20.055900000
C	-12.117700000	8.067400000	21.414100000
H	-11.117100000	7.630300000	21.369800000
H	-12.832700000	7.282300000	21.672200000
C	-12.144800000	9.160500000	22.513400000
H	-11.420200000	9.940300000	22.268400000
H	-13.140700000	9.606700000	22.558800000
C	-11.796200000	8.569900000	23.900900000
H	-10.797800000	8.130200000	23.880400000
H	-11.819600000	9.362400000	24.650500000
H	-12.522000000	7.802100000	24.173500000
C	-13.966300000	5.369000000	16.656500000
H	-14.960700000	5.816100000	16.705400000
H	-13.712400000	4.974500000	17.642200000
C	-10.987100000	5.918400000	16.303000000
H	-10.956100000	5.069800000	15.617300000
H	-10.848700000	5.532300000	17.314300000
C	-13.968900000	4.213300000	15.620300000
H	-14.624600000	4.477000000	14.787600000
H	-12.961200000	4.056800000	15.232800000
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C	-9.830300000	6.887800000	15.937000000
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H	-10.163600000	7.925600000	15.993900000
C	-8.612100000	6.706300000	16.884800000
H	-8.679600000	7.447400000	17.685300000
H	-8.635100000	5.710200000	17.333100000
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H	-7.233200000	7.823200000	15.621400000
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H	-4.582700000	7.538100000	15.736500000
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