Electronic Supporting Information (ESI)

Evolution of catalytic machinery: Three-component nanorotor catalyzes formation of four-component catalytic machinery

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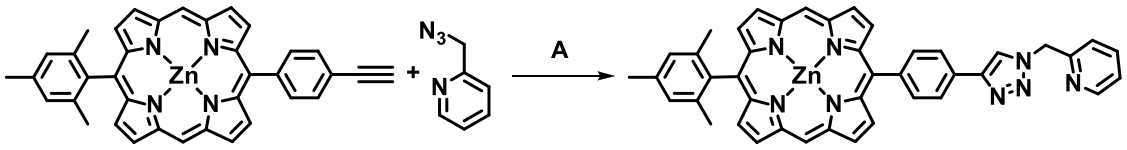
1. Synthesis

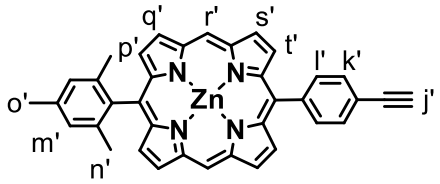
General Section

All solvents were dried by distillation prior to use while the commercial reagents **4**-**7** were used without any further purification. ^{1}H and ^{13}C NMR spectra were recorded on Bruker Avance (400 MHz) and Varian VNMR-S (600 MHz) spectrometers 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). The following abbreviations were utilized to describe peak patterns: s = singlet, d = doublet, t = triplet, dd = doublet of doublets, td = triplet of doublets, dt = doublet of triplets, br = broad and m = multiplet. Electrospray-ionization (ESI) mass spectra were recorded on a Thermo-Quest LCQ deca. Melting points were measured on a Büchi SMP-20 and were left uncorrected. Infrared spectra were recorded using a Perkin Elmer Spectrum-Two FT-IR spectrometer. Elemental analysis measurements were measured using the EA 3000 CHNS. Energy minimized structures were obtained through DFT computations using the B3LYP functional in combination with the 6-31G(d) and LanL2DZ (for the metal ions) basis set. UV-vis spectra were recorded on a Cary Win 50 (298 K). The numbering of the carbon skeleton in molecular formulae as shown in the manuscript does not comply with the IUPAC nomenclature rules; it is only used for assignments of NMR signals. Compounds **1**,[1] **2**,[2] **3**,[3] **Phen**,[4] **S**[5] and **R**[6] were synthesized according to literature known procedures.



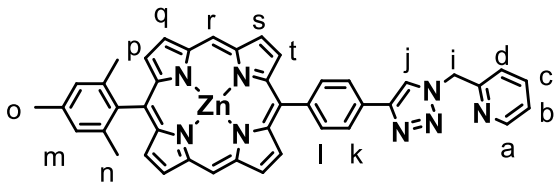
Scheme 1. Synthesis of ligand **P**. Reaction conditions: (A) $[Cu(CH_3CN)]PF_6$, CH_2Cl_2, room temperature, 24 h, 91%.

Zinc(II)-5-(4-ethynylphenyl)-15-(2,4,6-trimethylphenyl)porphyrin (1)



Compound **1** was prepared according to a literature method with all spectral data being in full agreement.[1] **MP** > 250 °C. **^{1}H NMR** (400 MHz, CD_2Cl_2) δ 10.32 (s, 2H, r'-H), 9.47 (d, ^3J = 4.5 Hz, 2H, s'-H), 9.44 (d, ^3J = 4.5 Hz, 2H, q'-H), 9.11 (d, ^3J = 4.5 Hz, 2H, t'-H), 8.96 (d, ^3J = 4.5 Hz, 2H, p'-H), 8.25 (d, ^3J = 8.2 Hz, 2H, l'-H), 7.95 (d, ^3J = 8.2 Hz, 2H, k'-H), 7.35 (s, 2H, m'-H), 3.41 (s, 1H, j'-H), 2.67 (s, 3H, o'-H), 1.82 (s, 6H, n'-H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 21.4, 21.7, 31.5, 65.8, 82.2, 94.6, 105.9, 118.5, 118.9, 121.8, 127.7, 129.9, 131.4, 131.8, 132.0, 132.2, 134.4, 137.5, 138.6, 139.3, 142.8, 149.3, 149.5, 149.6, 149.9 ppm.

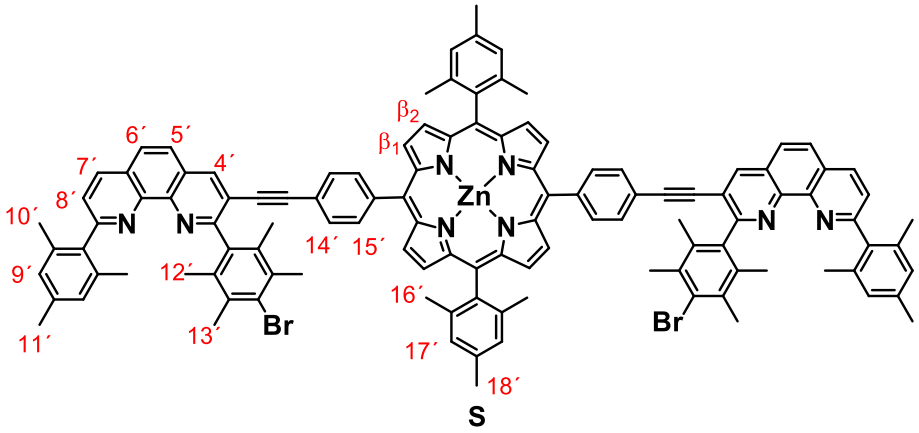
Synthesis of ZnPor Platform (P)



Porphyrin **1** (36.0 mg, 61.0 µmol), 2-pyridylmethyl azide (**2**) (16.0 mg, 122 µmol) and $[Cu(CH_3CN)_4]PF_6$ (4.50 mg, 6.10 mmol) were dissolved in 3 mL of CH_2Cl_2 and allowed to stir at room temperature for 24 h. The product was separated by column chromatography eluting firstly with DCM and then 30% EtOAc in DCM (R_f = 0.41) to give the product as a violet solid (40.0 mg, 55.5 mmol, 91%). **MP** > 250 °C. **IR** (KBr) $\tilde{\nu}$ 2919, 2850, 1609, 1518, 1461, 1438, 1392, 1355, 1057, 995, 850, 784, 722, 701 cm^{-1}; **^{1}H NMR** (400 MHz, CD_2Cl_2:THF-d_8, 80:20) δ 10.20 (s, 2H, r-H), 9.39 (d, ^3J = 4.4 Hz, 2H, s-H), 9.35 (d, ^3J = 4.4 Hz, 2H, q-H), 9.11 (d, ^3J = 4.4 Hz, 2H, t-H), 8.87 (d, ^3J = 4.4 Hz, 2H, p-H), 8.63 (dd, ^3J = 4.9 Hz, ^4J = 1.8 Hz, 1H, a-H), 8.31 (d, ^3J = 8.2 Hz, 2H, l-H), 8.29 (s, 1H, j-H), 8.26 (d, ^3J = 8.2 Hz, 2H, k-H), 7.78 (td, ^3J = 7.7 Hz, ^4J = 1.8 Hz, 1H, c-H), 7.36 (d, ^3J = 7.7 Hz, 1H, d-H), 7.32(s, 2H, m-H), 7.27−7.24 (m, 1H, b-H), 5.79 (s, 2H, i-H), 2.65 (s, 3H, o-H), 1.81 (s, 6H, n-H); **^{13}C NMR** (101 MHz, CD_2Cl_2) δ 155.3, 150.2, 150.2, 150.1, 149.8, 149.7, 148.3, 143.4, 139.7, 139.6, 137.8, 137.6, 135.6, 132.3, 132.2, 131.8, 131.2, 130.2, 128.0, 124.1, 123.7, 122.7, 121.2, 119.3, 118.1, 105.7, 56.0, 21.8, 21.5; **ESI-MS**:

m/z (%) 724.5 (100) $[M+H]^+$; **Anal. Calcd**. for $C_{43}H_{32}N_8Zn$: C, 71.12; H, 4.44; N, 15.43 found: C, 71.10; H, 4.35; N, 15.80.

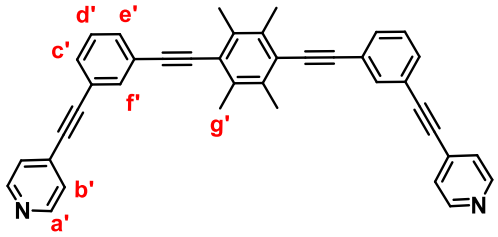
Synthesis of zinc(II)-*meso*-5,15-bis-{4-[2-(4-bromo-2,3,5,6-tetramethylphenyl)-9-(2,4,6-trimethylphenyl)-[1,10]phenanthrolinyl-3-ethinyl]phenyl}-10,20-bis-(2,4,6-trimethylphenyl)-porphyrin (Stator S). 5



Stator **S** was prepared according to a literature method.5

MP: >300 °C; **IR** (KBr)**:** $\tilde{\nu}$ = 3441, 2963, 2914, 2733, 2362, 2201, 1913, 1804, 1701, 1602, 1491, 1442, 1263, 1162, 1093, 994, 846, 802, 765, 722, 573 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 8.85 (d, 4H, ^3J = 4.6 Hz, β_1-H), 8.79 (d, 4H, ^3J = 4.6 Hz, β_2-H), 8.63 (s, 2H, 4´-H), 8.33 (d, ^3J = 8.4 Hz, 2H, 7´-H), 8.17 (d, ^3J = 8.0 Hz, 4H, 15´-H), 7.95 (d, 2H, ^3J = 9.0 Hz, 6´/5´-H), 7.92 (d, ^3J = 9.0 Hz, 2H, 5´/6´-H), 7.61 (d, ^3J = 8.4 Hz, 2H, 8´-H), 7.49 (d, ^3J = 8.0 Hz, 4H, 14´-H), 7.29 (s, 4 H, 17´-H), 6.96 (s, 4 H, 9´-H), 2.64 (s, 6H, 18´-H), 2.53 (s, 12H, 12´-H), 2.33 (s, 6H, 11´-H), 2.16 (s, 12H, 13´-H), 2.13 (s, 12H, 10´-H), 1.83 (s, 12H, 16´-H); **^{13}C NMR (100 MHz $CDCl_3$):** δ = 162.6, 160.7, 150.0, 149.7, 145.9, 144.7, 143.4, 139.2, 139.2, 138.9, 138.5, 137.9, 137.6, 137.5, 136.1, 136.0, 134.5, 133.8, 133.7, 132.1, 131.0, 129.7, 129.3, 128.5, 127.7, 127.7, 127.2, 127.0, 125.7, 125.2, 121.8, 120.2, 119.6, 119.3, 95.7, 87.8, 21.6, 21.5, 21.1, 21.1, 20.5, 18.7; **ESI-MS:** *m/z* (%) = 1825.6 (60) $[M+H]^+$, 913.4 (100) $[M+2H]^{2+}$; **UV-Vis:** λ_{abs} (CH_2Cl_2) = 422, 549, 595 nm; $\varepsilon_{422} = 2.17 \times 10^4\ M^{-1}cm^{-1}$.

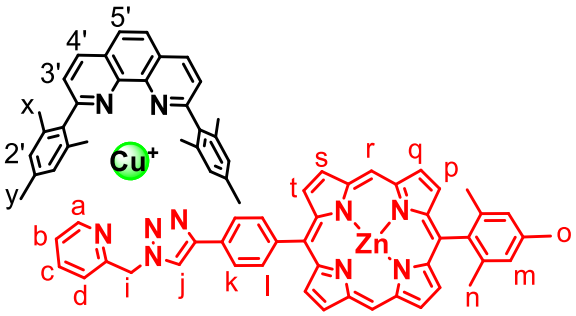
Spectroscopic data for rotator R[7]



Compound **R** was prepared according to a literature method.7 **MP:** 210-212 °C; **IR (KBr):** $\tilde{\nu}$ = 3050, 2923, 2211, 1593, 1569, 1537, 1489, 1478, 1404, 1375, 1315, 1214, 1090, 1066, 1014, 988, 936, 919, 820, 795, 748, 686, 646, 587, 565, 544, 533, 497 cm^{-1}; **^{1}H NMR (400 MHz, CD_2Cl_2):** δ = 8.61 (d, ^3J = 6.0 Hz, 4H, a´-H), 7.74 (t, ^4J = 1.6 Hz, 2H, f´-H), 7.57 (dt, ^3J = 8.0 Hz, ^4J = 1.6 Hz, 2H, e´/c´-H), 7.52 (dt, ^3J = 8.0 Hz, ^4J = 1.6 Hz, 2H, c´/e´-H), 7.40 (d, ^3J = 6.0 Hz, 4H, b´-H), 7.38 (t, ^3J = 8.0 Hz, 2H, d´-H), 2.51 (s, 12H, g´-H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 149.8, 135.8, 134.4, 131.9, 131.3, 131.1, 128.6, 125.5, 124.3, 123.2, 122.5, 97.1, 93.1, 89.5, 87.2, 18.4 ppm; **ESI-MS:** *m/z* (%) 537.4 (100) $[R + H]^+$.

2. Synthesis and characterization of complexes

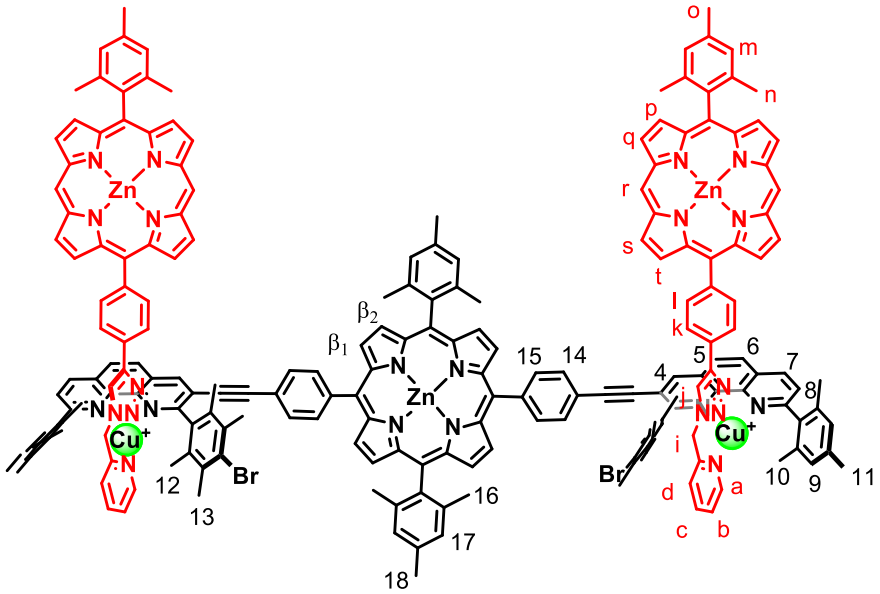
Complex C1 = Synthesis of model complex [Cu(**Phen**)(**P**)]PF_6



Compound **Phen** (430 µg, 1.03 µmol), product **P** (750 µg, 1.03 µmol) and $[Cu(CH_3CN)_4]PF_6$ (384 µg, 1.03 µmol) were dissolved in 550 µL of CH_2Cl_2 and sonicated for 1 min to quantitatively furnish [Cu(**Phen**)(**P**)]PF_6. **IR** (KBr) $\tilde{\nu}$ 2920, 2853,1610, 1589, 1439, 1388, 1385, 1057, 995, 842, 791, 557 cm^{-1}; **^{1}H NMR** (400 MHz, CD_2Cl_2): δ 10.33 (s, 2H, r-H), 9.48 (d, ^3J = 4.4 Hz, 2H, s-H), 9.44 (d, ^3J = 4.4 Hz, 2H, q-H), 9.17 (d, ^3J = 4.4 Hz, 2H, t-H), 8.96 (d, ^3J = 4.4 Hz, 2H, p-H), 8.69 (d, ^3J = 8.3 Hz, 2H, 4'-H), 8.33 (d, ^3J = 7.8 Hz, 2H, l-H), 8.19 (s, 2H, 5'-H), 8.14 (d, ^3J

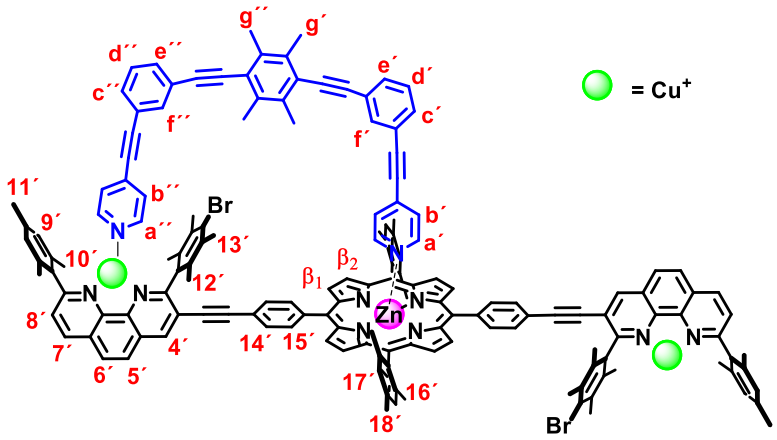
= 7.8 Hz, 2H, k-H), 8.13 (s, 1H, j-H) 7.89 (d, ^3J = 8.3 Hz, 2H, 3'-H), 7.80 (br s, 1H, c-H), 7.70 (br s, 1H, a-H), 7.46 (br s, 1H, d-H), 7.34 (s, 2H, m-H), 7.14 (br s, 1H, b-H), 6.73 (s, 4H, 2'-H), 4.36 (s, 2H, i-H), 2.66 (s, 3H, o-H), 2.24 (s, 6H, y-H), 1.94 (s, 12H, x-H), 1.80 (s, 6H, n-H); **ESI-MS**: *m/z* (%) 1205.3 (100) $[M - PF_6]^+$; **Anal. Calcd**. for $C_{81}H_{72}CuF_6N_{14}PZn \cdot 1/2CH_2Cl_2$: C, 62.83; H, 4.72; N, 12.59. Found: C, 62.61; H, 4.35; N, 12.39.

Complex C2 = Synthesis of Deck = $[Cu_2(\mathbf{S})(\mathbf{P})_2](PF_6)_2$



Stator **S** (1.17 mg, 0.641 µmol), product **P** (932 µg, 1.28 µmol) and $[Cu(CH_3CN)_4]PF_6$ (477 µg, 1.28 µmol) were dissolved in 550 µL of CH_2Cl_2 and sonicated for 1 min to quantitatively afford $[Cu_2(\mathbf{S})(\mathbf{P})_2](PF_6)_2$. **IR** (KBr) $\tilde{\nu}$ 2919, 2860, 2206, 1619, 1550, 1461, 1438, 1384, 1332, 1203, 1057, 995,844, 720, 557 cm^{-1}; **^{1}H NMR** (400 MHz, CD_2Cl_2) δ 10.30 (s, 4H, r-H), 9.46 (br s, 4H, s-H), 9.42 (d, ^3J = 4.5 Hz, 4H, q-H), 9.16 (d, ^3J = 4.5 Hz, 4H, t-H), 8.99 (s, 2H, 4-H), 8.95 (d, ^3J = 4.5 Hz, 4H, p-H), 8.83 (d, ^3J = 4.7 Hz, 4H, β_1-H), 8.76 (d, ^3J = 4.7 Hz, 1H, β_2-H), 8.73 (d, ^3J = 8.3 Hz, 2H, 7-H), 8.33 (br s, 4H, l-H), 8.26 (s, 4H, [5+6]-H), 8.17 (d, ^3J = 7.8 Hz, 4H, 15-H), 8.16 (s, 2H, j-H), 8.15 (br s, 4H, k-H), 7.93 (d, ^3J = 8.3 Hz, 2H, 8-H), 7.87 (br s, 4H, [a+c]-H), 7.51 (d, ^3J = 7.8 Hz, 4H, 14-H), 7.48 (br s, 2H, d-H), 7.34 (s, 4H, m-H), 7.29 (s, 4H, 17-H), 7.23 (s, 2H, b-H), 6.78 (s, 4H, 9-H), 4.43 (br s, 4H, i-H), 2.66 (s, 6H, o-H), 2.60 (s, 6H, 18-H), 2.32 (s,12H, 12-H), 2.29 (s, 6H, 11-H), 2.13 (s, 12H, 10-H), 1.95 (s, 12H, 13-H), 1.80 (s, 24H, [n+16]-H); **ESI-MS**: *m/z* (%) 1701.5 (25) $[M–\mathbf{2}PF_6]^{2+}$. **Anal. Calcd**. for $C_{218}H_{182}Br_2Cu_2F_{12}N_{32}P_2Zn_3 \cdot 2CH_3CN$: C, 64.95; H, 4.62; N, 11.60. Found: C, 65.03; H, 4.66; N, 11.29.

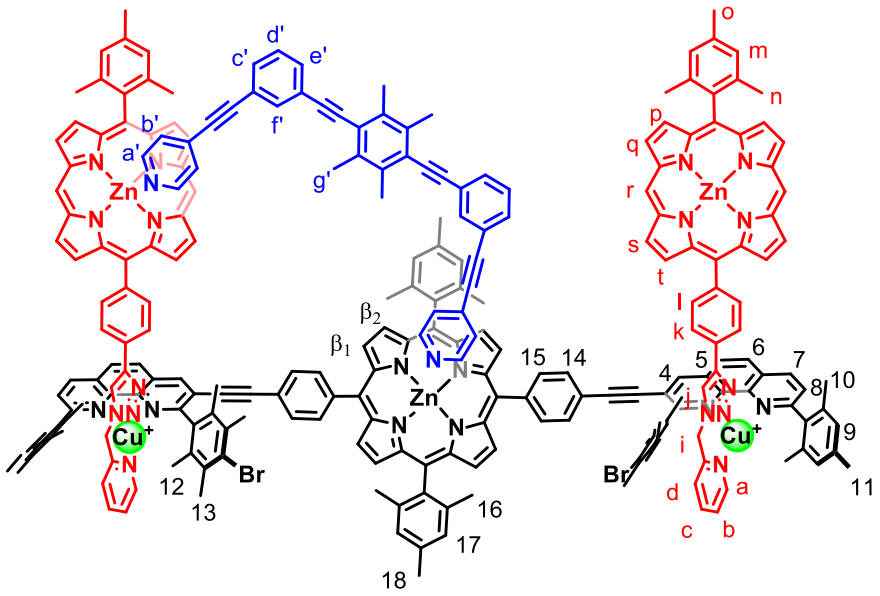
Complex C3 = Rotor $[Cu_2(\mathbf{S})(\mathbf{R})]^{2+}$



Compound **S** was prepared according to literature method.[5]

MP > 250 °C; **IR** (KBr): $\tilde{\nu}$ = 3036, 2919, 2209, 1605, 1491, 1459, 1382, 1336, 1203, 1064, 996, 843, 796, 719, 683, 623, 560 cm^{-1}; **^{1}H NMR** (400 MHz, CD_2Cl_2): δ 8.95 (s, 2H, 4´-H), 8.80 (d, 4H, ^3J = 4.4 Hz, β_1-H), 8.76 (d, ^3J = 8.4 Hz, 2H, 7´-H), 8.74 (d, 4H, ^3J = 4.4 Hz, β_2-H), 8.26 (d, 2H, ^3J = 8.8 Hz, 6´/5´-H), 8.23 (d, ^3J = 8.8 Hz, 2H, 5´/6´-H), 8.15 (d, ^3J = 7.8 Hz, 4H, 15´-H), 7.98 (d, ^3J = 8.4 Hz, 2H, 8´-H), 7.69 (brs, 2H, f´-, f´´-H), 7.56 (d, ^3J = 7.8 Hz, 2H, e´-, e´´-H), 7.47 (d, ^3J = 7.8 Hz, 2H, c´-, c´´-H), 7.36-7.42 (m, 6H, d´-, d´´-, 14´-H), 7.29 (s, 4H, 17´-H), 7.03 (s, 4H, 9´-H), 6.89 (brs, 4H, b´-H), 5.66 (brs at −60 °C, 4H, a´-H), 2.61 (s, 6H, 18´-H), 2.43 (s, 12H, g´´-, g´-H), 2.13 (s, 12H, 12´-H), 2.38 (s, 6H, 11´-H), 2.14 (s, 12H, 13´-H), 2.10 (s, 12H, 10´-H), 1.79 (s, 12H, 16´-H); **ESI-MS:** *m*/*z* (%) = 1244.7 (100) $[[Cu_2(\mathbf{S})(\mathbf{R})]^{2+}]$; **UV-Vis:** λ_{abs} (CH_2Cl_2) = 429, 559, 602, 607 nm; ε_{429} = 1.96×10^4 $M^{-1}cm^{-1}$; **Anal. Calcd**. for $C_{156}H_{122}Br_2Cu_2F_{12}N_{10}P_2Zn$: C, 67.42; H, 4.43; N, 5.04. Found: C, 67.50; H, 4.41; N, 5.26.

Complex C4 = Slider-on-deck $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$



In an NMR tube, stator **S** (1.17 mg, 0.641 μmol), product **P** (932 μg, 1.28 μmol), rotator **R** (344 μg, 0.641 μmol) and $[Cu(CH_3CN)_4]PF_6$ (477 μg, 1.28 μmol) were dissolved in 550 μL of CH_2Cl_2 and sonicated for 1 min to quantitatively afford $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$. **IR** (KBr) $\tilde{\nu}$ 2922, 2853, 2206, 1604, 1461, 1438, 1384, 1260, 1201, 1057, 994, 843, 794, 722, 557 cm^{-1}; **^{1}H NMR** (400 MHz, CD_2Cl_2) δ 10.22 (s, 4H, r-H), 9.42 (br s, 4H, s-H), 9.36 (br s, 4H, q-H), 9.13 (br s, 4H, t-H), 8.96 (s, 2H, 4-H), 8.90 (d, ^3J = 4.4 Hz, 4H, p-H), 8.78 (d, ^3J = 4.6 Hz, 4H, β_1-H), 8.71 (d, ^3J = 4.6 Hz, 4H, β_2-H), 8.71 (d, ^3J = 8.3 Hz, 2H, 7-H), 8.33 (d, ^3J = 7.5 Hz, 4H, l-H), 8.23 (s, 4H, [5+6]-H), 8.16 (d, ^3J = 7.9 Hz, 4H, 15-H), 8.15 (s, 2H, j-H), 8.14 (d, ^3J = 7.5 Hz, 4H, k-H), 7.92 (d, ^3J = 8.3 Hz, 2H, 8-H), 7.82 (br s, 4H, [a+c]-H), 7.48 (d, ^3J = 7.9 Hz, 4H, 14-H), 7.43 (br s, 2H, d-H), 7.35 (br s, 2H, d'-H), 7.32 (s, 4H, m-H), 7.27 (s, 4H, 17-H), 7.15 (br s, 6H, [b+c'+e']-H), 7.09 (s, 2H, f'-H), 6.79 (br s, 4H, 9-H), 5.77 (br s, 4H, b'-H), 4.37 (br s, 4H, i-H), 3.69 (br s, 4-H a'-H at –70 °C), 2.65 (s, 6H, o-H), 2.59 (s, 6H, 18-H), 2.30 (s, 6H, 11-H), 2.28 (s, 24H, [g'+12]-H), 2.11 (s, 12H, 10-H), 1.95 (s, 12H, 13-H), 1.78 (s, 24H, [n+16]-H); **ESI-MS**: *m/z* (%) 1970.8 (20) $[M - 2PF_6]^{2+}$. **Anal. Calcd.** for $C_{258}H_{210}Br_2Cu_2F_{12}N_{34}P_2Zn_3 \cdot CH_2Cl_2$: C, 66.98; H, 4.60; N, 10.25. Found: C, 67.05; H, 4.56; N, 9.96.

3. NMR spectra

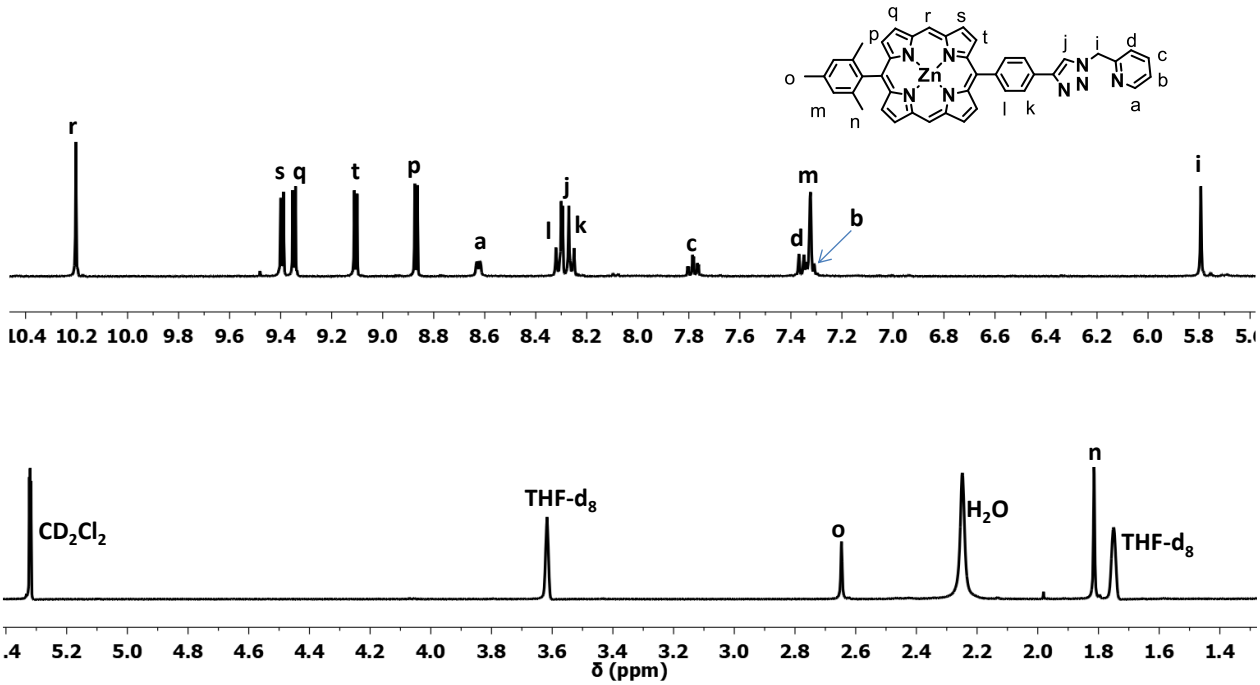


Figure S1. ^{1}H NMR (400 MHz, CD_2Cl_2:THF-d_8, 80:20) of compound **P**.

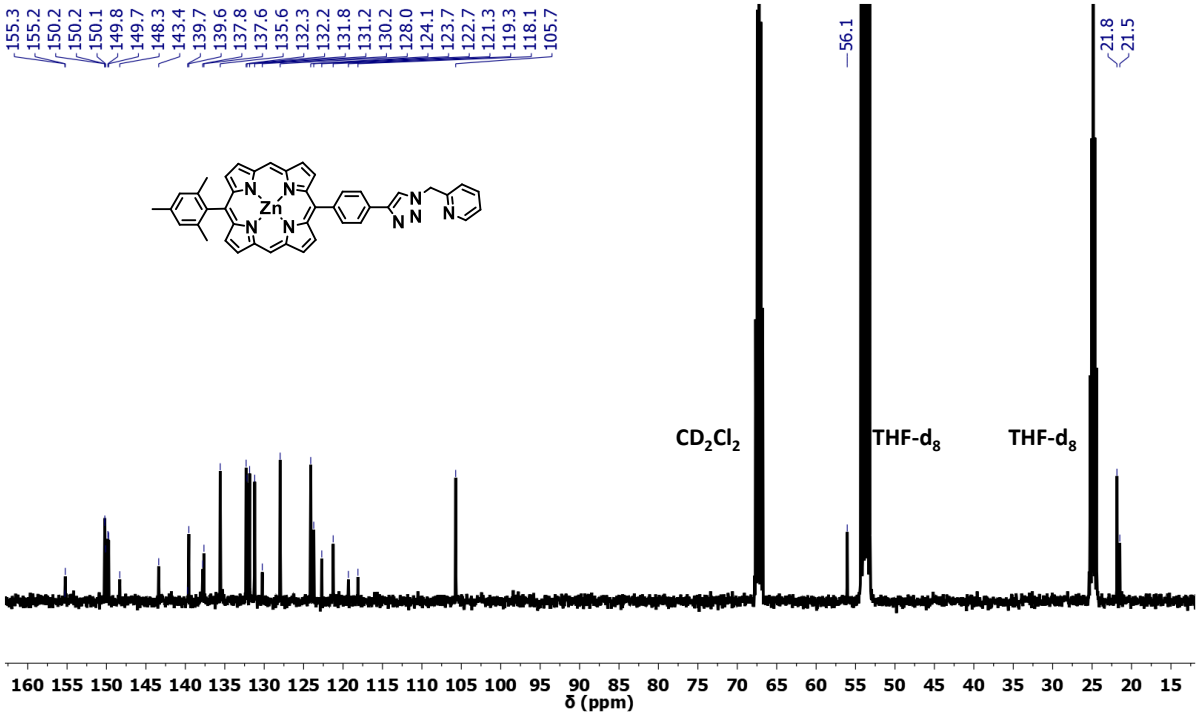


Figure S2. ^{13}C NMR (101 MHz, CD_2Cl_2:THF-d_8, 80:20) of compound **P**.

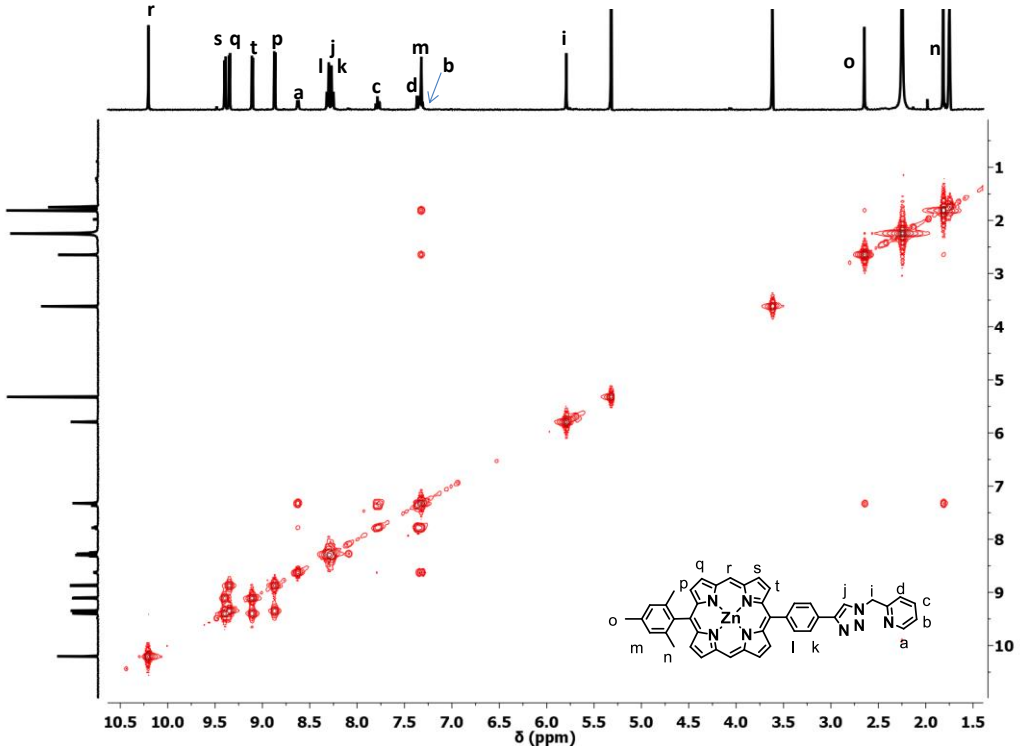


Figure S3. ^{1}H-^{1}H COSY (400 MHz, CD_2Cl_2:THF-d_8, 80:20) of compound **P**.

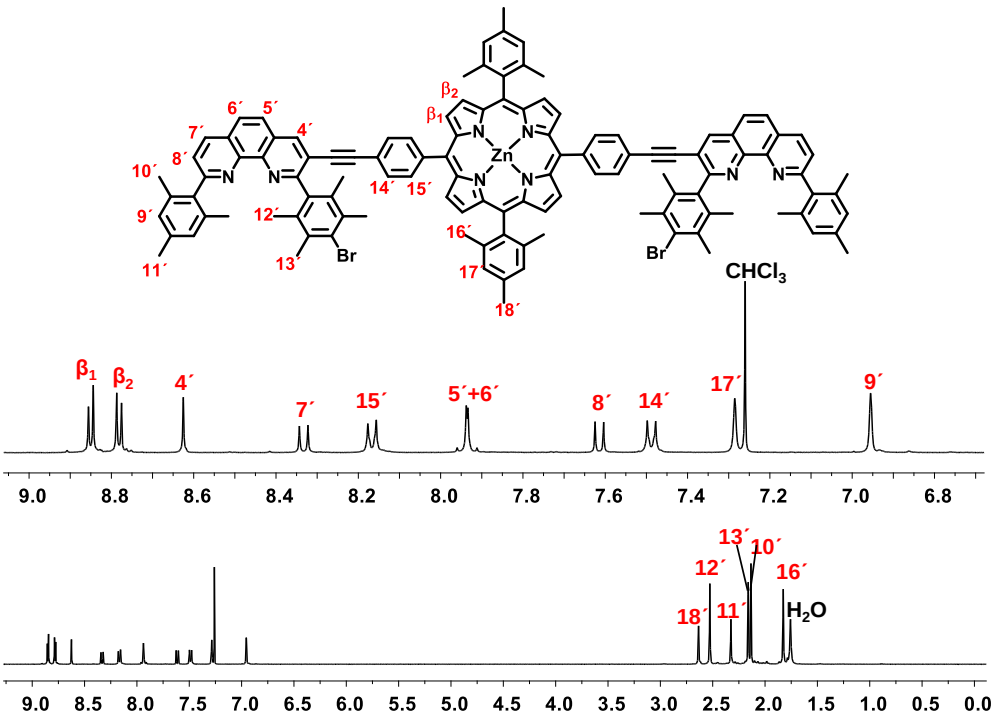


Figure S4. ^{1}H NMR spectrum of stator **S** in $CDCl_3$ (400 MHz, 298 K).

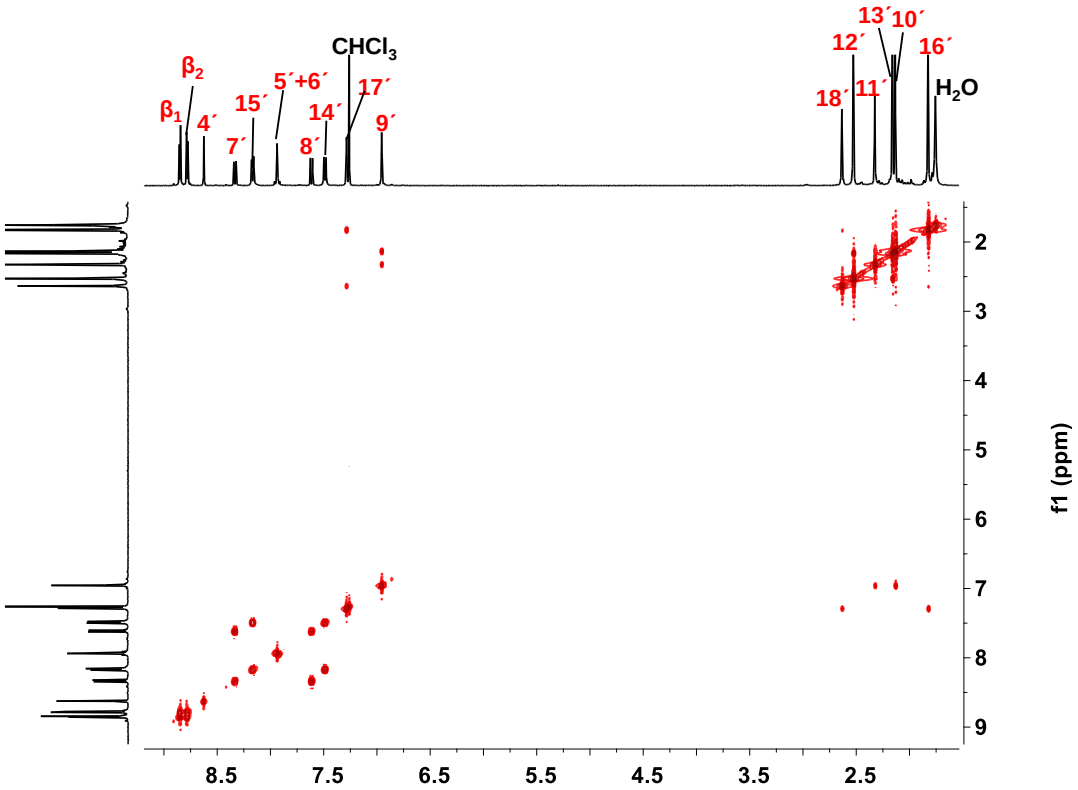


Figure S5. ^{1}H-^{1}H COSY spectrum of stator **S** in $CDCl_3$ (400 MHz, 298 K).

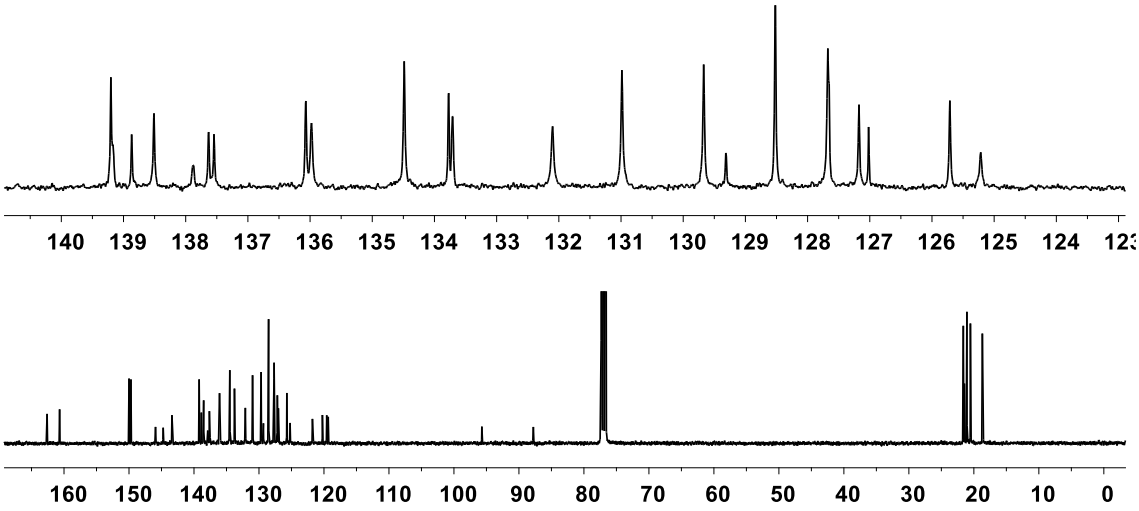


Figure S6. ^{13}C NMR spectrum of stator **S** in $CDCl_3$ (100 MHz, 298 K).

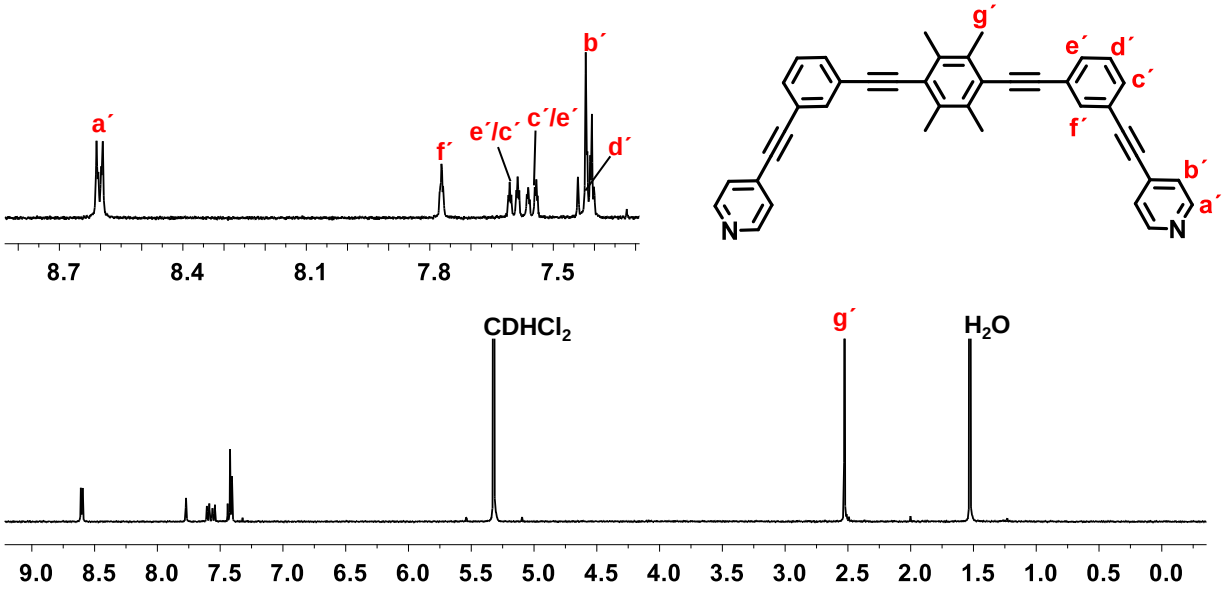


Figure S7. ^{1}H NMR spectrum of rotator ligand **R** in CD_2Cl_2 (400 MHz, 298 K).

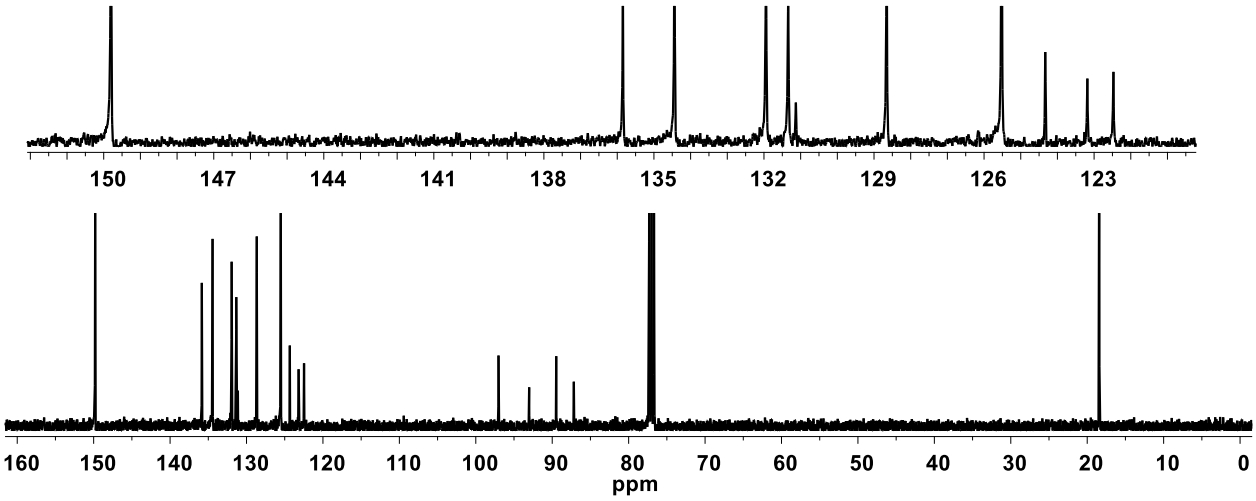


Figure S8. ^{13}C NMR spectrum of rotator **R** in $CDCl_3$ (100 MHz, 298 K).

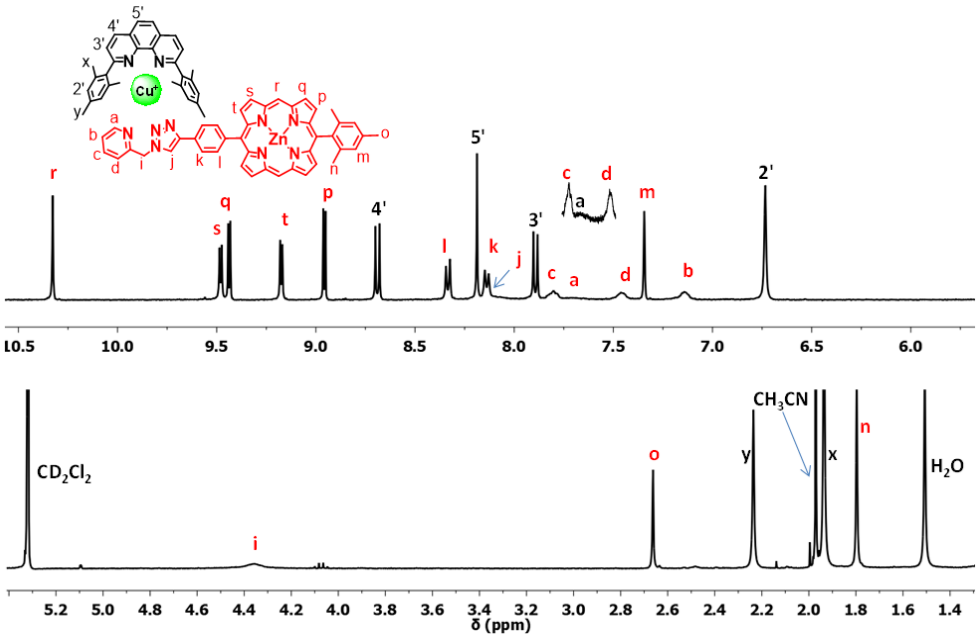


Figure S9. ^{1}H NMR (400 MHz, CD_2Cl_2) of [Cu(**Phen**)(**P**)]PF_6.

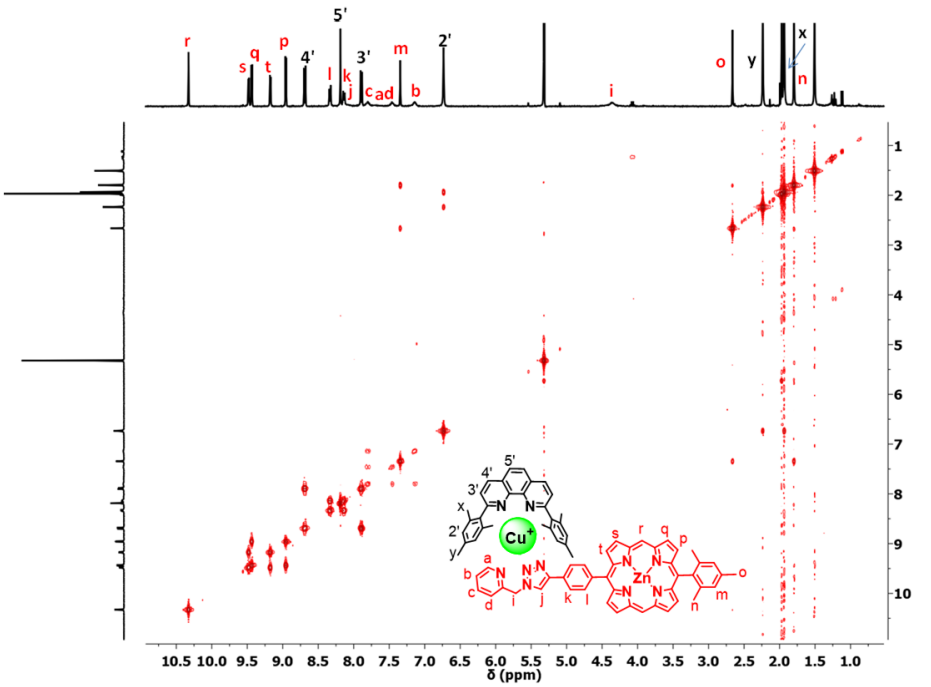


Figure S10. ^{1}H-^{1}H COSY (400 MHz, CD_2Cl_2) of [Cu(**phen**)(**P**)]PF_6.

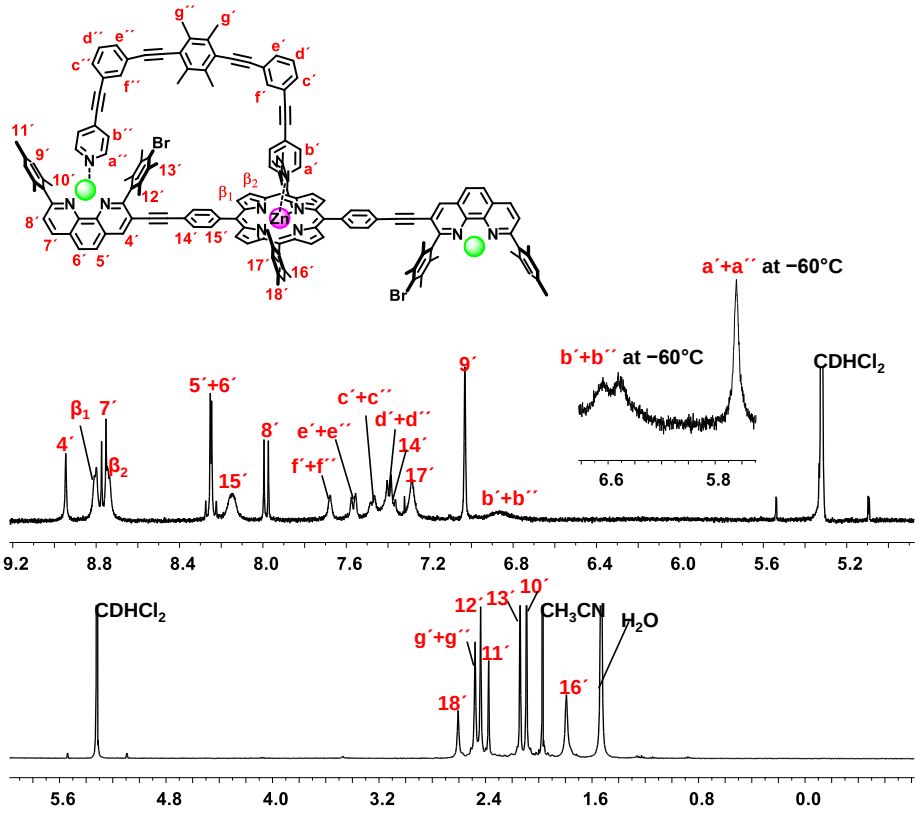


Figure S11. ^{1}H NMR spectrum (400 MHz, 298 K) of complex $[Cu_2(\mathbf{S})(\mathbf{R})]^{2+}$ in CD_2Cl_2.

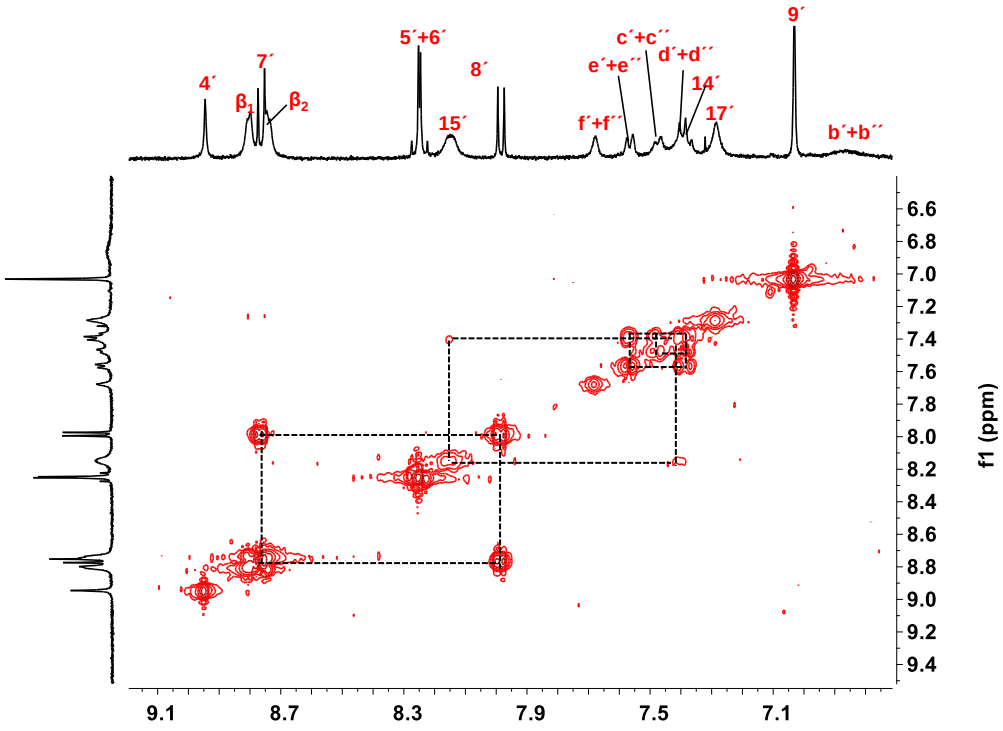


Figure S12. ^{1}H-^{1}H COSY spectrum (400 MHz, 298 K) of complex $[Cu_2(\mathbf{S})(\mathbf{R})]^{2+}$ in CD_2Cl_2.

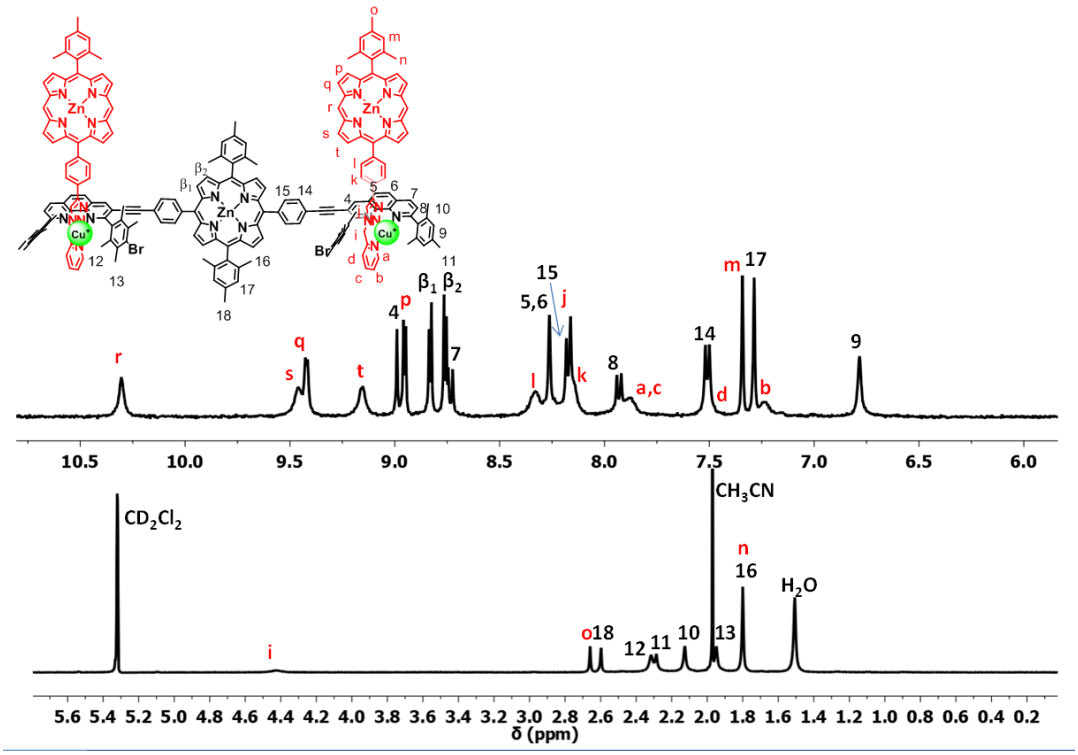


Figure S13. ^{1}H NMR (400 MHz, CD_2Cl_2) of $[Cu_2(\mathbf{S})(\mathbf{P})_2](PF_6)_2$.

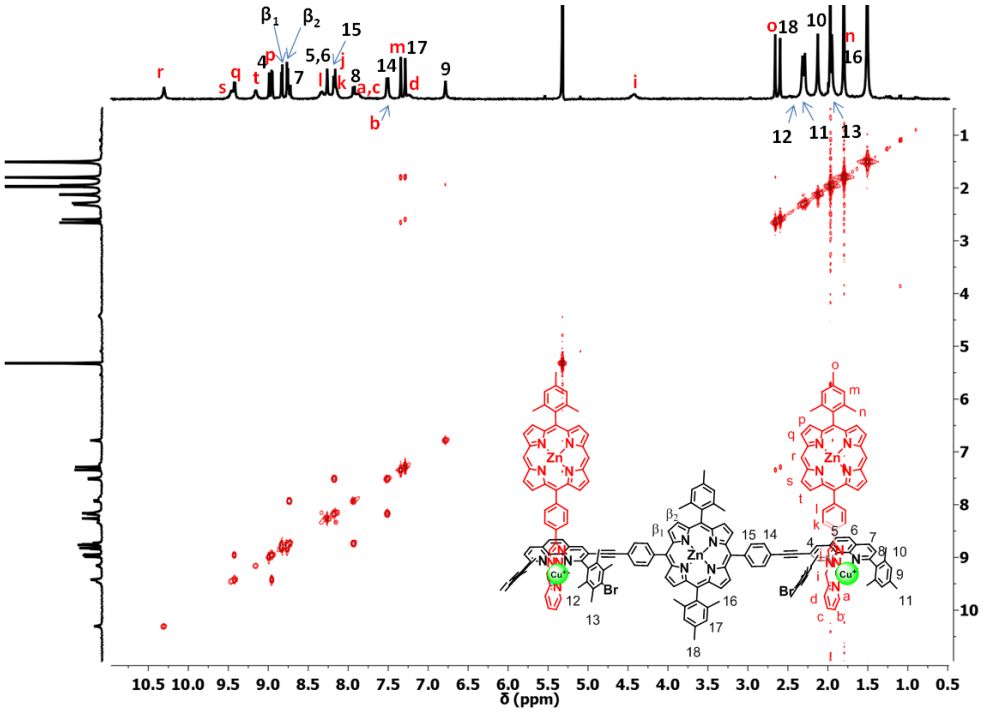


Figure S14. ^{1}H-^{1}H COSY (400 MHz, CD_2Cl_2) of $[Cu_2(\mathbf{S})(\mathbf{P})_2](PF_6)_2$.

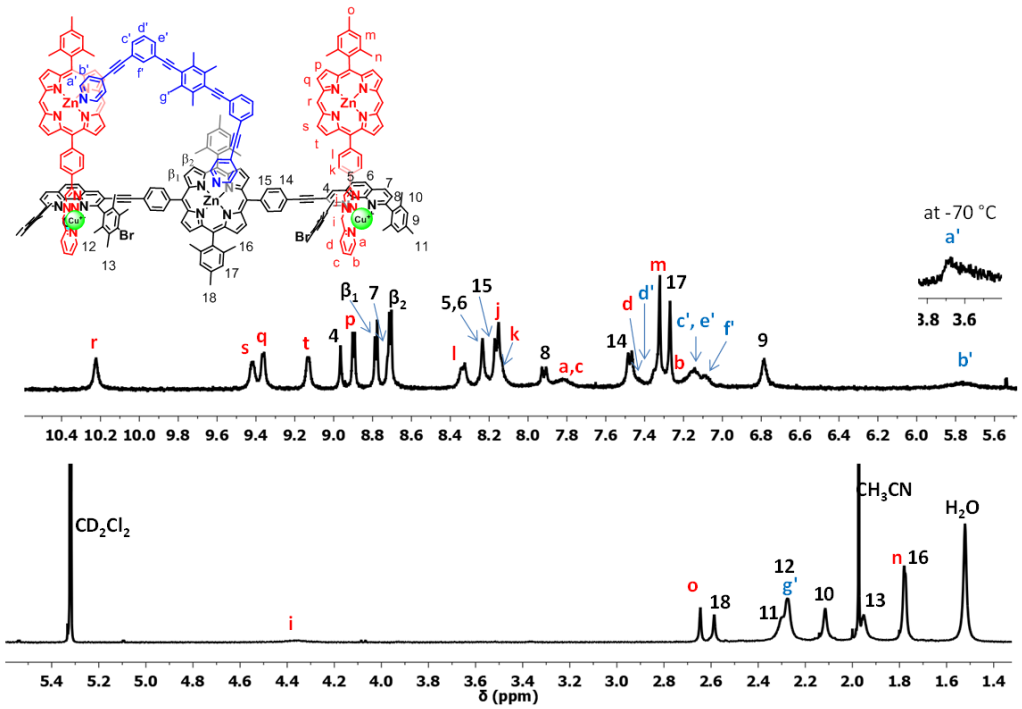


Figure S15. ^{1}H NMR (400 MHz, CD_2Cl_2) of $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$.

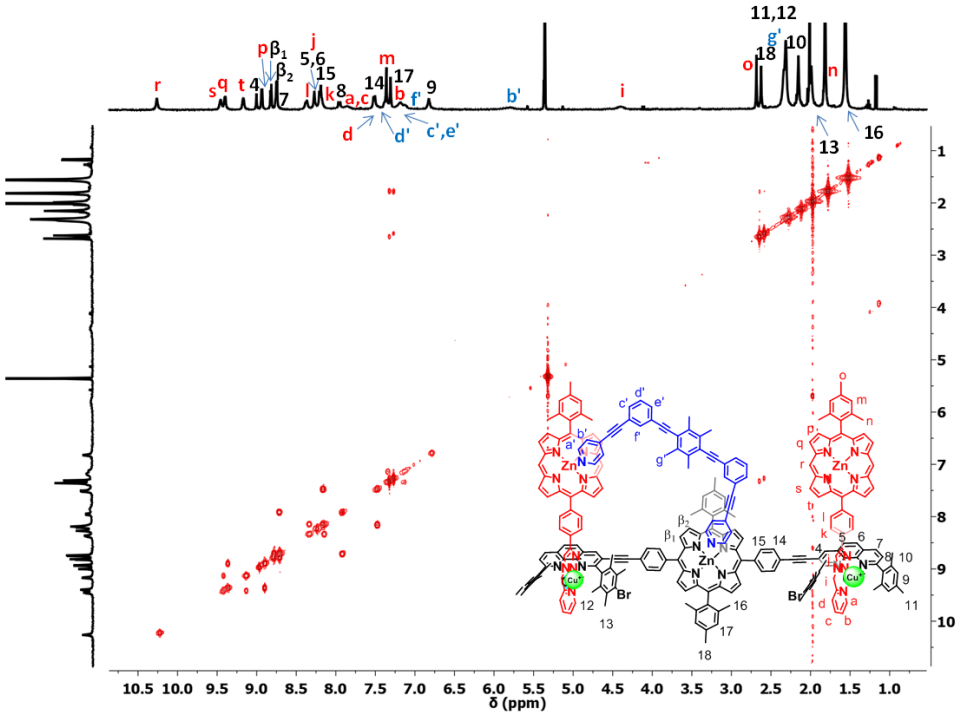


Figure S16. ^{1}H-^{1}H COSY (400 MHz, CD_2Cl_2) of $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$.

4. DOSY NMR spectra

Calculation of hydrodynamic radius from:

For $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$ and $[Cu_2(\mathbf{S})(\mathbf{P})_2](PF_6)_2$ the diffusion coefficient D was obtained from the DOSY spectrum. The corresponding hydrodynamic radius was calculated by using the Stokes-Einstein equation

$$r = k_B T/6\pi\eta D$$

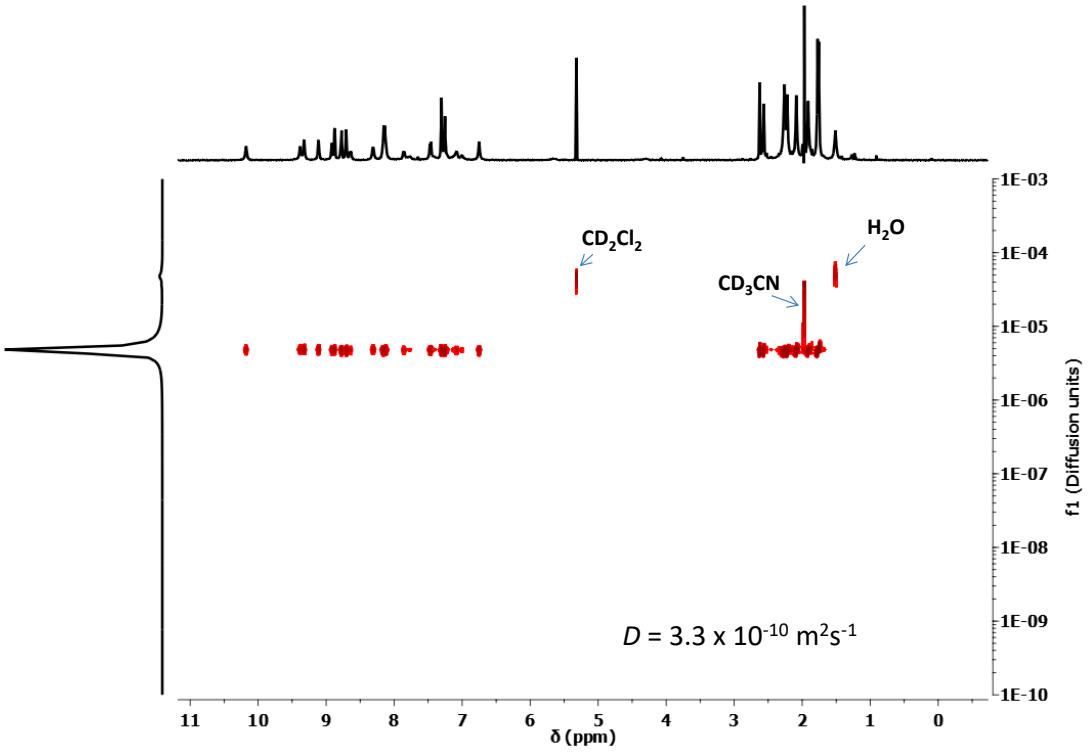


Figure S17. ^{1}H DOSY NMR (600 MHz, CD_2Cl_2) of $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$. D = 3.3 x 10^{-10} m^2s^{-1} and r = 16.1 Å.

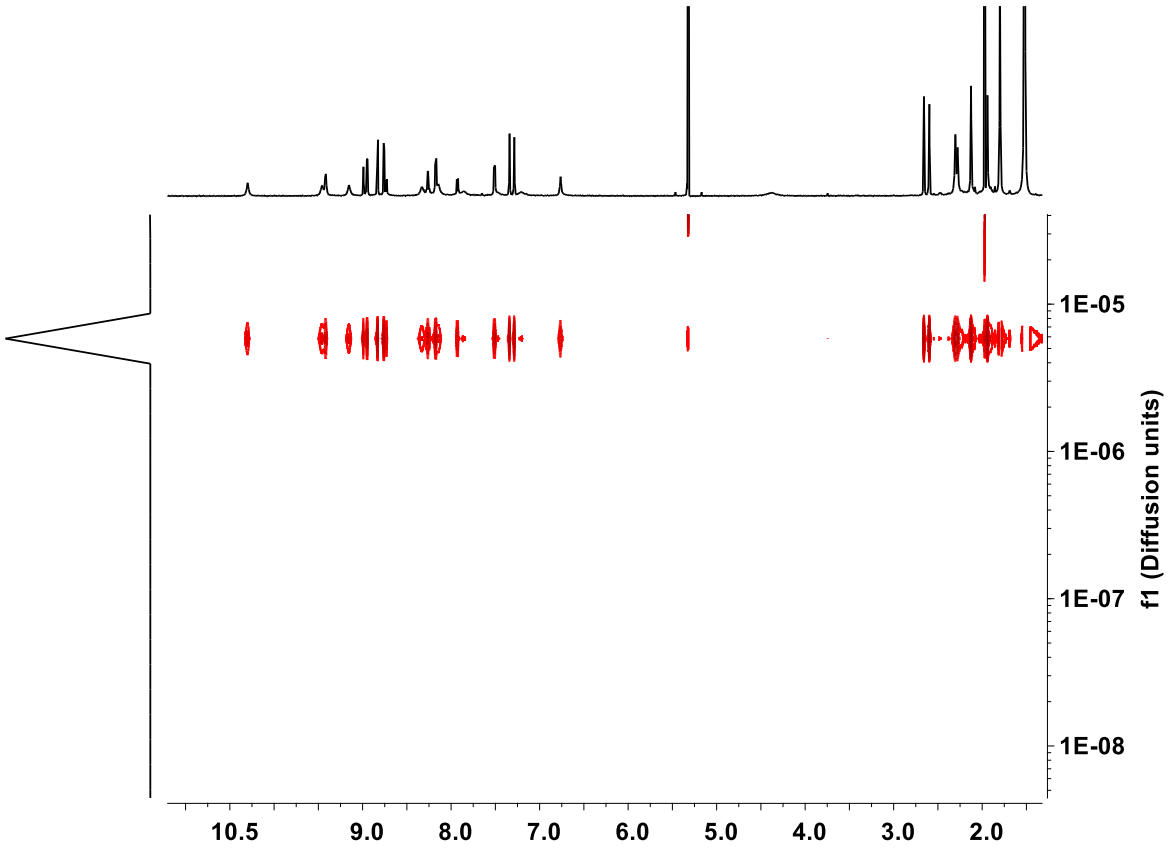


Figure S18. ^{1}H DOSY NMR (600 MHz, CD_2Cl_2) of deck $[Cu_2(\mathbf{S})(\mathbf{P})_2](PF_6)_2$. D = 3.9 x 10^{-10} m^2s^{-1}. r = 13.6 Å.

5. Catalysis

Procedure for the *in-situ* formation of the ZnPor deck P

A mixture of compounds **1** (4.0 mM), **2**, 2,9-dimesityl-1,10-phenanthroline (**Phen**) and $[Cu(CH_3CN)_4]PF_6$ and standard (trimethoxybenzene, **7**) in 1:1:1:1:1 ratio was heated at 50 °C for 24 h in CD_2Cl_2:$CDCl_3$ = 4:1 to quantitatively produce complex [Cu(**Phen**)(**P**)]PF_6.

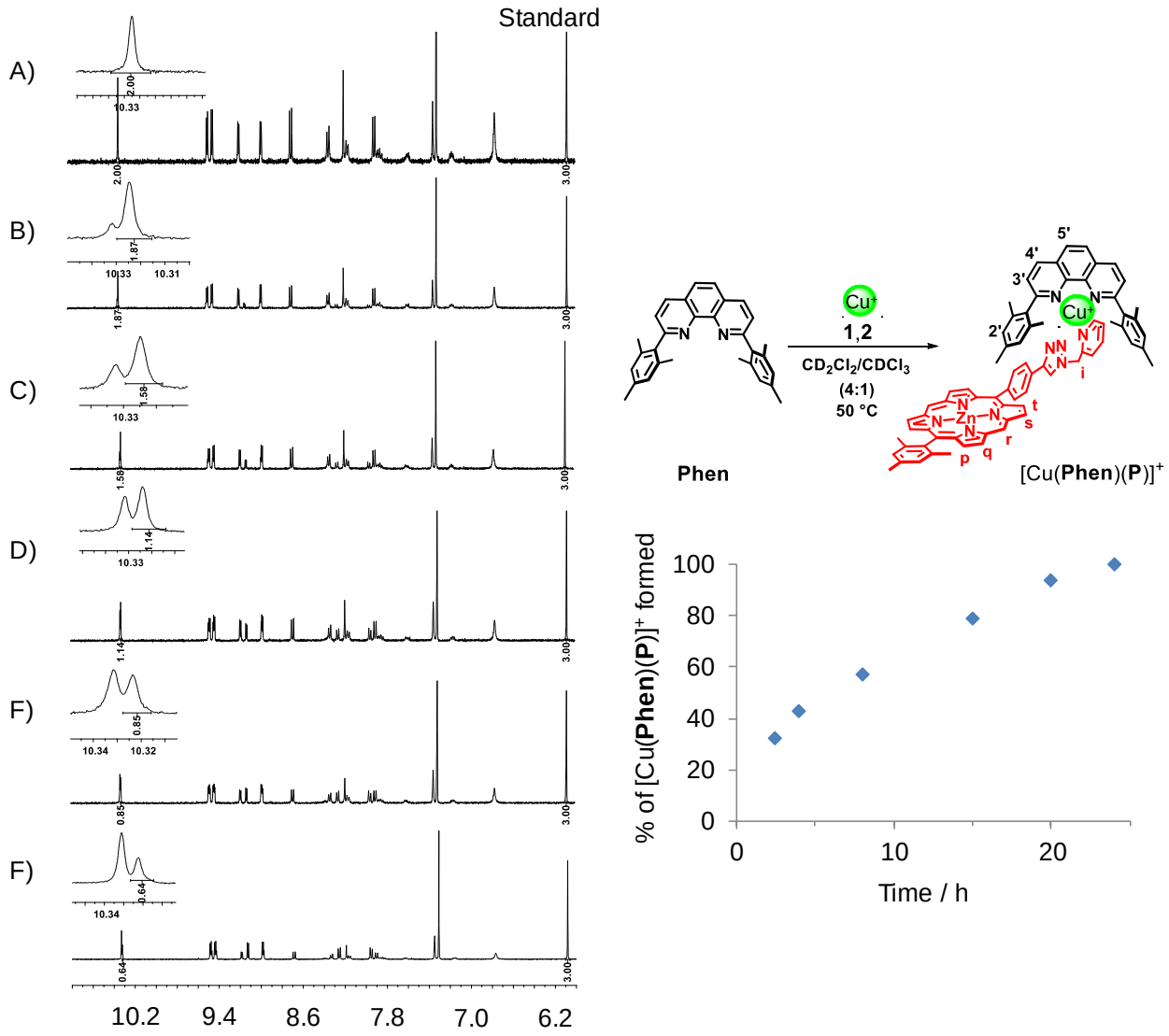


Figure S19. (A) ^{1}H NMR (400 MHz, CD_2Cl_2:$CDCl_3$ = 4:1, 298 K) spectra were recorded with time to monitor the formation of complex [Cu(**Phen**)(**P**)]PF_6. (B) Plot of formation of [Cu(**Phen**)(**P**)]PF_6 (%) vs time (h). Quantitative transformation was observed after 24 h.

Procedure for the *in-situ* formation of the slider-on-deck from the nanorotor

A mixture of compounds **1** (4.0 mM), **2**, **S**, **R**, [Cu(CH_3CN)$_4$]PF_6 and standard (trimethoxybenzene, **7**) in 2:2:1:1:2:10 ratio was heated at 50 °C for 24 h in CD_2Cl_2:$CDCl_3$ = 4:1 to produce the slider-on-deck [Cu_2(**S**)(**R**)(**P**)$_2$](PF_6)$_2$.

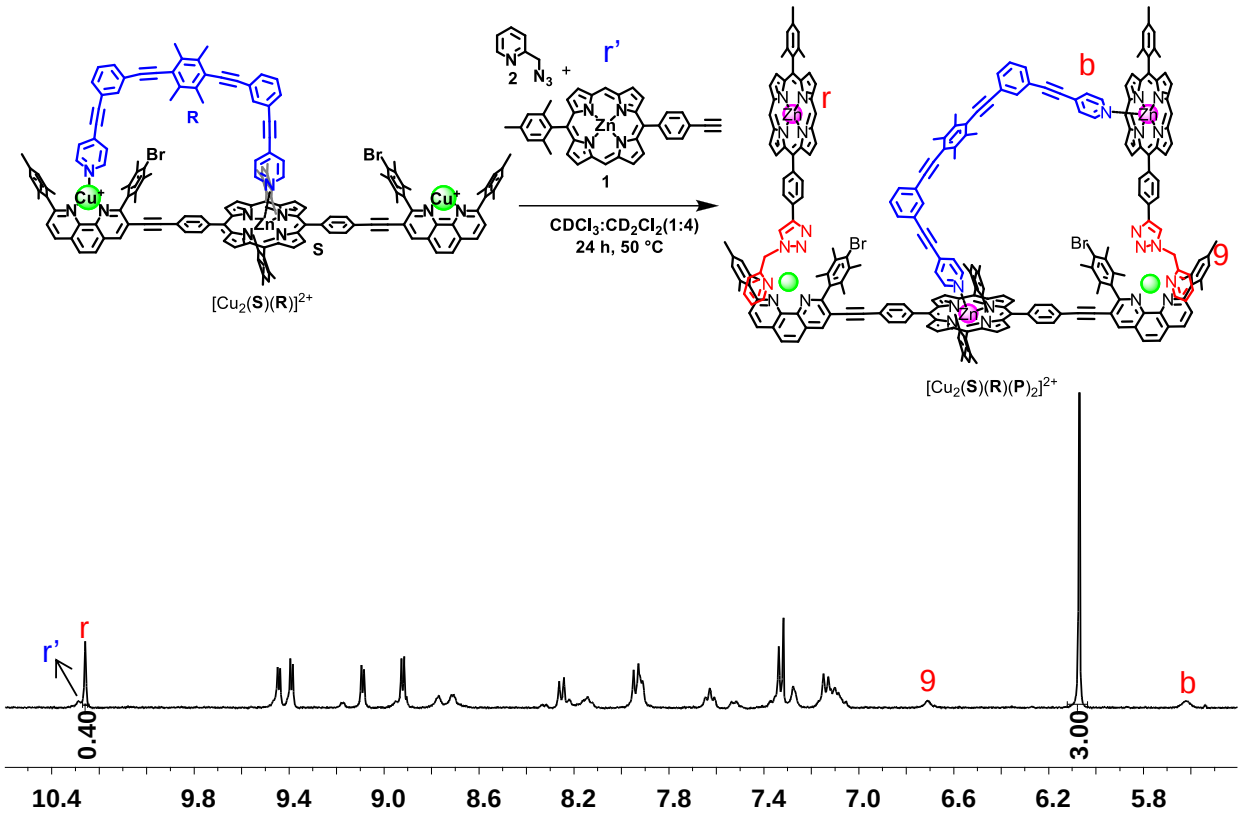


Figure S20. A mixture of compounds **1** (4.0 mM), **2**, **S**, **R** and $[Cu(CH_3CN)_4]PF_6$ and standard (trimethoxybenzene, **7**) in 2:2:1:1:2:10 ratio was heated at 50 °C for 24 h in CD_2Cl_2:$CDCl_3$ = 4:1 and to produce quantitative slider-on-deck $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$.

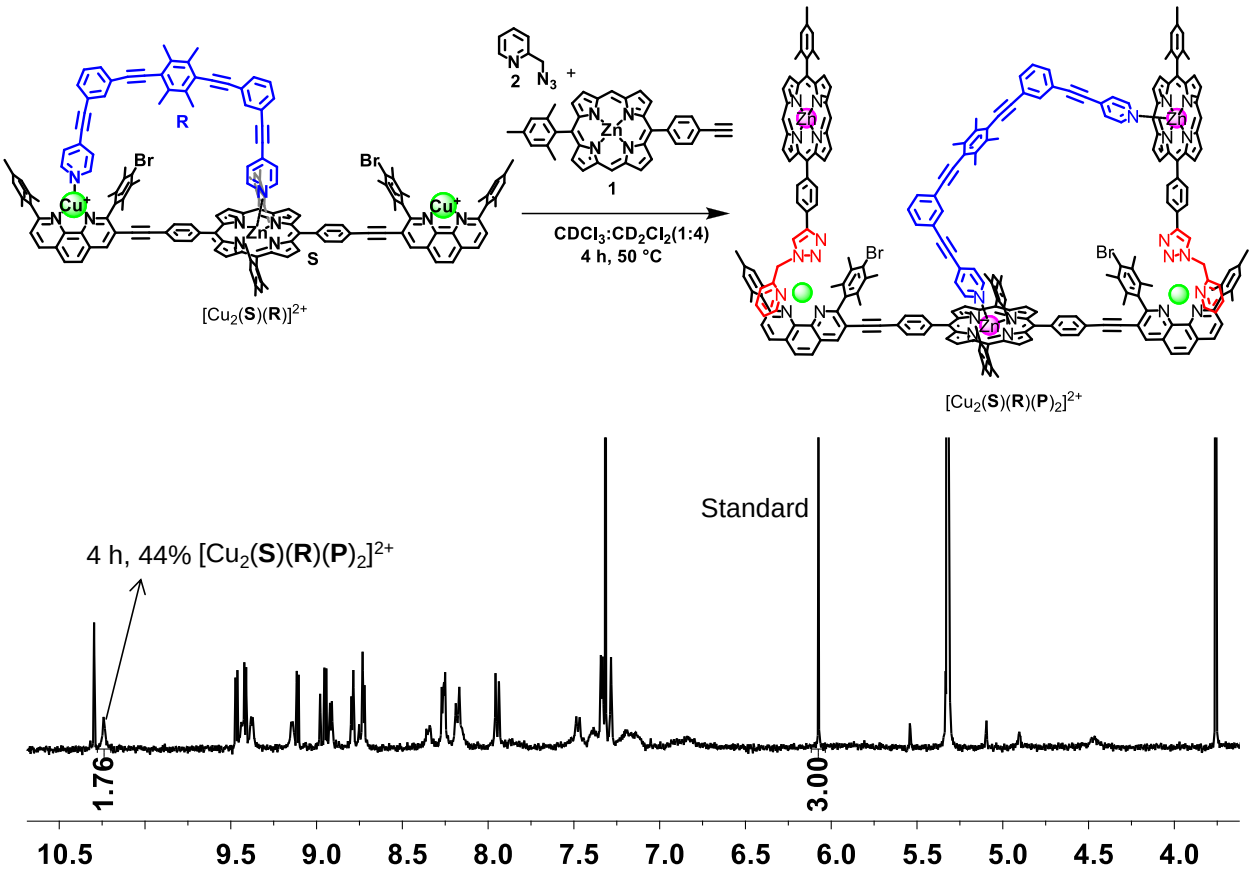


Figure S21. ^{1}H NMR (400 MHz, CD_2Cl_2:$CDCl_3$ = 4:1, 298 K) spectrum obtained after heating the reaction mixture of **S** (≈ 2.0 mM), **R**, $[Cu(CH_3CN)_4]PF_6$, **1**, **2** and standard (trimethoxy-benzene, **7**) in 1:1:2:2:2:2 ratio at 50 °C. After 4 h, product **P** had formed in 88% generating 44% of slider-on-deck $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$.

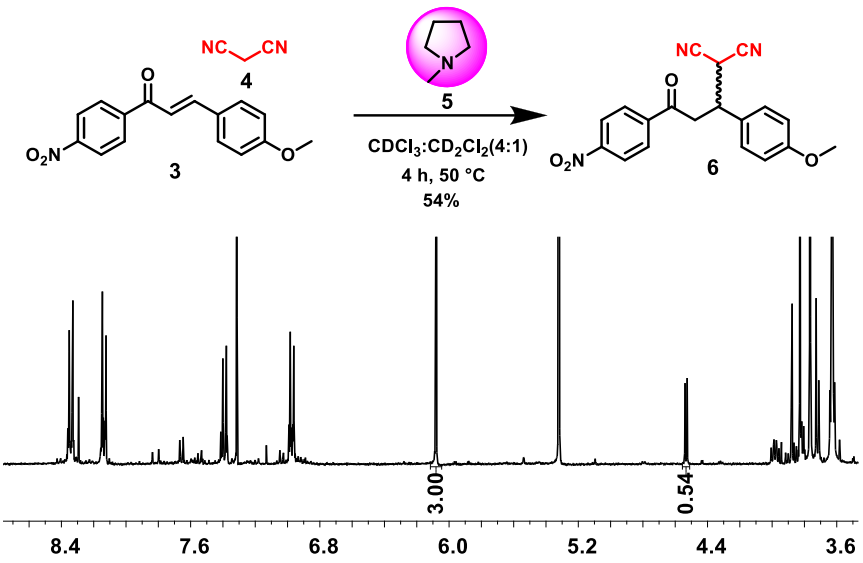


Figure S22. ^{1}H NMR (400 MHz, CD_2Cl_2:$CDCl_3$ = 4:1, 298 K) spectrum obtained after heating the reaction mixture of **3** (≈ 40 mM), **4**, **5** and standard (trimethoxybenzene, **7**) in 10:50:1:10 ratio at 50 °C. Product **6** was furnished after 4 h in 54% yield.

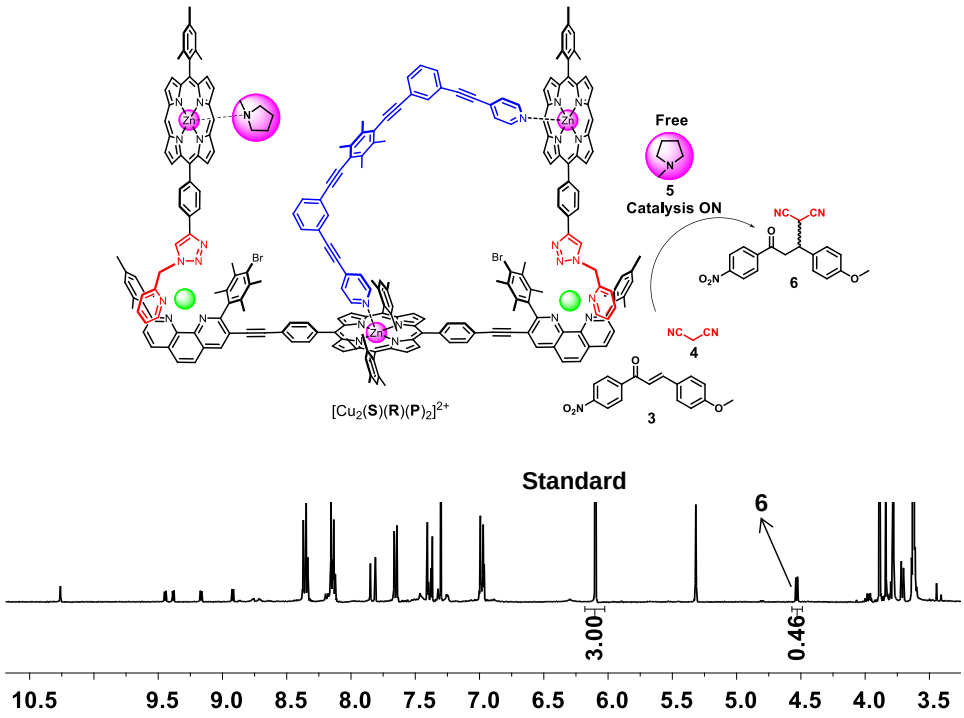


Figure S23. ^{1}H NMR (400 MHz, CD_2Cl_2:$CDCl_3$ = 4:1, 298 K) spectrum obtained after heating the reaction mixture of **S** (≈ 2.0 mM), **R**, $[Cu(CH_3CN)_4]PF_6$, **P**, **3** (≈ 40 mM), **4**, **5** and standard (trimethoxybenzene, **7**) in 1:2:2:2:20:100:2:20 ratio at 50 °C. Product **6** was furnished after 4 h in 46% yield.

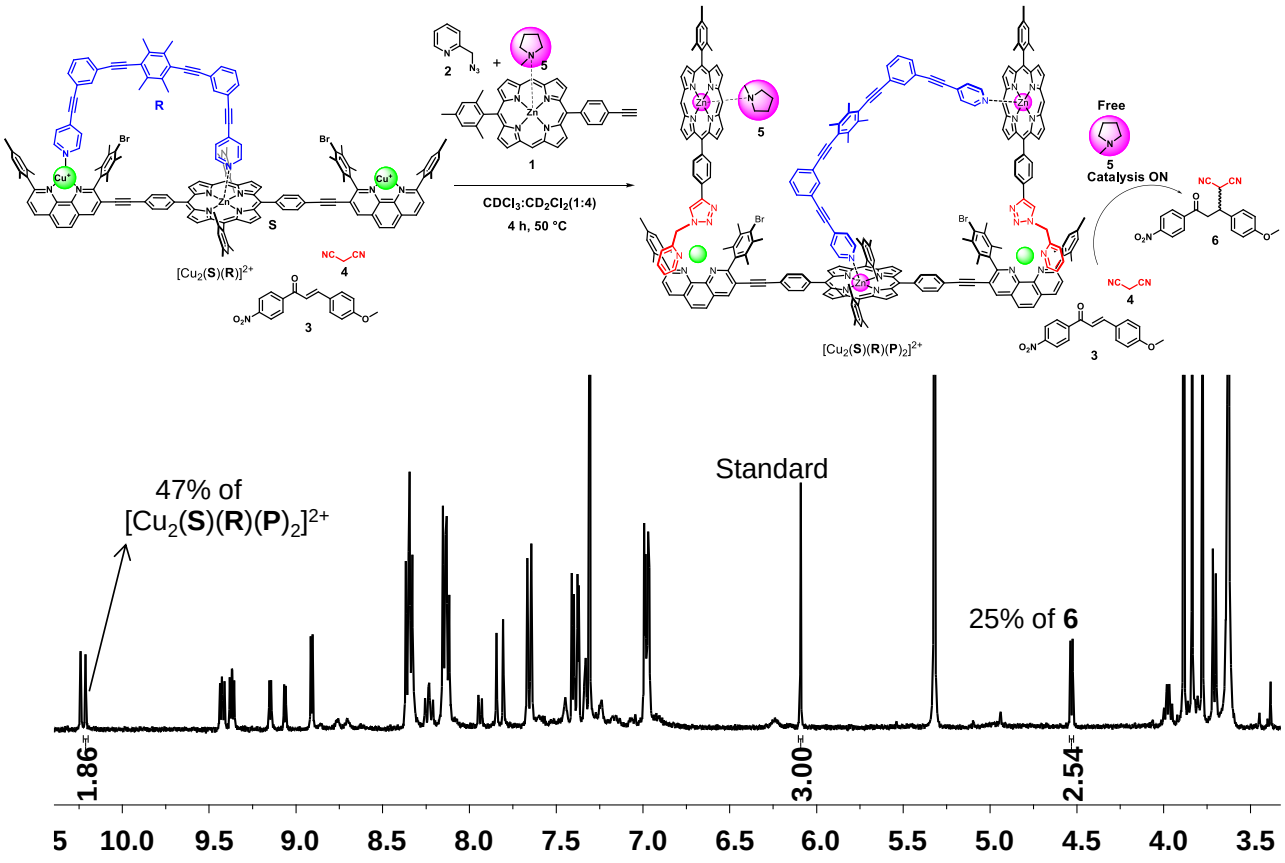


Figure S24. ^{1}H NMR (400 MHz, CD_2Cl_2:$CDCl_3$ = 4:1, 298 K) spectrum obtained after heating the reaction mixture of **S** (≈ 2.0 mM), **R**, $[Cu(CH_3CN)_4]PF_6$, **1**, **2**, **3** (≈ 40 mM), **4**, **5** and standard (trimethoxybenzene, **7**) in 1:1:2:2:2:20:100:2:2 ratio at 50 °C. 93% of the product **P** (≈ 47% of slider-on-deck $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$ and 25% of the product **6** were furnished after 4 h.

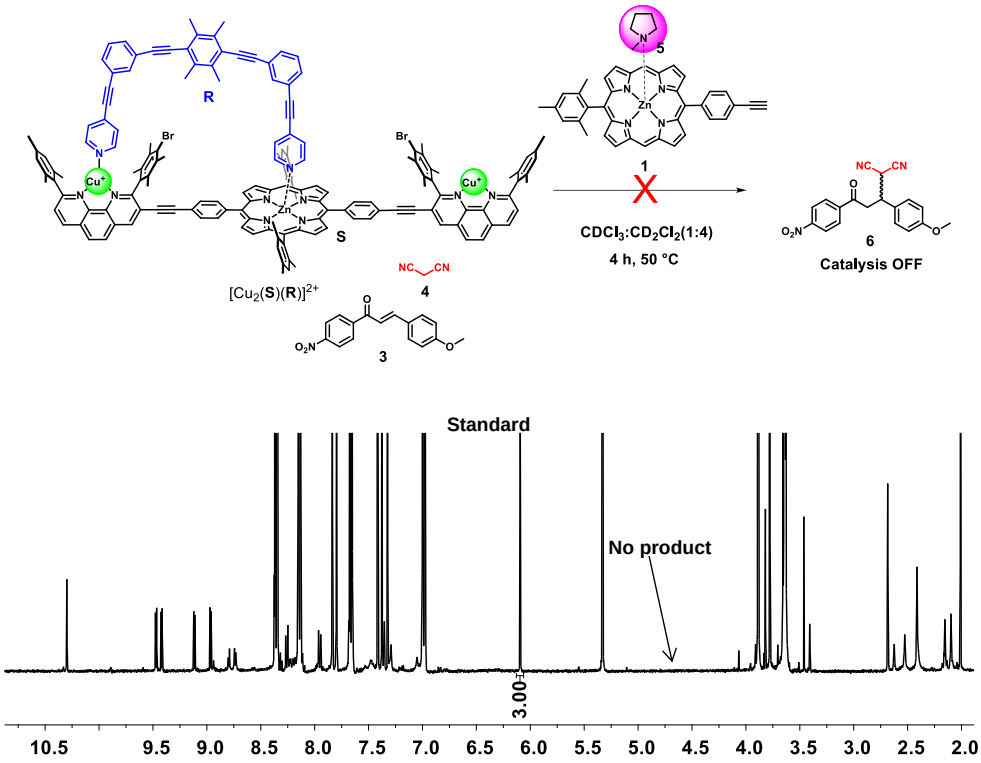


Figure S25. ^{1}H NMR (400 MHz, CD_2Cl_2:$CDCl_3$ = 4:1, 298 K) spectrum obtained after heating the reaction mixture of **S** (≈ 2.0 mM), **R**, $[Cu(CH_3CN)_4]PF_6$, **1**, **3** (≈ 40 mM), **4**, **5** and standard (trimethoxybenzene, **7**) in 1:1:2:2:20:100:2:20 ratio at 50 °C. Neither product **P** nor product **6** was furnished after 4 h.

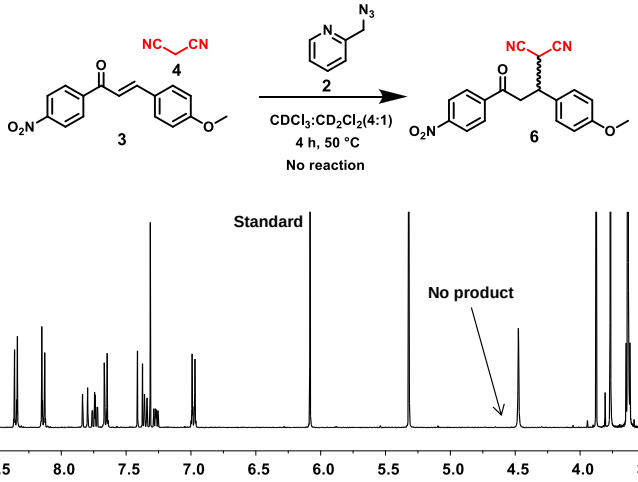
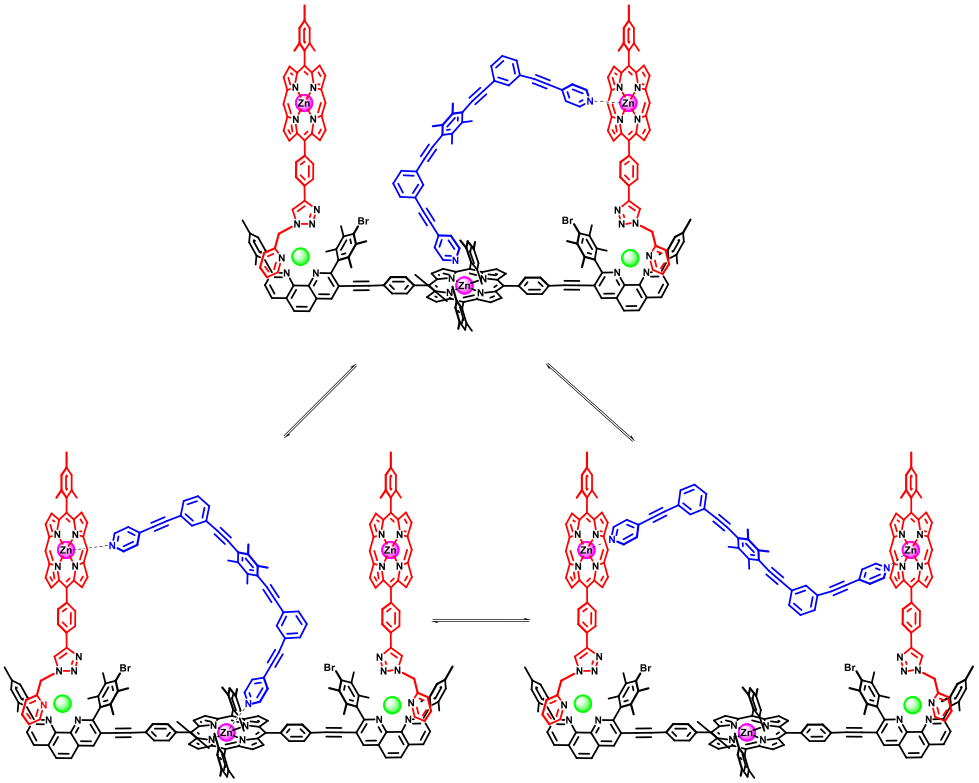


Figure S26. ^{1}H NMR (400 MHz, CD_2Cl_2:$CDCl_3$ = 4:1, 298 K) spectrum obtained after heating the reaction mixture of **3** (≈ 40 mM), **4**, **2** and standard (trimethoxybenzene, **7**) in 10:50:1:10 ratio at 50 °C. No product **6** was furnished after 4 h.

6. Variable temperature ^{1}H NMR

Three possible dynamic structures of slider-on-deck $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$



The kinetics of rotation was analyzed at various temperatures using the program WinDNMR[8] through simulation of the experimental ^{1}H NMR spectra. The spectral simulation providing rate constants was performed using the model of a 2-spin system with mutual exchange. Activation parameters were determined from an Eyring plot.

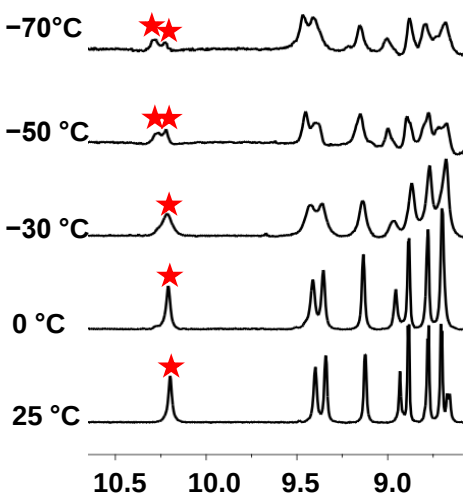


Figure S27. Partial ^{1}H VT-NMR (600 MHz, CD_2Cl_2) of $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$ showing splitting of r-H (red asterisk).

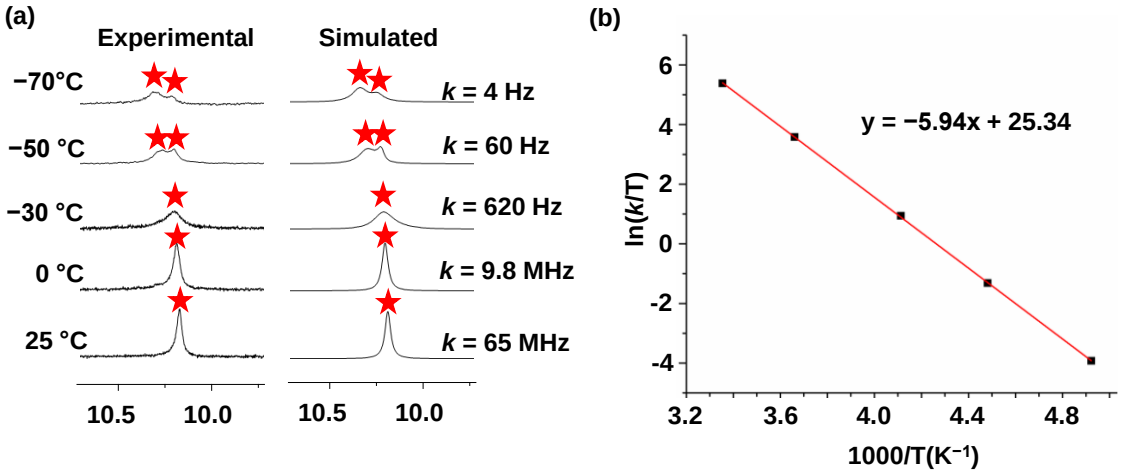


Figure S28. (a) Partial ^{1}H VT-NMR (600 MHz, CD_2Cl_2) of $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$ shows the splitting of proton r-H (red asterisk marked). (b) Eyring plot for exchange dynamics in slider-on-deck $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$. Activation parameters were determined to be $\Delta G^{\ddagger}$ = 45.5 kJ mol^{-1} $\Delta H^{\ddagger}$ = 49.4 ± 0.2 kJ mol^{-1} and $\Delta S^{\ddagger}$ = 13.1 ± 0.8 J mol^{-1} K^{-1}

7. ESI-MS

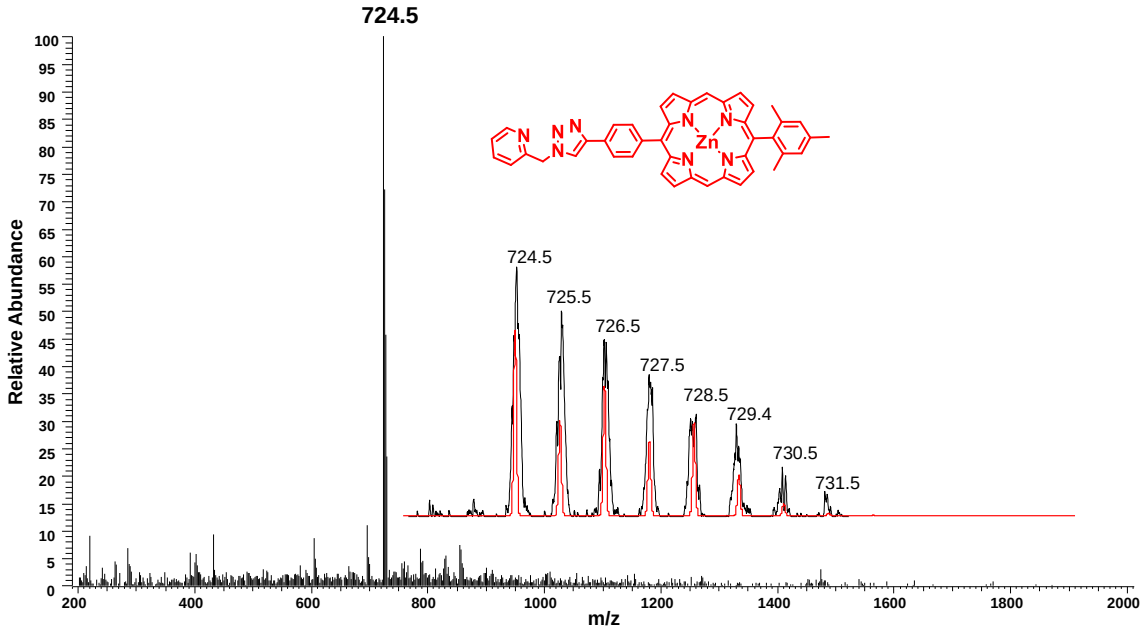


Figure S29. ESI-MS spectrum of [**P** + H]$^+$ in the presence of CH_3CO_2H in CH_2Cl_2.

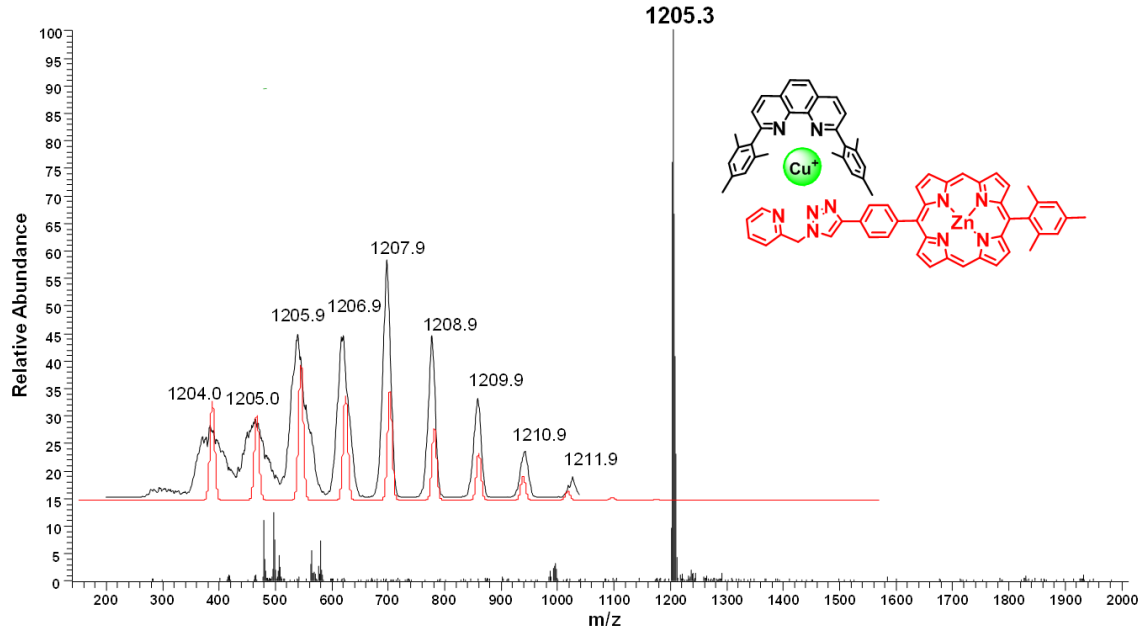


Figure S30. ESI-MS spectrum of complex [Cu(**Phen**)(**P**)]PF_6 in CH_2Cl_2 along with experimental (black) and calculated (red) isotopic distributions showing species [Cu(**Phen**)(**P**)]$^+$.

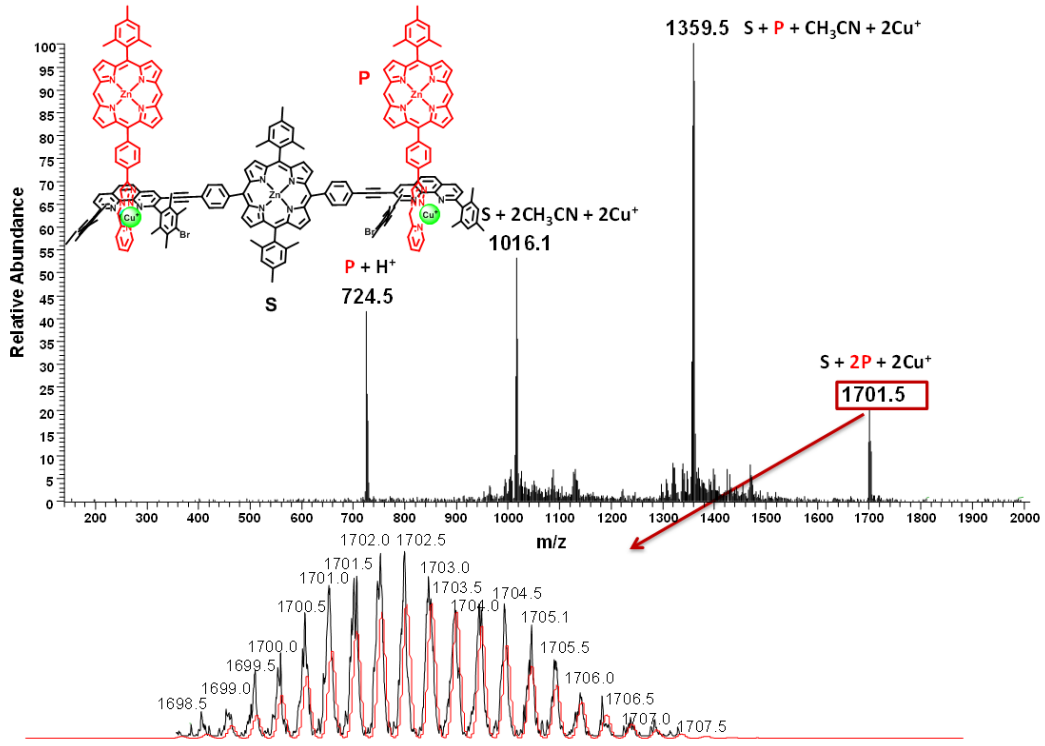


Figure S31. ESI-MS spectrum of complex $[Cu_2(\mathbf{S})(\mathbf{P})_2](PF_6)_2$ in CH_2Cl_2 along with experimental (black) and calculated (red) isotopic distributions showing species $[Cu_2(\mathbf{S})(\mathbf{P})_2]^{2+}$.

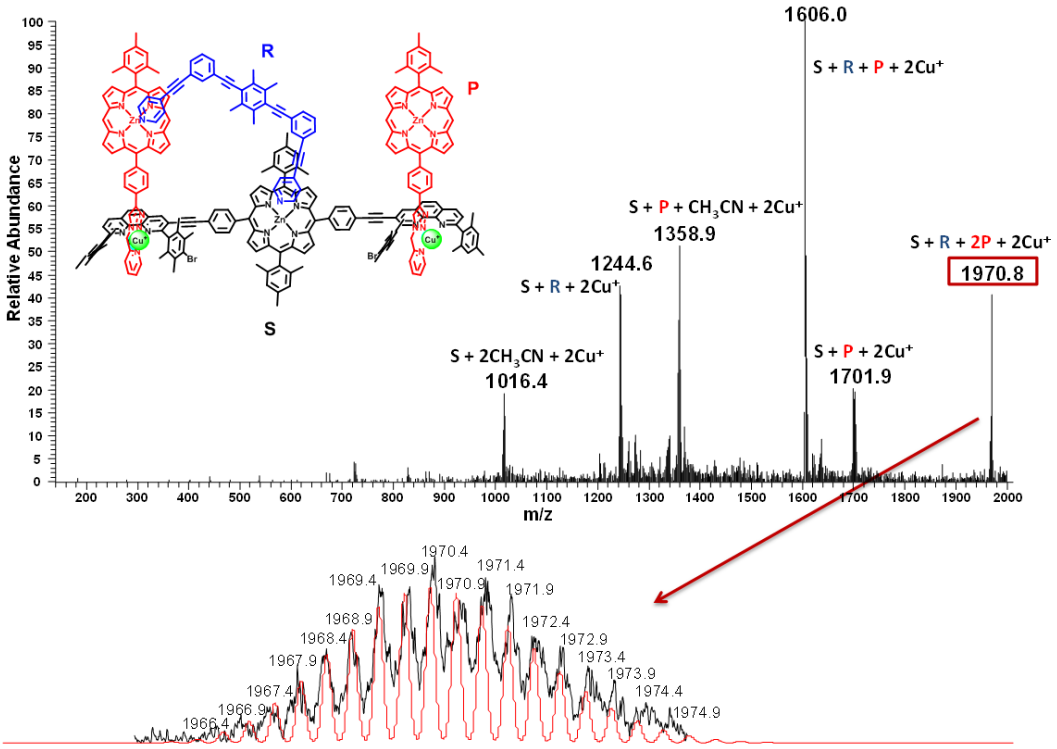


Figure S32. ESI-MS spectrum of complex $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$ in CH_2Cl_2 along with experimental (black) and calculated (red) isotopic distributions showing species $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2]^{2+}$.

8. UV-vis spectra

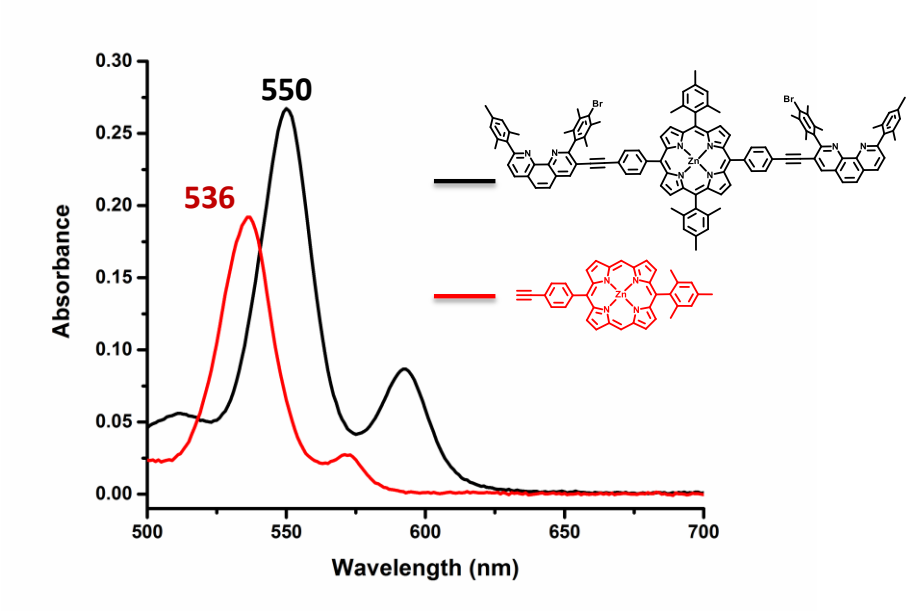


Figure S33. Comparison of UV-vis spectra of stator **S** and compound **1** in 1,1,2,2-tetrachloroethane (*c* = 1.00 mM, 298 K) in 1.0 mm cuvette.

9. Estimation of hydrodynamic radius and energy minimized structures

Stokes-Einstein Equation; $D = kT/6\pi\eta r$
D = diffusion coefficient
k = Boltzmann constant
T = temperature
η = viscosity of the solution
r = hydrodynamic radius of the particle

There are two possible slider-on-deck structures, **DS1** and **DS2**, see below.

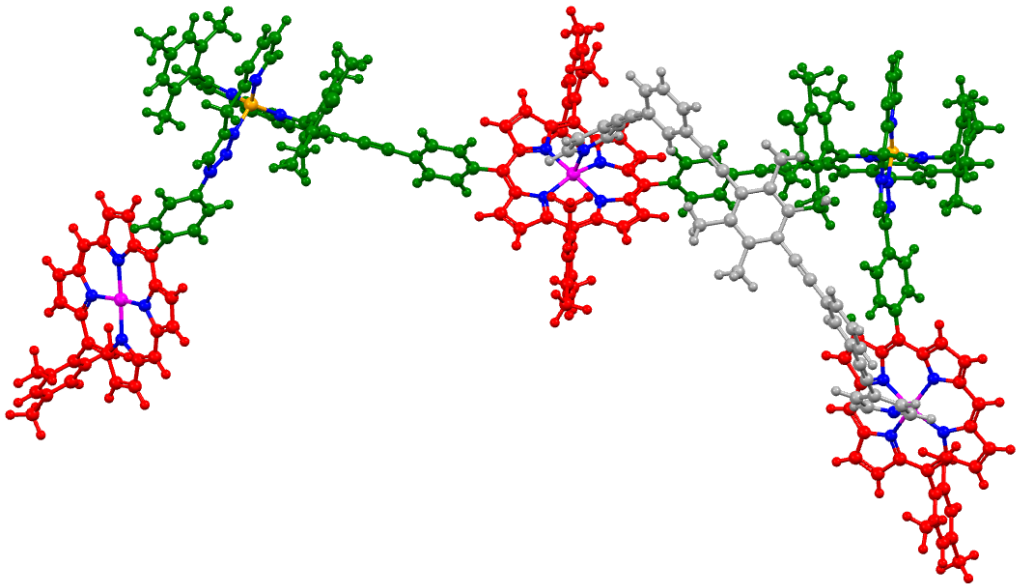


Figure S34. DFT-optimized structure of complex slider-on-deck **DS1** = $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$ (biped coordinated to the inner and one outer ZnPor unit) using B3LYP/6-31G(d)) and separately LanL2DZ basis set for copper(I)/zinc(II). Counter anions are not included. Hydrogens are omitted for clarity.

$D = 3.3 \times 10^{-10}$ m^2s^{-1} (from DOSY of the interconverting **DS1** ⇆ **DS2**)

The experimental hydrodynamic radius was calculated as

r_H = 16.1 Å

The radius calculated from the energy minimized structure:

r_H = 16.8 Å

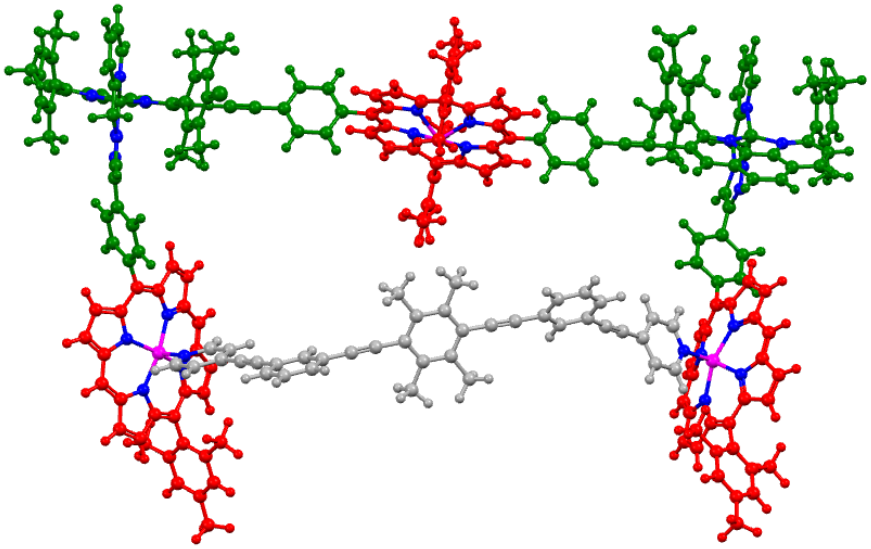


Figure S35. DFT-optimized structure of complex slider-on-deck **DS2** = $[Cu_2(\mathbf{S})(\mathbf{R})(\mathbf{P})_2](PF_6)_2$ (biped coordinated to both peripheral ZnPor units) using B3LYP/6-31G(d)) and separately LanL2DZ basis set for copper(I)/zinc(II). Counter anions are not included. Hydrogens are omitted for clarity.

$D = 3.3 \times 10^{-10}$ m^2s^{-1} (from DOSY of the interconverting **DS1** ⇆ **DS2**)

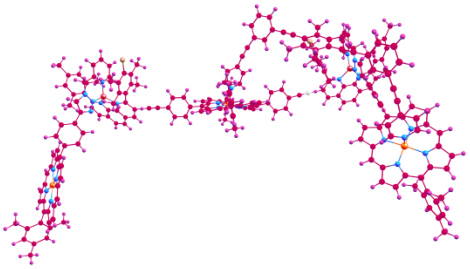
The experimental hydrodynamic radius was calculated as

$r_H = 16.1$ Å

The radius calculated from the energy minimized structure:

$r = 16.4$ Å

Coordinates:



DS1 = $[Cu_2(S)(R)(P)_2](PF_6)_2$

C	2.032500000	-6.252300000	-8.098700000
C	2.278200000	-4.872600000	-8.208300000
C	1.549200000	-6.770600000	-6.884800000
C	2.097100000	-4.018700000	-7.104300000
H	2.611300000	-4.477400000	-9.124400000
C	1.330900000	-5.928500000	-5.778700000
H	1.345700000	-7.799700000	-6.806400000
C	1.616700000	-4.549400000	-5.886300000
C	1.407800000	-3.667300000	-4.717600000
C	2.354600000	-3.553500000	-3.778100000
C	0.183600000	-2.893700000	-4.606300000
N	2.361300000	-2.678600000	-2.651300000
C	3.685500000	-4.139500000	-3.923300000
N	-0.219100000	-2.113100000	-3.491800000
C	-0.801100000	-2.915900000	-5.520000000
Zn	0.799900000	-1.798600000	-1.845700000
C	3.598500000	-2.590600000	-2.269300000
C	4.454200000	-3.509300000	-3.036900000
H	4.002200000	-4.839800000	-4.631500000
C	-1.594300000	-1.825100000	-3.717600000
C	-1.943300000	-2.229700000	-4.950300000
H	-0.810300000	-3.460500000	-6.413200000
N	1.961100000	-0.790200000	-0.617700000
N	-0.733400000	-0.766900000	-1.163900000
C	4.162300000	-1.717500000	-1.249000000
H	5.480900000	-3.660600000	-2.910000000
C	-2.552100000	-1.398900000	-2.709400000
H	-2.908000000	-2.233300000	-5.354600000
C	1.604100000	-0.036000000	0.378700000
C	3.380900000	-0.881200000	-0.558500000
C	-0.795400000	-0.171100000	0.124600000
C	-2.099000000	-0.931700000	-1.540400000
C	2.776900000	0.496000000	1.088200000
C	0.252100000	0.212300000	0.861600000
C	3.865800000	-0.007500000	0.507600000
C	-2.194400000	-0.002000000	0.529400000
C	-2.968800000	-0.469100000	-0.453100000
H	2.769200000	1.146900000	1.906700000
C	0.050700000	0.864800000	2.175700000
H	4.857600000	0.165500000	0.789000000
H	-2.536800000	0.406400000	1.429500000
H	-4.014600000	-0.474700000	-0.448100000
C	-0.052500000	2.271400000	2.258400000
C	-0.036600000	0.084900000	3.350100000
C	-0.224500000	2.884600000	3.513800000
C	0.024800000	3.139900000	1.021400000
C	-0.207000000	0.715500000	4.596400000
C	0.062400000	-1.422500000	3.303400000
C	-0.283400000	2.115600000	4.688800000
H	-0.304700000	3.931400000	3.577800000
H	0.993500000	3.007700000	0.537600000
H	-0.767700000	2.863200000	0.324800000
H	-0.093300000	4.192500000	1.281800000
H	-0.273500000	0.134900000	5.471200000
H	-0.698000000	-1.820400000	2.630700000
H	1.052600000	-1.710800000	2.949100000
H	-0.092800000	-1.852300000	4.293700000
C	-0.503600000	2.779500000	6.026100000
H	-1.573500000	2.910100000	6.194600000
H	-0.088000000	2.164800000	6.826100000
H	-0.015400000	3.754900000	6.046400000
C	2.212600000	-7.158800000	-9.291800000
H	1.255000000	-7.287000000	-9.798400000
H	2.931800000	-6.728500000	-9.990100000
H	2.580700000	-8.133600000	-8.968100000
C	2.375500000	-2.539800000	-7.270700000
H	1.432800000	-1.994600000	-7.333100000
H	2.952700000	-2.166700000	-6.424000000
H	2.946400000	-2.358200000	-8.182500000
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H	1.626800000	-6.518000000	-3.739800000
H	-0.020600000	-5.955000000	-4.109000000
H	0.507100000	-7.560200000	-4.636900000
C	-3.990800000	-1.640500000	-2.924500000
C	-4.582400000	-2.798600000	-2.385300000
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H	-4.010800000	-3.462700000	-1.804400000
C	-6.119600000	-1.051100000	-3.952100000
H	-4.332100000	0.099600000	-4.119300000
C	-6.705700000	-2.213600000	-3.419700000
H	-6.366900000	-3.951500000	-2.219700000
H	-6.689900000	-0.393500000	-4.542300000
C	5.619100000	-1.754800000	-1.023500000
C	6.465600000	-0.900800000	-1.754100000
C	6.177000000	-2.727000000	-0.172400000
C	7.860200000	-1.044200000	-1.663100000
H	6.058400000	-0.182700000	-2.405200000
C	7.571900000	-2.871400000	-0.082500000
H	5.551800000	-3.381100000	0.363000000
C	8.415300000	-2.042100000	-0.842400000
H	8.484100000	-0.428900000	-2.245400000
H	7.978600000	-3.630000000	0.521000000
C	-8.080800000	-2.500900000	-3.663900000
C	9.821300000	-2.278100000	-0.869900000
C	-9.243600000	-2.734000000	-3.876100000
C	11.011700000	-2.459400000	-0.913900000
H	-10.235500000	-2.895700000	-4.062300000
C	-11.263900000	-3.061400000	-4.258200000
C	-11.865000000	-2.498300000	-5.404800000
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C	-16.086900000	-2.882900000	-5.717900000
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C	13.062000000	-2.756600000	-1.124700000
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C	13.845700000	-3.356700000	-0.113700000
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H	15.246700000	-1.905000000	-4.540900000
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H	17.588700000	-2.562800000	-4.779300000
C	19.083600000	-3.878700000	-2.885600000
C	18.848100000	-4.723000000	-0.609000000
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H	19.660600000	-3.744100000	-3.753500000
H	20.613300000	-4.911000000	-1.807500000
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C	20.214200000	-6.781300000	2.900600000
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C	-18.300500000	3.860300000	1.469000000
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C	-14.175000000	6.802400000	-0.712300000
C	-13.256100000	5.687900000	-0.957700000
H	-13.483700000	3.602800000	-0.611600000
C	-19.261700000	5.815000000	0.937700000
C	-19.525000000	4.632500000	1.512200000
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N	-18.532200000	8.555700000	0.247100000
C	-13.703100000	8.162800000	-0.860600000
H	-12.284500000	5.754800000	-1.338900000
C	-20.252000000	6.846500000	0.758900000
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C	-19.863100000	8.077800000	0.429200000
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H	-13.180400000	10.933000000	-1.168100000
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H	-19.781900000	15.543000000	-4.083400000
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C	17.100500000	-4.461600000	3.883700000
C	15.301000000	-7.886700000	1.975900000
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C	15.629200000	-7.923400000	3.337600000
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N	17.249500000	-3.171200000	3.231100000
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C	17.858200000	-2.004000000	3.747600000
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H	18.339800000	2.860000000	0.537700000
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C	20.696600000	3.696200000	1.460300000
C	21.695000000	3.482300000	0.594200000
C	20.325700000	5.054000000	1.810800000
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N	20.868300000	6.245900000	1.259000000
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C	23.410500000	3.766200000	-0.715200000
C	23.218200000	2.322200000	-0.564900000
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C	20.092700000	7.295400000	1.817400000
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C	24.486300000	4.260300000	-1.545600000
H	23.793400000	1.568400000	-1.006400000
C	20.168900000	8.697600000	1.483900000
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C	24.412500000	7.719700000	-1.671900000

C	24.673300000	5.565800000	-1.725400000
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C	21.090300000	9.130800000	0.624200000
H	25.141900000	3.575400000	-2.002200000
H	19.499300000	9.378700000	1.924700000
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C	23.935800000	9.082900000	-1.495000000
C	25.752100000	6.107400000	-2.540400000
C	22.288800000	10.663200000	-0.532400000
C	21.234800000	10.545300000	0.279600000
H	26.201200000	8.129100000	-2.989900000
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H	26.492400000	5.575200000	-3.051400000
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H	20.630100000	11.329800000	0.616200000
C	24.339200000	10.622700000	-3.433400000
C	25.710800000	10.842000000	-1.419000000
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C	26.404400000	11.909200000	-2.019200000
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C	26.091000000	12.326600000	-3.324100000
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H	26.329100000	9.357800000	0.002200000
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C	26.814200000	13.498500000	-3.941500000
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H	27.836200000	13.552400000	-3.563000000
H	26.849500000	13.390600000	-5.026600000
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C	-0.994800000	-5.006900000	1.078400000
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C	-6.851100000	-1.960900000	6.526100000
C	-10.668100000	-1.671900000	6.244700000
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C	-8.964000000	0.046300000	7.004100000
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H	-6.762600000	-1.373900000	7.441300000
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H	-12.920500000	-3.782400000	6.248500000
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H	-13.347700000	2.253700000	5.727000000
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C	-15.131200000	4.149200000	6.283100000
H	-15.573500000	1.575600000	10.054000000
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C	-15.404000000	5.056800000	5.538200000
C	-15.687000000	6.054400000	4.558500000
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H	-17.793000000	6.162800000	4.928900000
C	-15.058100000	7.147000000	2.498400000
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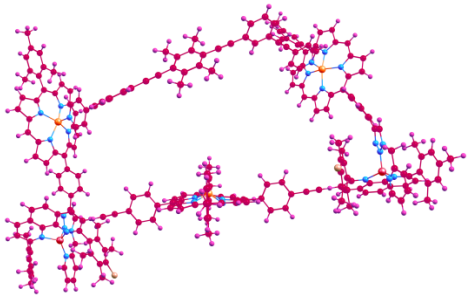

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C	0.166500000	9.590400000	-6.889100000
H	-1.283100000	8.564900000	-8.053100000
C	-4.622000000	10.663400000	-3.081400000
C	-5.722200000	10.322800000	-3.770200000
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H	1.000900000	9.581300000	-7.519300000
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C	-10.960600000	-6.256600000	0.256900000
C	-13.305100000	-6.377300000	-0.438300000
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C	-9.832900000	-5.558700000	0.986400000
C	-13.038100000	-7.600400000	-1.081900000
C	-14.716400000	-5.829600000	-0.463400000
C	-11.744400000	-8.150400000	-1.074800000
H	-9.749500000	-7.897100000	-0.370800000
H	-9.723300000	-4.540700000	0.609100000
H	-10.051400000	-5.524600000	2.054800000
H	-8.891500000	-6.087700000	0.836900000
H	-13.815400000	-8.114200000	-1.570500000
H	-15.152300000	-5.887000000	0.534600000
H	-14.708500000	-4.790600000	-0.795100000
H	-15.338900000	-6.405000000	-1.150600000
C	-11.484700000	-9.494100000	-1.710800000
H	-11.673300000	-10.282000000	-0.979900000
H	-12.141000000	-9.638300000	-2.570200000
H	-10.448900000	-9.558300000	-2.046800000
N	8.923400000	13.465400000	-14.936500000
C	8.071200000	13.209700000	-15.932900000
C	9.239600000	14.691900000	-14.557100000
C	7.523700000	14.297500000	-16.646700000
C	7.587900000	11.827900000	-16.400400000
C	8.744100000	15.816300000	-15.234600000
H	9.894100000	14.824600000	-13.748300000
C	7.872600000	15.613900000	-16.312300000
H	6.858100000	14.130700000	-17.444300000
H	6.503400000	11.800400000	-16.263600000
H	7.787600000	11.757900000	-17.473500000
N	8.126700000	10.620200000	-15.797500000
H	9.031500000	16.786100000	-14.951500000
H	7.486600000	16.427100000	-16.853700000
C	7.676500000	9.280500000	-15.930600000
N	9.074400000	10.583500000	-14.851000000
C	8.417700000	8.568200000	-15.065100000
H	6.896200000	8.930700000	-16.532300000
N	9.271300000	9.459200000	-14.392000000
C	8.395300000	7.167200000	-14.654100000
C	7.767300000	6.823700000	-13.442200000
C	9.342800000	6.291400000	-15.211800000
C	8.117200000	5.638900000	-12.771800000
H	7.102300000	7.496900000	-12.982500000
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C	9.113200000	4.795300000	-13.295400000
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H	10.439300000	4.488400000	-14.947500000
C	9.576200000	3.626200000	-12.513400000
C	10.687800000	3.669600000	-11.772500000
C	8.986100000	2.330400000	-12.741800000
N	11.353400000	2.578800000	-11.111800000
C	11.580200000	4.829400000	-11.830200000
N	9.246000000	1.122600000	-12.025900000
C	8.202300000	2.104000000	-13.809300000
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C	12.556100000	3.023600000	-10.904800000
C	12.748600000	4.402700000	-11.358900000
H	11.400400000	5.752200000	-12.286000000
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H	7.911000000	2.798100000	-14.535100000
N	12.484200000	0.189800000	-10.190300000
N	10.269800000	-1.161200000	-10.936900000
C	13.695100000	2.329600000	-10.365400000
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C	10.983900000	-2.277500000	-10.417200000
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C	14.385000000	-0.993000000	-9.641600000
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C	9.152300000	-3.226800000	-11.347600000
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C	-0.908200000	-0.991800000	5.343500000
C	0.112800000	-0.605800000	4.812100000
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C	1.935500000	-1.051300000	3.192000000
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C	3.052700000	-0.647000000	2.434500000
C	3.036200000	1.483200000	3.544300000
C	3.601900000	0.643900000	2.559200000
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C	5.590100000	1.361300000	0.912300000
C	6.709500000	1.791600000	0.070200000
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H	7.576000000	2.861600000	1.712600000
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C	9.614800000	0.193300000	-6.541500000
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H	9.733600000	-0.622800000	-5.886100000
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H	0.332800000	2.336800000	5.035600000
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C	3.665000000	-1.637900000	1.427100000
H	3.330900000	-1.395200000	0.440100000
H	4.732300000	-1.574400000	1.468100000
H	3.357200000	-2.632700000	1.673400000

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