Supporting Information

for

Reversible cargo shipping between orthogonal stations of a nanoscaffold upon redox input

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NMR Spectra

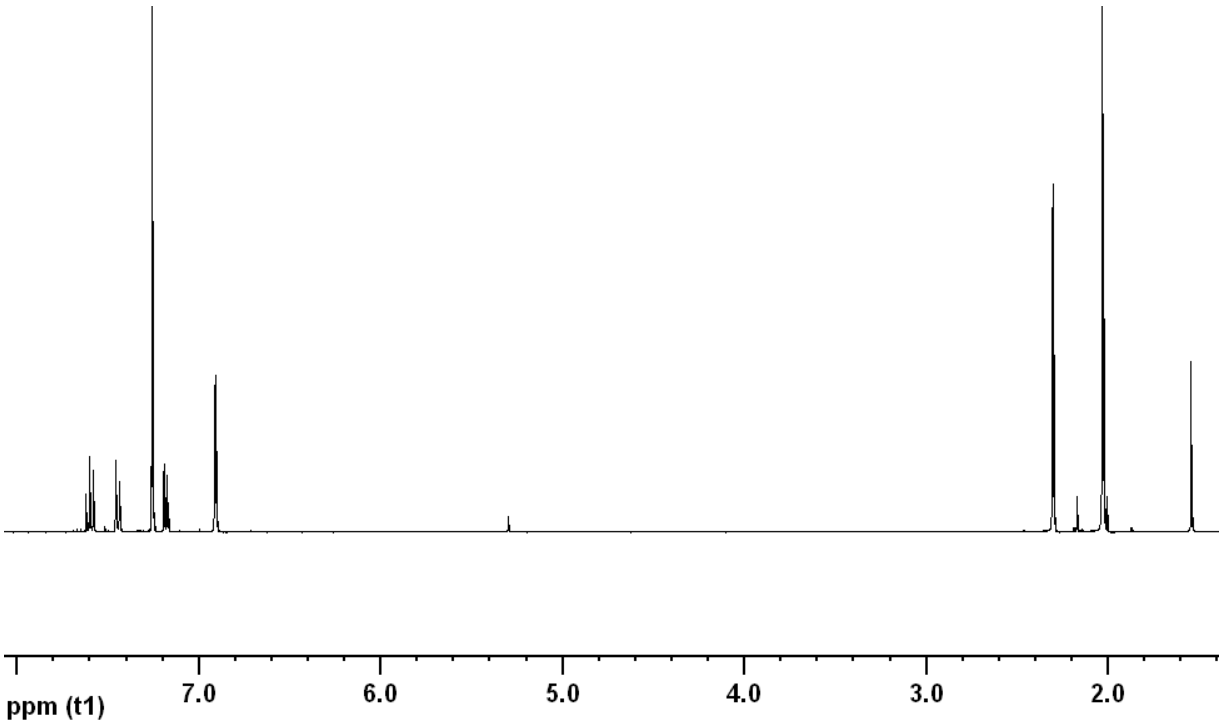

Figure S1. ^{1}H NMR spectrum of **6** ($CDCl_3$, 400 MHz, 298 K).

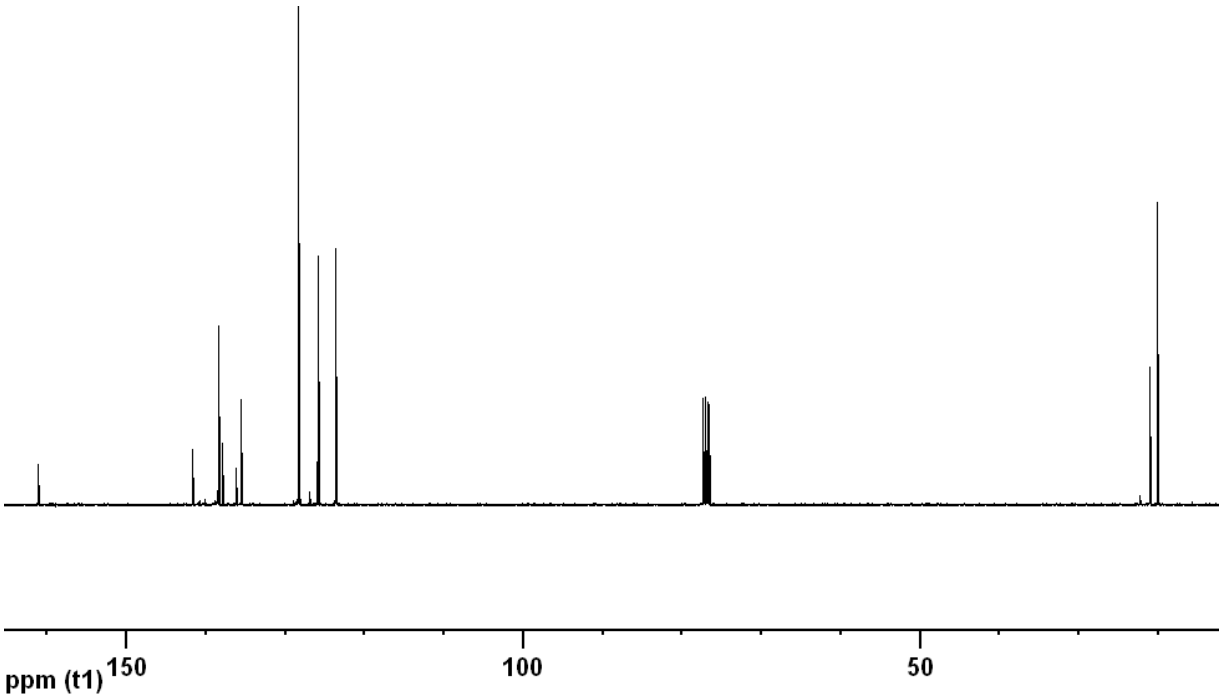

Figure S2. ^{13}C NMR spectrum of **6** ($CDCl_3$, 100 MHz, 298 K).

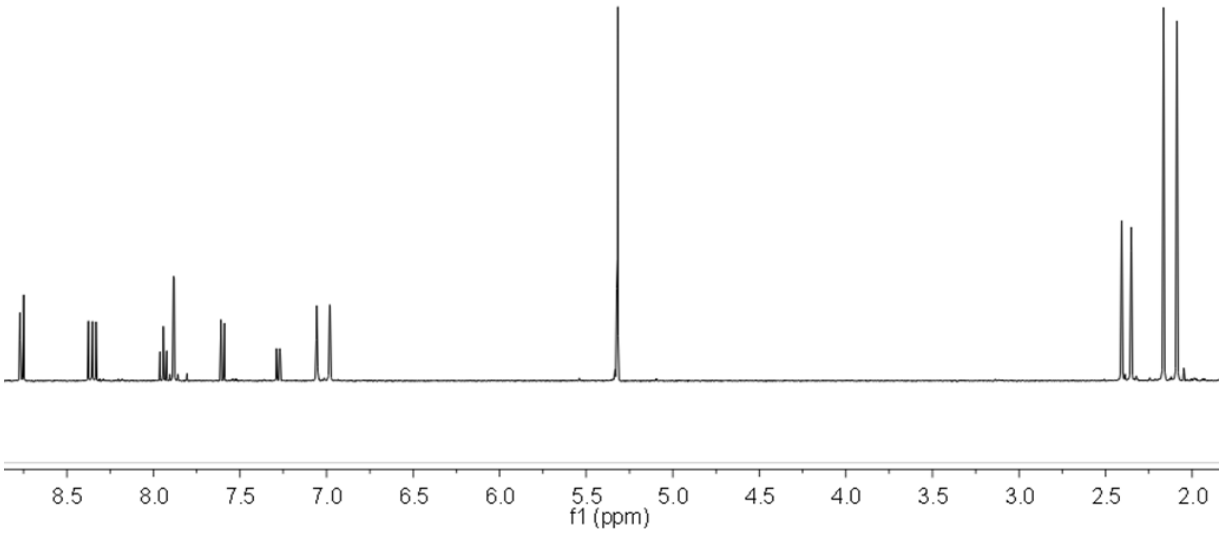

Figure S3. ^{1}H NMR spectrum of **5** (CD_2Cl_2, 400 MHz, 298 K).

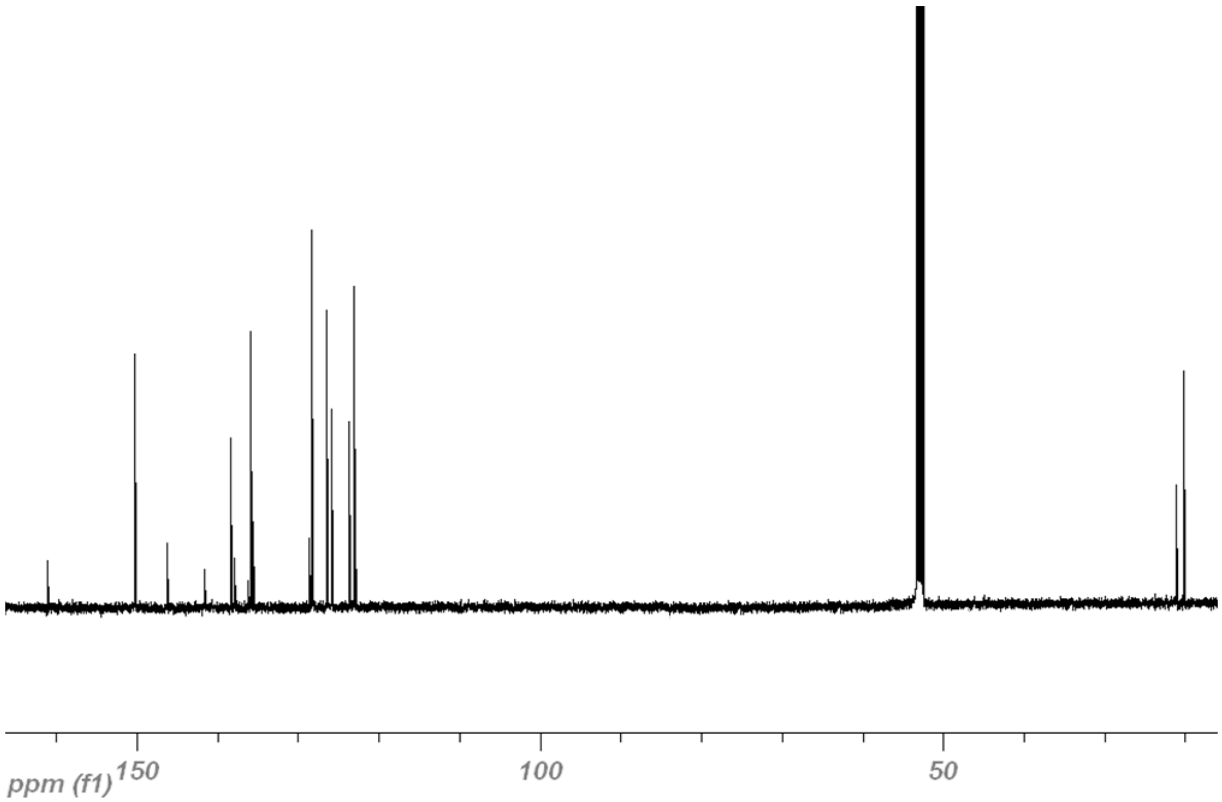

Figure S4. ^{13}C NMR spectrum of **5** (CD_2Cl_2, 100 MHz, 298 K).

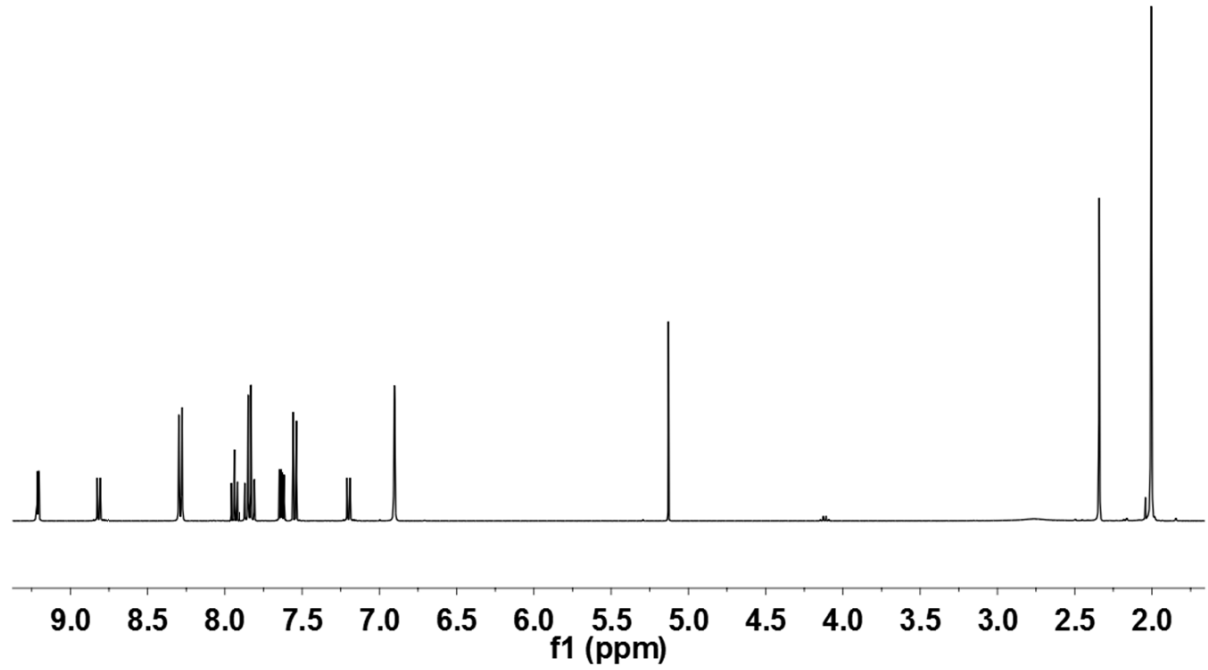

Figure S5. ^{1}H NMR spectrum of **7** (CD_2Cl_2, 400 MHz, 298 K).

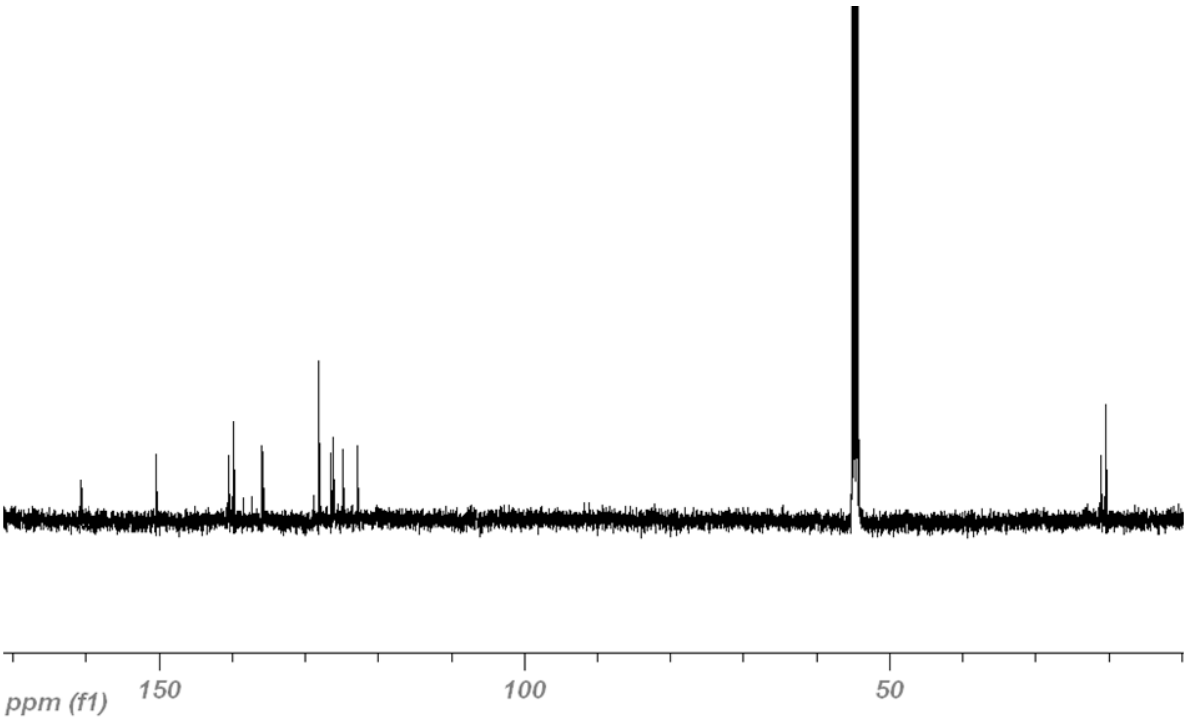

Figure S6. ^{13}C NMR spectrum of **7** (CD_2Cl_2, 100 MHz, 298 K).

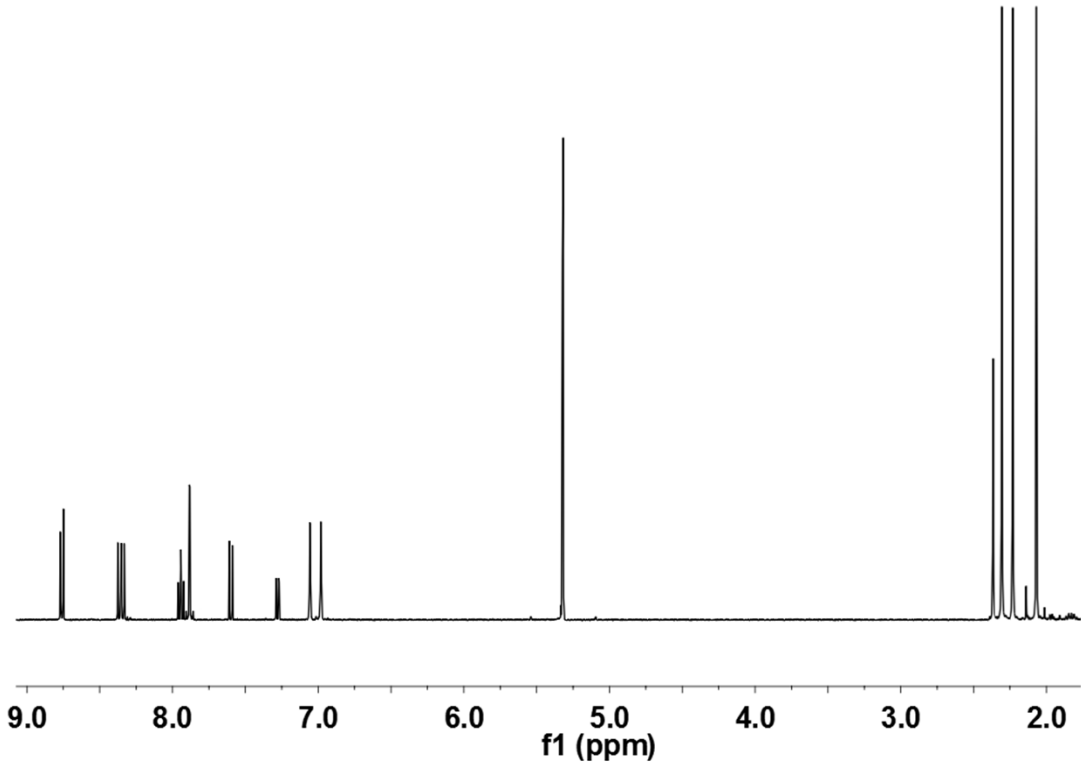

Figure S7. ^{1}H NMR spectrum of **8** (CD_2Cl_2, 400 MHz, 298 K).

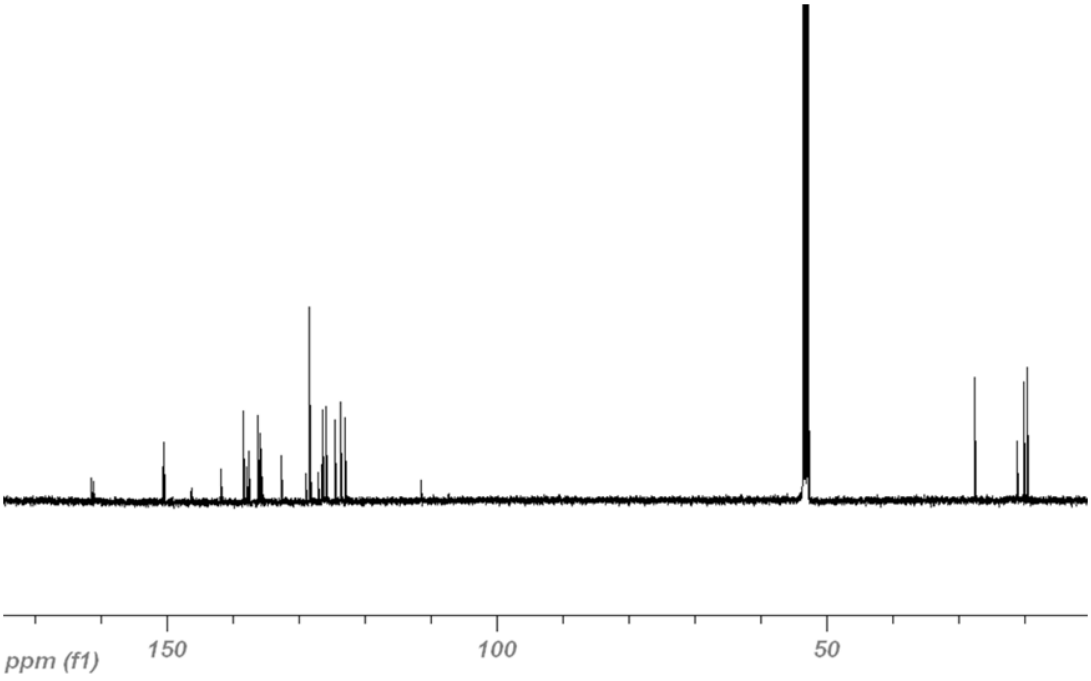

Figure S8. ^{13}C NMR spectrum of **8** (CD_2Cl_2, 100 MHz, 298 K).

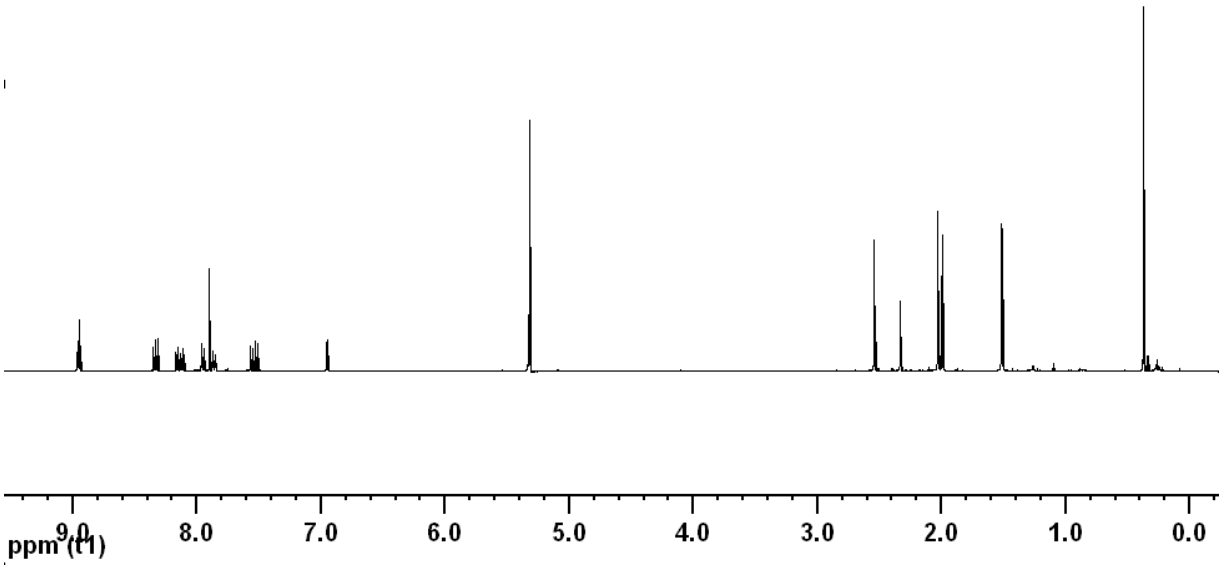

Figure S9. ^{1}H NMR spectrum of **10** (CD_2Cl_2, 400 MHz, 298 K).

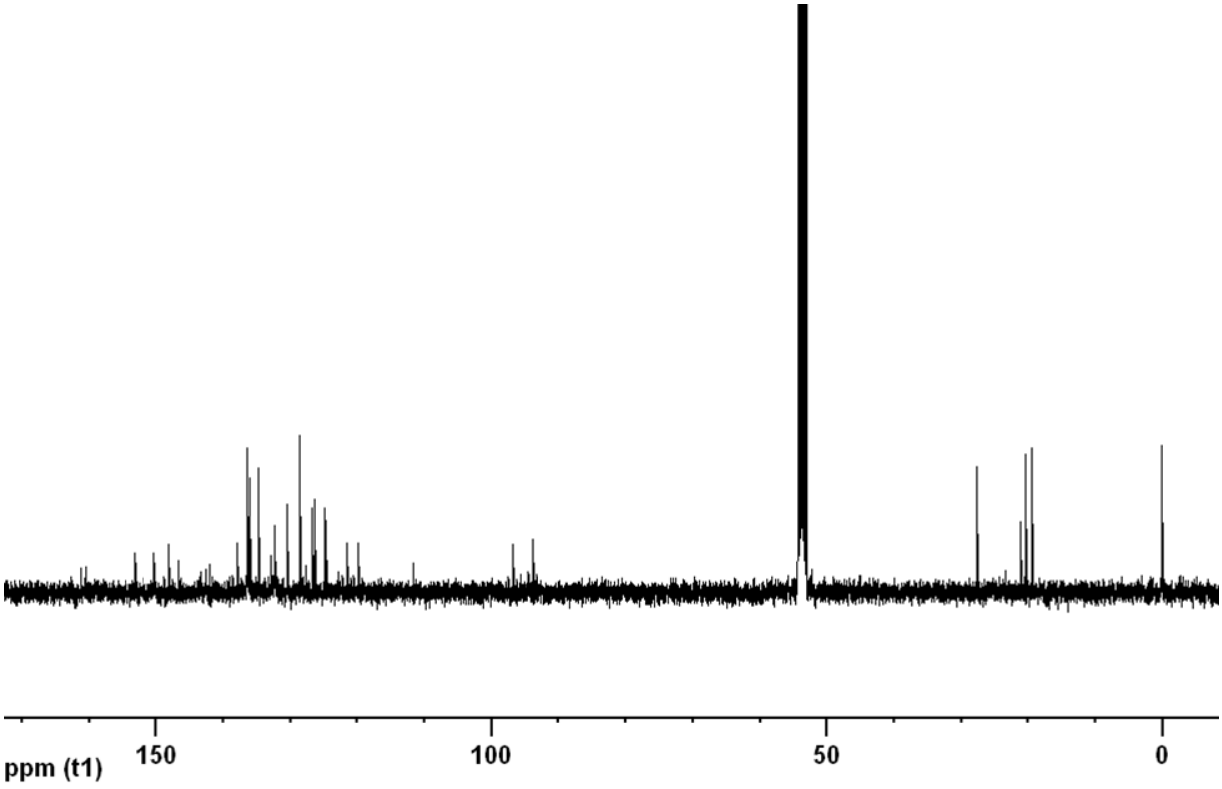

Figure S10. ^{13}C NMR spectrum of **10** (CD_2Cl_2, 100 MHz, 298 K).

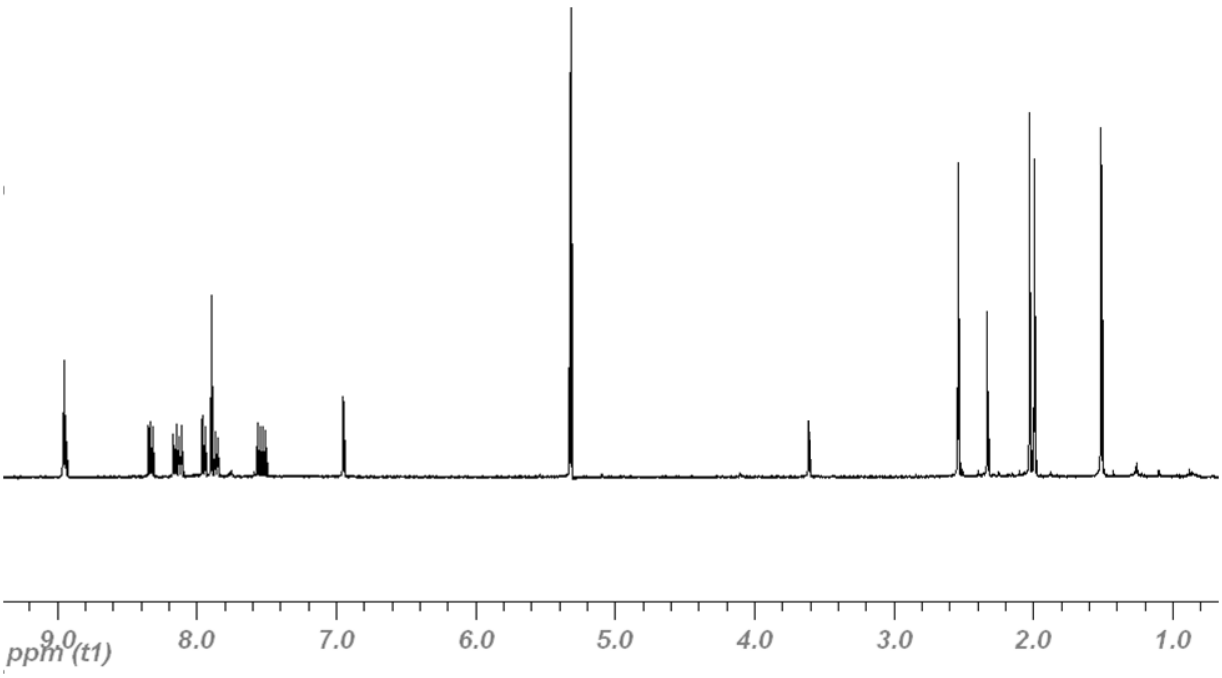

Figure S11. ^{1}H NMR spectrum of **11** (CD_2Cl_2, 400 MHz, 298 K).

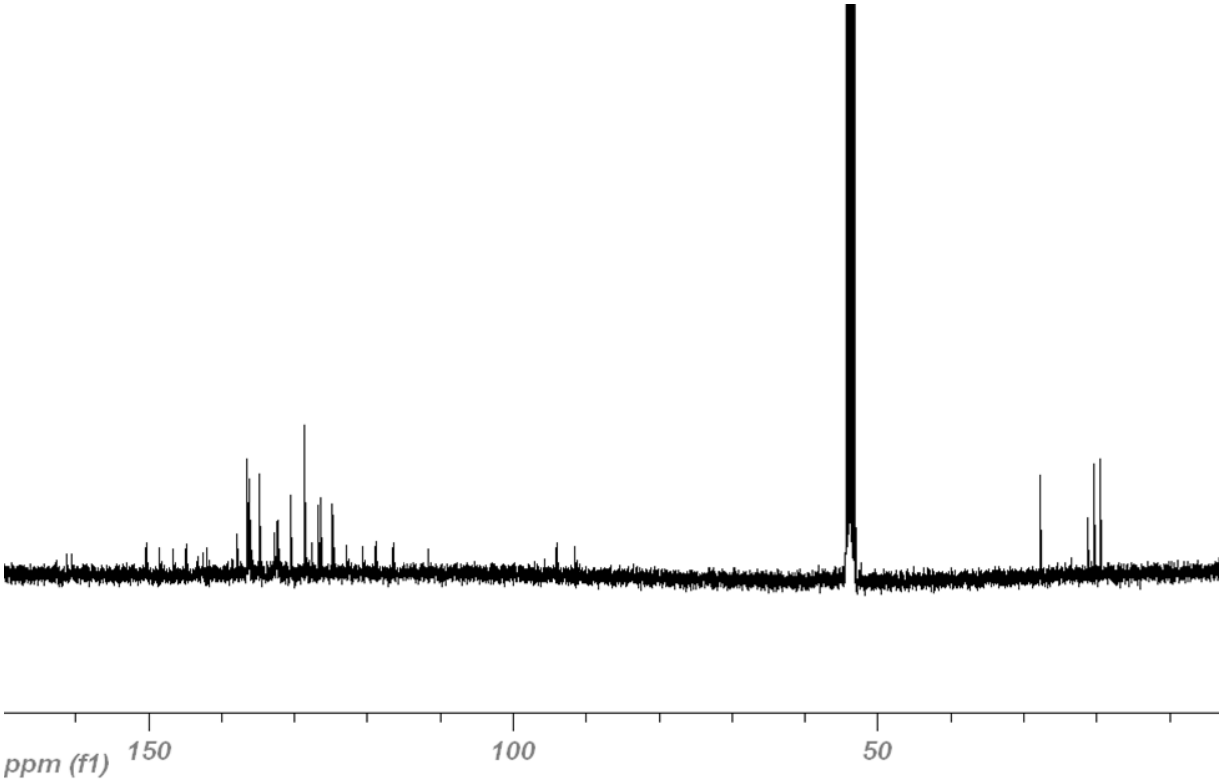

Figure S12. ^{13}C NMR spectrum of **11** (CD_2Cl_2, 100 MHz, 298 K).

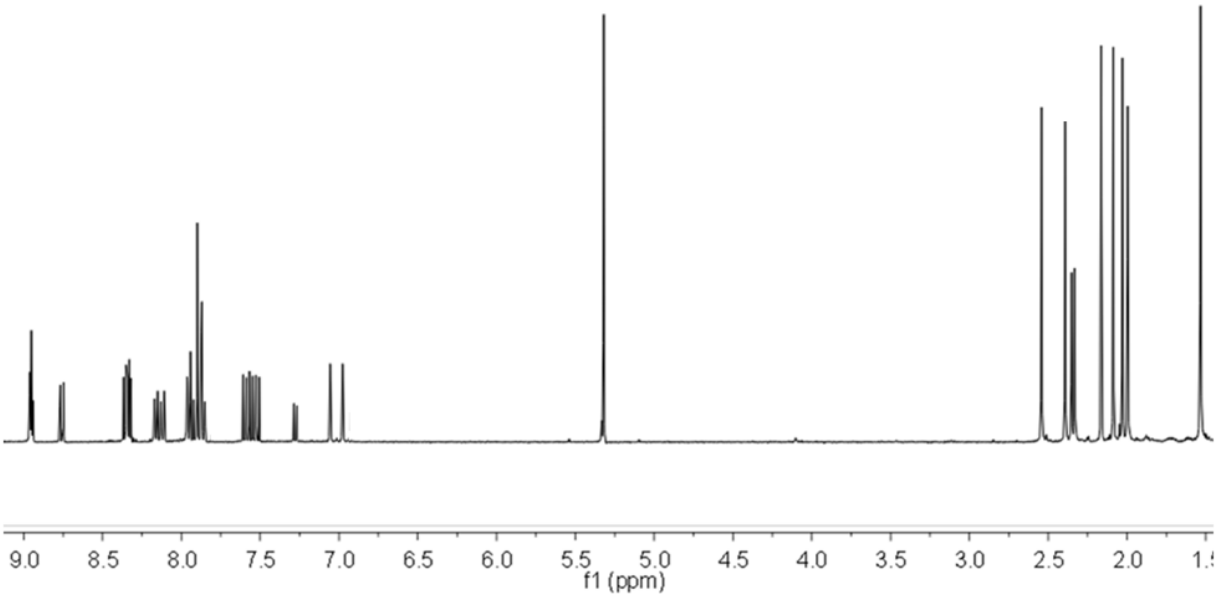

Figure S13. ^{1}H NMR spectrum of **2** (CD_2Cl_2, 400 MHz, 298 K).

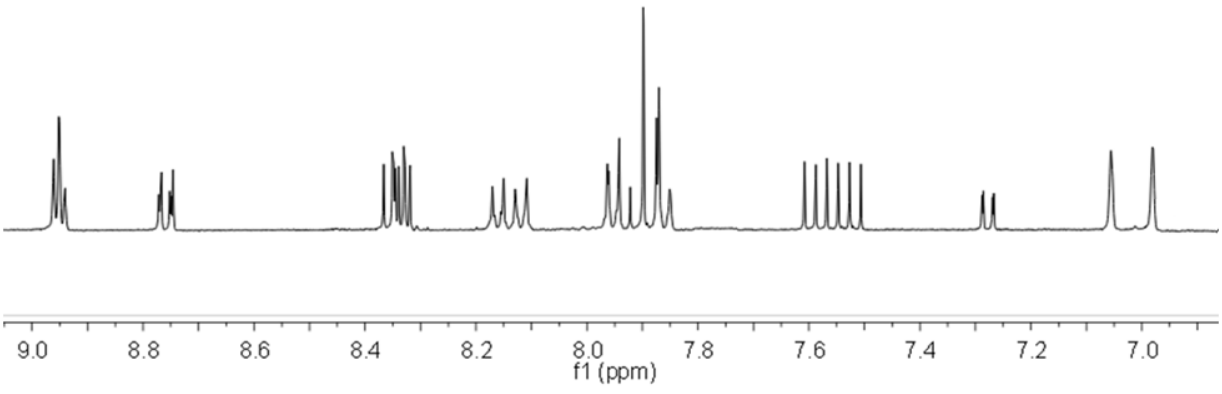

Figure S14. Expanded aromatic region of **2**.

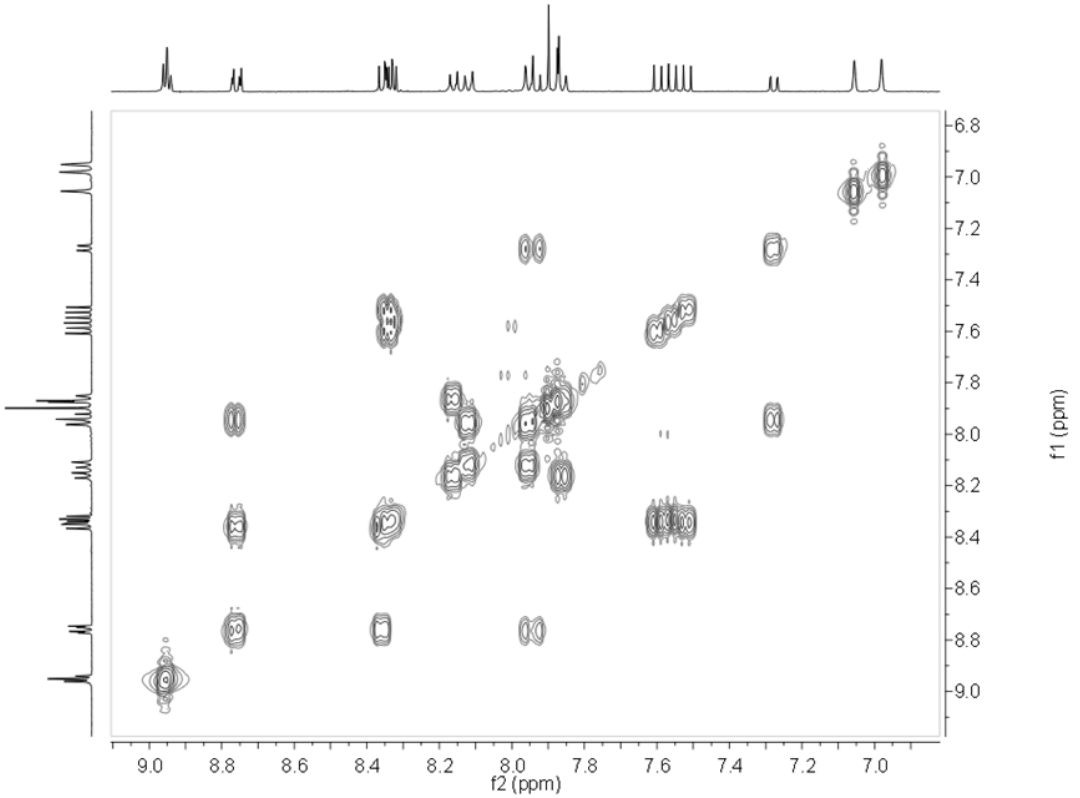

Figure S15. ^{1}H-^{1}H COSY spectrum of **2**.

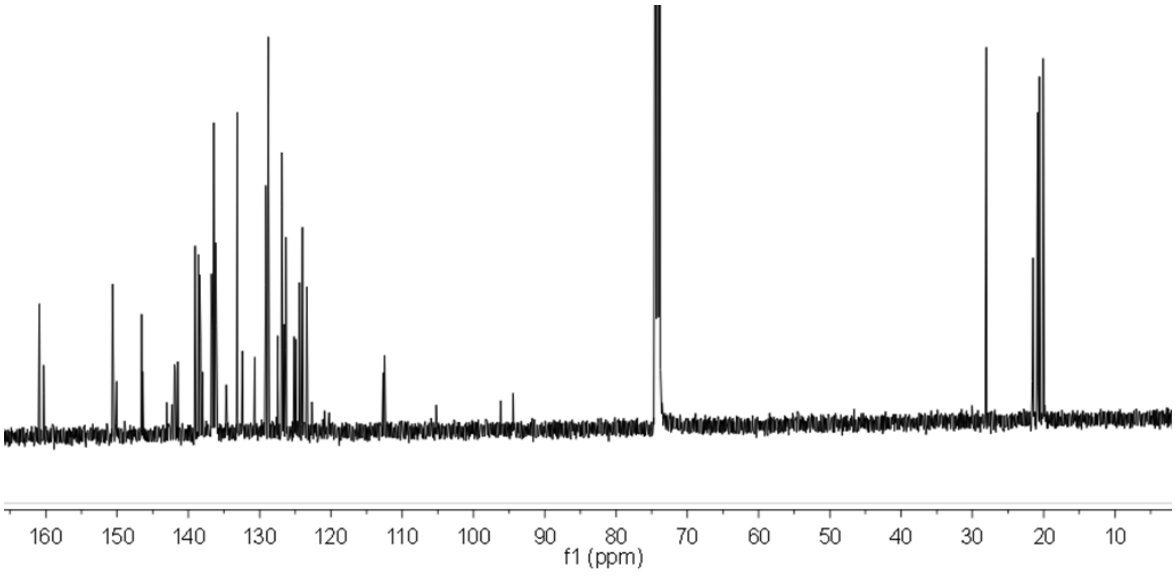

Figure S16. ^{13}C NMR spectrum of **2** (CD_2Cl_2, 100 MHz, 298 K).

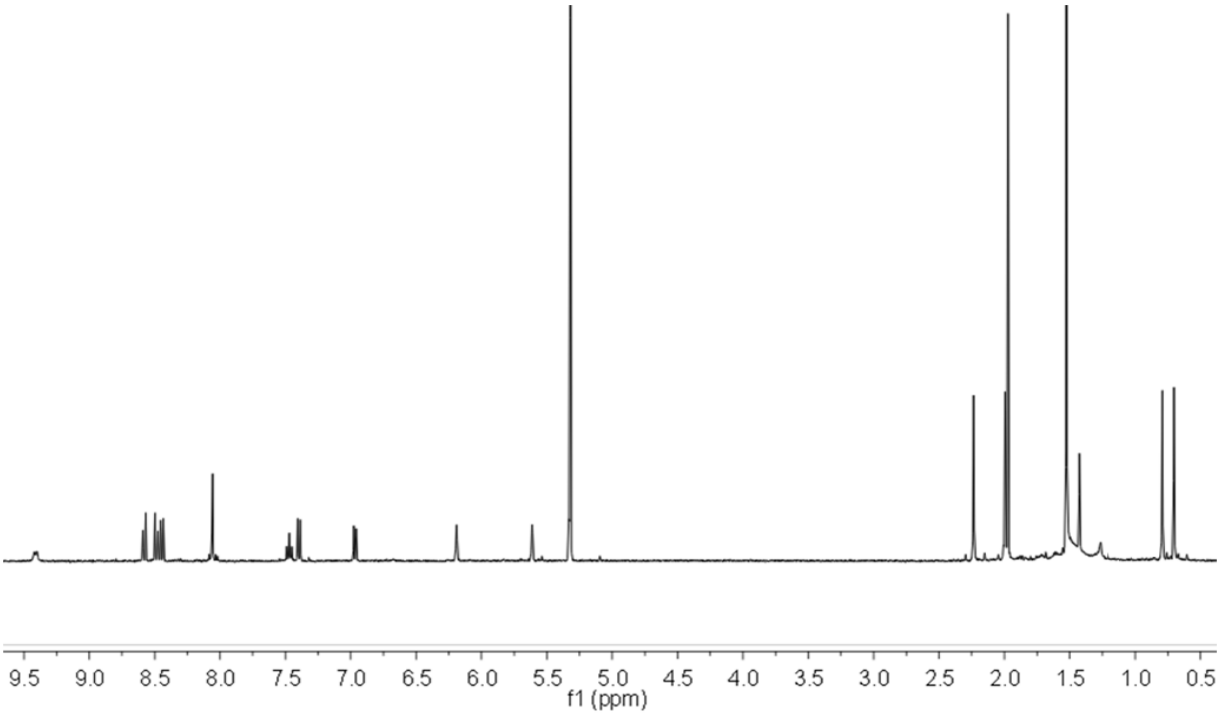

Figure S17. ^{1}H NMR spectrum of [Cu(**5**)$_2$]PF$_6$ (CD_2Cl_2, 400 MHz, 298 K).

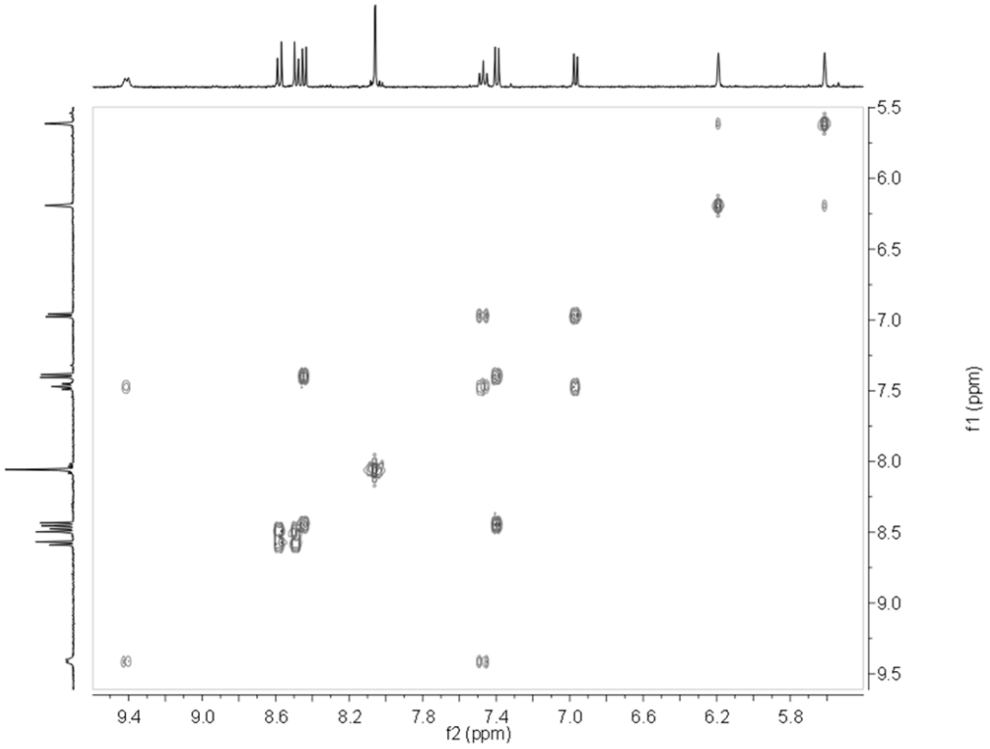

Figure S18. ^{1}H-^{1}H COSY spectrum of [Cu(**5**)$_2$]PF$_6$ (CD_2Cl_2, 400 MHz, 298 K).

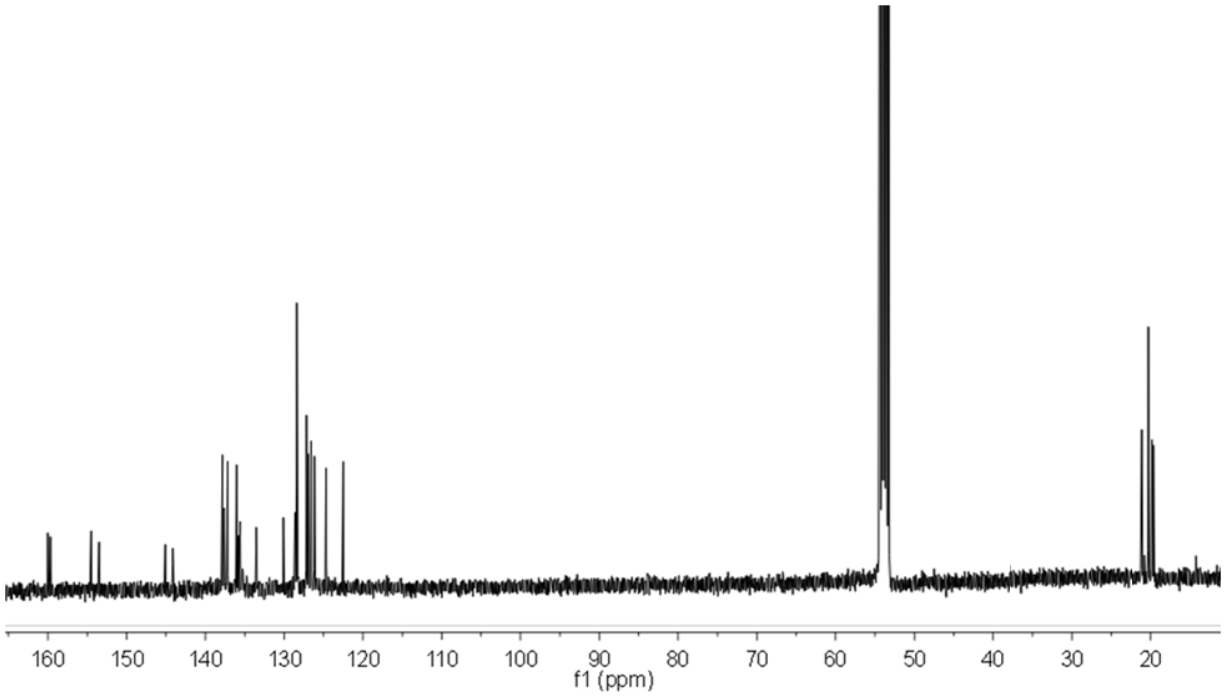

Figure S19. ^{13}C NMR spectrum of $[Cu(\mathbf{5})_2]PF_6$ (CD_2Cl_2, 100 MHz, 298 K).

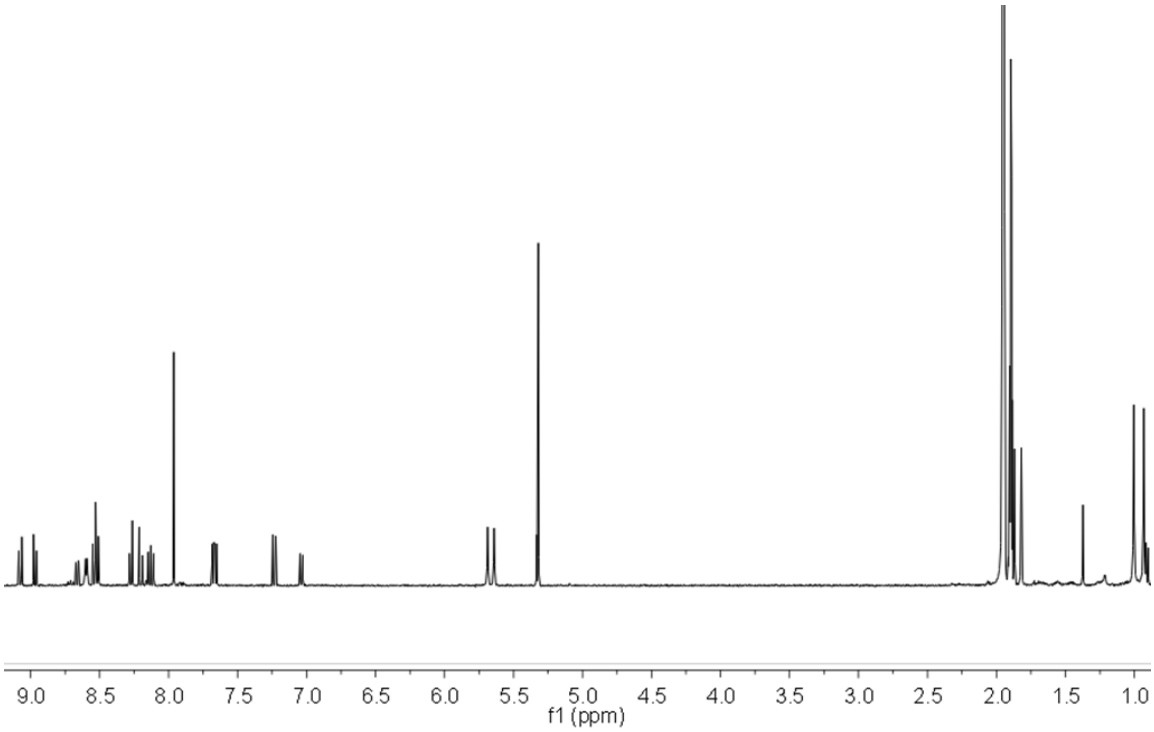

Figure S20. ^{1}H NMR spectrum of $[Zn(\mathbf{4})(\mathbf{5})](OTf)_2$ (CD_2Cl_2,:CD_3CN = 3:1, 400 MHz, 298 K).

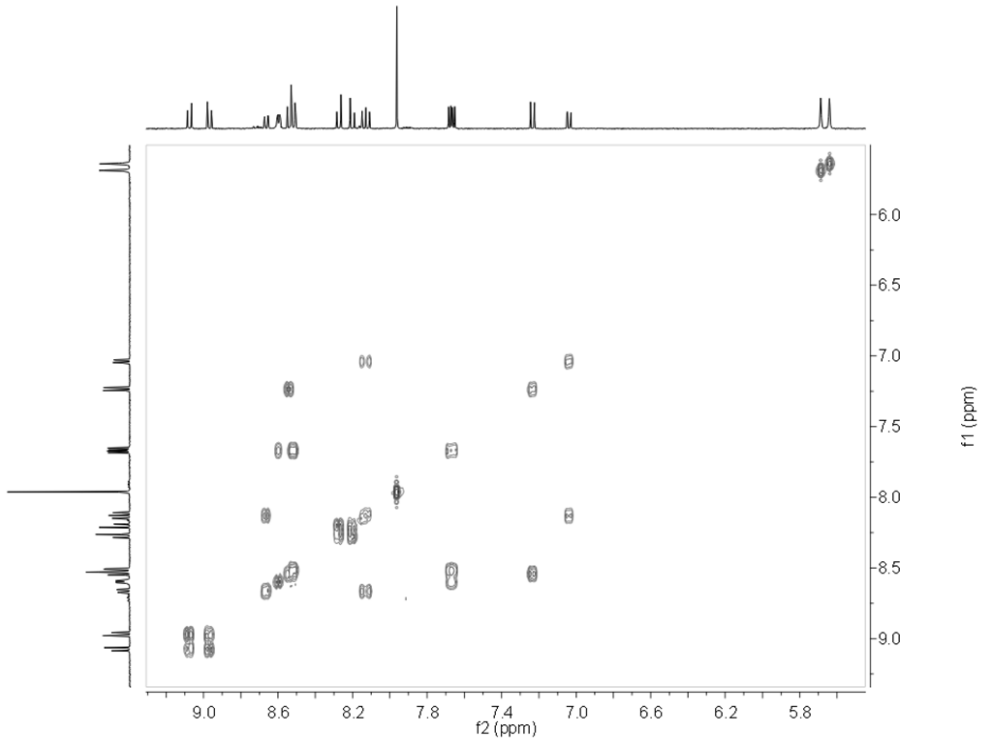

Figure S21. ^{1}H-^{1}H COSY spectrum of [Zn(**4**)(**5**)](OTf)$_2$ (CD_2Cl_2 : CD_3CN = 3:1, 400 MHz, 298 K).

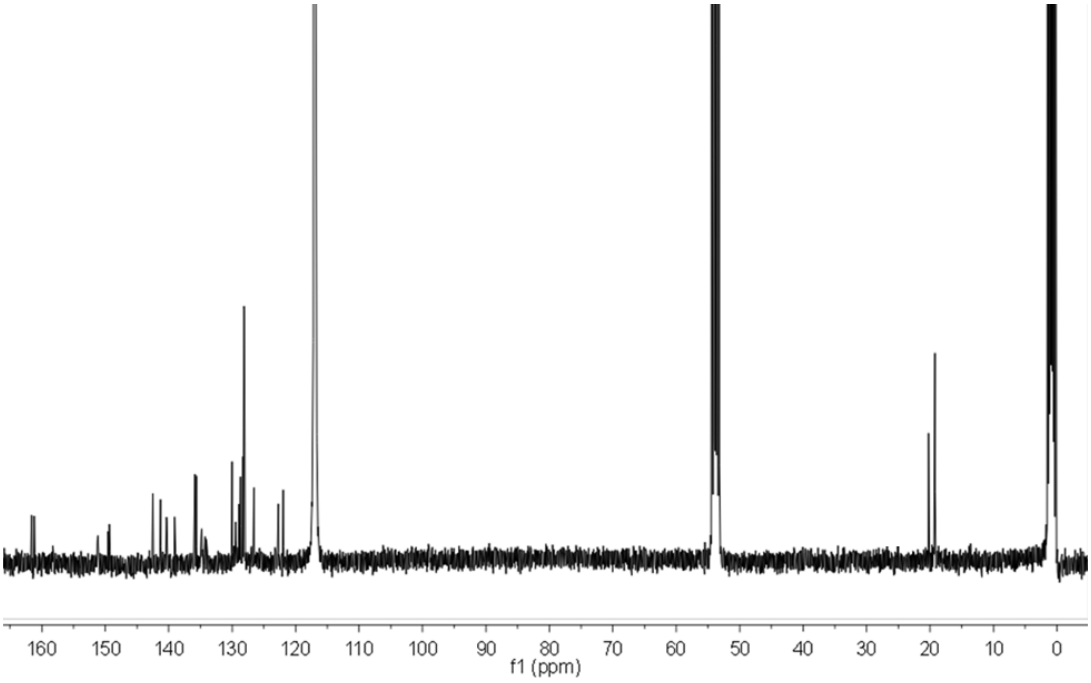

Figure S22. ^{13}C NMR spectrum of [Zn(**4**)(**5**)](OTf)$_2$ (CD_2Cl_2,:CD_3CN = 3:1, 100 MHz, 298 K).

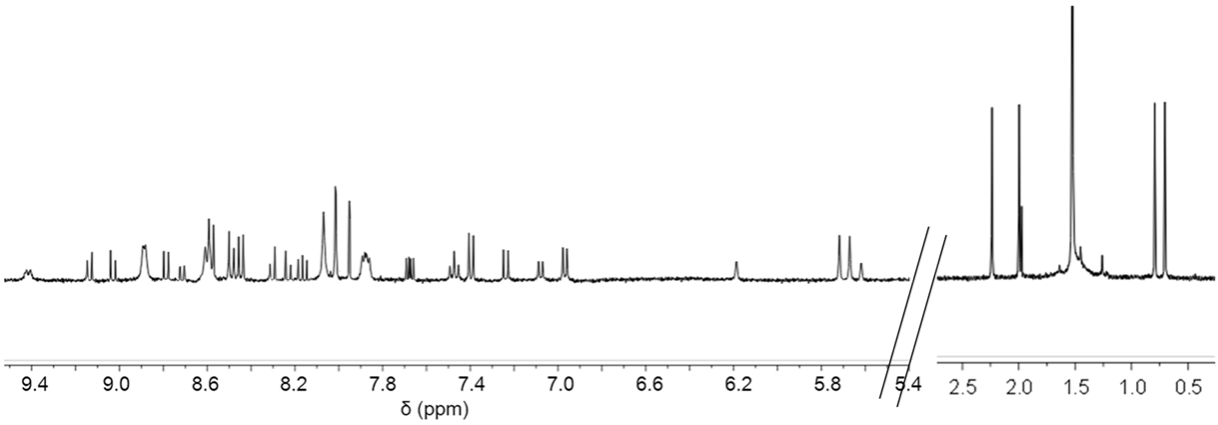

Figure S23. ^{1}H NMR spectrum of equimolar mixture of **4**, **5** and $[Cu(CH_3CN)_4]PF_6$ (CD_2Cl_2, 400 MHz, 298 K).

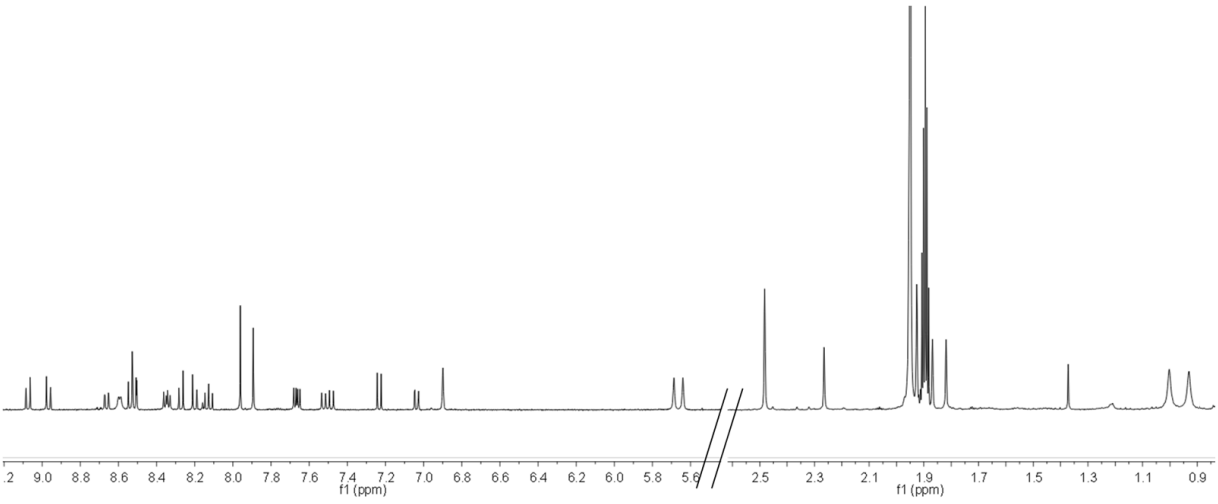

Figure S24. ^{1}H NMR spectrum of equimolar mixture of **3**, **4**, **5** and $Zn(OTf)_2$ (CD_2Cl_2:CD_3CN = 3:1, 400 MHz, 298 K).

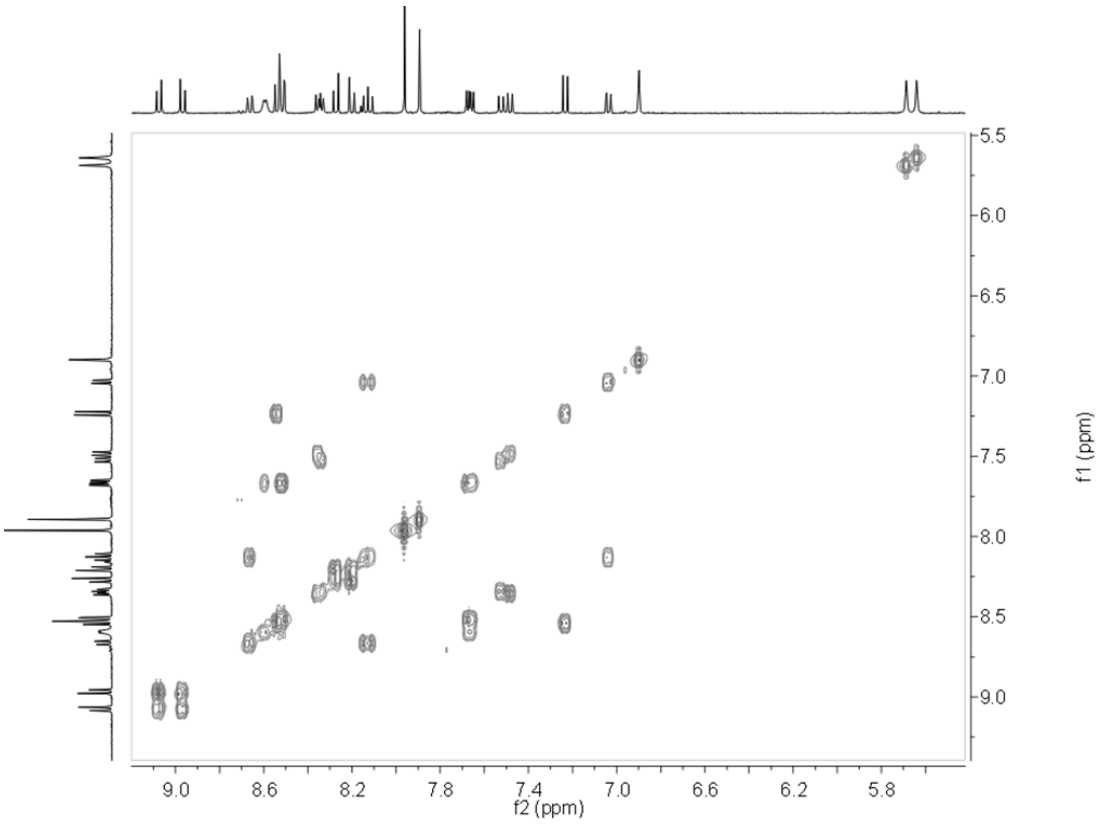

Figure S25. ^{1}H-^{1}H COSY spectrum of equimolar mixture of **3**, **4**, **5** and $Zn(OTf)_2$ (CD_2Cl_2:CD_3CN = 3:1, 400 MHz, 298 K).

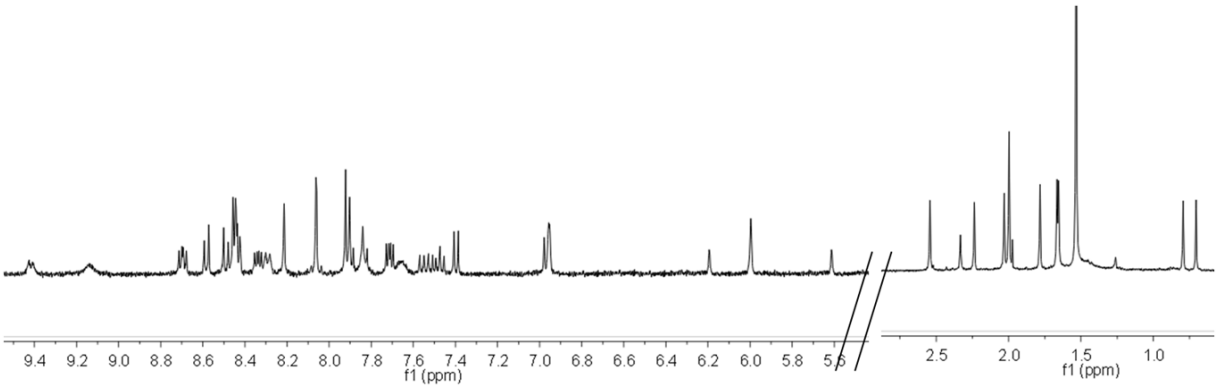

Figure S26. ^{1}H NMR spectrum of equimolar mixture of **3**, **4**, **5** and $[Cu(CH_3CN)_4]PF_6$ (CD_2Cl_2, 400 MHz, 298 K).

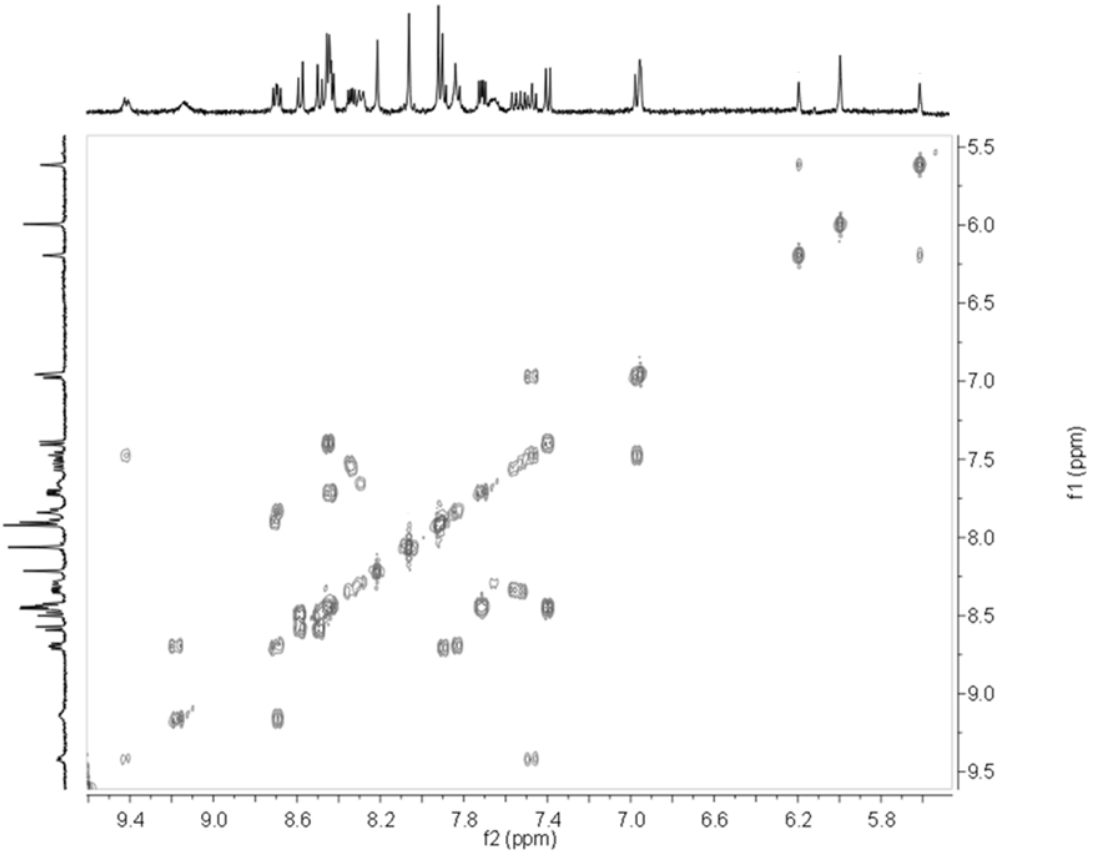

Figure S27. ^{1}H-^{1}H COSY spectrum of equimolar mixture of **3**, **4**, **5** and $[Cu(CH_3CN)_4]PF_6$ (CD_2Cl_2, 400 MHz, 298 K).

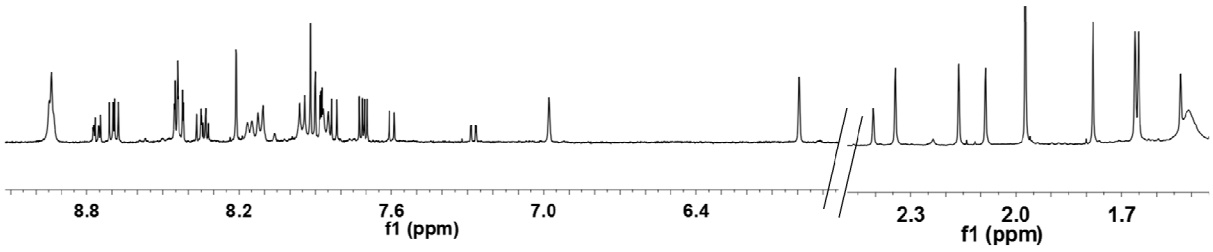

Figure S28. ^{1}H NMR spectrum of $^{Cu}\mathbf{1}_{phen}$ (CD_2Cl_2, 400 MHz, 298 K).

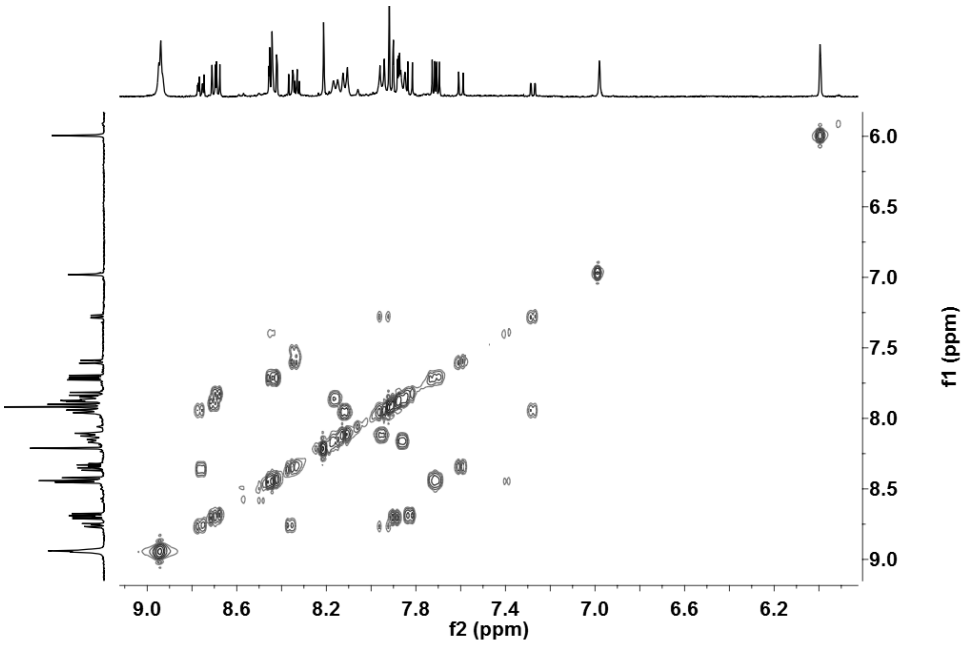

Figure S29. ^{1}H-^{1}H COSY spectrum of $^{Cu}\mathbf{1}_{phen}$ (CD_2Cl_2, 400 MHz, 298 K).

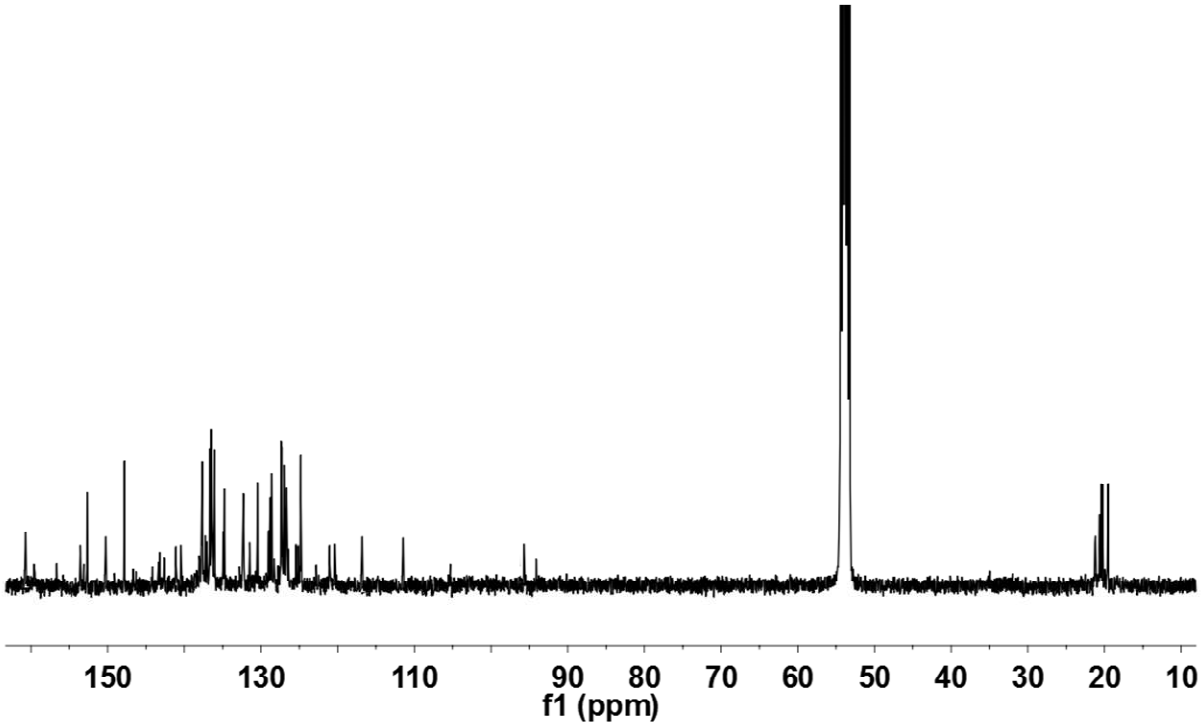

Figure S30. ^{13}C NMR spectrum of $^{Cu}\mathbf{1}_{phen}$ (CD_2Cl_2, 100 MHz, 298 K).

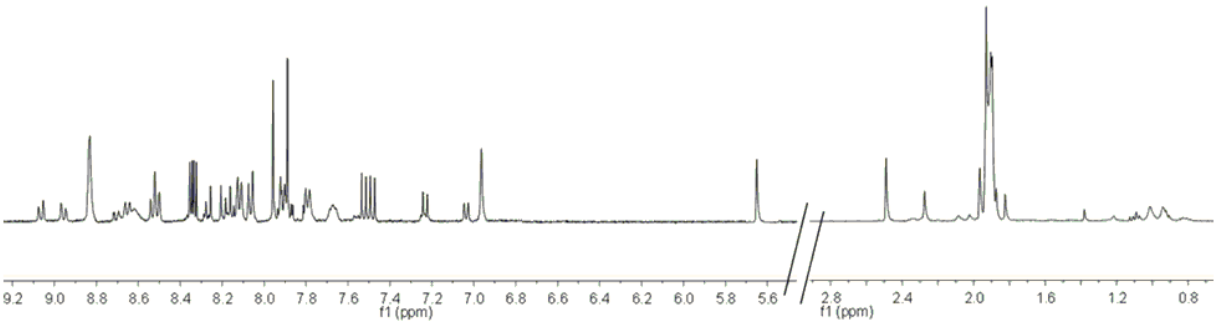

Figure S31. ^{1}H NMR spectrum of $^{Zn}\mathbf{1}_{terpy}$ (CD_2Cl_2:CD_3CN =3:1, 400 MHz, 298 K).

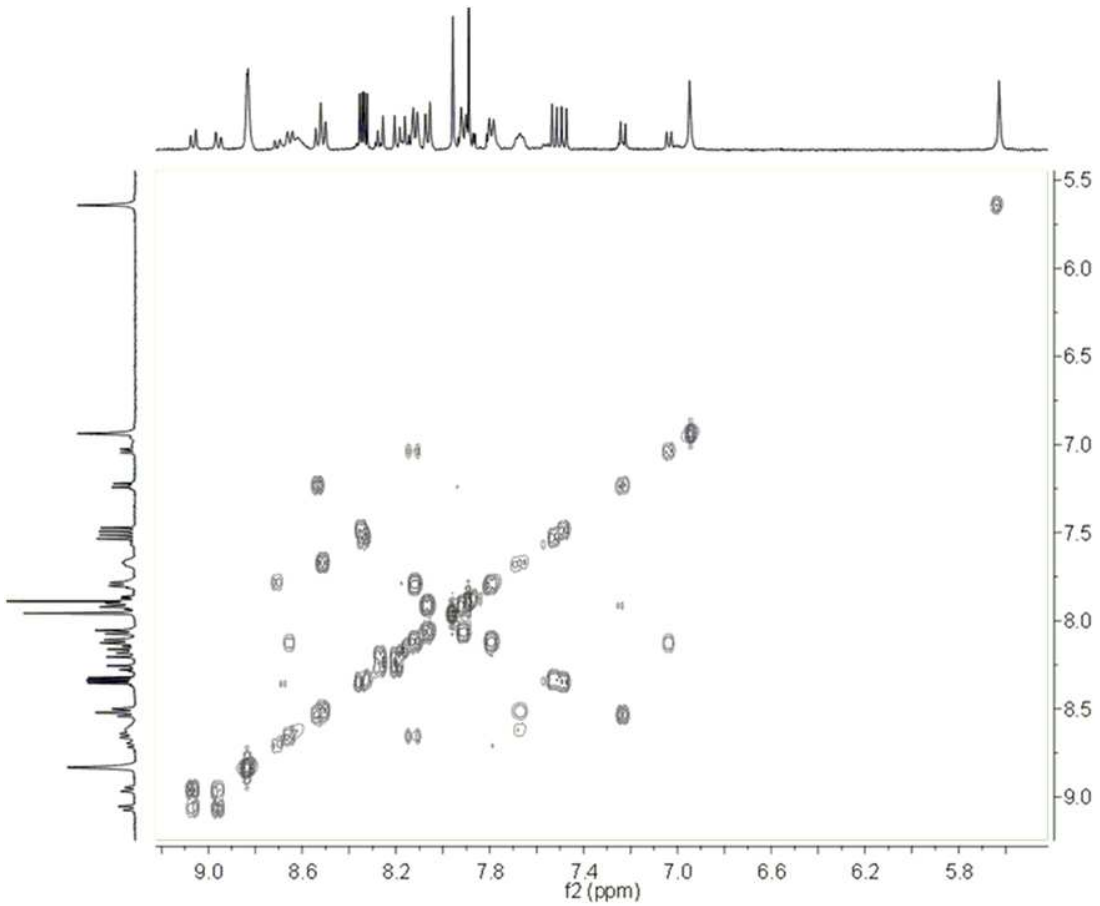

Figure S32. ^{1}H-^{1}H COSY spectrum of $^{Zn}\mathbf{1}_{terpy}$ (CD_2Cl_2:CD_3CN =3:1, 400 MHz, 298 K).

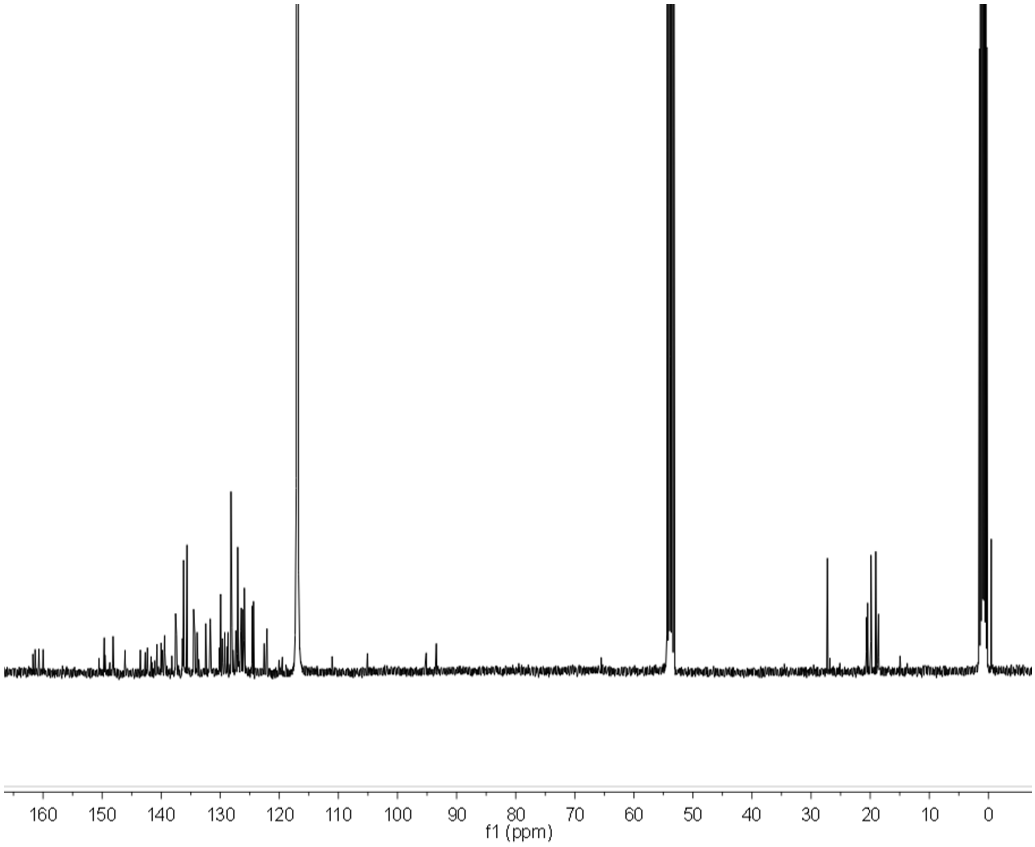

Figure S33. ^{13}C NMR spectrum of $^{Zn}\mathbf{1}_{terpy}$ (CD_2Cl_2:CD_3CN =3:1**,** 100 MHz, 298 K).

Table S1. ^{1}H NMR shifts of the aromatic protons of $[Zn(\mathbf{4})(\mathbf{5})]^{2+}$

Protons	δ / ppm of aromatic protons of **5**	δ / ppm of aromatic protons of **4**
3'-H	8.54	
4'-H	7.23	
5' or 6'-H	8.20	
6' or 5'-H	8.27	
7'-H	9.08	
8'-H	8.97	
12-H	8.66	

13-H	8.13	
14-H	7.04	
15-, 15'-H	5.64, 5.69	
2"-H		8.60
3"-H		7.67
4"-H		8.52
5"-H		7.96

Table S2. ^{1}H NMR shifts of the aromatic protons of **2**.

Protons	δ / ppm of aromatic prorons $PhenAr_2$	δ / ppm of aromatic prorons $TerpyAr_2$	δ / ppm of other aromatic protons
3 or 8-H	8.33		
4 or 7-H	7.52		
5, 6-H	7.90		
7 or 4-H	7.56		
8 or 3-H	8.34		
9-H	6.95		
3'-H		8.34	
4'-H		7.60	
5', 6'-H		7.87	
7'-H		8.76	
8'-H		8.36	
12-H		8.77	
13-H		7.94	

14-H		7.28	
15'-H		6.98	
10 or 11-H			8.12
11 or 10-H			7.95
16 or 17-H			8.16
17 or 16-H			7.86
β-H			8.95, 8.96

Table S3. ^{1}H NMR shifts of the aromatic protons of $^{Cu}\mathbf{1}_{phen}$.

Protons	δ / ppm of aromatic protons of $PhenAr_2$	δ / ppm of aromatic protons of $TerpyAr_2$	δ / ppm of other aromatic protons
3 or 8-H	8.69		
4 or 7-H	7.83		
5, 6-H	8.21		
7 or 4-H	7.89		
8 or 3-H	8.70		
9-H	6.00		
3'-H		8.34	
4'-H		7.60	
5'-, 6'-H		7.91	
7'-H		8.76	
8'-H		8.36	
12-H		8.77	
13-H		7.94	

14-H		7.27	
15'-H		6.97	
10 or 11-H			7.86
11 or 10-H			8.16
16 or 17-H			7.95
17 or 16-H			8.12
2''-H			8.45
3''-H			7.71
4''-H			8.42
5''-H			7.92
β-H			8.94, 8.95

Table S4. ^{1}H NMR shifts of the aromatic protons of $^{Zn}\mathbf{1}_{terpy}$.

Protons	δ / ppm of aromatic protons of $PhenAr_2$	δ / ppm of aromatic protons of $TerpyAr_2$	δ / ppm of other aromatic protons
3 or 8-H	8.33		
4 or 7-H	7.48		
5, 6-H	7.89		
7 or 4-H	7.53		
8 or 3-H	8.35		
9-H	6.91		
3'-H		8.51	
4'-H		7.24	
5' or 6'-H		8.19	

6' or 5'-H		8.27	
7'-H		9.06	
8'-H		8.96	
12-H		8.69	
13-H		8.16	
14-H		7.05	
15'-H		5.69	
10 or 11-H			7.91
11 or 10-H			8.06
16 or 17-H			7.79
17 or 16-H			8.12
2"-H			8.62
3"-H			7.68
4"-H			8.53
5"-H			7.96
β-H			8.85, 8.83

ESI-MS

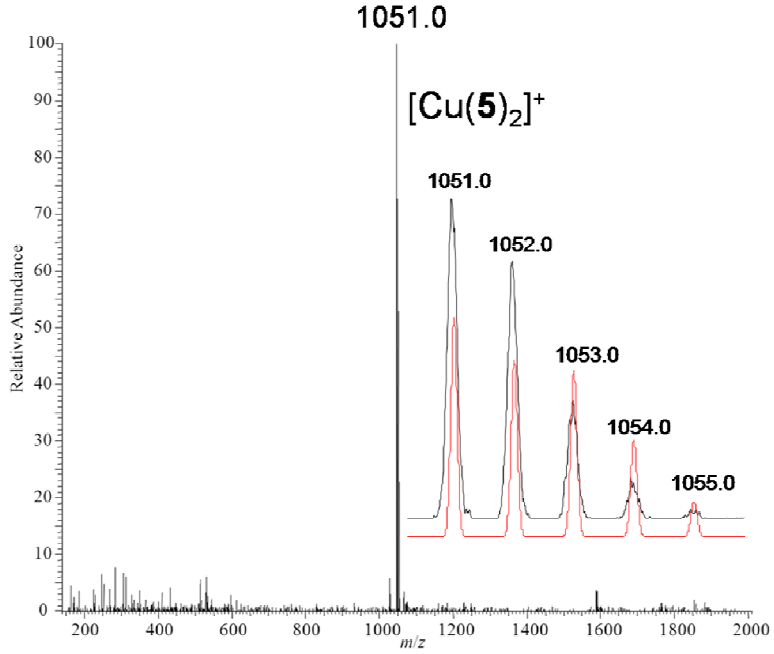

Figure S34. ESI-MS spectrum of $[Cu(\mathbf{5})_2]PF_6$ in CH_2Cl_2.

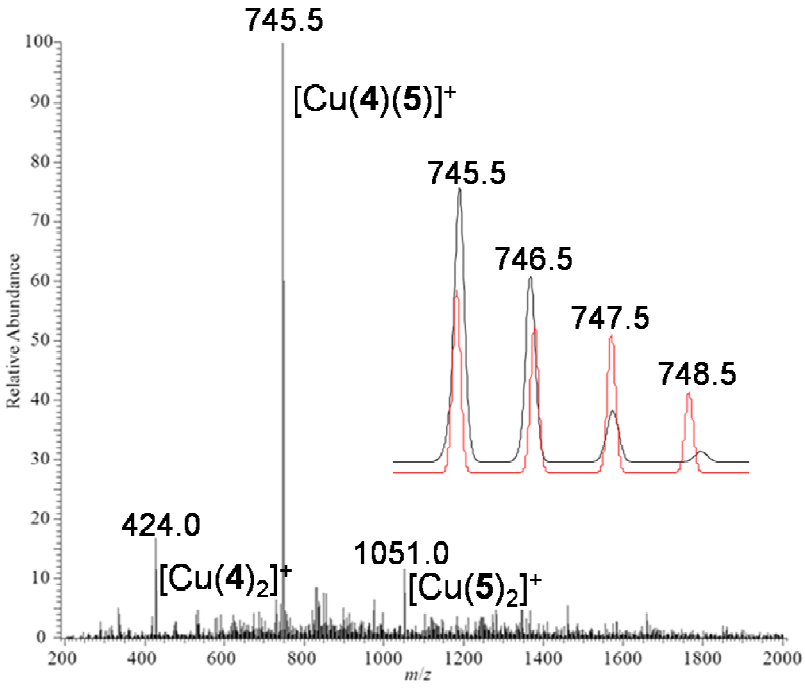

Figure S35. ESI-MS spectrum of a (1:1:1) mixture of **4**, **5** and $[Cu(CH_3CN)_4]PF_6$ in CH_2Cl_2.

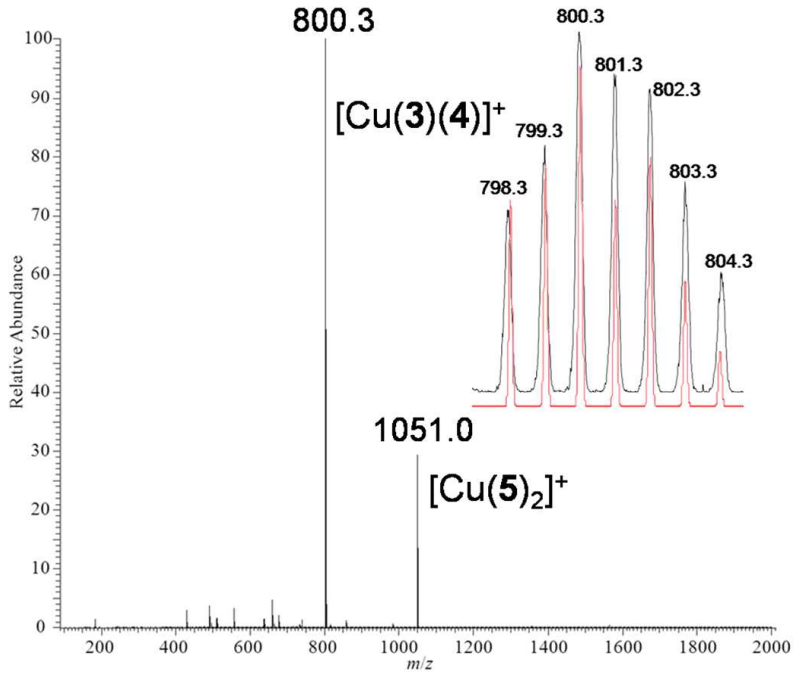

Figure S36. ESI-MS spectrum of a (1:1:1:1) mixture of **3**, **4**, **5** and $[Cu(CH_3CN)_4]PF_6$ in CH_2Cl_2.

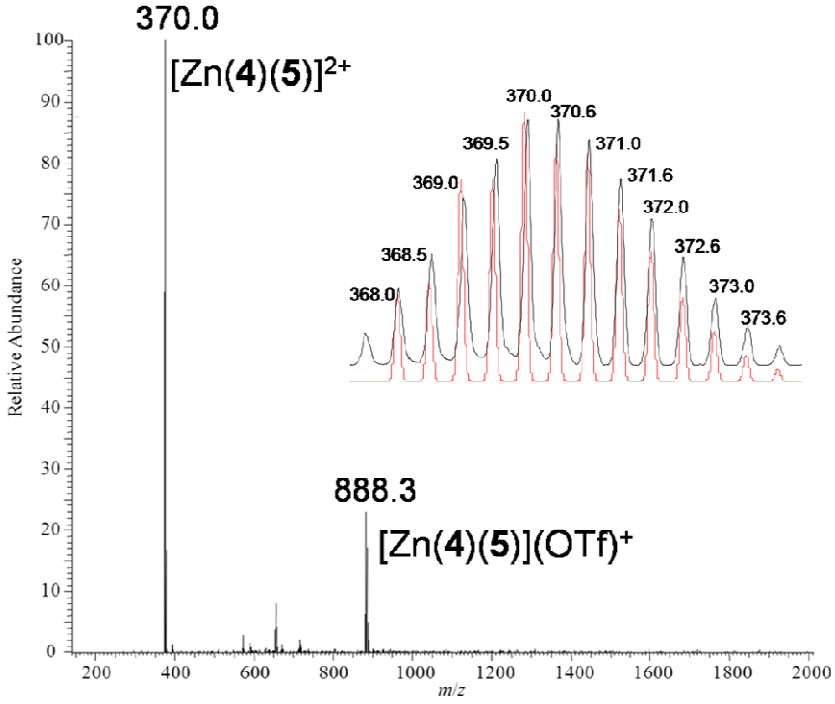

Figure S37. ESI-MS spectrum of a (1:1:1) mixture of **4**, **5** and $Zn(OTf)_2$ in CH_2Cl_2 : CH_3CN = 3:1.

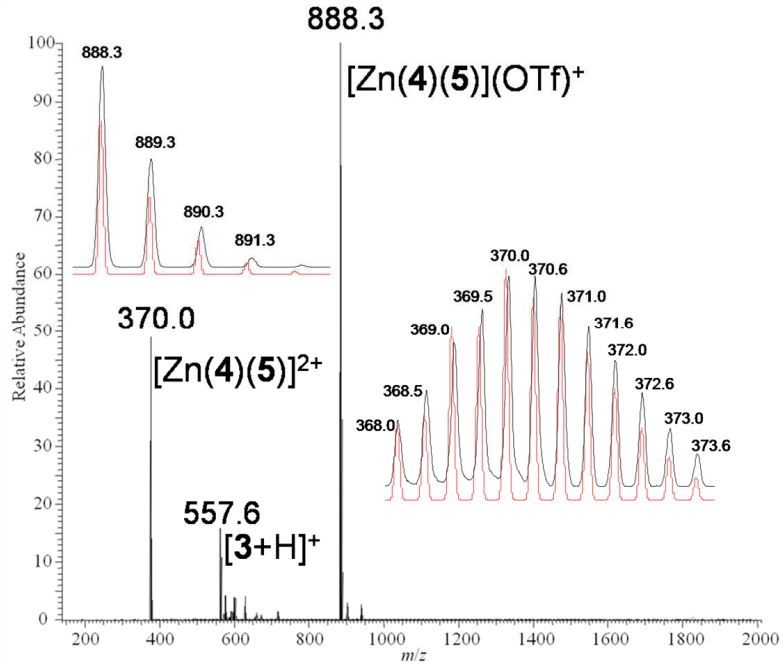

Figure S38. ESI-MS spectrum of a (1:1:1:1) mixture of **3**, **4**, **5** and $Zn(OTf)_2$ in CH_2Cl_2:CH_3CN = 3:1.

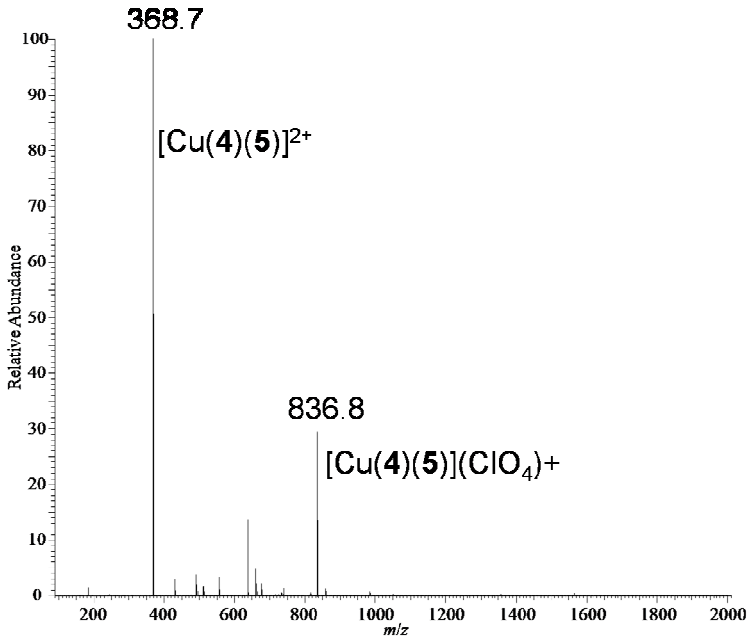

Figure S39. ESI-MS spectrum of a (1:1:1) mixture of **4**, **5** and $Cu(ClO_4)_2 \cdot 6H_2O$ in CH_2Cl_2 : CH_3CN = 3:1.

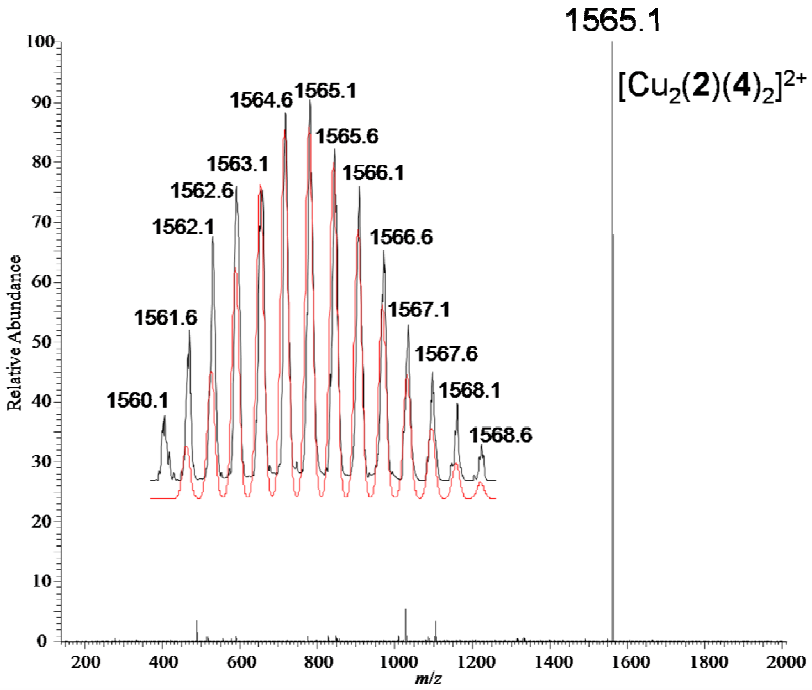

Figure S40. ESI-MS spectrum of $^{Cu}\mathbf{1}_{phen}$ = $[Cu_2(\mathbf{2})(\mathbf{4})_2](PF_6)_2$ in CH_2Cl_2.

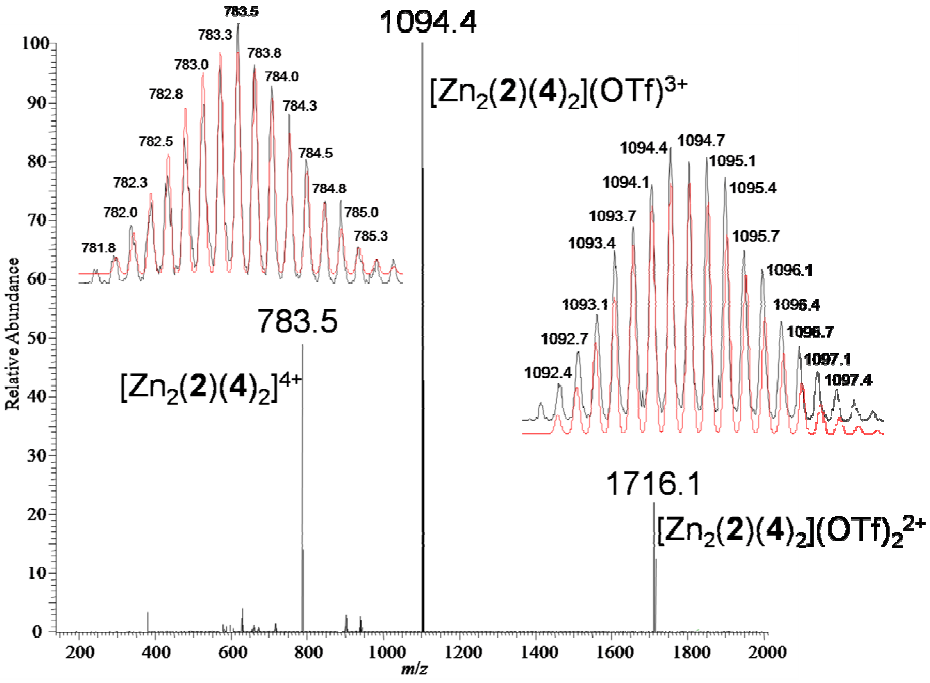

Figure S41. ESI-MS spectrum of $^{Zn}\mathbf{1}_{terpy}$ = $[Zn_2(\mathbf{2})(\mathbf{4})_2](OTf)_4$ in CH_2Cl_2:CH_3CN = 3:1.

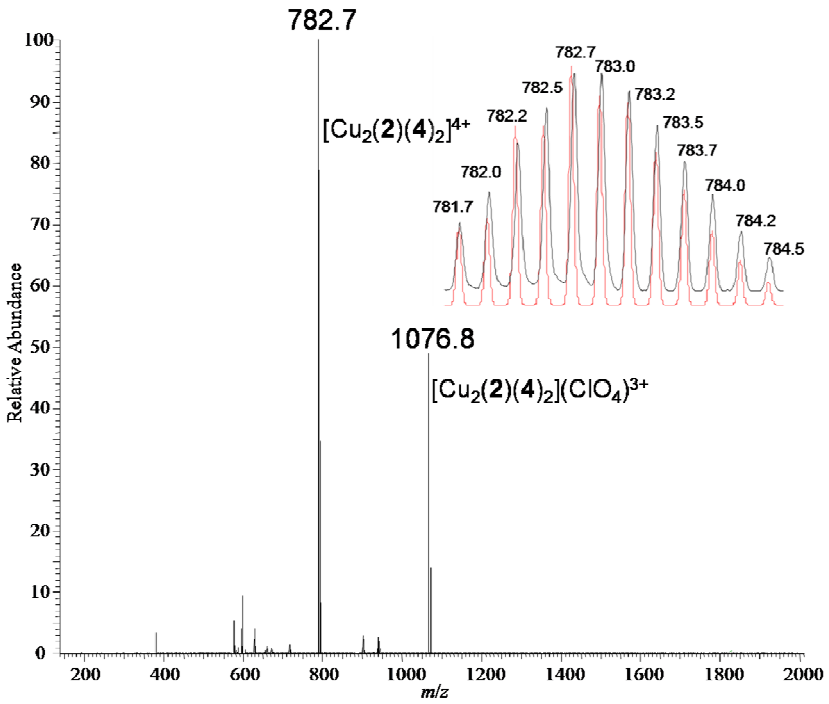

Figure S42. ESI-MS spectrum of $^{Cu}\mathbf{1}_{terpy}$ = $[Cu_2(\mathbf{2})(\mathbf{4})_2](ClO_4)_4$ in CH_2Cl_2:CH_3CN = 3:1.

Cyclic voltammetry

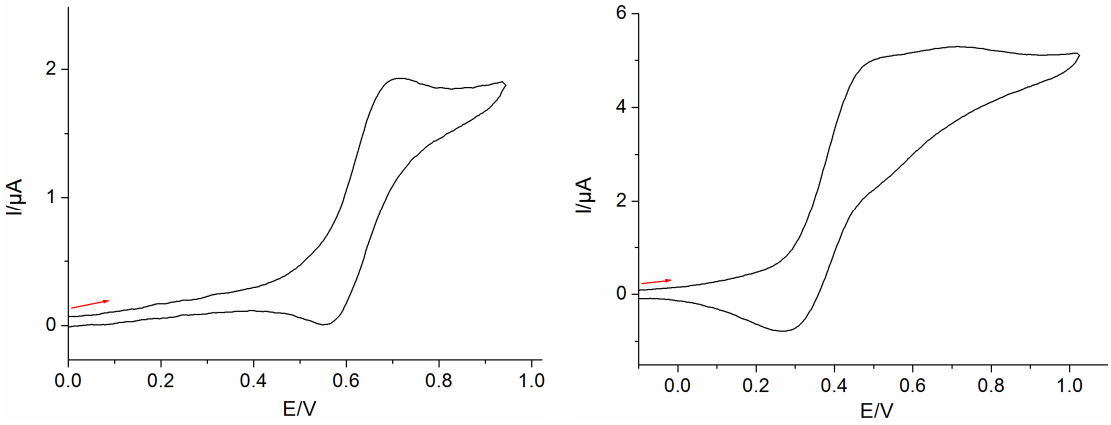

Figure S43. Cyclic voltammogram of (left) [Cu(**5**)$_2$](PF$_6$) and (right) equimolar mixture of **4**, **5** and Cu^+ in dry CH_2Cl_2 (scan rate = 100 mV/s). The experiment was carried out with 0.1 M *n*-Bu_4NPF_6 as electrolyte against a Ag wire as a quasi-reference electrode and triphenylpyrylium tetrafluoroborate as internal standard (scan rate = 100 mV/s).

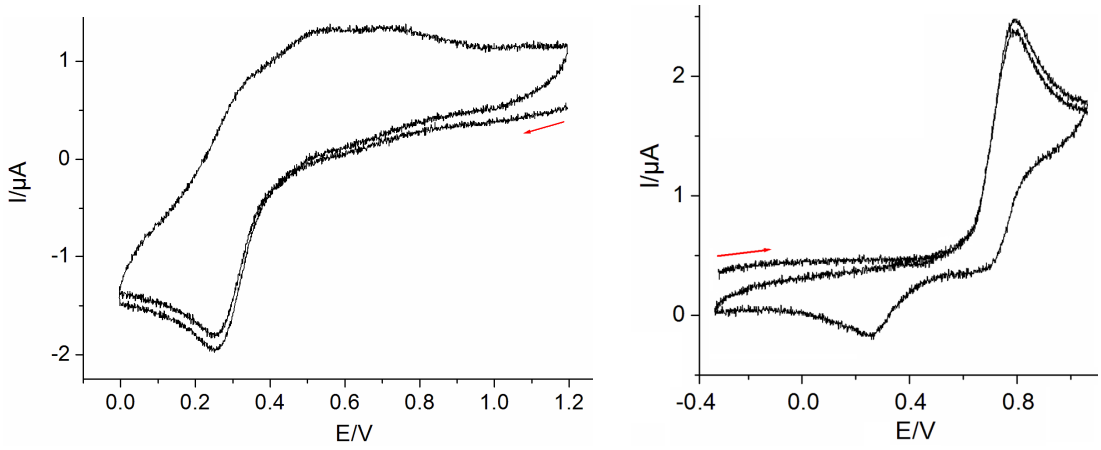

Figure S44. (Left) Cyclic voltammogram of (left) equimolar mixture of **4**, **5** and Cu^{2+} and (right) equimolar mixture of **3**, **4**, **5** and Cu^+ in dry CH_2Cl_2 (scan rate = 100 mV/s).

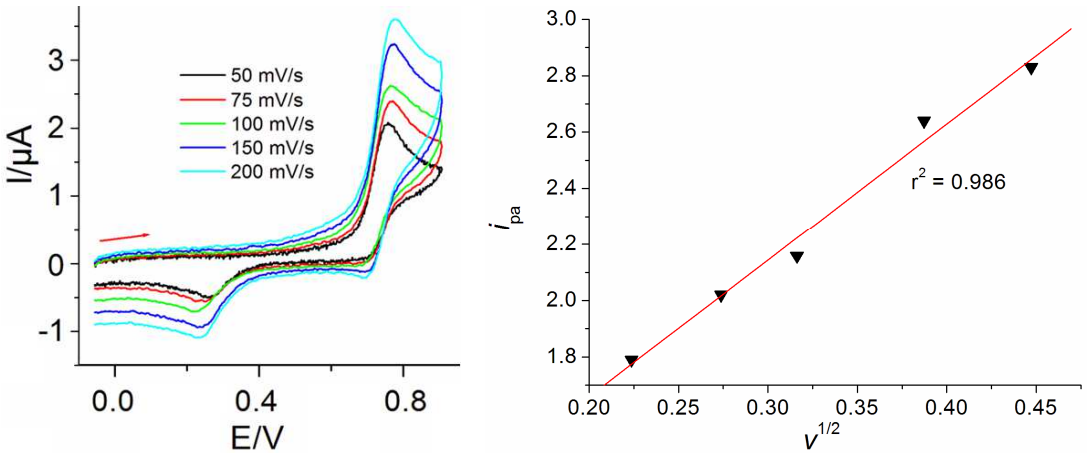

Figure S45. (Left) Cyclic voltammogram of equimolar mixture of **3**, **4**, **5** and Cu^{+} in dry CH_2Cl_2 at different scan rates. (Right) Randles-Sevcik plot i_{pa} (μA) vs $v^{1/2}$.

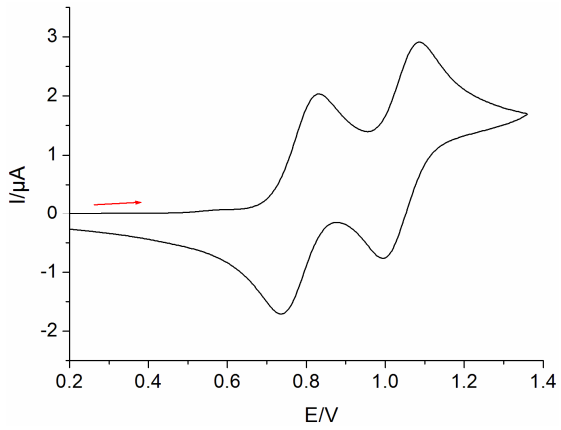

Figure S46. Cyclic voltammogram of zinc(II) tetraphenylporphyrin in dry CH_2Cl_2 (scan rate = 100 mV/s).

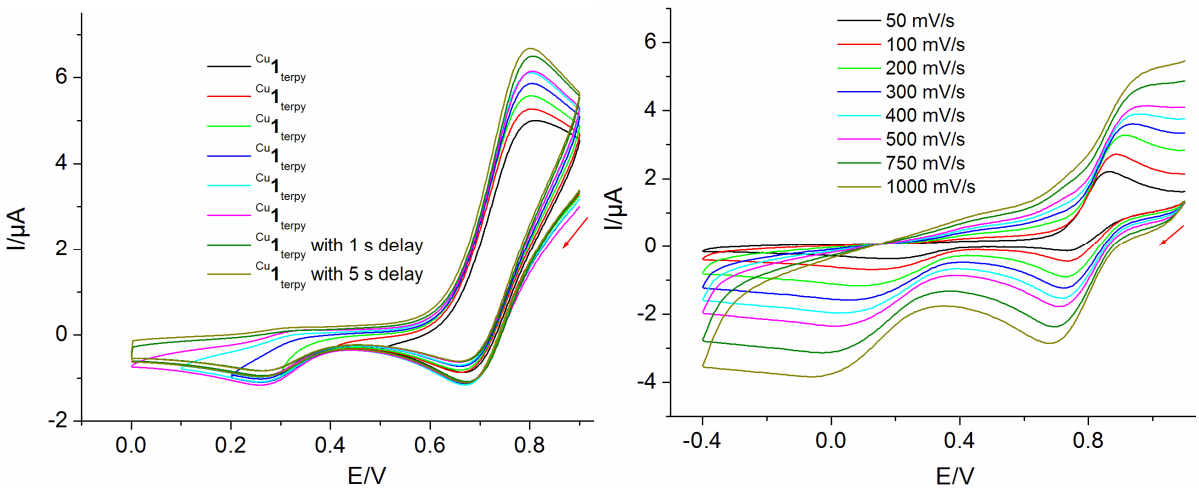

Figure S47. (Left) Cyclic voltammograms of complex $^{Cu}\mathbf{1}_{terpy}$ with cathodically shifted switching potential (ΔE = 100 mV) show the gradual increase of the anodic current (i_{pa}) in dry CH_2Cl_2 (scan rate = 100 mV/s). Last two measurements were done using a time delay at the switching potential (E). (Right) Cyclic voltammogram of $^{Cu}\mathbf{1}_{terpy}$ at various scan rates in dry CH_2Cl_2.

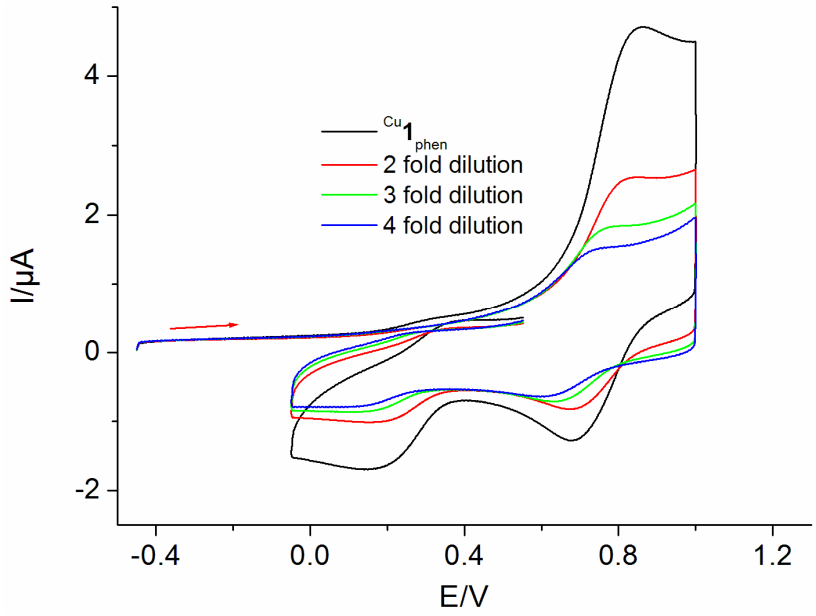

Figure S48. Concentration-dependent cyclic voltammograms of $^{Cu}\mathbf{1}_{phen}$ (scan rate = 500 mV/s). 5 s delay at the switching potential E = 1.00 V.

CV Simulations

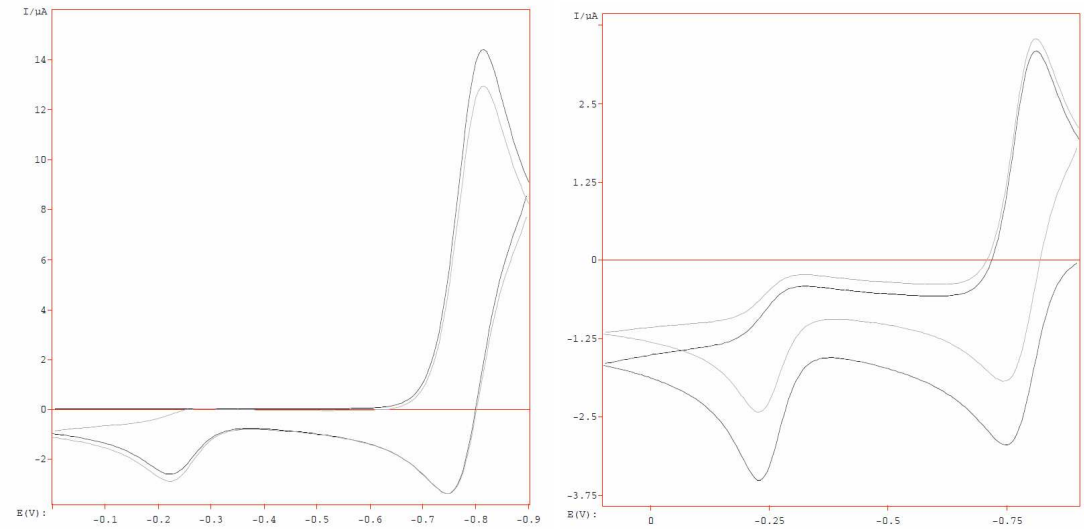

Figure S49. (left) Simulation of the cyclic voltammogram trace in Figure 6 (left) at v = 500 mV/s. (right) Simulation of the cyclic voltammogram trace in Figure 6 (right) at v = 100 mV/s.

The following mechanism was used (simulated as reduction mechanism) for both cyclic voltammetric traces using DigiSim 3®:

A + e = B (E = –0.79 V)

C + e = D (E = –0.79 V)

B = E (optimised for both scans!)

F + e = E (E = –0.24 V)

F = G (optimised for both scans!)

H + e = I (E = –1.05 V)

Rate constants after optimisation: k (B→E) = 10 s^{-1}; k (F→G) = 5 s^{-1}

The same rate constants could be applied for simulation of Figure S42 right.

DOSY

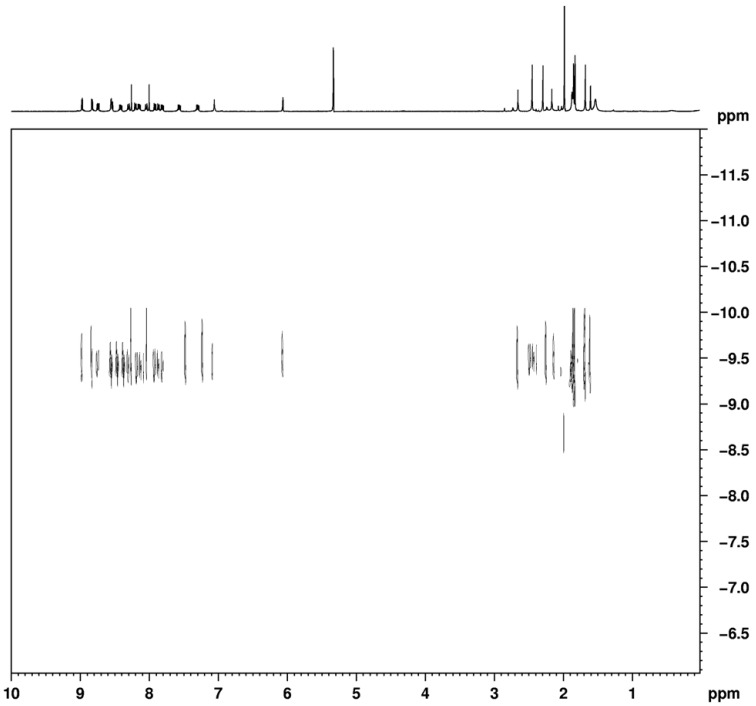

Figure S50. ^{1}H DOSY of $^{Cu}\mathbf{1}_{phen}$ = $[Cu_2(\mathbf{2})(\mathbf{4})_2](PF_6)_2$ (CD_2Cl_2 , 400 MHz, 298 K).

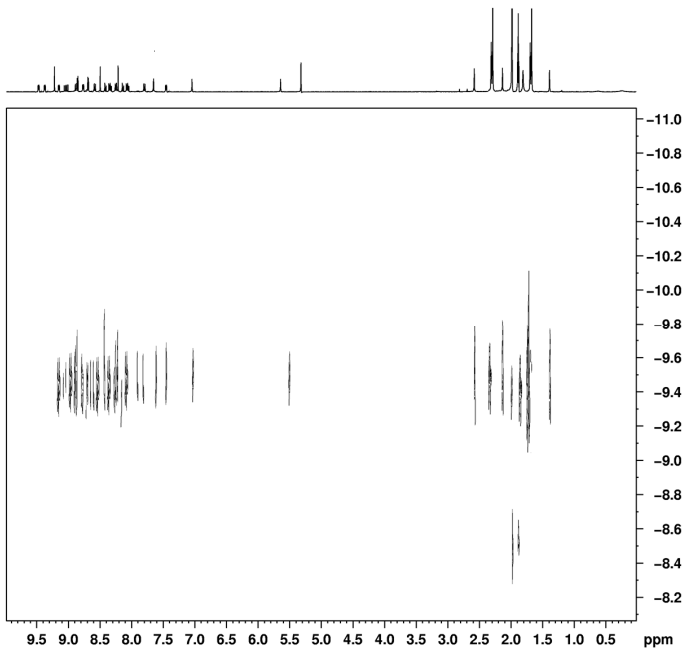

Figure S51. ^{1}H DOSY of $^{Zn}\mathbf{1}_{terpy}$ = $[Zn_2(\mathbf{2})(\mathbf{4})_2](OTf)_4$ (CD_2Cl_2:CD_3CN, 400 MHz, 298 K).

DFT Computations

All geometry optimizations, frequencies, and thermal energy corrections were performed with the B3LYP functional, 6-31G* basis set for all main group elements and LANL2DZ basis set for copper as implemented in Gaussian 09.[1]

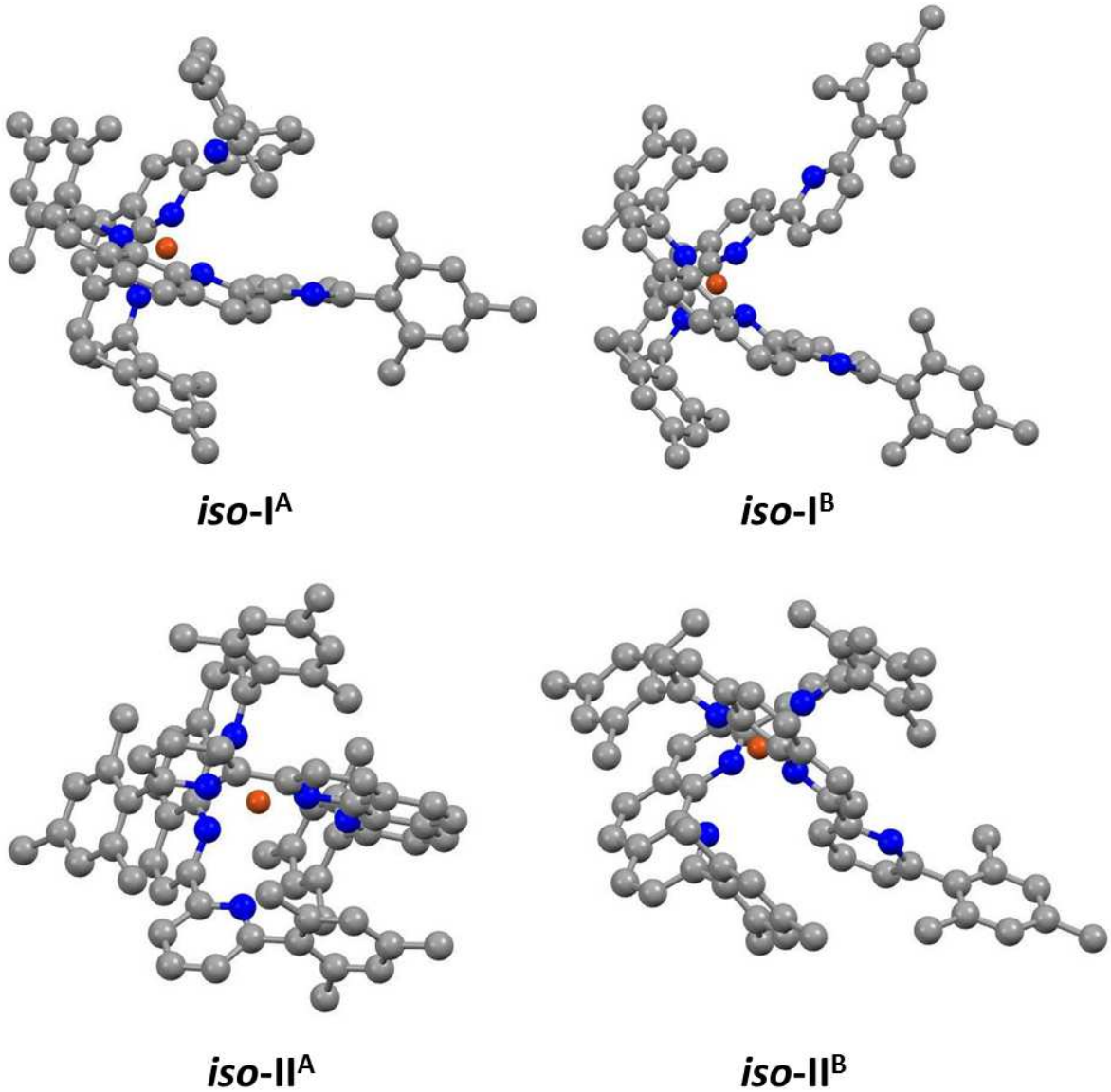

Figure S52. DFT optimised conformers of *iso*-**I** and *iso*-**II** of $[Cu(\mathbf{5})_2]^+$. Hydrogens are removed for clarity.

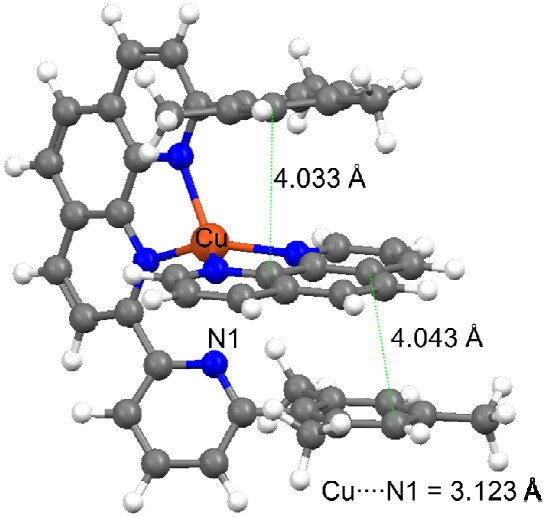

Figure S53. DFT optimised structure of $[Cu(\mathbf{4})(\mathbf{5})]^{+}$ showing strong π····π interaction.

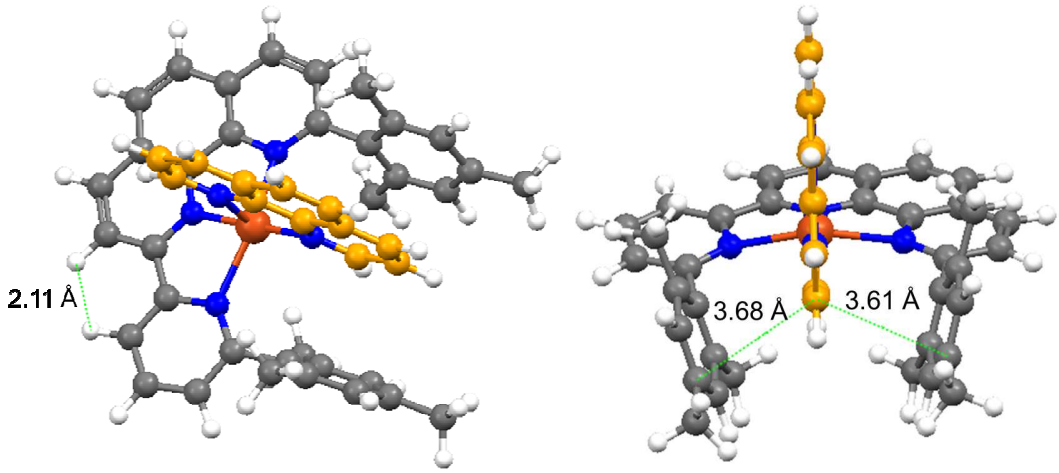

Figure S54. DFT optimised structure of $[Cu(\mathbf{4})(\mathbf{5})]^{2+}$ square pyramidal geometry of Cu^{2+}– two different views of the structure.

Table S5. X,Y,Z cartesian coordinates of *iso*-$\mathbf{I}^{A}$ of complex $[Cu(\mathbf{5})_2]^+$.

E(RB3LYP) = -3229.4590898

C	3.935000	-1.208100	-2.338000	H	-3.716900	3.110400	1.073400
C	2.586500	-1.542700	-2.281500	H	-2.532100	2.745600	-0.186800
C	4.553700	-0.674500	-1.193200	H	-3.951000	3.734200	-0.562100
C	1.877000	-1.324900	-1.100700	H	2.090700	-1.980500	-3.144200
C	2.551700	-0.756900	-0.016000	N	3.862600	-0.454300	-0.065900
C	1.900400	-0.472200	1.298300	H	0.835700	-1.609200	-1.017100
C	2.743600	-0.385900	2.434900	H	4.513600	-1.359700	-3.243600
C	2.202100	-0.103500	3.663100	C	6.010000	-0.329000	-1.193100
H	3.805600	-0.538400	2.295500	C	6.978000	-1.347400	-1.302700
C	0.028800	0.020800	2.599900	C	6.412100	1.021000	-1.082700
C	0.812600	0.118400	3.780800	C	8.333700	-0.995900	-1.305500
H	2.830400	-0.041300	4.547800	C	7.774500	1.324500	-1.101800
C	-1.400900	0.272400	2.695100	C	8.755000	0.331200	-1.211400
C	0.205600	0.436200	5.037700	H	9.079000	-1.784900	-1.379500
C	-1.961400	0.590100	3.961700	H	8.080600	2.366300	-1.028200
C	-1.132900	0.663500	5.127000	C	5.401000	2.139700	-0.957800
H	0.840400	0.495100	5.917400	H	4.646600	2.097300	-1.753100
C	-3.352200	0.824400	4.020300	H	4.858700	2.082100	-0.007500
C	-3.476500	0.446000	1.636300	H	5.894700	3.114800	-1.012300
H	-1.595600	0.907400	6.079200	C	6.599200	-2.811600	-1.394800
C	-4.102000	0.754400	2.869300	H	5.813800	-3.077500	-0.678900
H	-3.813900	1.066700	4.974000	H	6.229100	-3.082000	-2.392000
H	-5.169700	0.946300	2.880800	H	7.467300	-3.445700	-1.191100
N	-2.162100	0.198900	1.566500	C	10.221900	0.692300	-1.216200
N	0.575500	-0.283100	1.386800	H	10.524200	1.143100	-0.262500
C	-4.316000	0.451700	0.394500	H	10.851000	-0.187500	-1.382300
C	-5.121500	-0.658800	0.061000	H	10.450700	1.422100	-2.002200
C	-4.383500	1.634300	-0.372200	Cu	-0.962200	-0.469200	-0.068000
C	-5.934700	-0.586100	-1.073900	C	-2.358300	-2.465900	-1.720800
C	-5.214900	1.659300	-1.498100	C	-1.566300	-3.753100	0.052800
C	-5.993900	0.561600	-1.871000	C	-2.247200	-1.251600	-2.511400
H	-6.551000	-1.445000	-1.331300	C	-3.223400	-3.500700	-2.165200
H	-5.268800	2.573600	-2.085600	C	-2.436700	-4.812900	-0.301500
C	-6.915600	0.626900	-3.066500	C	-2.957300	-1.166800	-3.737600
H	-6.941300	-0.326400	-3.606300	C	-3.983800	-3.339300	-3.369700
H	-7.945700	0.850100	-2.759700	C	-3.265500	-4.683300	-1.394700
H	-6.609100	1.409500	-3.768100	H	-2.417400	-5.727700	0.281800
C	-5.136400	-1.916300	0.901300	C	-2.730700	-0.031800	-4.544100
H	-4.184700	-2.454700	0.846200	C	-3.846400	-2.220100	-4.132100
H	-5.319200	-1.700400	1.960300	C	-1.178600	0.783000	-2.883600
H	-5.922600	-2.597700	0.563200	H	-4.649700	-4.141500	-3.675200
C	-3.602600	2.869300	0.010200	H	-3.928500	-5.492400	-1.690400

C	-1.823400	0.919500	-4.135000
H	-3.260000	0.071500	-5.487500
H	-4.397100	-2.110500	-5.062200
H	-1.610700	1.789300	-4.746800
N	-1.571100	-2.595100	-0.619300
N	-1.415800	-0.259100	-2.079900
C	-0.170400	1.825500	-2.502800
C	0.930700	2.024300	-3.345300
C	1.831000	3.040800	-3.031800
H	1.078300	1.393800	-4.216400
C	0.444200	3.583900	-1.133000
C	1.580100	3.836500	-1.917900
H	2.701300	3.219700	-3.656900
H	2.238100	4.659900	-1.658900
N	-0.402700	2.574000	-1.414300
C	0.104200	4.489200	0.013100
C	0.764000	4.362100	1.249800
C	-0.864800	5.499100	-0.174300
C	0.419100	5.228200	2.294100
C	-1.174200	6.344500	0.894700
C	-0.545900	6.226300	2.139200
H	0.924000	5.120700	3.252100
H	-1.922500	7.121000	0.748900
C	1.841500	3.323100	1.464700
H	1.545600	2.344300	1.076700
H	2.775700	3.598200	0.957500
H	2.070300	3.212800	2.529000
C	-1.541200	5.702600	-1.512600
H	-0.817400	5.987100	-2.287200
H	-2.039200	4.791700	-1.860300
H	-2.289800	6.498200	-1.453100
C	-0.879700	7.172700	3.268700
H	-0.596000	6.754500	4.240000
H	-0.347700	8.126500	3.155800
H	-1.950300	7.403200	3.297100
C	-0.546400	-3.969400	1.131100
C	-0.850500	-3.757800	2.490400
C	0.722900	-4.463600	0.756500
C	0.143100	-3.986400	3.448400
C	1.684700	-4.675300	1.749100
C	1.419100	-4.438500	3.101200
H	-0.092500	-3.813600	4.496500
H	2.664400	-5.047600	1.457000
C	2.465300	-4.708300	4.156900
H	2.298800	-4.100600	5.052300
H	2.447100	-5.760400	4.470200
H	3.474100	-4.499600	3.785200
C	1.045100	-4.824800	-0.678000
H	0.497400	-5.723300	-0.991600
H	0.782200	-4.028600	-1.380600
H	2.112100	-5.034700	-0.794600
C	-2.226700	-3.317700	2.935000
H	-2.537800	-2.392100	2.443000
H	-2.986100	-4.076100	2.705100
H	-2.250300	-3.149000	4.015600

Table S6. X,Y,Z cartesian coordinates of *iso*-$\mathbf{I}^{B}$ of complex $[Cu(\mathbf{5})_2]^+$.

E(RB3LYP) = -3229.4653704

C	1.415400	3.737200	-2.158900	H	-2.548800	-2.679500	3.388200
C	1.223800	2.371000	-2.331600	H	-2.177300	-1.371200	2.265100
C	1.934200	4.205700	-0.937900	H	-3.841100	-1.944200	2.434000
C	1.531800	1.501200	-1.285700	H	0.839400	1.982400	-3.270900
C	2.013900	2.043200	-0.090200	N	2.219900	3.364200	0.066000
C	2.350700	1.219700	1.110500	H	1.410700	0.431000	-1.401100
C	3.242200	1.781000	2.060300	H	1.171000	4.441500	-2.947400
C	3.560600	1.075400	3.193400	C	2.172100	5.664900	-0.708600
H	3.644800	2.765900	1.863300	C	3.162900	6.345200	-1.447400
C	2.073700	-0.677700	2.433700	C	1.404400	6.357900	0.252300
C	2.972800	-0.189100	3.418500	C	3.362900	7.710100	-1.214000
H	4.251200	1.482900	3.927200	C	1.632800	7.723200	0.442900
C	1.402200	-1.943000	2.679100	C	2.604500	8.421600	-0.280900
C	3.252000	-0.955000	4.595600	H	4.137500	8.228800	-1.774900
C	1.691600	-2.663400	3.868700	H	1.034500	8.256000	1.179200
C	2.640400	-2.151800	4.811600	C	0.338800	5.661400	1.070800
H	3.958400	-0.554100	5.317100	H	-0.368200	5.111900	0.436900
C	1.000100	-3.876300	4.080600	H	0.780200	4.933800	1.761000
C	-0.202900	-3.510200	2.017300	H	-0.232100	6.386600	1.658400
H	2.847200	-2.730200	5.707600	C	4.035100	5.636300	-2.463300
C	0.054400	-4.290600	3.169600	H	4.425900	4.688300	-2.077000
H	1.204700	-4.459200	4.974900	H	3.490700	5.405500	-3.387700
H	-0.516700	-5.199600	3.325900	H	4.888700	6.262400	-2.739700
N	0.486300	-2.387000	1.773200	C	2.812500	9.903400	-0.074000
N	1.794800	0.013100	1.290900	H	2.614500	10.196000	0.962600
C	-1.324700	-3.896600	1.104000	H	3.835600	10.203800	-0.322400
C	-1.174800	-4.905500	0.132600	H	2.137100	10.489900	-0.711100
C	-2.581600	-3.279700	1.302400	Cu	0.632500	-1.317300	-0.022500
C	-2.278500	-5.247500	-0.659000	C	0.670400	-2.564100	-2.629400
C	-3.652000	-3.652600	0.487100	C	2.864100	-2.680800	-1.828000
C	-3.520900	-4.628900	-0.507500	C	-0.663300	-1.992700	-2.522300
H	-2.161900	-6.028600	-1.407100	C	0.967600	-3.431100	-3.716400
H	-4.618400	-3.177900	0.642900	C	3.220600	-3.568200	-2.870700
C	-4.694000	-5.000500	-1.383200	C	-1.614400	-2.314200	-3.527300
H	-4.504900	-5.924700	-1.937900	C	-0.034400	-3.747000	-4.689000
H	-5.606200	-5.140500	-0.792600	C	2.278400	-3.947700	-3.799800
H	-4.904800	-4.210100	-2.115600	H	4.243200	-3.925800	-2.928700
C	0.137200	-5.626500	-0.085400	C	-2.893300	-1.725000	-3.425400
H	0.853500	-5.004400	-0.634900	C	-1.277900	-3.202400	-4.598300
H	0.617300	-5.910400	0.857100	C	-2.169200	-0.592500	-1.419300
H	-0.017100	-6.539800	-0.667700	H	0.223900	-4.418600	-5.502800

C	-2.796000	-2.264000	2.403200
C	-3.167800	-0.871900	-2.387500
H	-3.646500	-1.947700	-4.176800
H	-2.039500	-3.428700	-5.339400
H	-4.132600	-0.396900	-2.271700
N	1.609000	-2.226400	-1.699500
N	-0.952500	-1.156100	-1.482400
C	-2.518600	0.375600	-0.334000
C	-1.575000	0.921200	0.541600
C	-2.005000	1.838900	1.499800
H	-0.529700	0.653900	0.470200
C	-4.240800	1.602800	0.633800
C	-3.350800	2.184800	1.554300
H	-1.290500	2.286300	2.185300
H	-3.717300	2.905900	2.278000
N	-3.819700	0.720900	-0.282800
C	-5.692200	1.974300	0.624800
C	-6.552200	1.508400	1.639700
C	-6.192900	2.796200	-0.406700
C	-7.902400	1.872100	1.602700
C	-7.547500	3.140800	-0.398700
C	-8.420900	2.692200	0.597100
H	-8.566700	1.501200	2.380500
H	-7.930300	3.778400	-1.193100
C	-6.056000	0.606900	2.750200
H	-5.528300	-0.268900	2.354100
H	-5.358000	1.121800	3.421700
H	-6.890600	0.247600	3.359300
C	-5.295000	3.317300	-1.507600
H	-4.421200	3.843800	-1.104100
H	-4.913400	2.503800	-2.135100
H	-5.836700	4.015600	-2.152300
C	-9.874800	3.102700	0.598600
H	-10.500200	2.363100	1.109300
H	-10.014600	4.060700	1.116700
H	-10.258000	3.227000	-0.419800
C	3.935000	-2.193500	-0.899200
C	4.280800	-2.919600	0.258200
C	4.669700	-1.042600	-1.261400
C	5.315700	-2.442800	1.070300
C	5.694200	-0.603500	-0.417800
C	6.027400	-1.281200	0.759400
H	5.580300	-3.004700	1.963600
H	6.257400	0.284100	-0.698600
C	7.123500	-0.769400	1.663700
H	7.510100	-1.560300	2.314100
H	2.535400	-4.624700	-4.610400
H	7.962100	-0.363500	1.087800
H	6.755700	0.038900	2.309900
C	4.422900	-0.318600	-2.567800
H	4.765700	-0.916600	-3.422400
H	3.364200	-0.100200	-2.733300
H	4.966700	0.630000	-2.594000
C	3.584900	-4.212300	0.618400
H	2.512200	-4.068000	0.776400
H	3.692900	-4.964400	-0.173100
H	4.004500	-4.637700	1.534800

Table S7. DFT Calculation. X,Y,*Z* cartesian coordinates of *iso*-**II**^{A} of complex $[Cu(\mathbf{5})_2]^+$.

E(RB3LYP) = -3229.45481745

C	-0.568100	-4.295500	-2.178700	H	-2.156000	3.021900	4.328700
C	-1.948000	-4.130000	-2.157900	H	-2.051800	1.423000	3.593200
C	0.260700	-3.174700	-2.016000	H	-1.897800	1.600900	5.346900
C	-2.464300	-2.846400	-2.012400	H	-2.613400	-4.983100	-2.251900
C	-1.573200	-1.771400	-1.883800	N	-0.239300	-1.932400	-1.862600
C	-2.143000	-0.389300	-1.823100	H	-3.534700	-2.685100	-1.959300
C	-3.221400	-0.090500	-2.692500	H	-0.122300	-5.275900	-2.314200
C	-3.806800	1.152100	-2.658500	C	1.750400	-3.356200	-2.021300
H	-3.558200	-0.841600	-3.397200	C	2.394700	-3.812300	-0.851500
C	-2.263000	1.745900	-0.891000	C	2.496200	-3.144100	-3.197900
C	-3.345000	2.113000	-1.735600	C	3.784000	-3.965700	-0.856600
H	-4.621400	1.403600	-3.332400	C	3.886600	-3.305300	-3.156300
C	-1.811100	2.697400	0.114700	C	4.553300	-3.698300	-1.993800
C	-3.937800	3.413500	-1.641400	H	4.276800	-4.314700	0.049000
C	-2.428600	3.977400	0.171400	H	4.460100	-3.134200	-4.065300
C	-3.488200	4.318000	-0.730500	C	1.835500	-2.850000	-4.527400
H	-4.757000	3.658000	-2.312000	H	1.546400	-3.785400	-5.026100
C	-1.969900	4.876900	1.156900	H	0.932000	-2.245200	-4.433100
C	-0.474900	3.158300	1.965700	H	2.524100	-2.329000	-5.200300
H	-3.934700	5.305900	-0.658300	C	1.604500	-4.188700	0.382200
C	-1.003900	4.470500	2.049300	H	0.844000	-3.442700	0.630000
H	-2.401700	5.872800	1.216100	H	1.081000	-5.143100	0.237500
H	-0.654900	5.130400	2.837000	H	2.264900	-4.310700	1.245900
N	-0.847100	2.315100	0.996000	C	6.058200	-3.825600	-1.961100
N	-1.664900	0.522300	-0.966800	H	6.519600	-2.921300	-1.541100
C	0.441200	2.708400	3.067000	H	6.377900	-4.669800	-1.340200
C	1.837000	2.897000	2.991400	H	6.472300	-3.968200	-2.964400
C	-0.141300	2.216500	4.253100	Cu	0.114100	0.440400	0.064500
C	2.628800	2.548300	4.089400	C	3.006300	0.558000	-0.502300
C	0.689500	1.893800	5.333000	C	2.077900	1.928000	-2.145100
C	2.076500	2.048300	5.273700	C	2.831600	-0.266800	0.686200
H	3.705600	2.691500	4.023100	C	4.320300	0.748400	-1.010900
H	0.234800	1.522100	6.248900	C	3.356900	2.147400	-2.715300
C	2.955100	1.716700	6.457800	C	3.988700	-0.805000	1.313700
H	3.777800	1.049600	6.174000	C	5.451700	0.151400	-0.366800
H	3.409500	2.621800	6.879800	C	4.467100	1.562900	-2.153200
H	2.386200	1.230900	7.256700	C	3.805200	-1.553900	2.493200
C	2.483100	3.510300	1.771900	C	5.292200	-0.590300	0.761300
H	2.152400	3.025900	0.849800	C	1.425200	-1.187200	2.305500
H	2.235600	4.576500	1.685100	H	6.438000	0.319800	-0.790100
H	3.573500	3.434000	1.826000	H	5.456900	1.724300	-2.572500

C	-1.639400	2.055500	4.386500
H	4.667500	-1.987000	2.993000
H	6.147200	-1.031300	1.266100
H	2.374000	-2.328300	3.882300
N	1.917300	1.148300	-1.069400
N	1.577000	-0.481800	1.177700
C	0.068800	-1.436600	2.887800
C	-0.076700	-1.376300	4.281800
C	-1.313500	-1.681500	4.841400
H	0.752800	-1.069200	4.907700
C	-2.133100	-2.083800	2.609000
C	-2.354500	-2.045700	3.995400
H	-1.459800	-1.638900	5.917100
H	-3.330600	-2.311400	4.389000
N	-0.941400	-1.771800	2.065300
C	-3.258800	-2.531600	1.722200
C	-3.372800	-3.894900	1.377000
C	-4.250300	-1.616100	1.320800
C	-4.480900	-4.314900	0.633900
C	-5.334700	-2.076500	0.563900
C	-5.477200	-3.424000	0.220300
H	-4.573900	-5.369500	0.381200
H	-6.098500	-1.365200	0.254600
C	-2.325000	-4.903600	1.791500
H	-1.380700	-4.735100	1.260600
H	-2.103100	-4.846900	2.863200
H	-2.657000	-5.922800	1.572000
C	-4.177700	-0.157400	1.715500
H	-4.406400	-0.017100	2.780400
H	-3.181000	0.259200	1.540800
H	-4.900800	0.436100	1.147400
C	-6.689800	-3.912700	-0.538900
H	-6.440100	-4.743300	-1.208100
H	-7.464800	-4.276300	0.148600
H	-7.139000	-3.114200	-1.138800
C	0.908200	2.594100	-2.812400
C	0.224500	1.908200	-3.837700
C	0.599600	3.945300	-2.543100
C	-0.781400	2.572800	-4.547600
C	-0.411100	4.569700	-3.281200
C	-1.117700	3.902800	-4.286200
H	-1.298300	2.039400	-5.342600
H	-0.640300	5.613000	-3.073100
C	0.602900	0.497200	-4.217500
H	1.566900	0.474100	-4.743900
H	0.693200	-0.150300	-3.340600
C	2.537200	-1.735200	2.990300
H	-0.142900	0.063300	-4.890900
C	1.324700	4.738800	-1.480300
H	0.946200	4.500900	-0.480100
H	2.400900	4.537400	-1.472200
H	1.187200	5.813100	-1.636800
C	-2.203000	4.606700	-5.066300
H	-1.873300	5.594900	-5.406700
H	-2.502700	4.030300	-5.947000
H	-3.097300	4.762800	-4.448800
H	3.441200	2.782500	-3.590700

Table S8. DFT Calculation. X,Y,*Z* cartesian coordinates of *iso*-**II**^{B} of complex $[Cu(\mathbf{5})_2]^+$.

E(RB3LYP) = -3229.4589363

C	0.133100	4.112100	-2.703000	C	-1.274500	-2.509600	3.355600
C	-0.440900	3.774100	-3.921400	H	-1.698900	-1.702300	2.751700
C	-0.035900	3.268700	-1.593200	H	-2.037600	-3.295700	3.424300
C	-1.195800	2.609300	-4.000500	H	-1.108400	-2.124600	4.366300
C	-1.375300	1.831900	-2.848800	C	1.331300	-4.651700	-0.463400
C	-2.219400	0.604100	-2.901300	H	0.729700	-5.566900	-0.537000
C	-3.198500	0.473300	-3.911600	H	0.958900	-3.960000	-1.225500
C	-3.965400	-0.664500	-3.960000	H	2.361000	-4.913600	-0.723200
H	-3.374100	1.277200	-4.615000	H	-0.296700	4.398900	-4.798000
C	-2.742600	-1.503100	-2.033400	N	-0.792700	2.150100	-1.668700
C	-3.750200	-1.695800	-3.024800	H	-1.618500	2.301700	-4.948900
H	-4.742100	-0.778500	-4.711100	H	0.727500	5.012900	-2.594000
C	-2.473700	-2.599500	-1.103100	C	0.679100	3.637100	-0.327400
C	-4.533300	-2.892700	-3.064500	C	2.077500	3.454300	-0.266200
C	-3.292500	-3.764700	-1.176200	C	0.006900	4.288100	0.728500
C	-4.325700	-3.884700	-2.159400	C	2.767200	3.874900	0.876100
H	-5.295800	-2.985900	-3.832700	C	0.739800	4.702200	1.844800
C	-3.027000	-4.811200	-0.266900	C	2.119000	4.497000	1.945600
C	-1.163700	-3.533700	0.572500	H	3.843300	3.722500	0.920800
H	-4.920200	-4.794100	-2.181000	H	0.218500	5.215100	2.650600
C	-1.971100	-4.698800	0.606300	C	-1.474300	4.579300	0.672100
H	-3.647500	-5.703800	-0.284300	H	-1.779900	4.966200	-0.306600
H	-1.725900	-5.495800	1.300900	H	-2.066100	3.678600	0.860300
N	-1.433300	-2.508000	-0.237700	H	-1.751300	5.322600	1.425900
N	-2.026700	-0.343500	-1.971200	C	2.861200	2.859200	-1.416100
C	0.065900	-3.506300	1.433900	H	2.328600	2.037000	-1.903100
C	0.011600	-3.034900	2.760000	H	3.069800	3.613100	-2.187000
C	1.262300	-4.056700	0.926300	H	3.821500	2.472400	-1.065900
C	1.169200	-3.082500	3.544100	C	2.882200	4.930000	3.174900
C	2.395200	-4.083900	1.746100	H	2.846700	4.157100	3.954700
C	2.372400	-3.601200	3.058100	H	3.937100	5.114800	2.948100
H	1.123800	-2.713200	4.566600	H	2.462200	5.844200	3.607800
H	3.317100	-4.505500	1.350700	Cu	-1.117800	0.456000	-0.242200
C	3.600000	-3.677100	3.935900	C	-1.430000	1.153900	2.539000
H	3.574000	-2.921800	4.728300	C	-3.594600	1.091800	1.656500
H	3.677200	-4.657600	4.424000	C	-0.012200	0.854000	2.391600
H	4.518100	-3.532200	3.356400	C	-1.892500	1.700800	3.767300
C	-4.114800	1.673300	2.839100	C	-5.054000	1.554600	-0.369100
C	0.845200	1.082900	3.501100	C	-5.165700	-0.625300	0.729500
C	-0.984000	1.940600	4.847600	C	-6.075400	1.141500	-1.233300
C	-3.271100	1.979200	3.881600	C	-6.185400	-0.991500	-0.153000

C	2.210800	0.760200	3.347300
C	0.334600	1.630500	4.720900
C	1.751600	0.071200	1.081900
H	-1.373700	2.361200	5.770400
H	-3.654500	2.414500	4.800900
C	2.660500	0.259500	2.152900
H	2.893400	0.914800	4.179100
H	1.026200	1.796400	5.542400
H	3.700500	0.013000	1.988700
N	-2.280600	0.874400	1.507700
N	0.449500	0.364800	1.206300
C	2.298400	-0.453800	-0.206200
C	1.490300	-1.022300	-1.196800
C	2.099900	-1.467500	-2.369300
H	0.428600	-1.161300	-1.035600
C	4.227600	-0.789300	-1.461600
C	3.478400	-1.350100	-2.511400
H	1.502900	-1.923600	-3.155000
H	3.980900	-1.706800	-3.404300
N	3.634700	-0.355300	-0.338600
C	5.717100	-0.675300	-1.553000
C	6.532000	-1.340800	-0.607400
C	6.316800	0.084600	-2.581100
C	7.920600	-1.233400	-0.711500
C	7.712900	0.175300	-2.633900
C	8.535500	-0.478800	-1.715800
H	8.541300	-1.756300	0.013500
H	8.167500	0.778100	-3.417500
C	5.949700	-2.183300	0.507200
H	5.557800	-1.560900	1.319700
H	5.119400	-2.808000	0.160900
H	6.716600	-2.840900	0.928900
C	5.512900	0.823800	-3.632700
H	5.235500	0.169700	-4.470000
H	4.585600	1.244700	-3.233400
H	6.102200	1.644900	-4.052900
C	10.040600	-0.397100	-1.815100
H	10.506000	-0.343000	-0.824800
H	10.452500	-1.282400	-2.317400
H	10.357800	0.480200	-2.387800
C	-4.584800	0.658700	0.612500
C	-6.659500	-0.123000	-1.141300
H	-6.435400	1.839800	-1.985900
H	-6.631200	-1.978900	-0.054400
C	-4.494900	2.951700	-0.504900
H	-4.531000	3.500500	0.443400
H	-3.448200	2.936300	-0.826000
H	-5.063500	3.527600	-1.241300
C	-4.724700	-1.600700	1.797400
H	-3.680600	-1.899900	1.662300
H	-4.807700	-1.171300	2.803000
H	-5.338300	-2.505800	1.772100
C	-7.793500	-0.531900	-2.051800
H	-8.757700	-0.480200	-1.530000
H	-7.862000	0.120600	-2.928200
H	-7.674300	-1.563700	-2.401600
H	-5.182800	1.850400	2.909800

Table S9. DFT Calculation. X,Y,Z cartesian coordinates of the complex [Cu(**4**)(**5**)]$^{+}$.

E(RB3LYP) = -2284.3803043

C	3.417500	-3.110400	1.657700	N	1.540000	-2.535400	0.274000
C	2.618000	-3.936100	2.440500	H	0.617200	-4.713600	2.695300
C	2.845200	-2.415500	0.577200	H	4.478200	-3.008700	1.861600
C	1.271400	-4.074900	2.110600	C	3.701200	-1.559700	-0.302700
C	0.778900	-3.360200	1.010600	C	4.390500	-0.450000	0.229900
C	-0.636100	-3.551700	0.577000	C	3.860700	-1.901300	-1.666900
C	-1.165600	-4.864100	0.542400	C	5.225700	0.297900	-0.609800
C	-2.456000	-5.071100	0.110200	C	4.712800	-1.130700	-2.461600
H	-0.535600	-5.699700	0.825600	C	5.412100	-0.029900	-1.953600
C	-2.646100	-2.681400	-0.206200	H	5.750300	1.156500	-0.195000
C	-3.242900	-3.967800	-0.282500	H	4.845200	-1.406900	-3.505900
H	-2.871800	-6.073700	0.059500	C	3.163800	-3.097700	-2.278500
C	-3.432700	-1.521200	-0.575400	H	3.368500	-4.015300	-1.713600
C	-4.592300	-4.110400	-0.744700	H	2.076500	-2.970300	-2.288900
C	-4.765800	-1.703200	-1.027000	H	3.503300	-3.257400	-3.306200
C	-5.324600	-3.021000	-1.106800	C	4.256400	-0.027700	1.679300
H	-5.018100	-5.108300	-0.799500	H	3.252500	-0.210200	2.074000
C	-5.493500	-0.545100	-1.377600	H	4.960600	-0.564200	2.328400
C	-3.566900	0.792900	-0.789600	H	4.474100	1.039700	1.788200
H	-6.346700	-3.131300	-1.457800	C	6.359800	0.757700	-2.827800
C	-4.898600	0.692000	-1.260000	H	5.968800	0.875500	-3.844600
H	-6.516500	-0.640800	-1.731700	H	6.551600	1.754800	-2.417800
H	-5.436100	1.599200	-1.515800	H	7.329400	0.250200	-2.914800
N	-2.858900	-0.294000	-0.464200	Cu	-0.801800	-0.469300	0.233000
N	-1.363600	-2.491400	0.209200	C	1.107800	1.724900	0.160700
C	-2.937100	2.141400	-0.635000	C	1.046600	0.785700	-1.947800
C	-2.314600	2.756800	-1.738700	C	0.678300	1.680900	1.541100
C	-3.024300	2.810800	0.603200	C	2.016100	2.730700	-0.255000
C	-1.757900	4.029800	-1.573200	C	1.945900	1.741700	-2.453700
C	-2.456400	4.082500	0.721100	H	0.655900	0.001200	-2.588700
C	-1.813100	4.708600	-0.352300	C	1.171900	2.645500	2.457500
H	-1.278500	4.507100	-2.425300	C	2.483600	3.699200	0.696400
H	-2.528900	4.602500	1.674200	C	2.426600	2.719600	-1.606400
C	-1.185200	6.073200	-0.188900	H	2.253100	1.693800	-3.492800
H	-1.062900	6.577000	-1.153000	C	0.740200	2.551200	3.799100
H	-1.791200	6.718800	0.455800	C	2.079200	3.658900	1.997700
H	-0.191000	5.997300	0.271400	C	-0.564500	0.632600	3.183700
C	-2.261700	2.079000	-3.090600	H	3.175000	4.466100	0.357900
H	-1.867600	1.059000	-3.021300	H	3.122600	3.474500	-1.962100
H	-3.258200	2.004900	-3.544600	C	-0.127200	1.540400	4.165300
H	-1.628300	2.640200	-3.783800	H	1.097600	3.272000	4.529700

C	-3.744300	2.191600	1.781300	H	2.442400	4.392300	2.712300
H	-4.812400	2.050700	1.572600	H	-1.248200	-0.171700	3.441200
H	-3.335800	1.207100	2.034600	H	-0.474100	1.436700	5.188100
H	-3.663900	2.829300	2.666400	N	0.627800	0.779200	-0.687000
H	3.037700	-4.474900	3.285200	N	-0.181900	0.696300	1.911600

Table S10. DFT Calculation. X,Y,Z cartesian coordinates of the complex $[Cu(\mathbf{4})(\mathbf{5})]^{2+}$.

E(UB3LYP) = -2284.0801083

C	0.687300	-4.714900	-0.752500	H	-0.584400	-6.452700	-0.663800
C	-0.532900	-5.368500	-0.675400	N	-0.389900	-2.573900	-0.681800
C	0.740400	-3.306800	-0.764100	H	-2.667500	-5.089000	-0.622400
C	-1.699200	-4.604000	-0.650400	H	1.613900	-5.272100	-0.832200
C	-1.593400	-3.215100	-0.669000	C	2.069700	-2.660500	-0.970700
C	-2.780700	-2.337800	-0.734000	C	3.068200	-2.761600	0.022300
C	-4.110900	-2.783800	-0.908600	C	2.368600	-2.101600	-2.236100
C	-5.133300	-1.859300	-1.001200	C	4.350200	-2.281300	-0.263500
H	-4.332200	-3.841200	-0.982800	C	3.668400	-1.643100	-2.474100
C	-3.499100	-0.102400	-0.783000	C	4.678600	-1.732800	-1.508300
C	-4.856700	-0.472800	-0.947800	H	5.119700	-2.357500	0.501600
H	-6.158100	-2.195100	-1.132500	H	3.906800	-1.233000	-3.452800
C	-3.104000	1.276200	-0.766900	C	1.344000	-2.037200	-3.350400
C	-5.847800	0.554200	-1.059800	H	0.909300	-3.022100	-3.558900
C	-4.108700	2.262400	-0.896200	H	0.508600	-1.365600	-3.115700
C	-5.483600	1.869900	-1.028400	H	1.803900	-1.681200	-4.275900
H	-6.888900	0.269900	-1.177400	C	2.794200	-3.381800	1.377100
C	-3.681100	3.609700	-0.908100	H	1.810800	-3.105000	1.772700
C	-1.378900	2.835200	-0.731200	H	2.826600	-4.478000	1.336400
H	-6.235000	2.648700	-1.118900	H	3.549900	-3.071400	2.104200
C	-2.335500	3.883500	-0.832500	C	6.089400	-1.293000	-1.817300
H	-4.409300	4.410700	-1.000600	H	6.616200	-0.958100	-0.917900
H	-1.973100	4.904500	-0.879200	H	6.668700	-2.124900	-2.237800
N	-1.768100	1.554600	-0.668700	H	6.110200	-0.483200	-2.553600
N	-2.524000	-1.029200	-0.662000	C	1.088000	0.246400	1.991900
C	0.063100	3.217200	-0.780800	C	2.071200	0.575800	-0.092000
C	0.769300	3.066500	-1.995800	C	-0.062400	-0.154900	2.756700
C	0.654300	3.878800	0.317500	C	2.260700	0.667000	2.665200
C	2.069300	3.577000	-2.080000	C	3.270400	1.008000	0.498100
C	1.958500	4.364900	0.184300	H	1.978600	0.521200	-1.168400
C	2.679700	4.240300	-1.009000	C	-0.010700	-0.128400	4.173400
H	2.608900	3.480400	-3.019500	C	2.281800	0.683300	4.100800
H	2.416000	4.873600	1.029900	C	3.366100	1.053600	1.873500
C	4.058500	4.839600	-1.148800	H	4.098100	1.295300	-0.138500

H	4.653300	4.316900	-1.904600	C	-1.172000	-0.534900	4.870600
H	3.993400	5.890100	-1.459700	C	1.192600	0.301100	4.826500
H	4.607000	4.819500	-0.201400	C	-2.244100	-0.924100	2.756500
C	0.141400	2.418500	-3.212500	H	3.189800	1.007700	4.600300
H	-0.108500	1.363300	-3.044200	H	4.281900	1.381600	2.357300
H	-0.789000	2.920900	-3.504200	C	-2.290000	-0.933000	4.162900
H	0.818900	2.465900	-4.068900	H	-1.175100	-0.530300	5.957000
C	-0.089600	4.078600	1.621300	H	1.219500	0.316400	5.911900
H	-0.860200	4.855200	1.537400	H	-3.108100	-1.230800	2.173800
H	-0.593000	3.163800	1.955600	H	-3.194900	-1.249300	4.670300
H	0.594900	4.394600	2.413500	N	1.013800	0.207400	0.628000
Cu	-0.744500	-0.409500	-0.103800	N	-1.167900	-0.548700	2.073100

1. Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.