SUPPORTING INFORMATION

Intramolecular electron transfer in Cu(II) complexes with aryl-1H-imidazo[4,5-*f*][1,10]phenanthroline derivatives

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Content

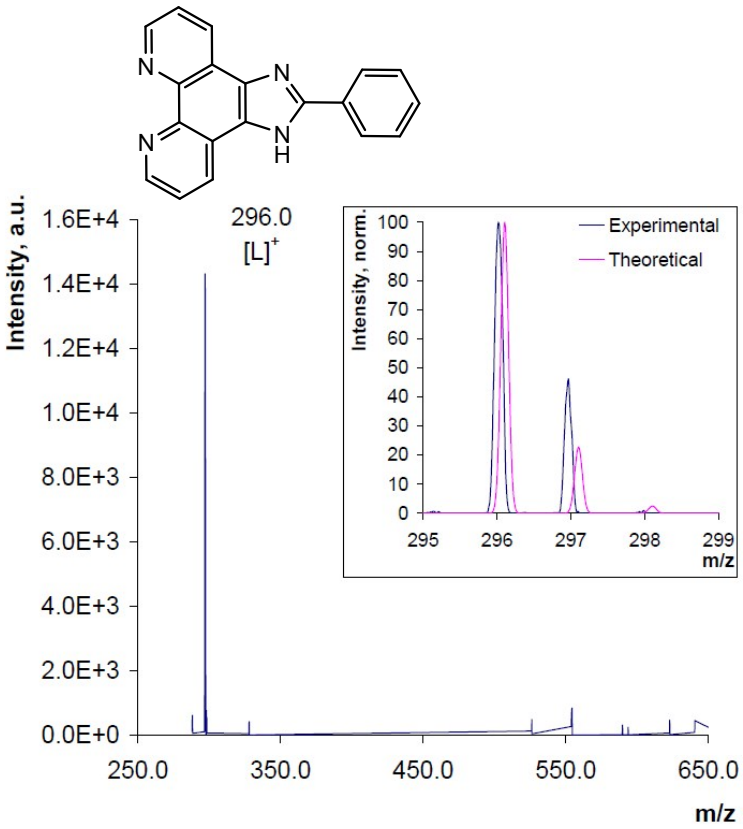


Fig. S1. ESI-MS of ligand **1**.

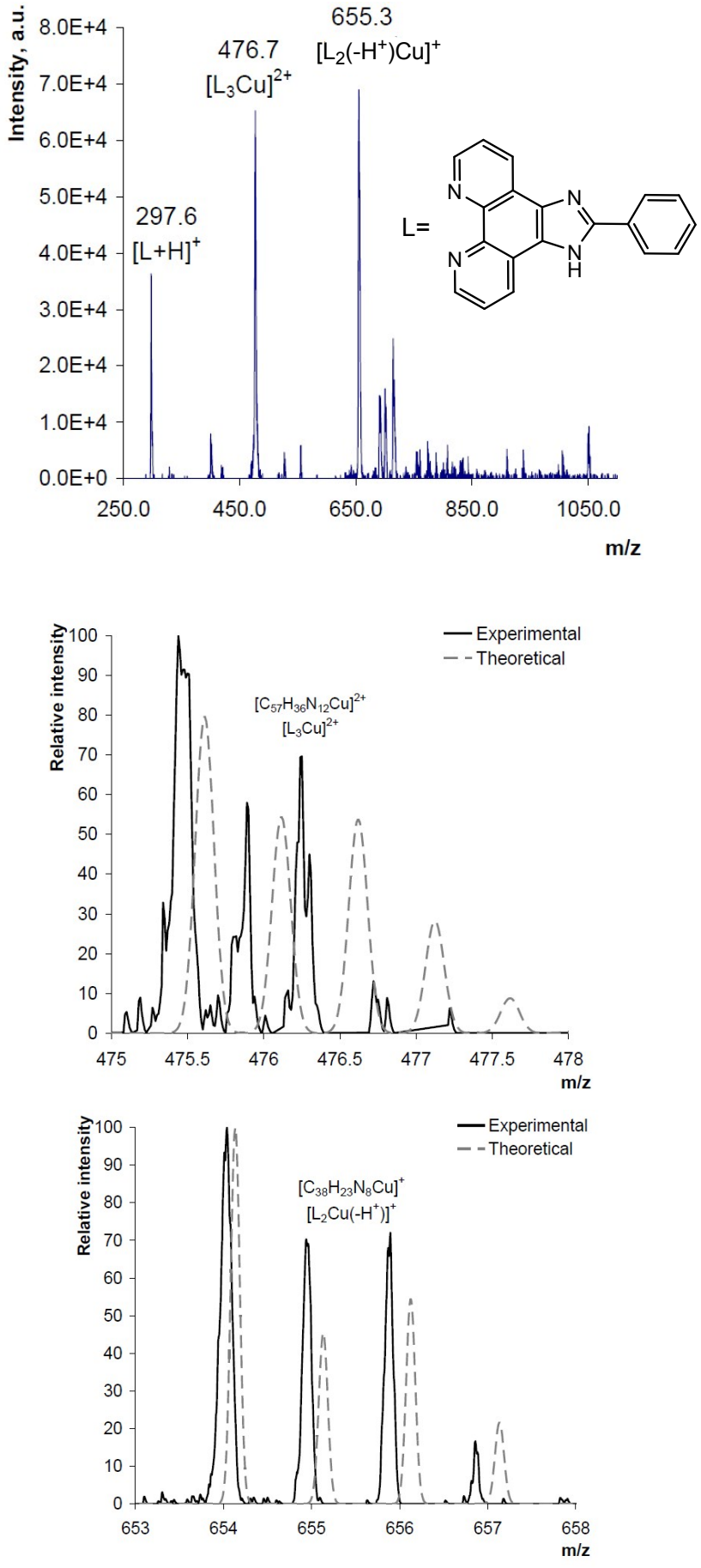


Fig. S2. ESI-MS of mixture ligand **1** with Cu^{2+}, ratio 3:1.

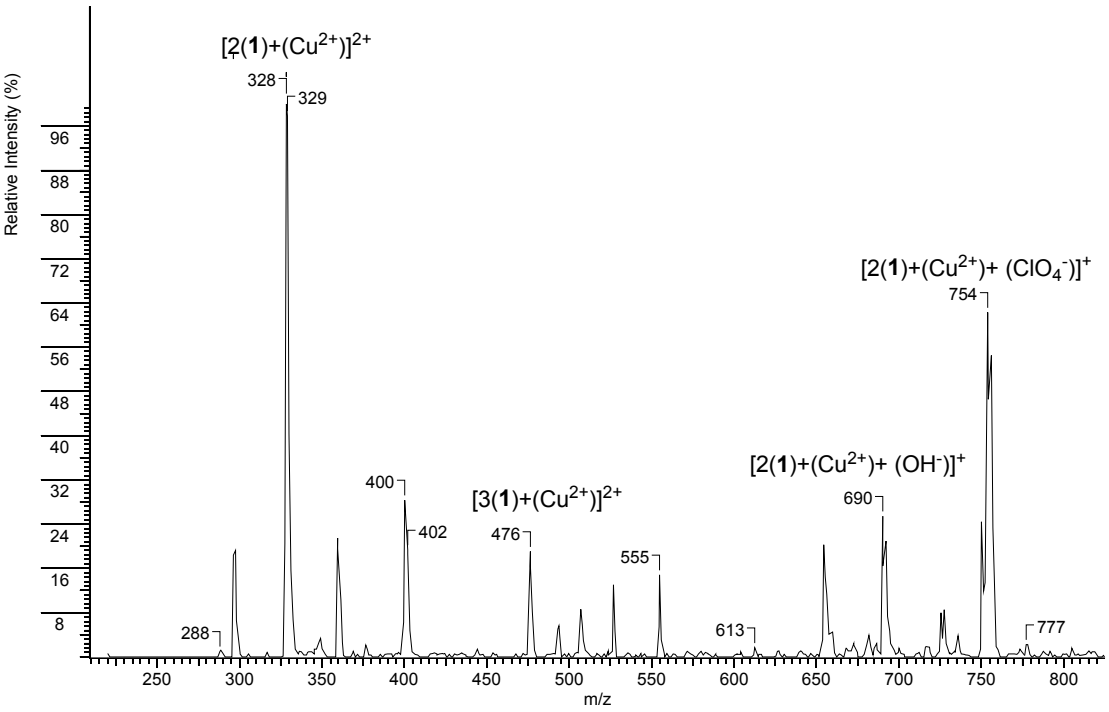


Fig. S3. ESI-MS of ligand **1** in the presence of 3-fold excess of $Cu(ClO_4)_2$.

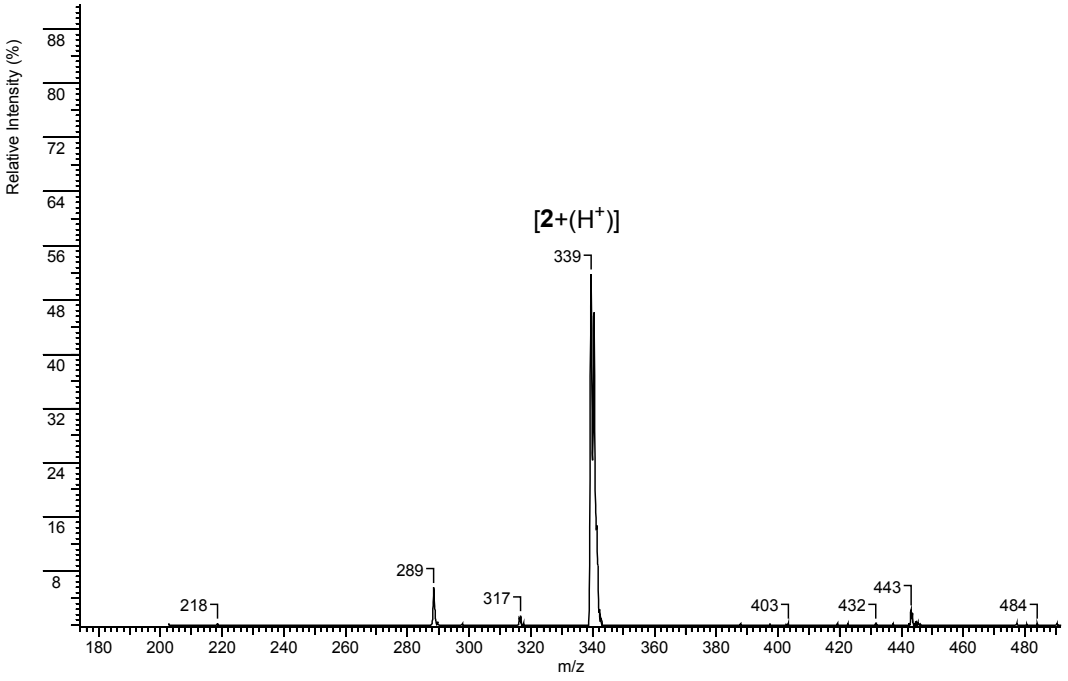


Fig. S4. ESI-MS of ligand **2**.

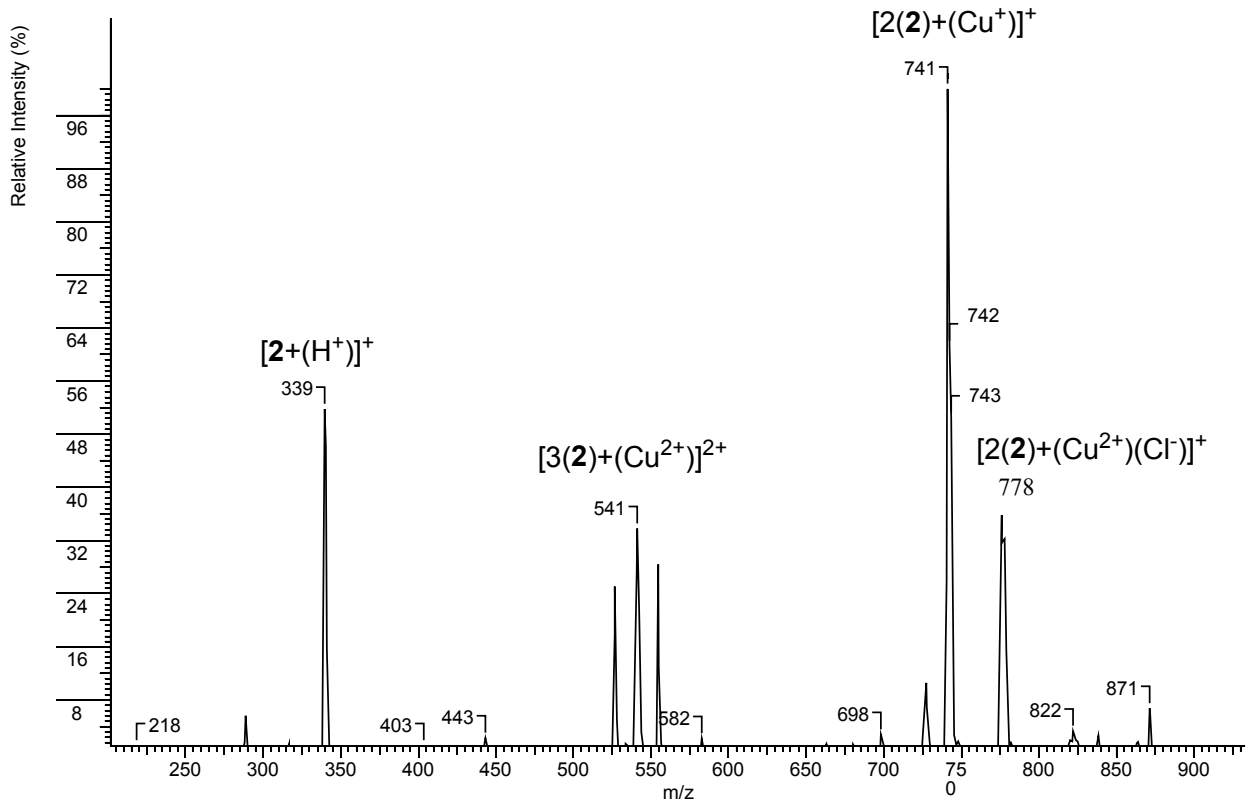


Fig. S5. ESI-MS of mixture ligand **2** with Cu^{2+}, ratio 3:1.

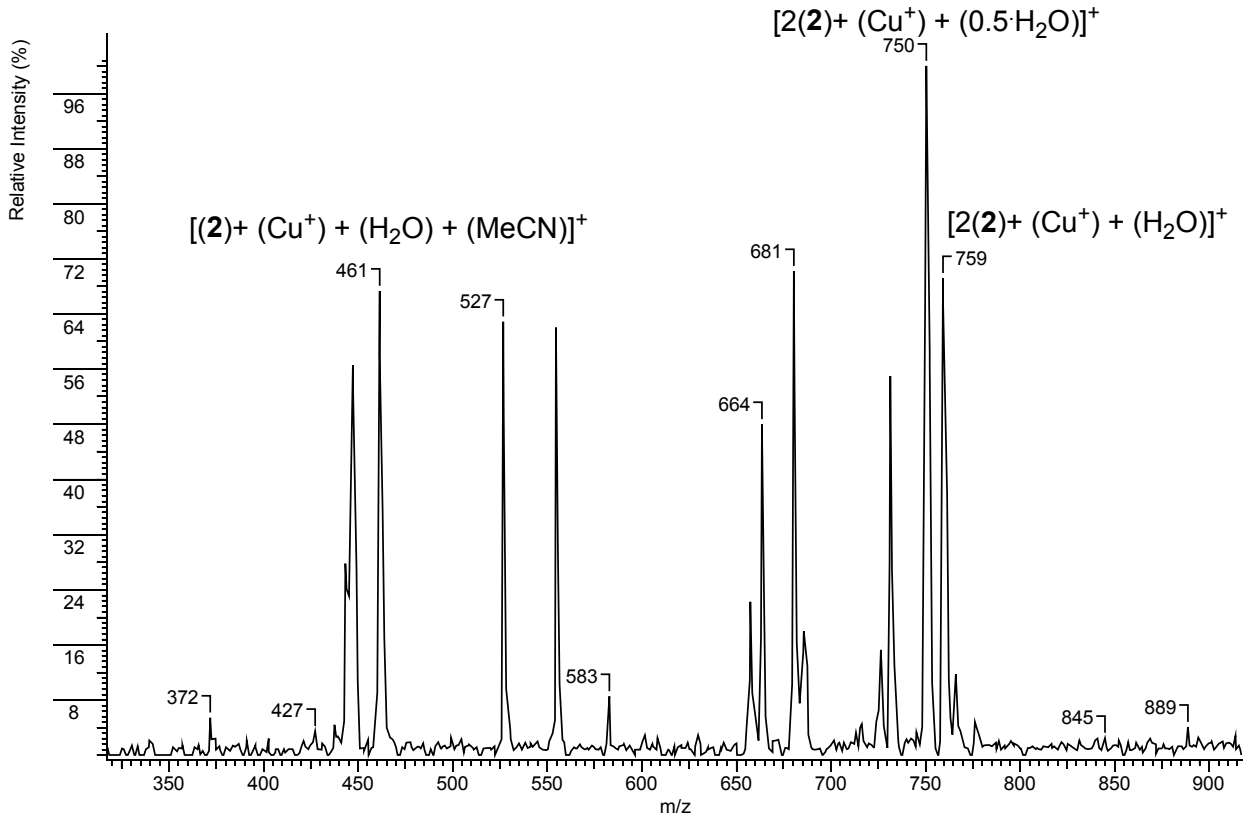


Fig. S6. ESI-MS of ligand **2** in the presence of 3-fold excess of $Cu(ClO_4)_2$.

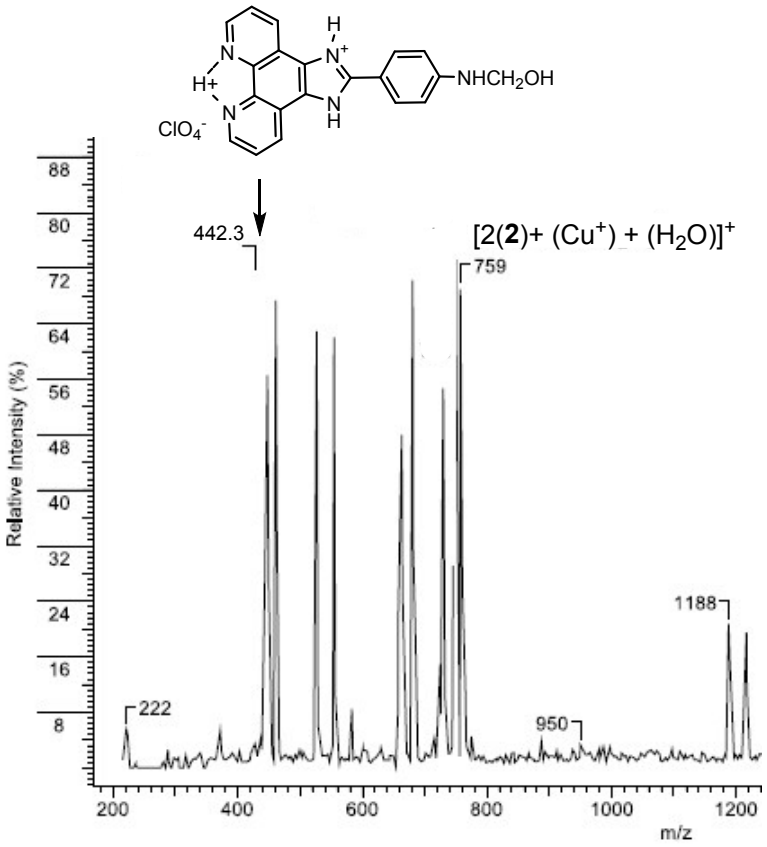


Fig. S7. ESI-MS of ligand **3** in the presence of 3-fold excess of $Cu(ClO_4)_2$ after keeping during 48 hours.

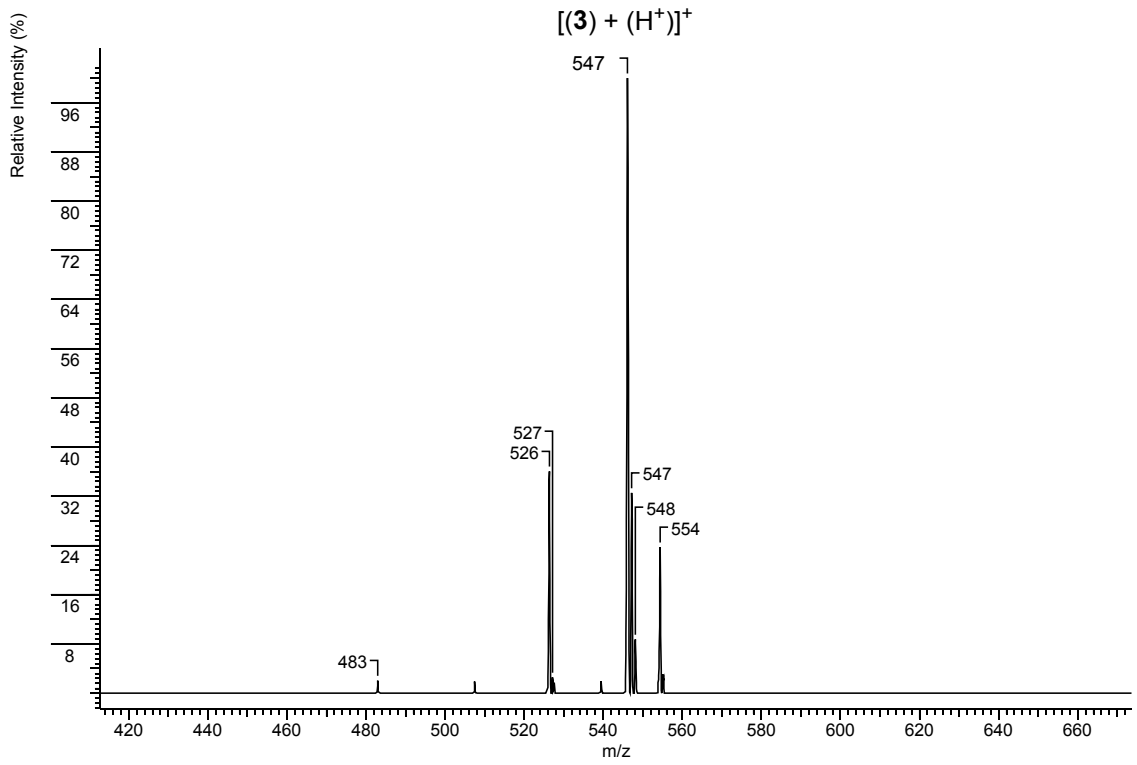


Fig. S8. ESI-MS of ligand **3**.

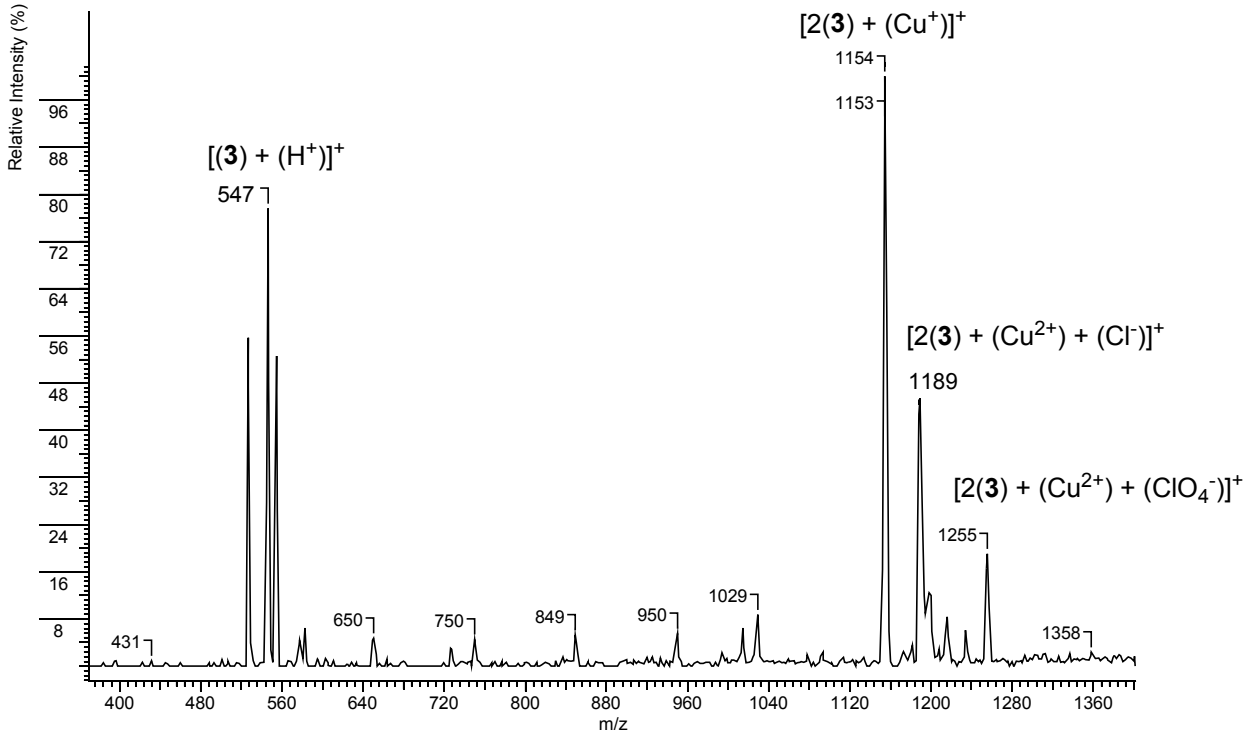


Fig. S9. ESI-MS of mixture ligand **3** with Cu^{2+}, ratio 3:1.

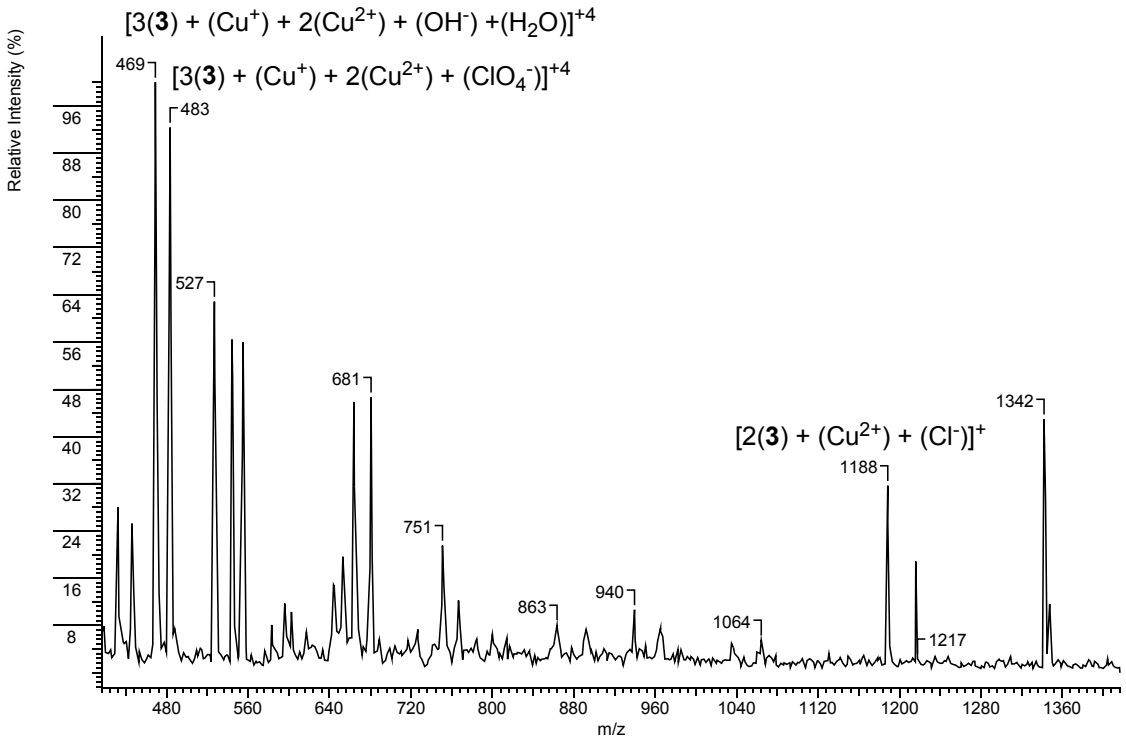


Fig. S10. ESI-MS of ligand **3** in the presence of 3-fold excess of $Cu(ClO_4)_2$.

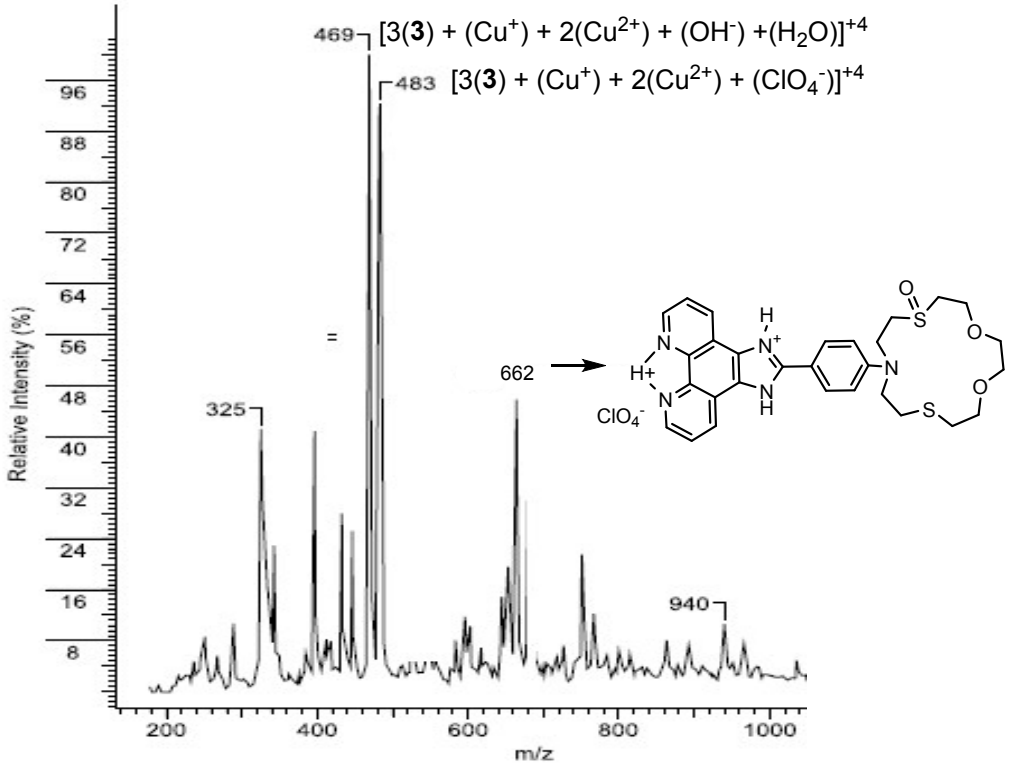


Fig. S11. ESI-MS of ligand **3** in the presence of 3-fold excess of $Cu(ClO_4)_2$ after keeping during 48 hours.

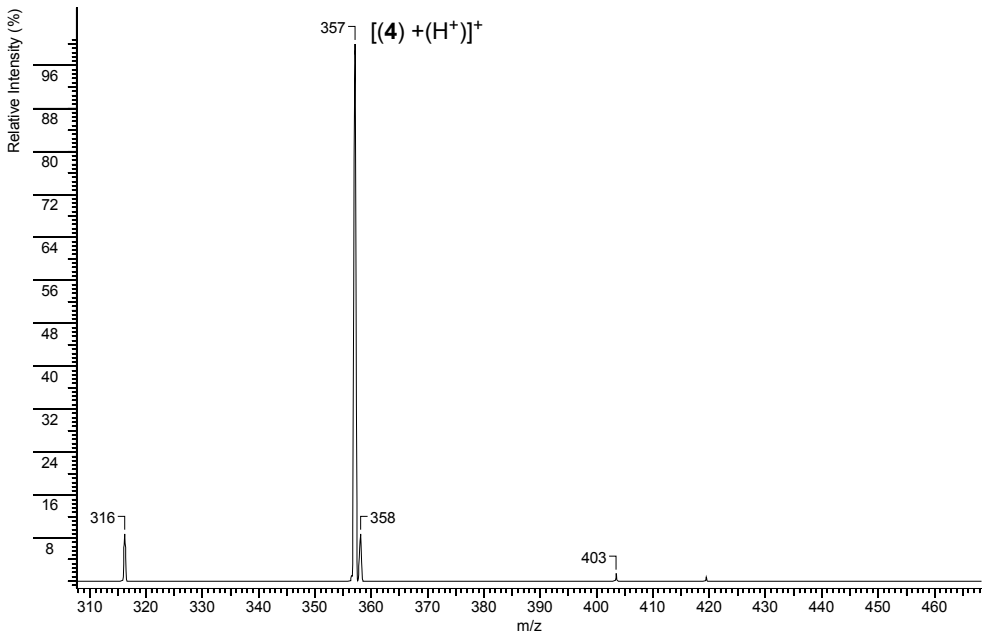


Fig. S12. ESI-MS of ligand **4**.

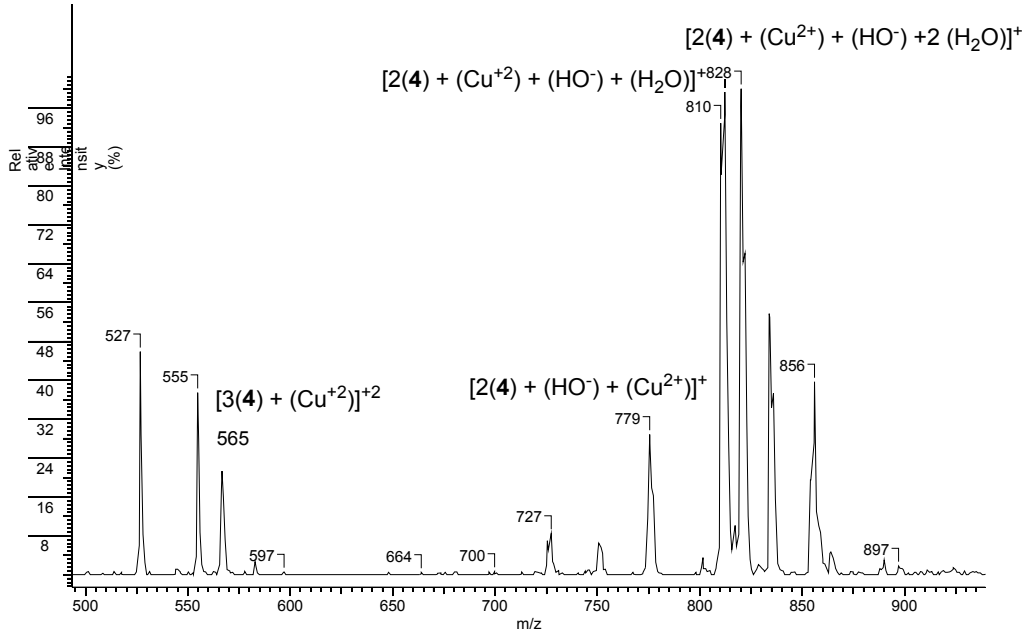


Fig. S13. ESI-MS of mixture ligand **4** with Cu^{2+}, ratio 3:1.

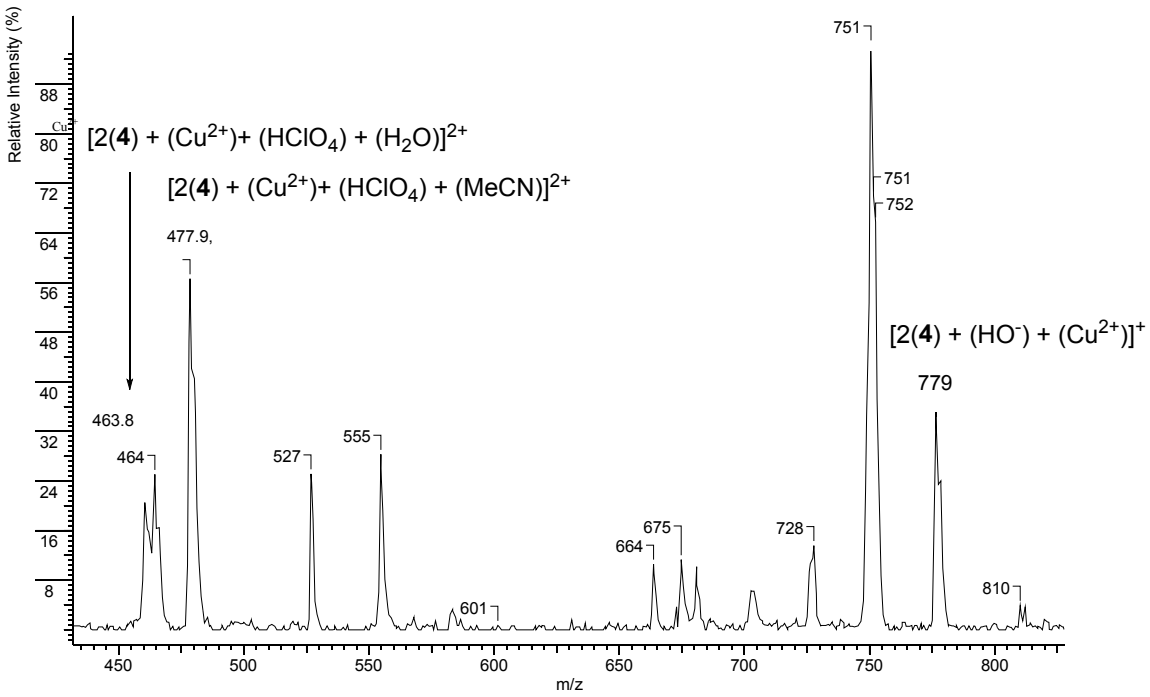


Fig. S14. ESI-MS of ligand **4** in the presence of 3-fold excess of $Cu(ClO_4)_2$.

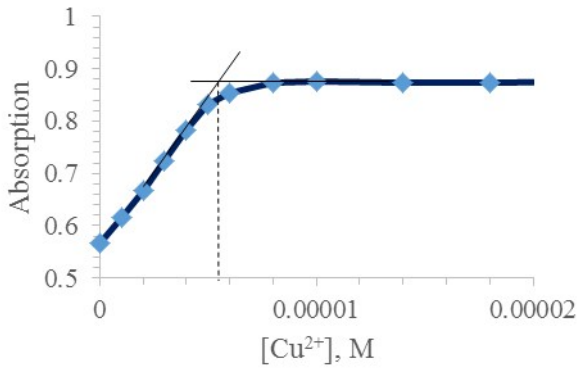


Fig. S15. The titration curve of ligand **1** (C_1 = 1.67•10^{-5} M) with copper (II) perchlorate at 280 nm in MeCN.

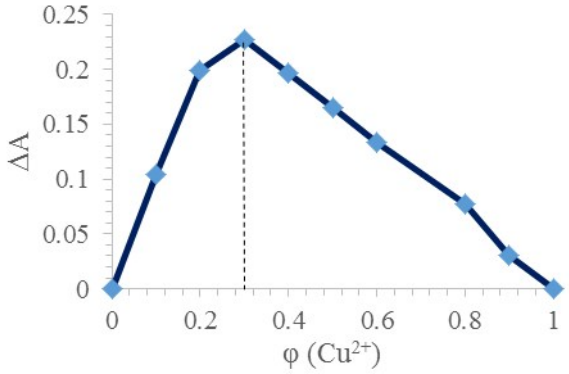


Fig. S16. Isomolar series of the **1** and Cu(II) solutions in MeCN (total concentration 1.67·10^{-5} M). φ - mole fraction of Cu^{2+}. A – absorption at 308 nm.

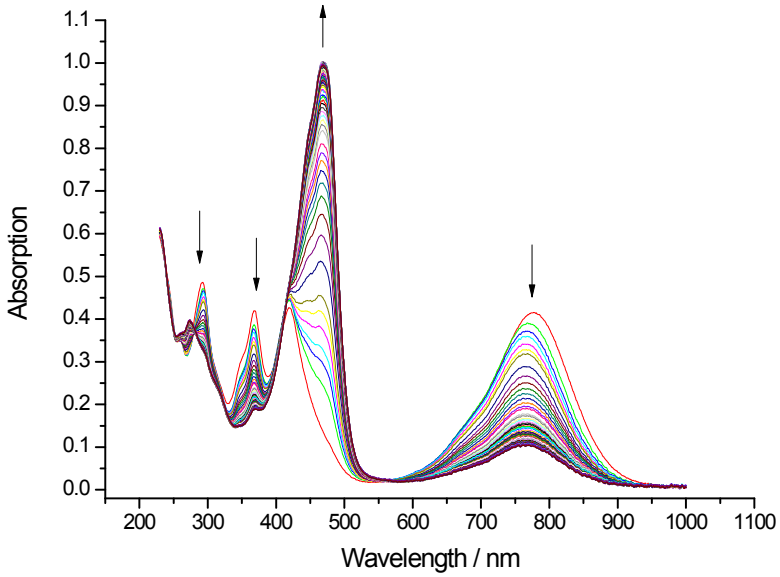


Fig.S17. Variation of electronic absorption spectra of 2×10^{-5} mol·L^{-1} **2** in the presence of 2×10^{-4} mol·L^{-1} $Cu(ClO_4)_2$ on time. Spectra were recorded during 80 min at intervals of 10-60 sec. Solvent – acetonitrile, T = 294K.

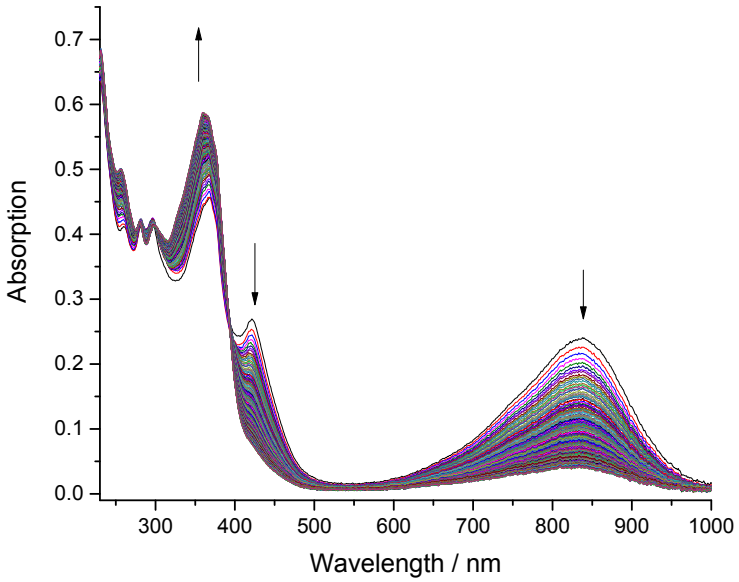


Fig. S18. Variation of electronic absorption spectra of 2×10^{-5} mol·L^{-1} **3** in the presence of 2×10^{-4} mol·L^{-1} $Cu(ClO_4)_2$ on time. Spectra were recorded during 40 min at intervals of 10 sec. Solvent – acetonitrile, T = 294K.

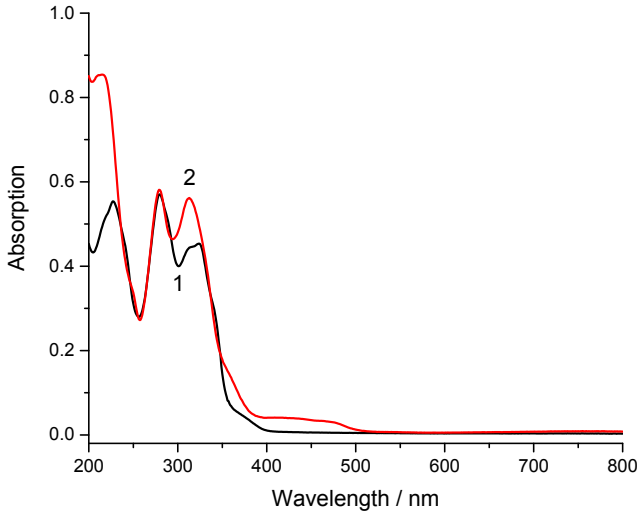


Fig. S19. Electronic absorption spectra of 2×10^{-5} mol·L^{-1} of **4** alone (1) and in the presence of 2×10^{-4} mol·L^{-1} (2) $Cu(ClO_4)_2$**.** Spectrum (2) was recorded in 30 sec after $Cu(ClO_4)_2$ addition. Solvent – acetonitrile, T = 294K.

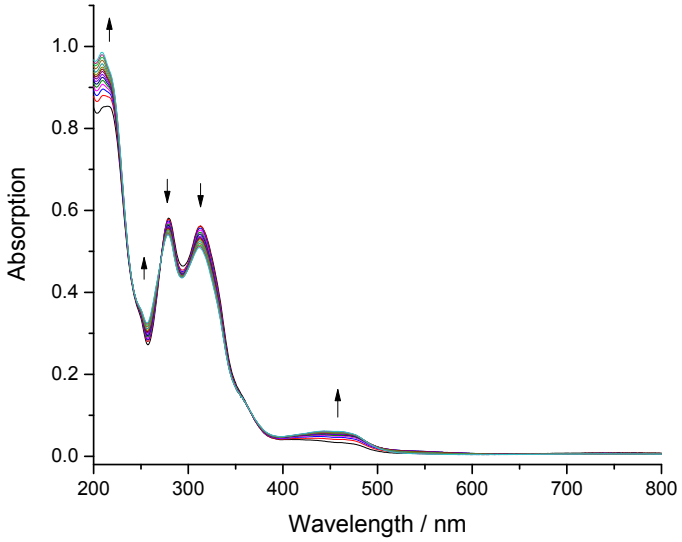


Fig. S20. Variation of electronic absorption spectra of 2×10^{-5} mol·L^{-1} **4** in the presence of 2×10^{-4} mol·L^{-1} $Cu(ClO_4)_2$ on time. Spectra were recorded during 48 min at intervals of 3 min. Solvent – acetonitrile, T = 294K.

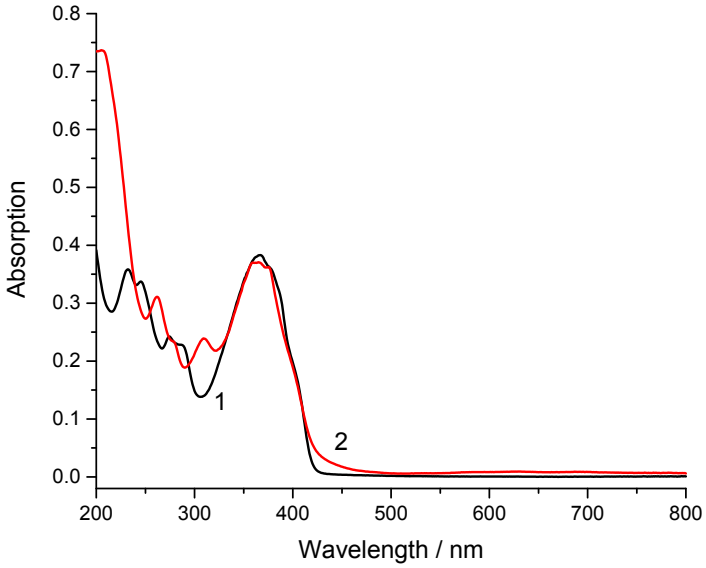


Fig. S21. Electronic absorption spectra of 2×10^{-5} mol·L^{-1} of **5** alone (1) and in the presence of 2×10^{-4} mol·L^{-1} (2) $Cu(ClO_4)_2$**.** Spectrum (2) was recorded in 30 sec after $Cu(ClO_4)_2$ addition. Solvent – acetonitrile, T = 294K.

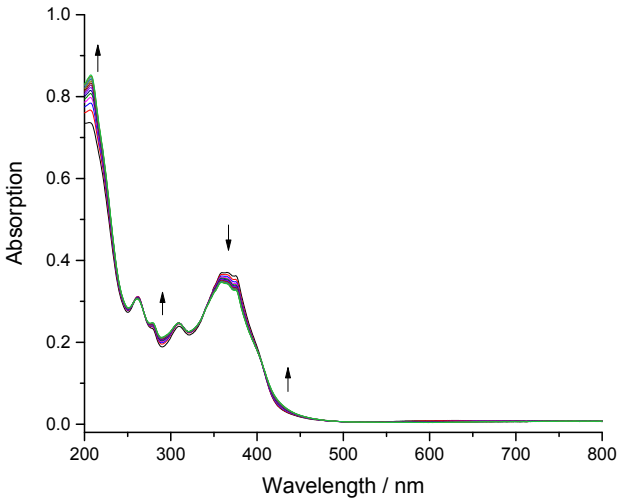


Fig. S22. Variation of electronic absorption spectra of 2×10^{-5} mol·L^{-1} **5** in the presence of 2×10^{-4} mol·L^{-1} $Cu(ClO_4)_2$ on time. Spectra were recorded during 42 min at intervals of 3 min. Solvent – acetonitrile, T = 294K.

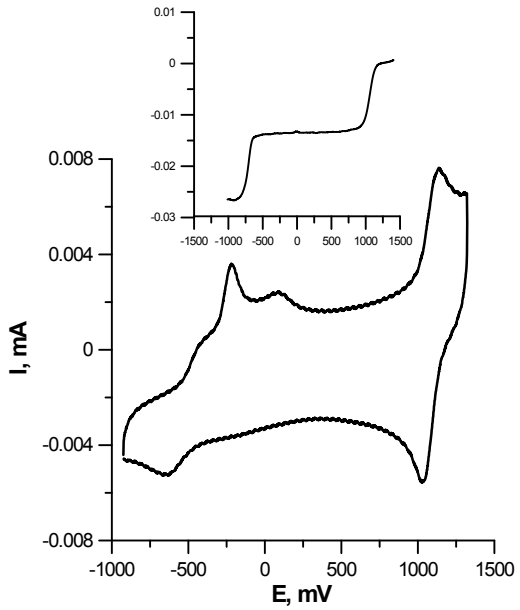


Fig. S23. Cyclic voltammogram of $1.67 \cdot 10^{-4}$M solution of $Cu(ClO_4)_2 \cdot 6H_2O$ in CH_3CN. Inset Scan rate dependence of Cu^{2+}/Cu^{+} redox couple obtained on a rotating disk electrode.

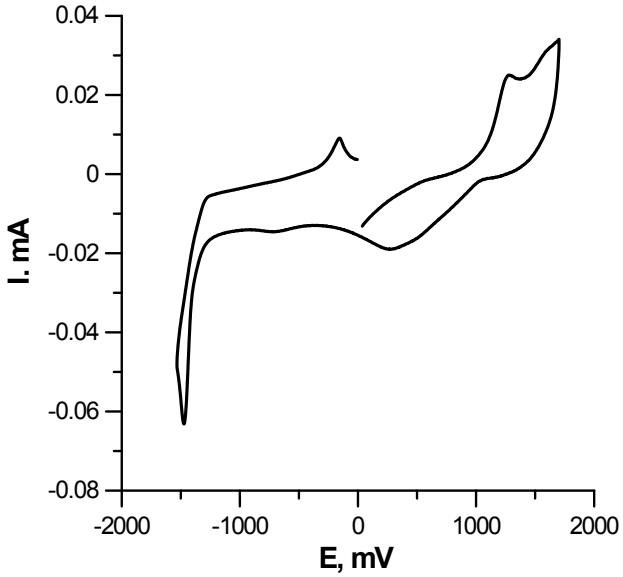


Fig. S24. Cyclic voltammogram of $1.67 \cdot 10^{-4}$M solution of ligand **3** in the presence of 3-fold excess of copper(II) in 0.1 M TBAP in MeCN at 100 mV/s.

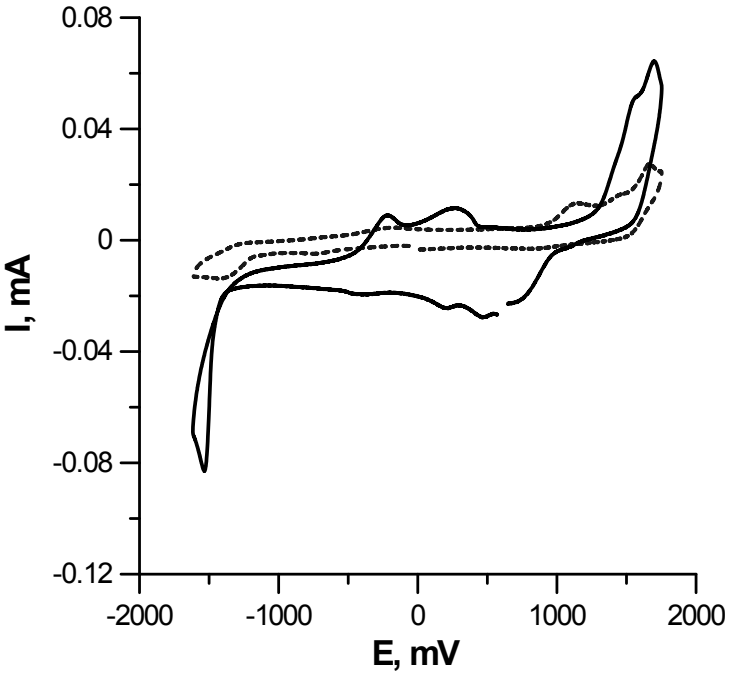


Fig. S25. Cyclic voltammogram of $1.67 \cdot 10^{-4}$M solution of ligand **1** (dashed line) and in the presence of 3-fold excess of copper(II) (solid line) recorded after keeping for 4 hours in 0.1 M TBAP in MeCN at 100 mV/s.

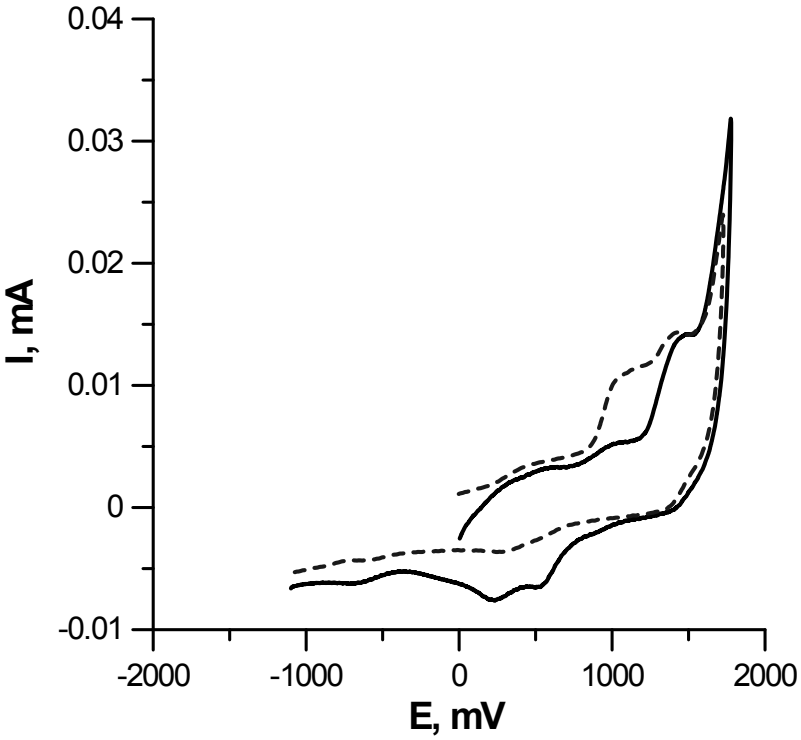


Fig. S26. Cyclic voltammogram of $1.67 \cdot 10^{-4}$M solution of ligand **4** (dashed line) and in the presence of 3-fold excess of copper(II) (solid line) recorded after keeping for 4 hours in 0.1 M TBAP in MeCN at 100 mV/s.

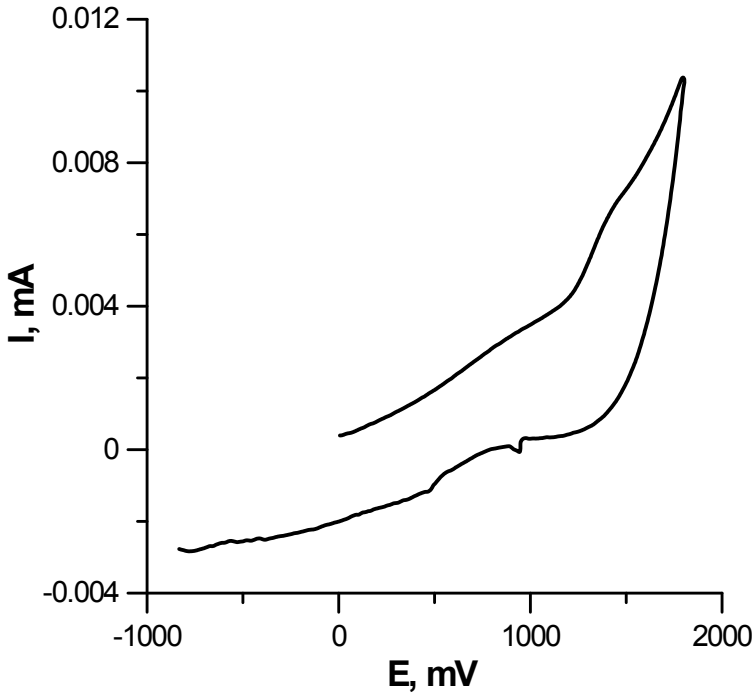


Fig. S27. Cyclic voltammogram of $1.67 \cdot 10^{-4}$M solution of ligand **5** in 0.1 M TBAP in MeCN at 100 mV/s. The measurement is accompanied by radical polymerization of thiophene derivative on electrode which makes electrochemical analysis ddifficult.

Mode of complexation of 2 with Cu(II)

The methodology level used in our calculations have been tested with a model compounds consisting of copper complexed with two phenanthroline ligand ($Cu(phen)_2$). In order to check the accuracy of our DFT calculation based on PBEPB1 functional, 6-31G(d) and LanL2DZ basis set, we have optimized the structures of $Cu(phen)_2^{2+}$, and $Cu(phen)_2^{+}$ and compared them with the available experimental and theoretical data [Cu-phen]. The optimized geometries are displayed found in **Figure S28** and are found in very good agreement with previous experimental findings [1].

[1] Howell, S. L.; Gordon, K. C. J. Phys. Chem. A 2004, 108, 2536-2544; Chen, L. X.; Shaw, G. B.; Novozhilova, I.; Liu, T.; Jennings, G.; Attenkofer, K.; Meyer, G. J.; Coppens, P. J. Am. Chem. Soc. 2003, 125, 7022-7034; Philip Coppens, I. V. N. Int. J. Quantum Chem. 2005, 101, 611-623; Wang, X. J.; Wang, W.; Koyama, M.; Kubo, M.; Miyamoto, A. J. Photochem. Photobiol., A 2006, 179, 149-155.

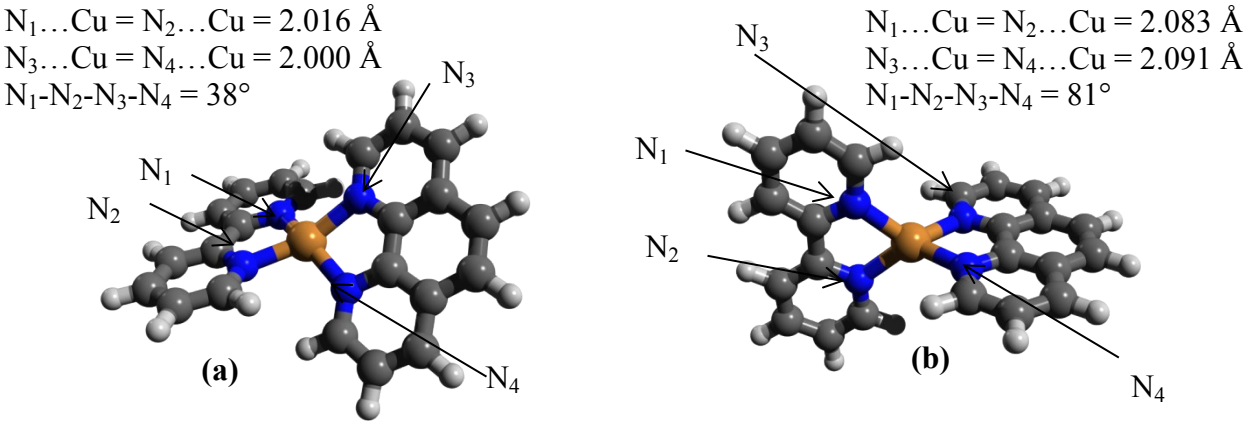


Fig. S28. The optimized structure of (a) $Cu(phen)_2^{2+}$ and (b) $Cu(phen)_2^{+}$.

Table S1. Selected bond lengths and dihedral angles of the complexes $\mathbf{2_2}$·$Cu^{2+}(Phen_2)$, $\mathbf{2_2}$·$Cu^{2+}(PhenIm_2)$, $\mathbf{2_2}$·$Cu^{2+}(Im_4)$, $\mathbf{2_2}$·$Cu^{+}(Phen_2)$, $\mathbf{2_2}$·$Cu^{+}(PhenIm_2)$ and $\mathbf{2_2}$·$Cu^{+}(Im_4)$.

	$\mathbf{2_2}$·$Cu^{2+}(Phen_2)$	$\mathbf{2_2}$·$Cu^{2+}(PhenIm_2)$	$\mathbf{2_2}$·$Cu^{2+}(Im_4)$
Cu-N1	2.088	2.024	2.109
Cu-N2	2.081	2.036	2.126
Cu-N3	2.085	2.014	2.109
Cu-N3	2.100	2.026	2.126
NN-NN angle	80.8°	26.2°	1.6°
	$\mathbf{2_2}$·$Cu^{+}(Phen_2)$	$\mathbf{2_2}$·$Cu^{+}(PhenIm_2)$	$\mathbf{2_2}$·$Cu^{+}(Im_4)$
Cu-N1	2.093	2.184	1.922
Cu-N2	2.084	2.198	1.922
Cu-N3	2.084	2.124	4.456
Cu-N3	2.093	2.133	4.4525
NN-NN angle	81.2	49.5	3.7

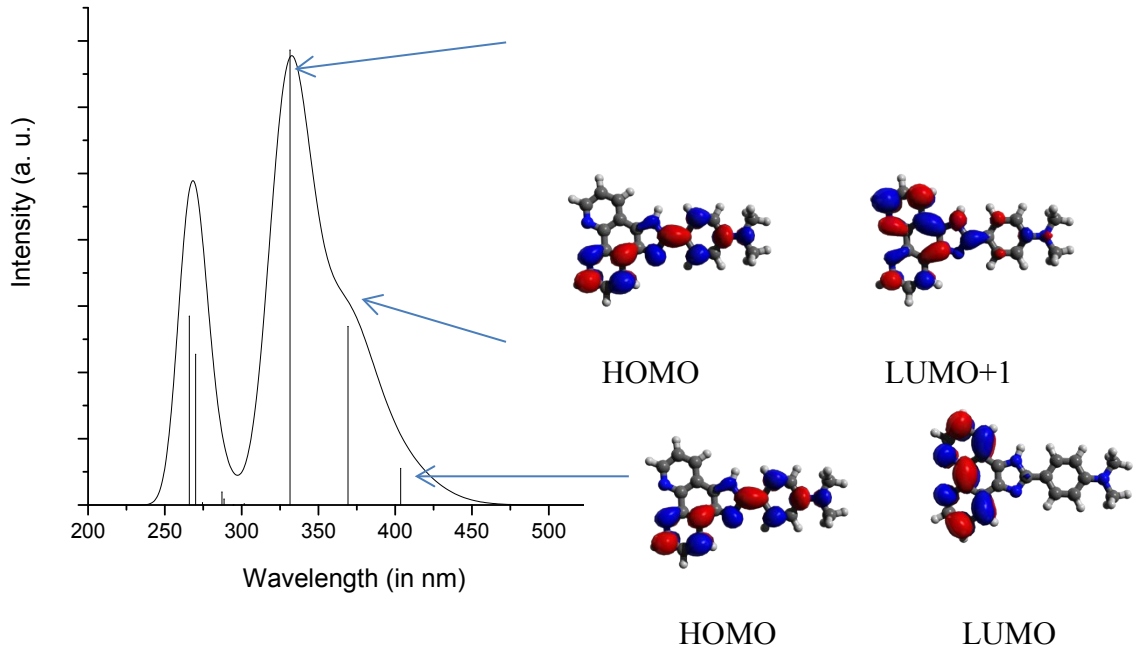


Figure S29. Calculated absorption spectrum of compound **2** representing main orbitals implied in the electronic excitations.

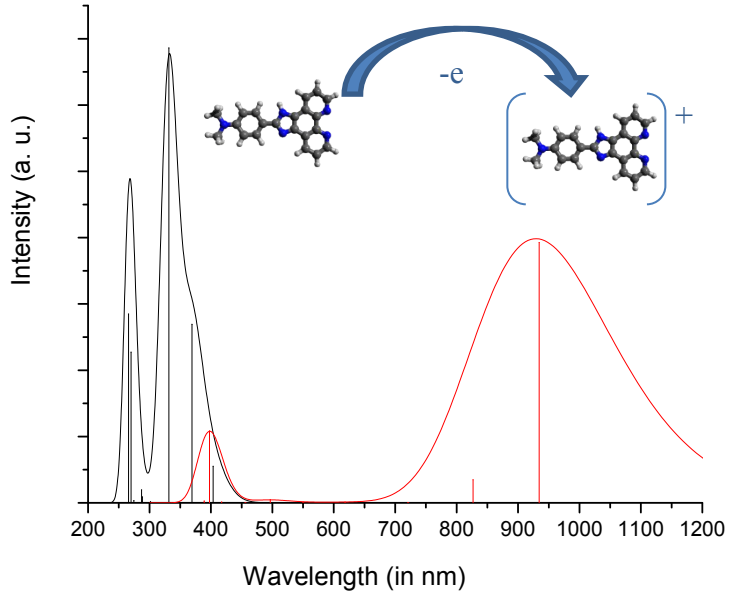


Figure S30. Comparison of the calculated absorption spectra of **2** in neutral (black curve) and cationic states (red curve).

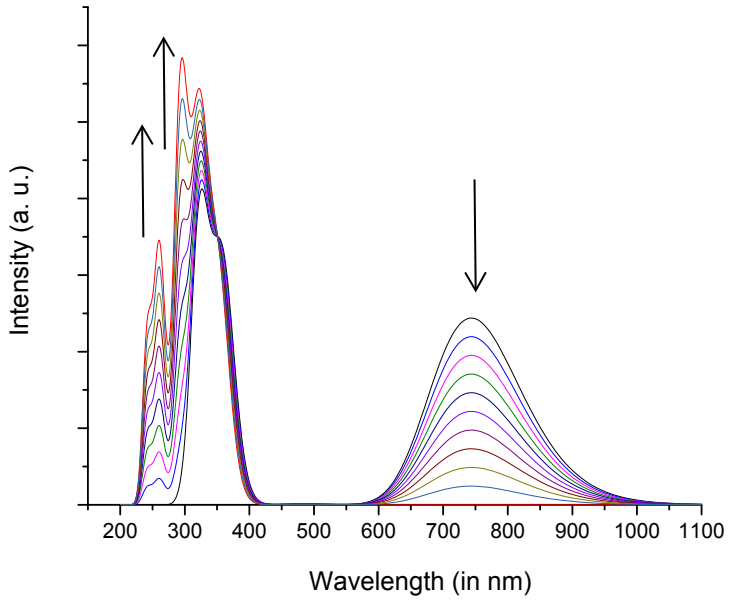


Figure S31. Expected evolution of the absorption spectra obtained from the reduction of the 2_2-Cu^{2+} complex. The spectra were obtained by summing the spectra of using the equation 2_2-Cu^{2+} and 2_2-Cu^{2+} using the following equation: 1-x (2_2-Cu^{2+}) + x 2_2-Cu^{+} ($0 \leq x \leq 1$). The black arrow displays the expected evolution of the absorption spectrum upon reduction of the 2_2-Cu^{2+} complex.

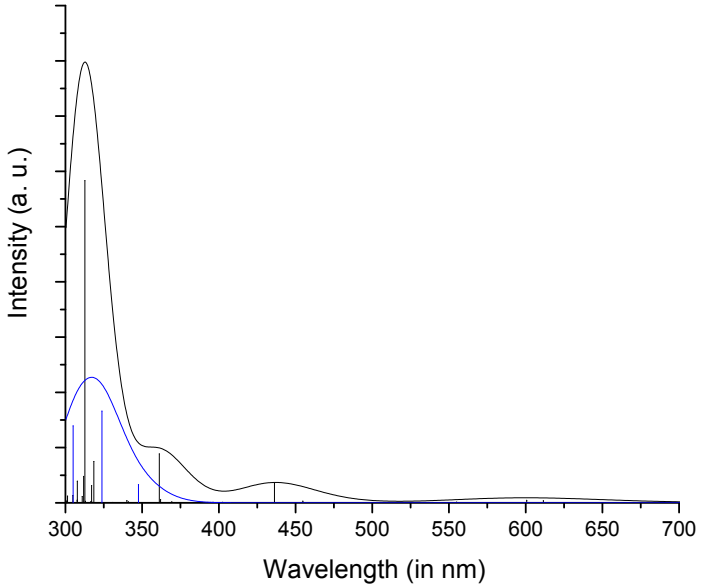
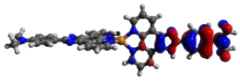
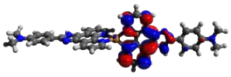
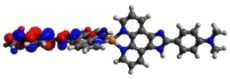
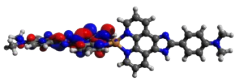
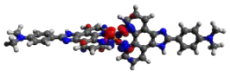
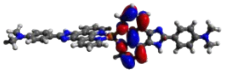
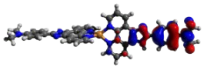
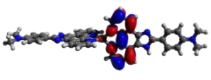
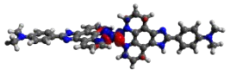
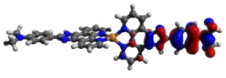
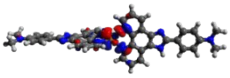
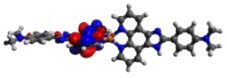


Figure S32. B3LYP calculated absorption spectra of ligand **1** (blue curve) and the complexes Cu^{2+}(1-Phen)$_2$ (black curve).

Figure S33 Main calculated molecular orbitals implied in the lowest allowed electronic transitions for $Cu^{2+}(2)_2$ and $Cu^{+}(2)_2$ complexes (B3LYP level of calculations).

$Cu^{2+}(\mathbf{2})_2$			
			
H(α)	L+4(α)	H(β)	L+2(β)
			
H-1(α)	L+2(α)	H-1(β)	L+1(β)
			
H-2(α)	L(α)	H-2(β)	L(β)

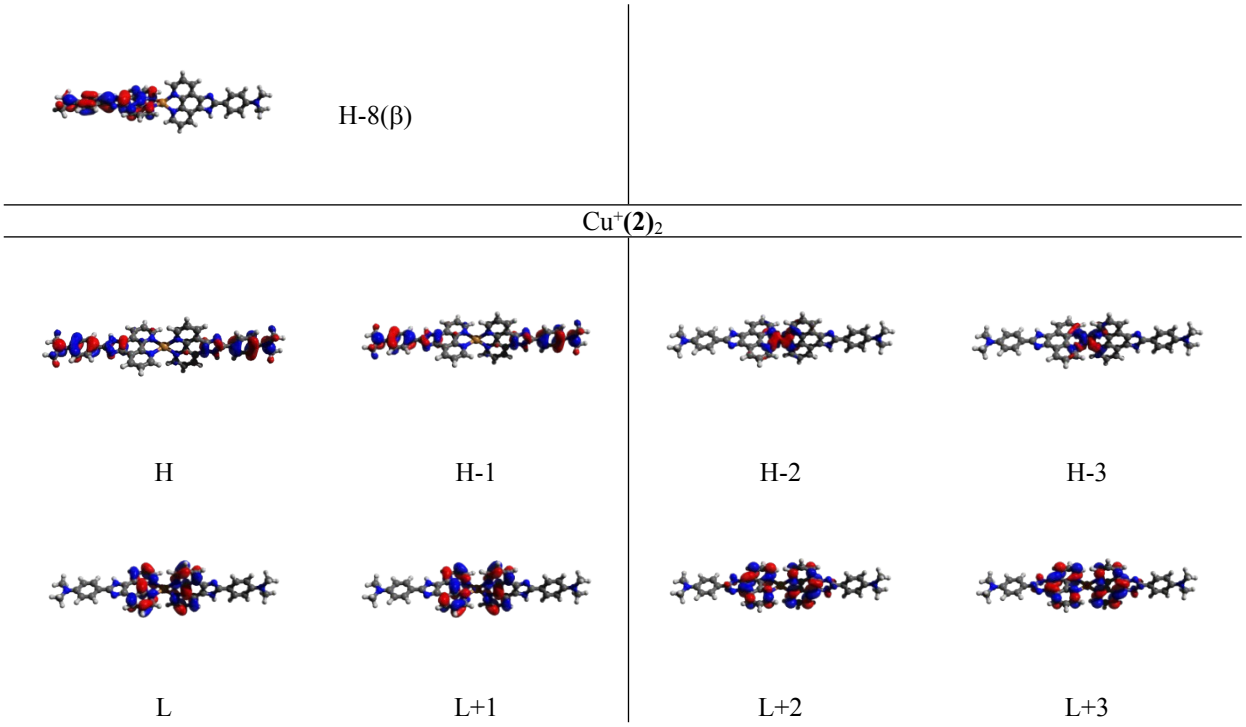


Table S2. Selected computed UV-vis energies transitions in acetonitrile for $Cu^{2+}(2\text{-Phen})_2$ complex.

States	λ_{calc} (nm)	Oscillator strength (*f*)	Assignment*	Character**
B3LYP				
S_8	751	0.599	H-7(β)→L(β)	MLCT
S_{21}	479	0.221	H-1(α)→L(α), H(α)→L+2(α), H-2(β)→L+2(β)	MLCT + π→π*
S_{22}	479	0.134	H-2(α)→L+2(α), HOMO(α)→L+4(α), HOMO(β)→L+2(β)	MLCT
S_{26}	465	0.028	H-1(α)→LUMO(α), HOMO(α)→L+2(α), H-1(β)→L+1(β)	π→π*
M062X				
S_2	743	0.673	H-3(β)→LUMO(β), H-2(β)→LUMO(β)	MLCT
S_{13}	361	0.575	H-1(α)→LUMO(α), H-1(α)→L+1(α)	π→π*
S_{14}	351	0.245	HOMO(α)→L+2(α) (37%), HOMO(β)→L+2(β) (37%)	π→π*
S_{23}	327	0.403	H-7(α)→LUMO(α) (12%), H-	π→π*

			1(α)->L+1(α) (13%), H-1(α)->L+3(α) (16%)	
S_{24}	322	0.567	HOMO(α)→L+4(α) (37%), HOMO(β)→L+4(β) (37%)	π→π*
MPW1PW91				
S_4	782	0.616	H-5(β)→LUMO(β) (92%)	MLCT
S_{19}	447	0.203	HOMO(α)→L+2(α) (43%), HOMO(β)→L+2(β) (44%)	
S_{26}	423	0.241	H-1(α)→LUMO(α) (30%), H-1(β)→L+1(β) (39%)	

* H=HOMO, L=LUMO ** MLCT = ligand to metal charge transfer

Table S3. Selected computed UV-vis energies transitions in acetonitrile for $Cu^{+}(2\text{-Phen})_2$ complex.

States	λ_{calc} (nm)	Oscillator strength (*f*)	Assignment		Character*
B3LYP					
S_2	475	0.252	H-1→L+1	HOMO->LUMO	
S_7	436	0.325	H-3→LUMO	H-2→L+1	
S_8	406	0.309	H-1→L+2	HOMO→L+3	
M062X					
S_1	352	0.772	H-1→L+1	HOMO→LUMO	
S_5	322	1.262	H-1→L+2	HOMO→L+3	
S_7	294	1.471	H-1→L+4	HOMO→L+5	
MPW1PW91					
S_2	446	0.338	H-1→L+1	HOMO→LUMO	
S_8	385	0.4202	H-1→L+2	HOMO→L+3	

Cartesian coordinates of the optimized studied complexes

$Cu^{2+}(Phen)_2$

1	29	0	0.035996	0.042548	-0.060468
2	7	0	0.049241	0.568051	1.886112
3	6	0	1.238845	0.279426	2.466037
4	6	0	-0.933958	1.053856	2.632802
5	6	0	2.249163	-0.294272	1.634997
6	6	0	1.499366	0.517957	3.828120
7	1	0	-1.880445	1.246702	2.138456
8	6	0	-0.771153	1.310081	4.001637
9	6	0	3.520833	-0.577642	2.166594
10	7	0	1.924126	-0.538567	0.342928
11	6	0	0.445741	1.054248	4.597189
12	6	0	2.795771	0.207044	4.350951
13	1	0	-1.603465	1.710718	4.568529
14	6	0	4.480484	-1.111176	1.281375
15	6	0	3.768251	-0.311911	3.551822
16	6	0	2.848349	-1.022638	-0.476658
17	1	0	0.599626	1.256276	5.653133
18	6	0	4.146631	-1.321619	-0.039693
19	1	0	5.475987	-1.346840	1.645996
20	1	0	2.558387	-1.179294	-1.510479
21	1	0	4.865515	-1.718930	-0.746777
22	7	0	-1.344681	1.249591	-0.858110

23	6	0	-1.631420	2.485141	-0.438685
24	6	0	-1.898794	0.770863	-1.991714
25	6	0	-2.519430	3.305728	-1.121143
26	1	0	-1.128802	2.822617	0.461316
27	6	0	-2.796289	1.539243	-2.725125
28	6	0	-1.464736	-0.585481	-2.374980
29	6	0	-3.113694	2.818131	-2.278942
30	1	0	-2.729608	4.301301	-0.748153
31	6	0	-2.012023	-1.311684	-3.427076
32	7	0	-0.483261	-1.109034	-1.610862
33	1	0	-3.812714	3.429266	-2.840375
34	6	0	-1.539029	-2.595110	-3.680989
35	6	0	-0.041833	-2.349097	-1.839130
36	6	0	-0.542489	-3.129144	-2.872834
37	1	0	-1.956008	-3.173666	-4.498744
38	1	0	0.725276	-2.723639	-1.169968
39	1	0	-0.156910	-4.129834	-3.029070
40	1	0	-2.804428	-0.893885	-4.036002
41	1	0	-3.235733	1.157404	-3.638547
42	1	0	4.750886	-0.537419	3.954235
43	1	0	2.989057	0.398138	5.401895

$Cu^{+}(Phen)_2$

1	29	0	0.040666	0.041590	-0.055050
2	7	0	-0.010554	0.013663	2.034912
3	6	0	1.233276	-0.004965	2.568907
4	6	0	-1.052306	0.014487	2.855032
5	6	0	2.354523	-0.004969	1.663743
6	6	0	1.464469	-0.023639	3.962404
7	1	0	-2.033555	0.028962	2.389562
8	6	0	-0.924846	-0.002017	4.252422
9	6	0	3.667879	-0.027296	2.183580
10	7	0	2.094902	0.016393	0.335308
11	6	0	0.336327	-0.021246	4.807260
12	6	0	2.808570	-0.044926	4.455803
13	1	0	-1.814601	0.000302	4.872648
14	6	0	4.731632	-0.027808	1.258967
15	6	0	3.866735	-0.047109	3.601532
16	6	0	3.116277	0.016240	-0.510037
17	1	0	0.472784	-0.034766	5.885101
18	6	0	4.455301	-0.006111	-0.090827
19	1	0	5.756403	-0.045070	1.619641
20	1	0	2.868266	0.034463	-1.567337
21	1	0	5.249225	-0.005747	-0.829768
22	7	0	-0.952383	1.400809	-1.281877
23	6	0	-0.886606	2.733085	-1.207438
24	6	0	-1.714925	0.831299	-2.234609
25	6	0	-1.573256	3.573015	-2.075467
26	1	0	-0.257361	3.136391	-0.419571
27	6	0	-2.434430	1.607985	-3.144708
28	6	0	-1.735356	-0.653583	-2.250174
29	6	0	-2.361838	2.993173	-3.063169
30	1	0	-1.487515	4.649473	-1.974787
31	6	0	-2.489336	-1.390866	-3.165123
32	7	0	-0.977233	-1.263755	-1.319334
33	1	0	-2.915760	3.609213	-3.764675
34	6	0	-2.454279	-2.778933	-3.113152
35	6	0	-0.946569	-2.598611	-1.274132
36	6	0	-1.667734	-3.400893	-2.149754
37	1	0	-3.035963	-3.364602	-3.818192

38	1	0	-0.317932	-3.035560	-0.503919
39	1	0	-1.610224	-4.481184	-2.072844
40	1	0	-3.099965	-0.897494	-3.911703
41	1	0	-3.045541	1.147269	-3.911485
42	1	0	4.884306	-0.063761	3.981275
43	1	0	2.965194	-0.059513	5.530599

Ligand 2

1	6	0	-0.025048	0.141939	0.037442
2	6	0	-0.025884	0.180606	1.440579
3	6	0	2.264006	0.079771	1.563181
4	6	0	2.371641	0.036462	0.142861
5	6	0	1.186032	0.069358	-0.614383
6	6	0	3.469007	0.047052	2.397959
7	6	0	4.395396	0.060907	4.495949
8	1	0	4.228099	0.097016	5.571877
9	6	0	5.706290	-0.011355	3.997046
10	6	0	5.882757	-0.055880	2.631738
11	6	0	4.753073	-0.027211	1.796779
12	6	0	4.834604	-0.068802	0.369216
13	6	0	3.683743	-0.037453	-0.404364
14	1	0	-0.959964	0.168958	-0.513023
15	1	0	-0.970398	0.238351	1.979960
16	1	0	1.224860	0.037635	-1.699792
17	1	0	6.550891	-0.031089	4.678651
18	1	0	6.871081	-0.112384	2.185063
19	7	0	3.313746	0.089477	3.736328
20	7	0	1.069357	0.151108	2.180743
21	6	0	5.502454	-0.153344	-1.662326
22	7	0	5.951458	-0.140545	-0.414792
23	7	0	4.133011	-0.092829	-1.698645
24	1	0	3.562567	-0.076807	-2.530374
25	6	0	6.343148	-0.221023	-2.847581
26	6	0	7.738463	-0.229319	-2.700332
27	6	0	5.831451	-0.282163	-4.151252
28	6	0	8.583866	-0.290586	-3.791272
29	1	0	8.156151	-0.186070	-1.698940
30	6	0	6.664179	-0.343930	-5.255145
31	1	0	4.758864	-0.288722	-4.329656
32	6	0	8.071238	-0.345677	-5.109859
33	1	0	9.654430	-0.294906	-3.621080
34	1	0	6.216328	-0.393998	-6.240836
35	7	0	8.900398	-0.397708	-6.195022
36	6	0	8.344901	-0.490316	-7.526795
37	1	0	9.157599	-0.503877	-8.253543
38	1	0	7.751877	-1.405520	-7.662503
39	1	0	7.701892	0.369433	-7.756347
40	6	0	10.333734	-0.443318	-6.008578
41	1	0	10.820309	-0.478034	-6.983647
42	1	0	10.701426	0.445996	-5.479957
43	1	0	10.645979	-1.330727	-5.440788

Ligand 1

1	7	0	3.918379	-1.287974	-0.007701
2	6	0	3.975994	-2.609103	-0.013287
3	6	0	2.709493	-0.695375	-0.003885
4	6	0	2.847645	-3.443385	-0.015489
5	1	0	4.973018	-3.047427	-0.016130
6	6	0	1.504593	-1.454182	-0.006294
7	6	0	2.663435	0.771507	0.003200

8	6	0	1.601076	-2.857222	-0.012075
9	1	0	2.962534	-4.522455	-0.019687
10	6	0	0.281459	-0.722804	-0.002131
11	6	0	1.416132	1.447937	0.007586
12	7	0	3.833064	1.440405	0.005317
13	1	0	0.705017	-3.471644	-0.013462
14	6	0	0.219306	0.663356	0.004687
15	7	0	-1.025454	-1.130745	-0.002755
16	6	0	1.414937	2.852485	0.013784
17	6	0	3.800984	2.762255	0.011184
18	7	0	-1.076949	1.093754	0.007736
19	6	0	-1.809573	-0.008109	0.002448
20	1	0	-1.353109	-2.084882	-0.019250
21	6	0	2.619445	3.520990	0.015469
22	1	0	0.467278	3.382904	0.016937
23	1	0	4.766720	3.266276	0.012560
24	6	0	-3.271419	-0.033066	0.001834
25	1	0	2.665582	4.605443	0.019990
26	6	0	-3.962402	1.185826	-0.050312
27	6	0	-4.003307	-1.226568	0.052579
28	6	0	-5.350708	1.208484	-0.053100
29	1	0	-3.391247	2.107876	-0.089048
30	6	0	-5.393903	-1.198912	0.048571
31	1	0	-3.501970	-2.189391	0.100804
32	6	0	-6.072876	0.016328	-0.004452
33	1	0	-5.872409	2.160579	-0.094418
34	1	0	-5.947553	-2.132576	0.088832
35	1	0	-7.159012	0.034565	-0.007197

Cu^{2+}(2-Phen)$_2$

1	29	0	-0.000034	0.048212	-0.000154
2	7	0	-1.619832	-0.889001	-0.922497
3	6	0	-2.812443	-0.446769	-0.465369
4	6	0	-1.604464	-1.830814	-1.858509
5	6	0	-2.793463	0.584582	0.561801
6	6	0	-4.033585	-0.957235	-0.955943
7	1	0	-0.624843	-2.157638	-2.195341
8	6	0	-2.768786	-2.391237	-2.400262
9	6	0	-4.000071	1.106195	1.099196
10	7	0	-1.585529	1.018384	0.977979
11	6	0	-3.994796	-1.951571	-1.945983
12	6	0	-5.244868	-0.424539	-0.408536
13	1	0	-2.692186	-3.158158	-3.163764
14	6	0	-3.903408	2.099524	2.090635
15	6	0	-5.208228	0.564805	0.576492
16	6	0	-1.521344	1.957153	1.914794
17	1	0	-4.927254	-2.352263	-2.331349
18	7	0	-6.519508	-0.756790	-0.721530
19	6	0	-2.658426	2.526841	2.500816
20	1	0	-4.799014	2.528267	2.532049
21	7	0	-6.521281	0.823248	0.853249
22	1	0	-0.526126	2.271728	2.215079
23	6	0	-7.284731	0.006068	0.049728
24	1	0	-2.549335	3.290423	3.263500
25	1	0	-6.871941	1.490551	1.522510
26	6	0	-8.727983	-0.017619	0.046689
27	6	0	-9.388068	-0.902252	-0.830555
28	6	0	-9.516529	0.800107	0.877900
29	6	0	-10.759326	-0.970000	-0.879108
30	1	0	-8.786560	-1.535738	-1.473893
31	6	0	-10.891354	0.745084	0.842021
32	1	0	-9.057829	1.498804	1.572885

33	6	0	-11.560472	-0.145477	-0.041758
34	1	0	-11.224183	-1.664340	-1.568368
35	1	0	-11.458661	1.392287	1.499633
36	7	0	-12.914353	-0.205656	-0.083885
37	6	0	-13.717679	0.643867	0.777712
38	6	0	-13.582504	-1.122321	-0.991457
39	1	0	-14.772809	0.448094	0.591715
40	1	0	-13.513241	0.440237	1.835494
41	1	0	-13.526032	1.704462	0.576553
42	1	0	-14.660444	-1.019740	-0.874429
43	1	0	-13.328064	-0.900729	-2.034542
44	1	0	-13.311086	-2.161854	-0.773300
45	7	0	1.585584	1.018551	-0.978039
46	6	0	1.521435	1.957772	-1.914402
47	6	0	2.793500	0.584833	-0.561737
48	6	0	2.658546	2.528016	-2.499830
49	1	0	0.526230	2.272270	-2.214810
50	6	0	4.000131	1.106856	-1.098676
51	6	0	2.812429	-0.446810	0.465140
52	6	0	3.903514	2.100685	-2.089617
53	1	0	2.549490	3.292027	-3.262089
54	6	0	5.208262	0.565336	-0.576051
55	6	0	4.033549	-0.957282	0.955764
56	7	0	1.619792	-0.889320	0.921924
57	1	0	4.799141	2.529842	-2.530584
58	6	0	5.244859	-0.424330	0.408656
59	7	0	6.521325	0.823959	-0.852580
60	6	0	3.994705	-1.951894	1.945524
61	6	0	1.604372	-1.831419	1.857649
62	7	0	6.519488	-0.756642	0.721634
63	6	0	7.284742	0.006474	-0.049337
64	1	0	6.871997	1.491030	-1.522065
65	6	0	2.768666	-2.391850	2.399451
66	1	0	4.927142	-2.352589	2.330937
67	1	0	0.624727	-2.158530	2.194132
68	6	0	8.727992	-0.017294	-0.046345
69	1	0	2.692027	-3.159018	3.162701
70	6	0	9.388050	-0.902735	0.830102
71	6	0	9.516561	0.801018	-0.876961
72	6	0	10.759304	-0.970711	0.878452
73	1	0	8.786521	-1.536714	1.472936
74	6	0	10.891382	0.745791	-0.841258
75	1	0	9.057883	1.500371	-1.571301
76	6	0	11.560473	-0.145594	0.041709
77	1	0	11.224136	-1.665705	1.567068
78	1	0	11.458708	1.393441	-1.498413
79	7	0	12.914350	-0.205977	0.083646
80	6	0	13.717695	0.644079	-0.777413
81	6	0	13.582479	-1.123767	0.990096
82	1	0	14.772823	0.448446	-0.591258
83	1	0	13.513512	0.440887	-1.835333
84	1	0	13.525812	1.704542	-0.575810
85	1	0	14.660417	-1.021377	0.872888
86	1	0	13.328395	-0.903175	2.033481
87	1	0	13.310695	-2.162998	0.770951

Cu^{2+}(1-Phen)$_2$

1	29	0	0.000000	0.000000	0.189881
2	7	0	1.505000	-1.245823	-0.285432
3	6	0	2.713900	-0.654895	-0.134197
4	6	0	1.431877	-2.469598	-0.794344

5	6	0	2.719622	0.690142	0.378782
6	6	0	3.911402	-1.318563	-0.462892
7	1	0	0.440648	-2.891633	-0.921552
8	6	0	2.575862	-3.192346	-1.158194
9	6	0	3.926787	1.384269	0.623996
10	7	0	1.512748	1.250917	0.620250
11	6	0	3.819232	-2.621376	-0.983935
12	6	0	5.130818	-0.605753	-0.242853
13	1	0	2.465581	-4.190080	-1.567016
14	6	0	3.831008	2.676841	1.176374
15	6	0	5.119809	0.685570	0.284039
16	6	0	1.440405	2.465780	1.150014
17	1	0	4.727018	-3.155259	-1.245971
18	7	0	6.402404	-1.023809	-0.482256
19	6	0	2.588672	3.209768	1.448190
20	1	0	4.726317	3.249820	1.395930
21	7	0	6.436993	1.038144	0.357295
22	1	0	0.449290	2.860279	1.347024
23	6	0	7.176118	-0.014021	-0.114020
24	1	0	2.485735	4.197052	1.883065
25	1	0	6.800946	1.927659	0.666562
26	6	0	8.634581	-0.012194	-0.200832
27	6	0	9.267965	-1.101706	-0.815168
28	6	0	9.414217	1.035172	0.307164
29	6	0	10.652074	-1.139222	-0.921196
30	1	0	8.658634	-1.910107	-1.206230
31	6	0	10.799838	0.992996	0.197229
32	1	0	8.956343	1.887822	0.800827
33	6	0	11.422797	-0.091808	-0.416854
34	1	0	11.131843	-1.987687	-1.400516
35	1	0	11.393650	1.810212	0.595878
36	7	0	-1.512749	-1.250940	0.620271
37	6	0	-1.440417	-2.465807	1.150017
38	6	0	-2.719624	-0.690130	0.378850
39	6	0	-2.588691	-3.209776	1.448229
40	1	0	-0.449306	-2.860339	1.346980
41	6	0	-3.926792	-1.384242	0.624089
42	6	0	-2.713897	0.654909	-0.134110
43	6	0	-3.831021	-2.676822	1.176456
44	1	0	-2.485753	-4.197063	1.883095
45	6	0	-5.119816	-0.685533	0.284164
46	6	0	-3.911398	1.318590	-0.462782
47	7	0	-1.504992	1.245838	-0.285362
48	1	0	-4.726338	-3.249780	1.396036
49	6	0	-5.130817	0.605791	-0.242733
50	7	0	-6.436998	-1.038100	0.357417
51	6	0	-3.819231	2.621406	-0.983824
52	6	0	-1.431875	2.469609	-0.794274
53	7	0	-6.402399	1.023858	-0.482129
54	6	0	-7.176114	0.014046	-0.113959
55	1	0	-6.800966	-1.927590	0.666740
56	6	0	-2.575863	3.192367	-1.158104
57	1	0	-4.727024	3.155287	-1.245841
58	1	0	-0.440648	2.891645	-0.921497
59	6	0	-8.634571	0.012191	-0.200846
60	1	0	-2.465575	4.190101	-1.566924
61	6	0	-9.267941	1.101635	-0.815317
62	6	0	-9.414212	-1.035144	0.307206
63	6	0	-10.652045	1.139118	-0.921416
64	1	0	-8.658602	1.910008	-1.206425
65	6	0	-10.799828	-0.993002	0.197197
66	1	0	-8.956341	-1.887737	0.800970
67	6	0	-11.422774	0.091738	-0.417013
68	1	0	-11.131806	1.987527	-1.400842

69	1	0	-11.393648	-1.810191	0.595889
70	1	0	12.505347	-0.121415	-0.500841
71	1	0	-12.505320	0.121317	-0.501059

Cu^{2+}(2-Phen)(2-Im)$_2$

1	29	0	0.709309	0.268305	-0.108205
2	7	0	-0.851253	0.905590	1.034401
3	6	0	-2.049232	0.684922	0.441098
4	6	0	-0.809158	1.430496	2.252554
5	6	0	-2.020068	0.124812	-0.880604
6	6	0	-3.266008	0.998611	1.079027
7	1	0	0.174044	1.596955	2.678398
8	6	0	-1.974052	1.762476	2.957927
9	6	0	-3.209505	-0.126146	-1.604732
10	7	0	-0.798193	-0.142339	-1.394822
11	6	0	-3.204341	1.548419	2.372151
12	6	0	-4.468220	0.736061	0.352818
13	1	0	-1.889206	2.186880	3.951736
14	6	0	-3.073569	-0.666634	-2.900051
15	6	0	-4.420013	0.200446	-0.935191
16	6	0	-0.687212	-0.640649	-2.618392
17	1	0	-4.125708	1.798533	2.888262
18	7	0	-5.751291	0.948824	0.747647
19	6	0	-1.814895	-0.913916	-3.404904
20	1	0	-3.951594	-0.887912	-3.498909
21	7	0	-5.729881	0.097885	-1.311945
22	1	0	0.317097	-0.834351	-2.977399
23	6	0	-6.503108	0.555726	-0.274693
24	1	0	-1.682254	-1.322928	-4.399855
25	1	0	-6.070202	-0.233316	-2.202292
26	6	0	-7.952851	0.596061	-0.301983
27	6	0	-8.644871	1.133600	0.795412
28	6	0	-8.714533	0.115399	-1.377989
29	6	0	-10.023764	1.193459	0.823237
30	1	0	-8.074557	1.509690	1.639334
31	6	0	-10.096004	0.167589	-1.365568
32	1	0	-8.236056	-0.318937	-2.252367
33	6	0	-10.797539	0.710307	-0.261320
34	1	0	-10.509181	1.618332	1.694175
35	1	0	-10.637671	-0.218188	-2.221157
36	7	0	-12.159945	0.763890	-0.242523
37	6	0	-12.921697	0.251485	-1.361026
38	6	0	-12.848775	1.325790	0.899304
39	1	0	-13.985195	0.374908	-1.155591
40	1	0	-12.690894	0.789231	-2.290267
41	1	0	-12.730058	-0.817011	-1.526832
42	1	0	-13.923842	1.285934	0.722825
43	1	0	-12.634792	0.766158	1.819641
44	1	0	-12.571192	2.375255	1.063987
45	7	0	7.156047	-0.953457	-3.034375
46	6	0	7.775660	-2.116555	-3.136368
47	6	0	5.889104	-0.939219	-2.581928
48	6	0	7.191439	-3.349556	-2.804958
49	1	0	8.800256	-2.085416	-3.503540
50	6	0	5.215232	-2.131389	-2.209704
51	6	0	5.196881	0.350699	-2.513300
52	6	0	5.896861	-3.355186	-2.335051
53	1	0	7.753572	-4.270713	-2.916545
54	6	0	3.887364	-1.990041	-1.712150
55	6	0	3.859753	0.430721	-2.033900
56	7	0	5.860589	1.434837	-2.954875

57	1	0	5.415484	-4.290920	-2.065673
58	6	0	3.245833	-0.775207	-1.562681
59	7	0	2.999354	-2.934643	-1.270220
60	6	0	3.210754	1.673009	-2.117268
61	6	0	5.234826	2.598632	-2.973730
62	7	0	1.998971	-0.992091	-1.004330
63	6	0	1.870592	-2.319725	-0.847916
64	1	0	3.166537	-3.927121	-1.181979
65	6	0	3.897283	2.770581	-2.587623
66	1	0	2.166309	1.763378	-1.839342
67	1	0	5.810676	3.450680	-3.331350
68	6	0	0.709028	-3.066657	-0.396074
69	1	0	3.420244	3.742066	-2.665759
70	6	0	0.379372	-4.280264	-1.023934
71	6	0	-0.129435	-2.627781	0.638164
72	6	0	-0.732826	-5.009295	-0.651642
73	1	0	0.982536	-4.645219	-1.851142
74	6	0	-1.249025	-3.340961	1.021205
75	1	0	0.120934	-1.736173	1.207259
76	6	0	-1.590516	-4.559552	0.383203
77	1	0	-0.948552	-5.929648	-1.181203
78	1	0	-1.850479	-2.962043	1.838920
79	7	0	-2.691651	-5.268549	0.750843
80	6	0	-3.570443	-4.762360	1.784368
81	6	0	-3.001524	-6.520996	0.093420
82	1	0	-4.407173	-5.449616	1.909058
83	1	0	-3.055025	-4.676301	2.749986
84	1	0	-3.976660	-3.776956	1.521241
85	1	0	-3.898644	-6.947246	0.542366
86	1	0	-3.191251	-6.381706	-0.979162
87	1	0	-2.187306	-7.247761	0.207917
88	6	0	5.721871	5.847715	2.395904
89	6	0	4.939447	6.837883	1.780039
90	6	0	3.376335	5.323837	1.063930
91	6	0	4.093332	4.254481	1.656389
92	6	0	5.292041	4.540894	2.333146
93	6	0	2.129408	5.062750	0.339497
94	6	0	0.397407	5.921126	-0.900084
95	1	0	-0.065763	6.804262	-1.336883
96	6	0	-0.191394	4.661104	-1.076318
97	6	0	0.423403	3.570822	-0.501356
98	6	0	1.608940	3.741334	0.234326
99	6	0	2.344377	2.682467	0.865839
100	6	0	3.531650	2.951637	1.520955
101	1	0	6.640659	6.113935	2.907620
102	1	0	5.257267	7.878577	1.818043
103	1	0	5.871284	3.748798	2.798652
104	1	0	-1.106198	4.552990	-1.649402
105	1	0	-0.020369	2.587820	-0.615549
106	7	0	1.513947	6.118489	-0.222291
107	7	0	3.810497	6.595359	1.136904
108	6	0	3.114807	0.776037	1.616799
109	7	0	2.101704	1.315569	0.926952
110	7	0	3.989716	1.742317	1.970569
111	1	0	4.801236	1.575487	2.549868
112	6	0	3.318839	-0.618935	1.990373
113	6	0	2.364951	-1.326801	2.734170
114	6	0	4.524137	-1.265647	1.675630
115	6	0	2.582128	-2.637938	3.117522
116	1	0	1.455912	-0.831117	3.064509
117	6	0	4.751176	-2.578033	2.046465

118	1	0	5.287722	-0.739328	1.108327
119	6	0	3.779010	-3.311717	2.770945
120	1	0	1.821132	-3.138802	3.704043
121	1	0	5.689781	-3.041125	1.765811
122	7	0	3.990538	-4.609480	3.127134
123	6	0	5.233552	-5.264218	2.778859
124	6	0	2.977455	-5.333781	3.864691
125	1	0	5.209921	-6.291579	3.142486
126	1	0	5.385025	-5.293073	1.691658
127	1	0	6.098623	-4.763097	3.232783
128	1	0	3.317939	-6.356332	4.028221
129	1	0	2.784083	-4.879443	4.845550
130	1	0	2.029516	-5.376106	3.312381

Cu^{2+}(2- Im)$_4$

1	29	0	0.000009	-0.437285	0.000006
2	7	0	-2.937584	-4.513976	3.606631
3	6	0	-3.235201	-3.405727	2.905210
4	6	0	-1.669981	-4.831415	3.800569
5	6	0	-4.653741	-3.084183	2.752172
6	6	0	-2.225486	-2.568563	2.344444
7	1	0	-1.479868	-5.741010	4.368013
8	6	0	-0.602262	-4.056785	3.330598
9	6	0	-5.033492	-1.915187	2.052472
10	7	0	-5.561746	-3.913358	3.299259
11	6	0	-0.893341	-2.922410	2.604257
12	6	0	-2.635037	-1.418573	1.578881
13	1	0	0.423956	-4.341754	3.538980
14	6	0	-6.402999	-1.619125	1.928832
15	6	0	-3.984510	-1.122884	1.503845
16	6	0	-6.842133	-3.612863	3.169692
17	1	0	-0.103233	-2.274702	2.256705
18	7	0	-1.919880	-0.439555	0.873700
19	6	0	-7.319206	-2.477598	2.494283
20	1	0	-6.737973	-0.736198	1.392266
21	7	0	-4.074034	0.044113	0.803196
22	1	0	-7.547641	-4.307030	3.623567
23	6	0	-2.834638	0.452849	0.453554
24	1	0	-8.385294	-2.290295	2.421514
25	1	0	-4.902094	0.608582	0.673685
26	6	0	-2.701165	1.748040	-0.200829
27	6	0	-1.781579	2.712170	0.235983
28	6	0	-3.683875	2.154701	-1.122727
29	6	0	-1.844551	4.018541	-0.212623
30	1	0	-1.042422	2.457442	0.988027
31	6	0	-3.745201	3.451903	-1.593526
32	1	0	-4.411440	1.435517	-1.491727
33	6	0	-2.832594	4.436374	-1.136495
34	1	0	-1.137999	4.733195	0.189992
35	1	0	-4.513725	3.707931	-2.313048
36	7	0	-2.904978	5.725631	-1.566598
37	6	0	-3.952792	6.128490	-2.481833
38	6	0	-1.948878	6.703649	-1.092418
39	1	0	-3.860065	7.195777	-2.682504
40	1	0	-3.882757	5.596005	-3.439431
41	1	0	-4.949445	5.947758	-2.059047
42	1	0	-2.162853	7.666475	-1.556540
43	1	0	-2.002883	6.832474	-0.002948
44	1	0	-0.920389	6.422420	-1.355951
45	7	0	5.850608	-2.675679	3.514843

46	6	0	6.533579	-2.007298	4.427941
47	6	0	4.660887	-2.185954	3.120339
48	6	0	6.093118	-0.813055	5.021406
49	1	0	7.493156	-2.432487	4.717731
50	6	0	4.134351	-0.983586	3.653178
51	6	0	3.889801	-2.947420	2.135867
52	6	0	4.878762	-0.296215	4.628399
53	1	0	6.702157	-0.313975	5.767625
54	6	0	2.875665	-0.550924	3.143418
55	6	0	2.648419	-2.452326	1.642015
56	7	0	4.388185	-4.136159	1.751664
57	1	0	4.510552	0.629723	5.060311
58	6	0	2.179470	-1.186311	2.133531
59	7	0	2.093617	0.504317	3.520663
60	6	0	1.932239	-3.282598	0.766382
61	6	0	3.687410	-4.884326	0.918252
62	7	0	1.001830	-0.480873	1.875076
63	6	0	0.967605	0.519117	2.774514
64	1	0	2.250577	1.132128	4.297098
65	6	0	2.437677	-4.511195	0.405144
66	1	0	0.970383	-2.963587	0.379725
67	1	0	4.127273	-5.840071	0.638692
68	6	0	-0.062474	1.507471	3.080882
69	1	0	1.893580	-5.168829	-0.264552
70	6	0	-1.368032	1.134815	3.431849
71	6	0	0.291140	2.859884	3.211525
72	6	0	-2.301503	2.075421	3.824555
73	1	0	-1.647976	0.087717	3.430696
74	6	0	-0.633803	3.812823	3.595810
75	1	0	1.303989	3.175038	2.977545
76	6	0	-1.970648	3.451921	3.894784
77	1	0	-3.293934	1.736427	4.097797
78	1	0	-0.316041	4.846666	3.663976
79	7	0	-2.895082	4.386638	4.248480
80	6	0	-2.523089	5.783599	4.320461
81	6	0	-4.249341	3.985439	4.565614
82	1	0	-3.399155	6.373363	4.590688
83	1	0	-1.747571	5.961598	5.077257
84	1	0	-2.151482	6.150906	3.354411
85	1	0	-4.840645	4.872515	4.792971
86	1	0	-4.724217	3.468503	3.721561
87	1	0	-4.283916	3.321071	5.439243
88	6	0	7.319652	-2.476413	-2.494163
89	6	0	6.842754	-3.611705	-3.169652
90	6	0	4.654276	-3.083268	-2.752287
91	6	0	5.033848	-1.914280	-2.052477
92	6	0	6.403315	-1.618069	-1.928729
93	6	0	3.235780	-3.404926	-2.905483
94	6	0	1.670776	-4.830610	-3.801234
95	1	0	1.480804	-5.740158	-4.368799
96	6	0	0.602938	-4.056104	-3.331320
97	6	0	0.893841	-2.921810	-2.604783
98	6	0	2.225932	-2.567914	-2.344733
99	6	0	2.635298	-1.417981	-1.578987
100	6	0	3.984738	-1.122145	-1.503856
101	1	0	8.385714	-2.288992	-2.421317
102	1	0	7.548374	-4.305771	-3.623506
103	1	0	6.738163	-0.735132	-1.392101
104	1	0	-0.423229	-4.341103	-3.539906
105	1	0	0.103650	-2.274189	-2.257250
106	7	0	2.938329	-4.513107	-3.607082

107	7	0	5.562409	-3.912327	-3.299343
108	6	0	2.834632	0.453386	-0.453539
109	7	0	1.919997	-0.439083	-0.873781
110	7	0	4.074101	0.044798	-0.803093
111	1	0	4.902093	0.609344	-0.673489
112	6	0	2.700926	1.748530	0.200876
113	6	0	1.781113	2.712460	-0.235897
114	6	0	3.683521	2.155359	1.122816
115	6	0	1.843781	4.018823	0.212762
116	1	0	1.042008	2.457570	-0.987940
117	6	0	3.744538	3.452554	1.593679
118	1	0	4.411203	1.436308	1.491848
119	6	0	2.831743	4.436843	1.136641
120	1	0	1.137047	4.733325	-0.189804
121	1	0	4.512960	3.708716	2.313262
122	6	0	-6.092893	-0.813437	-5.021612
123	6	0	-6.533213	-2.007752	-4.428190
124	6	0	-4.660511	-2.186224	-3.120578
125	6	0	-4.134117	-0.983775	-3.653373
126	6	0	-4.878605	-0.296460	-4.628575
127	6	0	-3.889334	-2.947644	-2.136136
128	6	0	-3.686689	-4.884585	-0.918625
129	1	0	-4.126440	-5.840391	-0.639098
130	6	0	-2.436977	-4.511349	-0.405549
131	6	0	-1.931688	-3.282673	-0.766739
132	6	0	-2.648002	-2.452425	-1.642278
133	6	0	-2.179236	-1.186311	-2.133709
134	6	0	-2.875494	-0.550968	-3.143576
135	1	0	-6.701988	-0.314408	-5.767819
136	1	0	-7.492737	-2.433048	-4.717999
137	1	0	-4.510503	0.629538	-5.060447
138	1	0	-1.892777	-5.168956	0.264087
139	1	0	-0.969838	-2.963579	-0.380129
140	7	0	-4.387574	-4.136455	-1.751985
141	7	0	-5.850167	-2.676080	-3.515107
142	6	0	-0.967595	0.519323	-2.774548
143	7	0	-1.001699	-0.480724	-1.875181
144	7	0	-2.093585	0.504411	-3.520735
145	1	0	-2.250579	1.132204	-4.297177
146	6	0	0.062318	1.507893	-3.080778
147	6	0	-0.291549	2.860253	-3.211263
148	6	0	1.367975	1.135526	-3.431674
149	6	0	0.633237	3.813417	-3.595361
150	1	0	-1.304472	3.175175	-2.977297
151	6	0	2.301287	2.076363	-3.824207
152	1	0	1.648124	0.088483	-3.430594
153	6	0	1.970166	3.452804	-3.894304
154	1	0	0.315283	4.847210	-3.663393
155	1	0	3.293812	1.737601	-4.097398
156	7	0	2.903878	5.726114	1.566739
157	6	0	1.947313	6.703841	1.092903
158	6	0	3.951307	6.129077	2.482367
159	1	0	2.161146	7.666731	1.556957
160	1	0	2.000947	6.832702	0.003423
161	1	0	0.918987	6.422288	1.356739
162	1	0	3.858471	7.196379	2.682908
163	1	0	3.880947	5.596653	3.439982
164	1	0	4.948119	5.948368	2.059960
165	7	0	2.894435	4.387742	-4.247857
166	6	0	2.522187	5.784646	-4.319621
167	6	0	4.248794	3.986850	-4.564951

168	1	0	3.398160	6.374620	-4.589689
169	1	0	1.746680	5.962630	-5.076435
170	1	0	2.150450	6.151718	-3.353534
171	1	0	4.839925	4.874067	-4.792211
172	1	0	4.723739	3.469944	-3.720917
173	1	0	4.283551	3.322562	-5.438633

$Cu^{+}(2\text{-Phen})_2$

1	29	0	0.000003	0.000712	0.068536
2	7	0	-1.625489	-0.918343	0.994110
3	6	0	-2.812701	-0.463482	0.530927
4	6	0	-1.619517	-1.856780	1.932439
5	6	0	-2.780145	0.563983	-0.495314
6	6	0	-4.043431	-0.960742	1.018416
7	1	0	-0.644371	-2.191328	2.274126
8	6	0	-2.792170	-2.404432	2.471428
9	6	0	-3.980944	1.095215	-1.034617
10	7	0	-1.565523	0.986877	-0.908958
11	6	0	-4.011684	-1.954087	2.011755
12	6	0	-5.246185	-0.418927	0.465643
13	1	0	-2.725234	-3.169721	3.237277
14	6	0	-3.872714	2.089934	-2.025030
15	6	0	-5.195182	0.564446	-0.516251
16	6	0	-1.489675	1.925134	-1.844024
17	1	0	-4.946134	-2.348409	2.398717
18	7	0	-6.535494	-0.739096	0.772627
19	6	0	-2.622382	2.505512	-2.430085
20	1	0	-4.763557	2.526738	-2.466019
21	7	0	-6.506555	0.836826	-0.801422
22	1	0	-0.491371	2.231211	-2.142380
23	6	0	-7.282874	0.032454	-0.006646
24	1	0	-2.504667	3.269813	-3.190531
25	1	0	-6.844919	1.499356	-1.482866
26	6	0	-8.735887	0.035097	-0.027863
27	6	0	-9.437964	-0.862295	0.791746
28	6	0	-9.489929	0.899233	-0.835113
29	6	0	-10.818689	-0.901747	0.808634
30	1	0	-8.874183	-1.540696	1.424941
31	6	0	-10.873249	0.872788	-0.830259
32	1	0	-9.004423	1.620530	-1.487894
33	6	0	-11.584315	-0.031725	-0.005923
34	1	0	-11.310791	-1.614986	1.459974
35	1	0	-11.406903	1.563133	-1.473203
36	7	0	-12.949262	-0.063802	0.004149
37	6	0	-13.701373	0.841003	-0.836896
38	6	0	-13.645769	-1.005045	0.853264
39	1	0	-14.767277	0.671546	-0.682114
40	1	0	-13.487385	1.891119	-0.596803
41	1	0	-13.483952	0.682934	-1.901939
42	1	0	-14.720477	-0.884541	0.714608
43	1	0	-13.386863	-2.043484	0.606772
44	1	0	-13.420346	-0.839746	1.915468
45	7	0	1.565302	-0.985597	-0.909230
46	6	0	1.489226	-1.923759	-1.844372
47	6	0	2.780023	-0.563131	-0.495448
48	6	0	2.621796	-2.504475	-2.430364
49	1	0	0.490847	-2.229467	-2.142855
50	6	0	3.980698	-1.094667	-1.034730
51	6	0	2.812814	0.464180	0.530940
52	6	0	3.872228	-2.089301	-2.025202

53	1	0	2.503901	-3.268712	-3.190847
54	6	0	5.195062	-0.564277	-0.516267
55	6	0	4.043662	0.960997	1.018582
56	7	0	1.625708	0.919322	0.994125
57	1	0	4.762965	-2.526367	-2.466145
58	6	0	5.246288	0.418948	0.465765
59	7	0	6.506376	-0.836918	-0.801470
60	6	0	4.012155	1.954162	2.012109
61	6	0	1.619965	1.857594	1.932623
62	7	0	6.535668	0.738765	0.772815
63	6	0	7.282874	-0.032842	-0.006569
64	1	0	6.844597	-1.499352	-1.483082
65	6	0	2.792749	2.404787	2.471792
66	1	0	4.946701	2.348136	2.399193
67	1	0	0.644900	2.192408	2.274278
68	6	0	8.735885	-0.035777	-0.027815
69	1	0	2.725994	3.169952	3.237781
70	6	0	9.438170	0.861661	0.791564
71	6	0	9.489725	-0.900245	-0.834896
72	6	0	10.818904	0.900852	0.808383
73	1	0	8.874550	1.540333	1.424613
74	6	0	10.873049	-0.874074	-0.830101
75	1	0	9.004040	-1.621600	-1.487477
76	6	0	11.584327	0.030490	-0.006000
77	1	0	11.311173	1.614169	1.459512
78	1	0	11.406537	-1.564688	-1.472892
79	7	0	12.949280	0.062314	0.004016
80	6	0	13.701203	-0.842705	-0.836965
81	6	0	13.645984	1.003678	0.852835
82	1	0	14.767139	-0.673377	-0.682268
83	1	0	13.487086	-1.892759	-0.596720
84	1	0	13.483739	-0.684746	-1.902016
85	1	0	14.720667	0.882916	0.714206
86	1	0	13.387278	2.042096	0.606042
87	1	0	13.420540	0.838734	1.915089

Cu^{+}(2-Phen)(2-Im)$_2$

1	29	0	-0.796855	0.229335	-0.037315
2	7	0	1.003758	0.277497	-1.296719
3	6	0	2.160315	0.335811	-0.599590
4	6	0	1.054087	0.267343	-2.621495
5	6	0	2.069911	0.398833	0.850911
6	6	0	3.419718	0.340490	-1.245880
7	1	0	0.099494	0.242359	-3.140574
8	6	0	2.255335	0.285113	-3.344268
9	6	0	3.243125	0.416576	1.652209
10	7	0	0.836178	0.452954	1.395969
11	6	0	3.446523	0.310853	-2.650519
12	6	0	4.591175	0.368668	-0.426650
13	1	0	2.232720	0.270113	-4.428688
14	6	0	3.084723	0.462558	3.050163
15	6	0	4.485315	0.395168	0.959199
16	6	0	0.714248	0.486870	2.715351
17	1	0	4.403298	0.313202	-3.163416
18	7	0	5.897109	0.365727	-0.819112
19	6	0	1.814175	0.490506	3.583561
20	1	0	3.952224	0.475192	3.703251
21	7	0	5.779855	0.407574	1.404840
22	1	0	-0.298735	0.514715	3.107053
23	6	0	6.600555	0.389794	0.305757

24	1	0	1.656408	0.523427	4.656133
25	1	0	6.079573	0.438432	2.367591
26	6	0	8.051757	0.397374	0.380099
27	6	0	8.802508	0.413903	-0.805815
28	6	0	8.757037	0.388598	1.592240
29	6	0	10.183871	0.423893	-0.789934
30	1	0	8.276507	0.419779	-1.755753
31	6	0	10.139994	0.398593	1.625934
32	1	0	8.231765	0.370188	2.543879
33	6	0	10.900072	0.417938	0.432135
34	1	0	10.715966	0.437534	-1.734235
35	1	0	10.635538	0.390035	2.589704
36	7	0	12.265148	0.429891	0.458328
37	6	0	12.965166	0.423123	1.723926
38	6	0	13.013835	0.444437	-0.779238
39	1	0	14.039493	0.439453	1.538869
40	1	0	12.712953	1.301889	2.332651
41	1	0	12.736135	-0.476271	2.311525
42	1	0	14.080268	0.451253	-0.552216
43	1	0	12.803594	-0.442139	-1.392528
44	1	0	12.789723	1.336251	-1.379860
45	7	0	-6.890314	-0.530751	3.550434
46	6	0	-7.612771	-1.617586	3.760626
47	6	0	-5.681718	-0.663579	2.972223
48	6	0	-7.197031	-2.914732	3.419686
49	1	0	-8.584704	-1.466796	4.228327
50	6	0	-5.173941	-1.932433	2.584754
51	6	0	-4.879426	0.544173	2.762517
52	6	0	-5.964421	-3.071191	2.825431
53	1	0	-7.837475	-3.767192	3.621208
54	6	0	-3.892854	-1.951911	1.964752
55	6	0	-3.601536	0.465469	2.140354
56	7	0	-5.391563	1.711749	3.197128
57	1	0	-5.610917	-4.059672	2.545777
58	6	0	-3.139432	-0.820528	1.702730
59	7	0	-3.146073	-2.997728	1.495834
60	6	0	-2.856165	1.652368	2.031953
61	6	0	-4.673316	2.811941	3.054815
62	7	0	-1.969248	-1.171851	1.062764
63	6	0	-1.991894	-2.503592	0.964950
64	1	0	-3.421133	-3.968195	1.477904
65	6	0	-3.390527	2.837606	2.487766
66	1	0	-1.863393	1.627910	1.590309
67	1	0	-5.126423	3.734174	3.416144
68	6	0	-0.968546	-3.383826	0.422913
69	1	0	-2.838134	3.769094	2.414821
70	6	0	-0.943728	-4.752233	0.741826
71	6	0	0.031241	-2.912977	-0.438219
72	6	0	0.012799	-5.604642	0.221341
73	1	0	-1.662926	-5.172113	1.440491
74	6	0	0.997970	-3.747988	-0.965602
75	1	0	0.048950	-1.862913	-0.713991
76	6	0	1.016365	-5.129669	-0.657375
77	1	0	-0.009882	-6.647966	0.513511
78	1	0	1.740708	-3.324162	-1.632080
79	7	0	1.959688	-5.964681	-1.179835
80	6	0	2.994279	-5.437817	-2.043214
81	6	0	1.951441	-7.371102	-0.840672
82	1	0	3.656582	-6.249938	-2.343836
83	1	0	2.573820	-4.989017	-2.952986
84	1	0	3.600028	-4.676233	-1.534030

85	1	0	2.759958	-7.871995	-1.373658
86	1	0	2.101579	-7.533458	0.235381
87	1	0	1.007341	-7.850337	-1.130928
88	6	0	-5.340872	6.394071	-2.341979
89	6	0	-4.363953	7.294692	-1.888255
90	6	0	-2.906447	5.615125	-1.327065
91	6	0	-3.827065	4.625232	-1.764273
92	6	0	-5.067410	5.045702	-2.277939
93	6	0	-1.605276	5.220033	-0.781179
94	6	0	0.410705	5.868997	0.103554
95	1	0	1.053287	6.692712	0.411775
96	6	0	0.857829	4.545620	0.235572
97	6	0	0.016599	3.529875	-0.163436
98	6	0	-1.250083	3.846236	-0.682443
99	6	0	-2.198565	2.867258	-1.126684
100	6	0	-3.419562	3.265928	-1.642951
101	1	0	-6.285692	6.759237	-2.731122
102	1	0	-4.555694	8.365990	-1.928895
103	1	0	-5.801107	4.319530	-2.616105
104	1	0	1.842985	4.335332	0.640053
105	1	0	0.316842	2.489882	-0.086688
106	7	0	-0.771216	6.201187	-0.386162
107	7	0	-3.192031	6.928863	-1.398211
108	6	0	-3.260044	1.056891	-1.656545
109	7	0	-2.114380	1.489797	-1.127134
110	7	0	-4.070340	2.105414	-1.967653
111	1	0	-4.951743	2.022287	-2.453319
112	6	0	-3.652360	-0.319221	-1.911967
113	6	0	-2.703212	-1.292074	-2.252393
114	6	0	-4.996078	-0.717449	-1.844164
115	6	0	-3.065578	-2.601401	-2.507177
116	1	0	-1.656988	-1.012189	-2.334613
117	6	0	-5.375687	-2.024761	-2.090822
118	1	0	-5.763490	-0.003141	-1.555364
119	6	0	-4.418268	-3.011545	-2.429701
120	1	0	-2.290440	-3.312395	-2.767139
121	1	0	-6.424166	-2.285301	-2.005311
122	7	0	-4.782082	-4.305450	-2.670115
123	6	0	-6.165435	-4.705443	-2.532341
124	6	0	-3.767132	-5.306709	-2.918188
125	1	0	-6.259176	-5.761497	-2.786964
126	1	0	-6.534573	-4.566827	-1.506255
127	1	0	-6.815911	-4.137885	-3.209672
128	1	0	-4.248072	-6.274209	-3.064719
129	1	0	-3.188283	-5.078492	-3.822420
130	1	0	-3.065389	-5.397211	-2.076993

$Cu^{+}(2\text{-}Im)_4$

1	29	0	-0.001906	-0.331626	-0.002063
2	7	0	-0.628093	-5.144142	3.110116
3	6	0	-1.320053	-4.006357	2.914484
4	6	0	0.599143	-5.231235	2.628645
5	6	0	-2.666440	-3.930089	3.488643
6	6	0	-0.775319	-2.907572	2.192503
7	1	0	1.122031	-6.169861	2.805686
8	6	0	1.238757	-4.194981	1.932554
9	6	0	-3.443322	-2.752435	3.335638
10	7	0	-3.127851	-4.999621	4.163205
11	6	0	0.542538	-3.025852	1.716814
12	6	0	-1.598632	-1.745818	2.024791

13	1	0	2.257803	-4.318341	1.581052
14	6	0	-4.727028	-2.715195	3.908710
15	6	0	-2.857512	-1.688613	2.591799
16	6	0	-4.337250	-4.937260	4.692805
17	1	0	1.016014	-2.195518	1.197627
18	7	0	-1.349646	-0.563160	1.348601
19	6	0	-5.180677	-3.818577	4.596652
20	1	0	-5.353645	-1.834047	3.807039
21	7	0	-3.350505	-0.450862	2.268030
22	1	0	-4.673528	-5.822868	5.229852
23	6	0	-2.424600	0.211817	1.531759
24	1	0	-6.164744	-3.832211	5.053319
25	1	0	-4.211739	-0.039083	2.598670
26	6	0	-2.623227	1.577603	1.084203
27	6	0	-1.563021	2.495790	1.062969
28	6	0	-3.900900	2.037959	0.728540
29	6	0	-1.769150	3.817289	0.710367
30	1	0	-0.569588	2.181117	1.373456
31	6	0	-4.117160	3.352616	0.364048
32	1	0	-4.739978	1.346986	0.700232
33	6	0	-3.055600	4.290910	0.353114
34	1	0	-0.925610	4.495727	0.738890
35	1	0	-5.117930	3.652927	0.077163
36	7	0	-3.265934	5.595657	0.018777
37	6	0	-4.583350	6.036638	-0.387747
38	6	0	-2.152267	6.516472	-0.050620
39	1	0	-4.556337	7.108993	-0.582040
40	1	0	-4.921307	5.532057	-1.303662
41	1	0	-5.326603	5.855651	0.398623
42	1	0	-2.523610	7.506358	-0.316660
43	1	0	-1.637762	6.599457	0.915353
44	1	0	-1.416452	6.213956	-0.809052
45	7	0	9.396296	-0.601186	0.589603
46	6	0	10.159639	0.403909	0.983567
47	6	0	8.084713	-0.573672	0.893216
48	6	0	9.686625	1.511817	1.704447
49	1	0	11.214082	0.341044	0.718007
50	6	0	7.508027	0.504777	1.623959
51	6	0	7.250289	-1.692216	0.443166
52	6	0	8.348001	1.560049	2.026069
53	1	0	10.365393	2.306151	1.997783
54	6	0	6.111981	0.429553	1.895054
55	6	0	5.862479	-1.714689	0.743043
56	7	0	7.840490	-2.679141	-0.260603
57	1	0	7.946424	2.401953	2.583524
58	6	0	5.309294	-0.628708	1.493146
59	7	0	5.262774	1.279725	2.554267
60	6	0	5.096621	-2.797481	0.279150
61	6	0	7.094502	-3.687086	-0.679281
62	7	0	4.014375	-0.442124	1.893781
63	6	0	4.012110	0.719790	2.531398
64	1	0	5.515039	2.130951	3.033572
65	6	0	5.714529	-3.796939	-0.440234
66	1	0	4.031935	-2.821258	0.490983
67	1	0	7.608399	-4.463723	-1.244555
68	6	0	2.850211	1.352417	3.138103
69	1	0	5.158766	-4.648420	-0.820146
70	6	0	1.724414	0.585881	3.471264
71	6	0	2.796385	2.729197	3.396445
72	6	0	0.605073	1.156344	4.051192
73	1	0	1.738711	-0.482336	3.275331

74	6	0	1.681027	3.316303	3.969296
75	1	0	3.626912	3.373453	3.117915
76	6	0	0.552413	2.543368	4.330602
77	1	0	-0.237012	0.516993	4.289786
78	1	0	1.686214	4.387726	4.132137
79	7	0	-0.541124	3.113986	4.925948
80	6	0	-0.633314	4.554487	5.022665
81	6	0	-1.725140	2.319719	5.168774
82	1	0	-1.562746	4.819048	5.528264
83	1	0	0.194546	4.967859	5.611158
84	1	0	-0.629058	5.039601	4.034969
85	1	0	-2.457697	2.926604	5.702618
86	1	0	-2.188715	1.960722	4.237672
87	1	0	-1.495150	1.450236	5.795478
88	6	0	5.183293	-3.823300	-4.590266
89	6	0	4.339946	-4.942001	-4.686870
90	6	0	2.667322	-3.933791	-3.486093
91	6	0	3.443965	-2.755982	-3.332950
92	6	0	4.728600	-2.719314	-3.903979
93	6	0	1.320104	-4.009619	-2.913825
94	6	0	-0.599430	-5.234315	-2.629556
95	1	0	-1.122018	-6.173139	-2.806439
96	6	0	-1.240130	-4.197402	-1.935436
97	6	0	-0.544290	-3.028023	-1.719824
98	6	0	0.774254	-2.910185	-2.193710
99	6	0	1.597246	-1.748241	-2.025890
100	6	0	2.856969	-1.691439	-2.591068
101	1	0	6.168103	-3.837371	-5.045315
102	1	0	4.676996	-5.828048	-5.222708
103	1	0	5.355123	-1.838129	-3.802035
104	1	0	-2.259683	-4.320467	-1.585311
105	1	0	-1.018562	-2.197168	-1.202199
106	7	0	0.628499	-5.147644	-3.109330
107	7	0	3.129731	-5.003881	-4.159079
108	6	0	2.422242	0.209918	-1.533415
109	7	0	1.347123	-0.565041	-1.351145
110	7	0	3.349322	-0.453307	-2.267743
111	1	0	4.211014	-0.041722	-2.597443
112	6	0	2.619955	1.576190	-1.086881
113	6	0	1.559686	2.494378	-1.068771
114	6	0	3.896939	2.036996	-0.729321
115	6	0	1.765157	3.816359	-0.717546
116	1	0	0.566828	2.179293	-1.380690
117	6	0	4.112509	3.352138	-0.366173
118	1	0	4.735953	1.346063	-0.698500
119	6	0	3.050948	4.290476	-0.358587
120	1	0	0.921666	4.494754	-0.748561
121	1	0	5.112743	3.652831	-0.077819
122	6	0	-9.683754	1.509181	-1.700854
123	6	0	-10.156718	0.401885	-0.979001
124	6	0	-8.082040	-0.576263	-0.889106
125	6	0	-7.505420	0.501544	-1.620829
126	6	0	-8.345283	1.556802	-2.023204
127	6	0	-7.247696	-1.694757	-0.438787
128	6	0	-7.091977	-3.689029	0.684739
129	1	0	-7.605840	-4.465189	1.250699
130	6	0	-5.712152	-3.799418	0.445117
131	6	0	-5.094284	-2.800550	-0.275119
132	6	0	-5.860015	-1.717772	-0.739262
133	6	0	-5.306861	-0.632364	-1.490238
134	6	0	-6.109521	0.425781	-1.892516

135	1	0	-10.362439	2.303526	-1.994351
136	1	0	-11.211039	0.339516	-0.712840
137	1	0	-7.943742	2.398215	-2.581426
138	1	0	-5.156462	-4.650853	0.825242
139	1	0	-4.029715	-2.824797	-0.487449
140	7	0	-7.837864	-2.681116	0.265807
141	7	0	-9.393472	-0.603185	-0.584786
142	6	0	-4.009848	0.715346	-2.529716
143	7	0	-4.012008	-0.446178	-1.891377
144	7	0	-5.260440	1.275400	-2.552552
145	1	0	-5.512691	2.126417	-3.032240
146	6	0	-2.848253	1.347679	-3.137361
147	6	0	-2.793740	2.724779	-3.393884
148	6	0	-1.723674	0.580678	-3.473524
149	6	0	-1.678859	3.311794	-3.967758
150	1	0	-3.623254	3.369281	-3.112929
151	6	0	-0.604846	1.151047	-4.054555
152	1	0	-1.738527	-0.487827	-3.279217
153	6	0	-0.551447	2.538446	-4.331937
154	1	0	-1.683444	4.383444	-4.129148
155	1	0	0.236283	0.511330	-4.295515
156	7	0	3.260745	5.595691	-0.025821
157	6	0	2.147317	6.517141	0.038585
158	6	0	4.577619	6.037315	0.381733
159	1	0	2.518437	7.507544	0.303007
160	1	0	1.635090	6.597878	-0.928798
161	1	0	1.409618	6.216889	0.796062
162	1	0	4.550153	7.109797	0.575228
163	1	0	4.914590	5.533512	1.298418
164	1	0	5.321845	5.855832	-0.403630
165	7	0	0.541711	3.109061	-4.927909
166	6	0	0.634656	4.549591	-5.023282
167	6	0	1.724389	2.313980	-5.174475
168	1	0	1.564026	4.814142	-5.528995
169	1	0	-0.193248	4.964079	-5.610966
170	1	0	0.631138	5.033688	-4.035093
171	1	0	2.456867	2.921254	-5.707973
172	1	0	2.188941	1.952250	-4.244915
173	1	0	1.492440	1.446203	-5.802836