Supplementary Material

Effects of the Ligand Linkers on Stability of Mixed-Valence Cu(I)Cu(II) and Catalytic Aerobic Alcohol Oxidation Activity

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Table of Contents

Contents Page

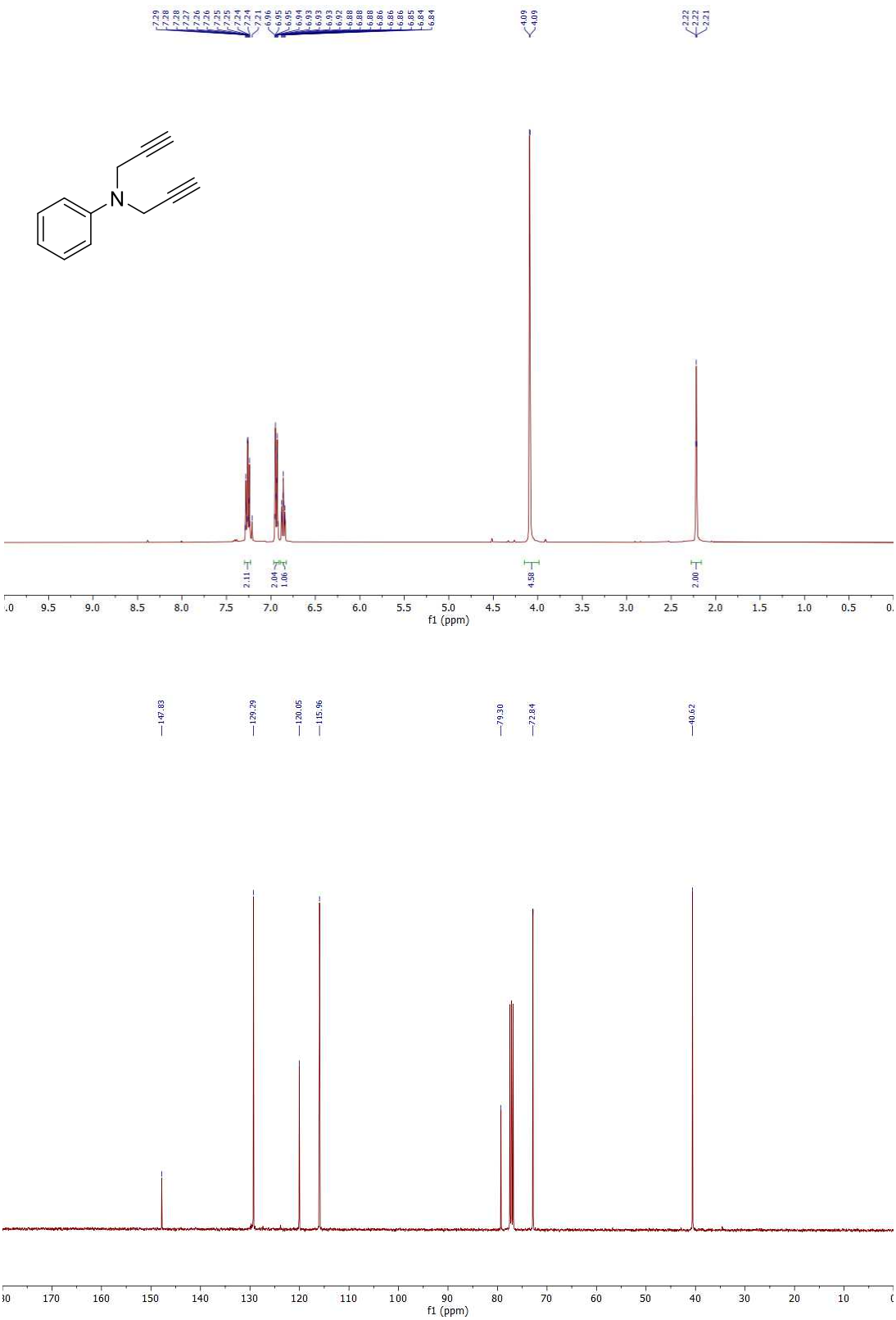
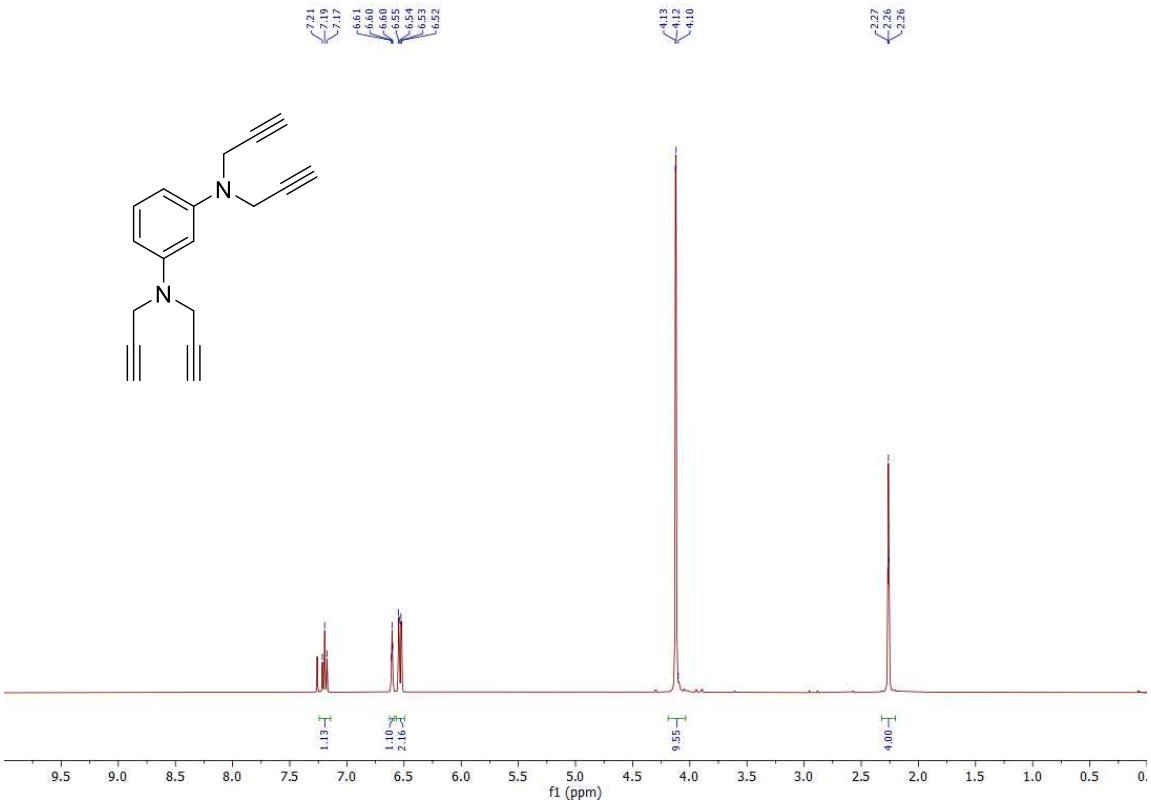


Figure S1 ^{1}H and $^{13}C\{^{1}H\}$ spectra NMR of compound **DP1** in $CDCl_3$



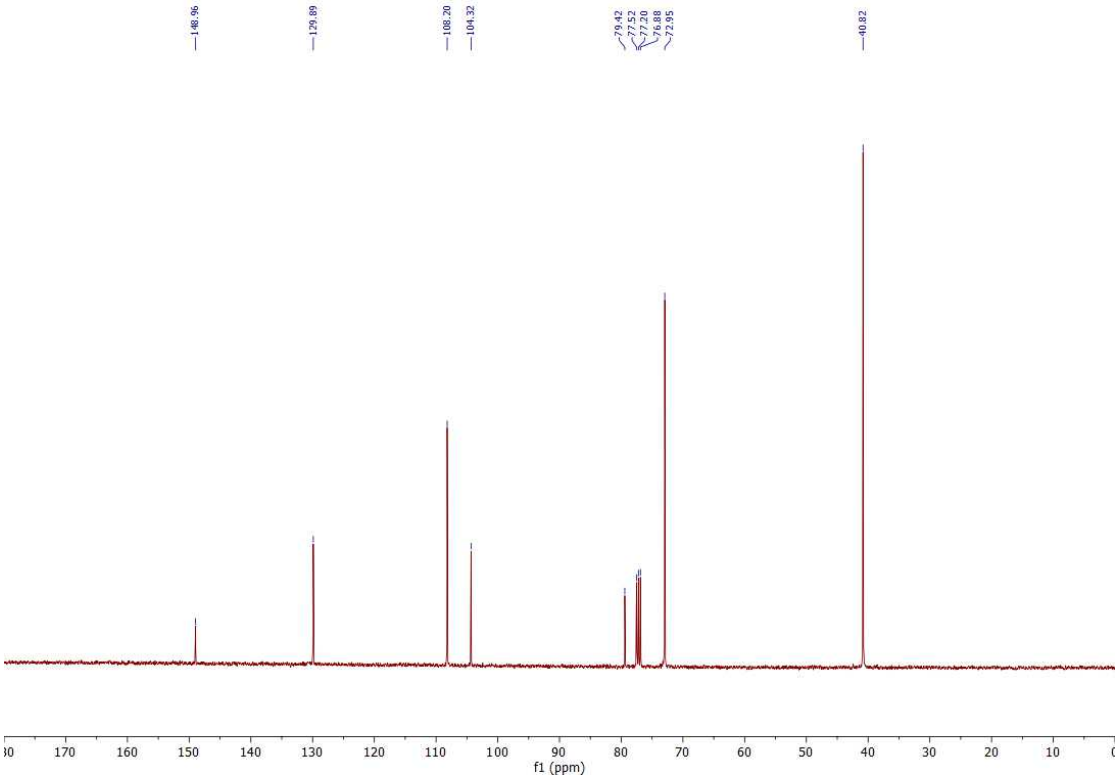


Figure S2 ^{1}H and $^{13}C\{^{1}H\}$ spectra NMR of compound **TP2** in $CDCl_3$

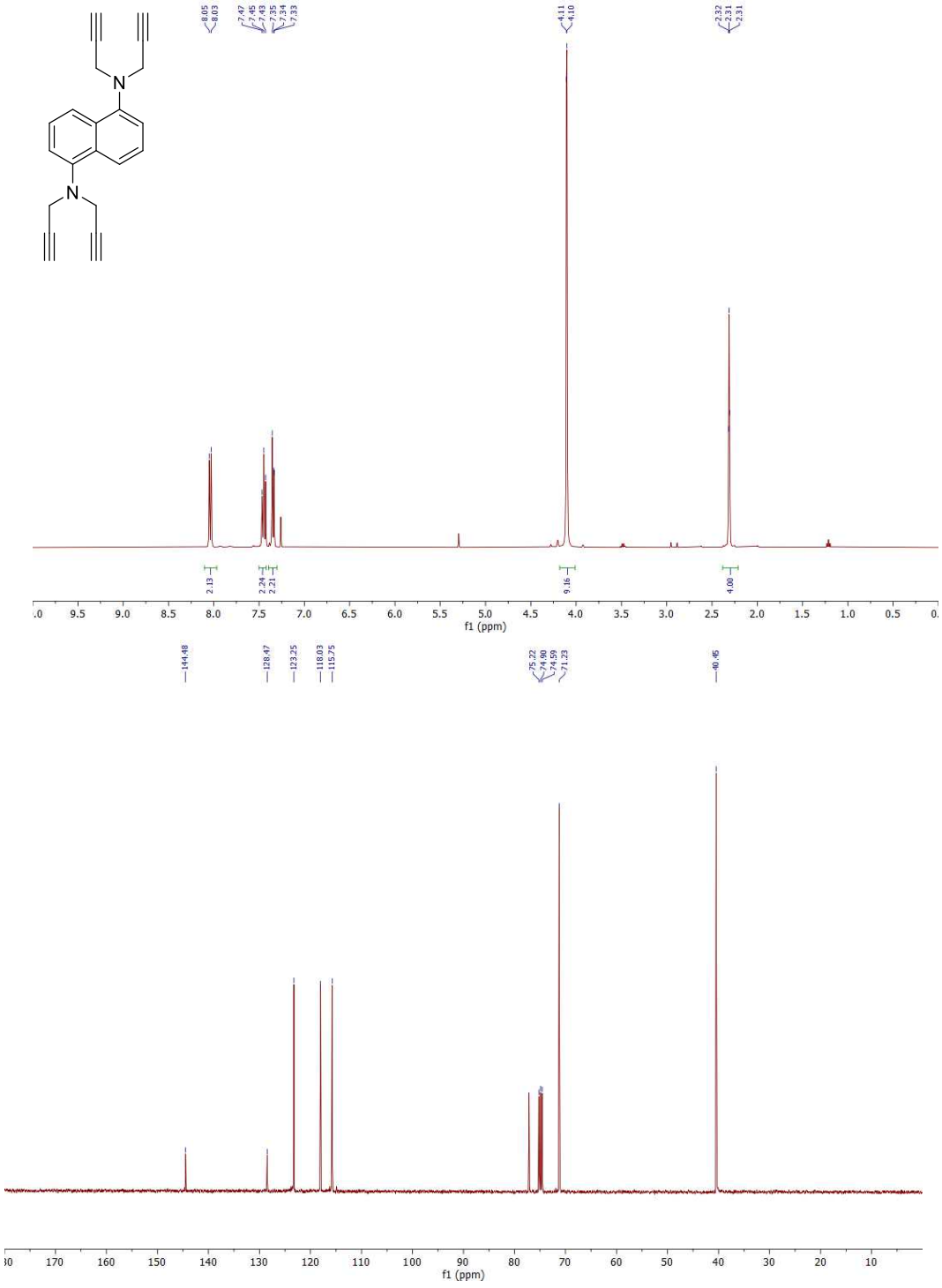


Figure S3 ^{1}H and $^{13}C\{^{1}H\}$ spectra NMR of compound **TP3** in $CDCl_3$

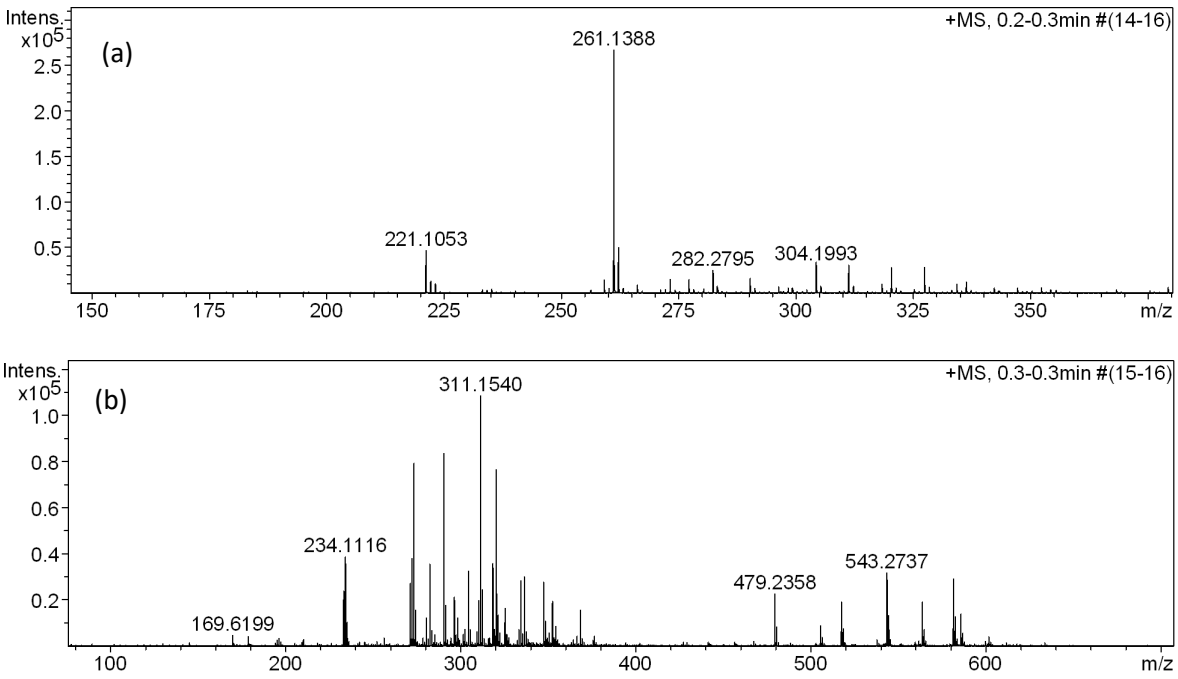


Figure S4 ESI-MS spectra of compounds **TP2** (a) and **TP3** (b)

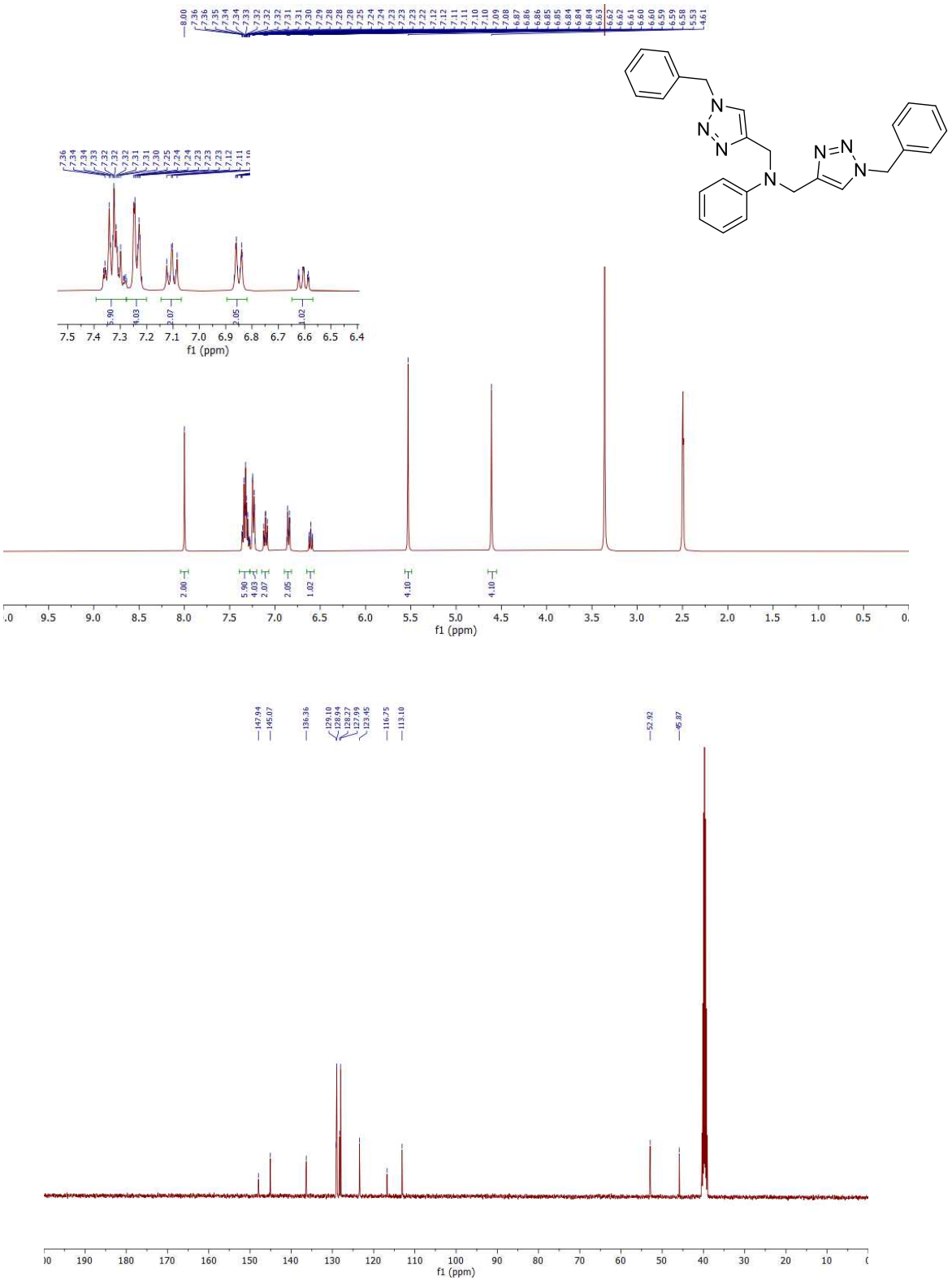


Figure S5 ^{1}H NMR and ^{13}C{^{1}H} NMR spectrum of **L1** in DMSO-d_6.

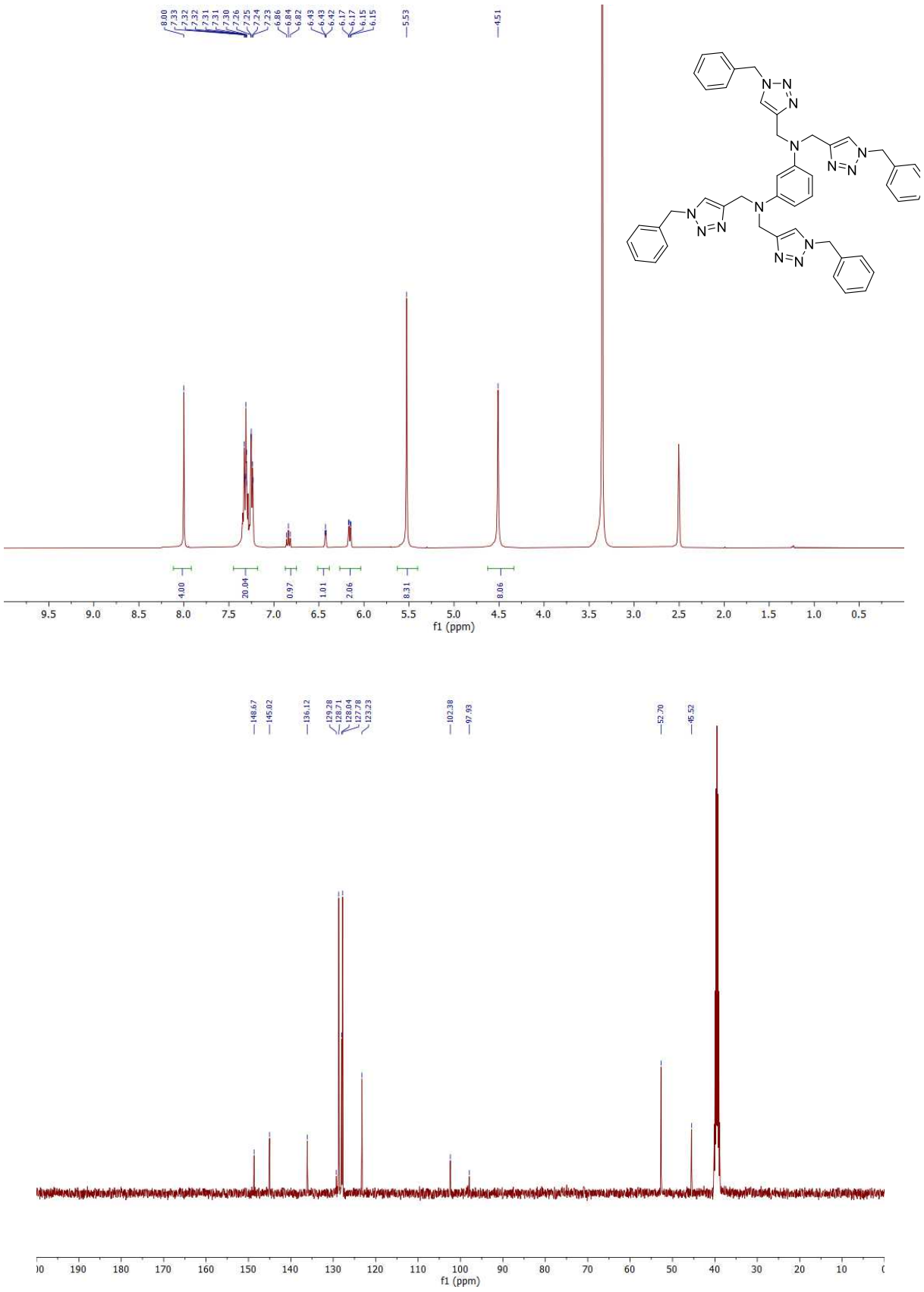


Figure S6 ^{1}H NMR and ^{13}C{^{1}H} NMR spectrum of **L2** in DMSO-d_6.

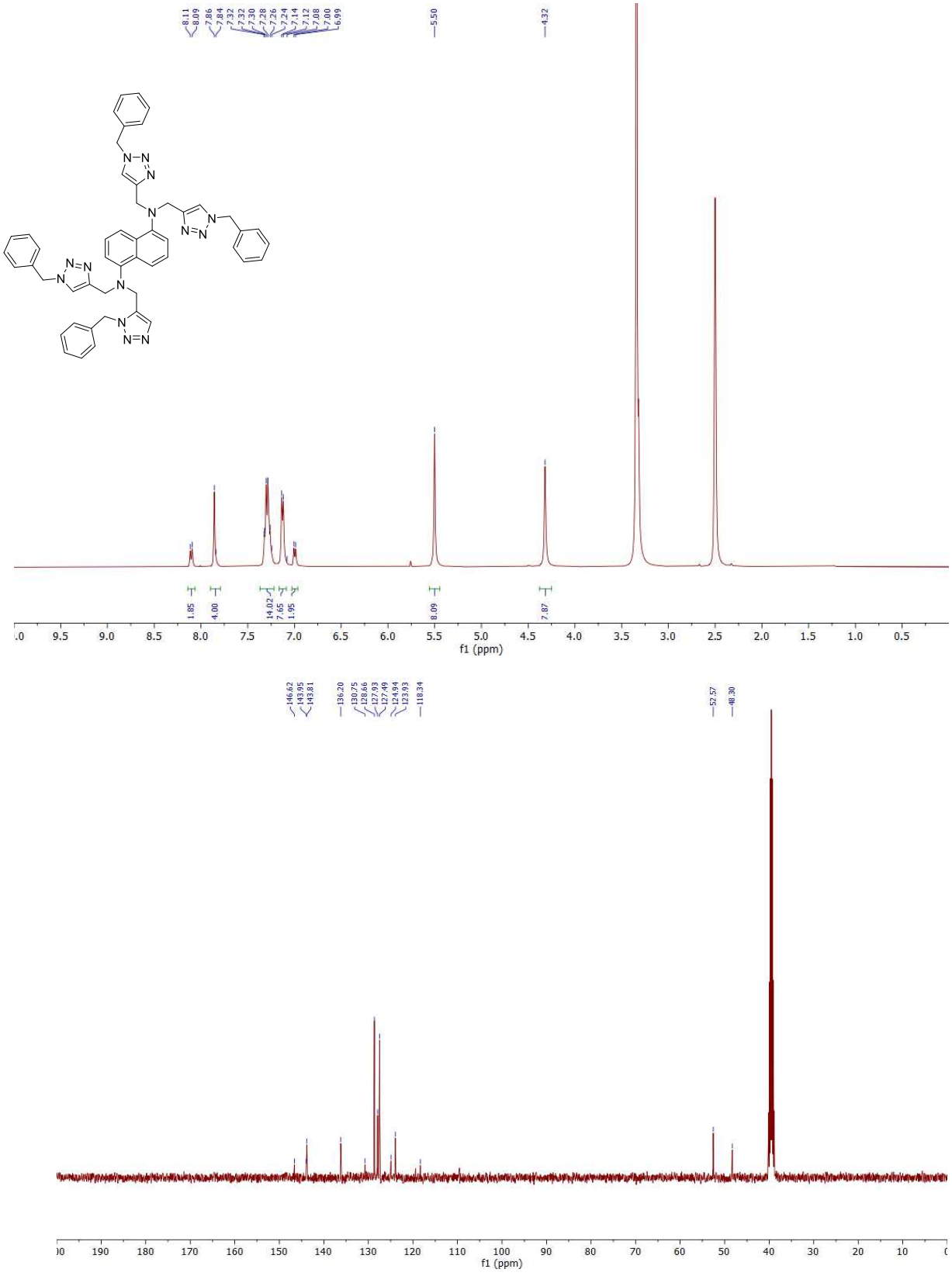


Figure S7 ^{1}H NMR and ^{13}C{^{1}H} NMR spectrum of **L3** in DMSO-d_6.

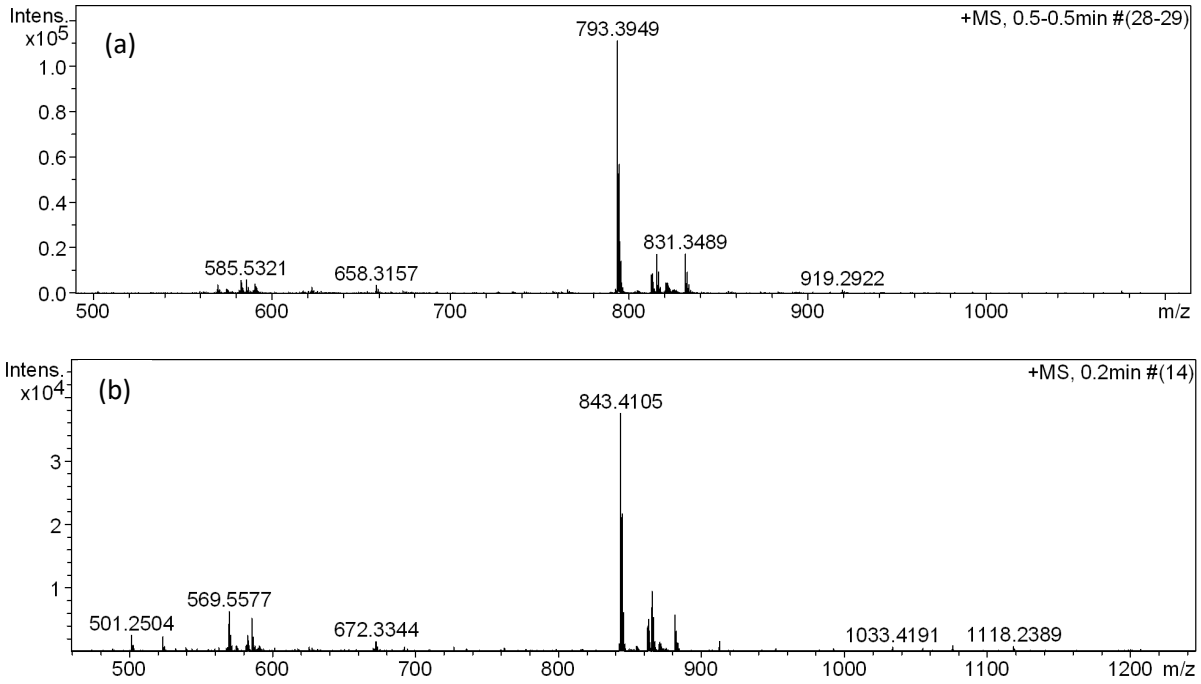


Figure S8. ESI-MS spectra of **L2** (a) and **L3** (b)

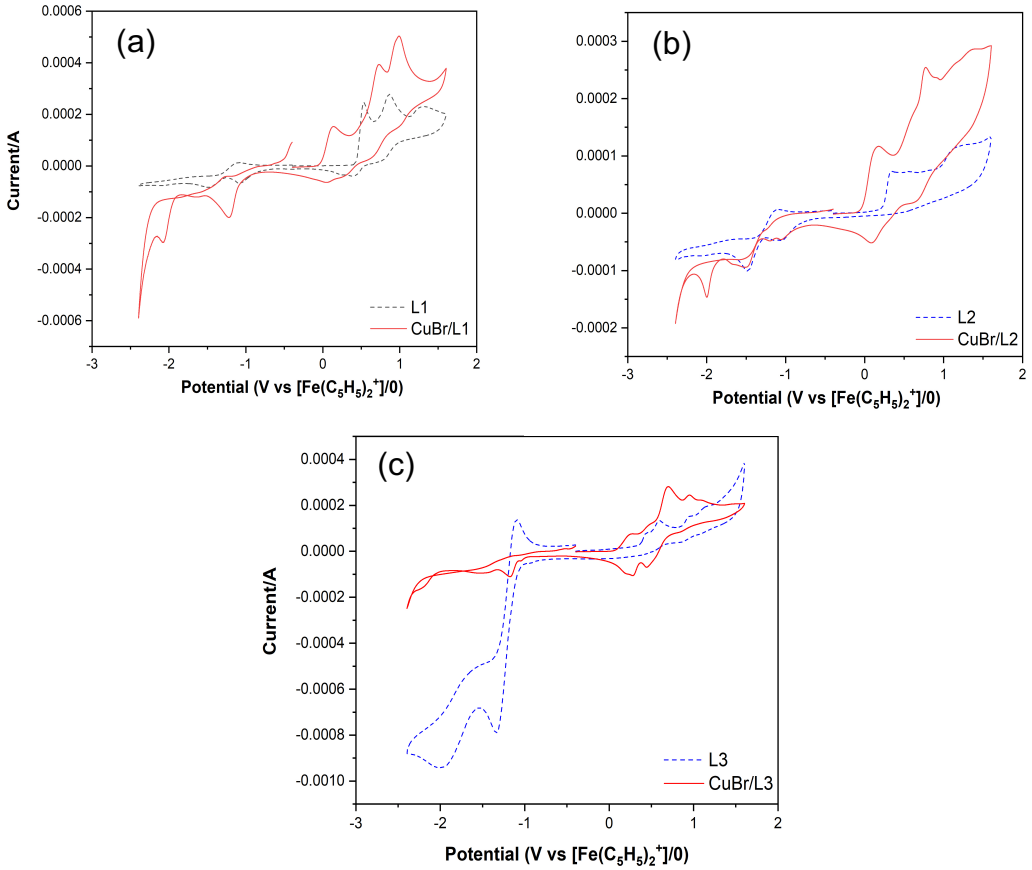


Figure S9 Overlaid CV of CuBr/**Ln** and **Ln** where **Ln** = **L1** (a), **L2** (b), and **L3** (c)

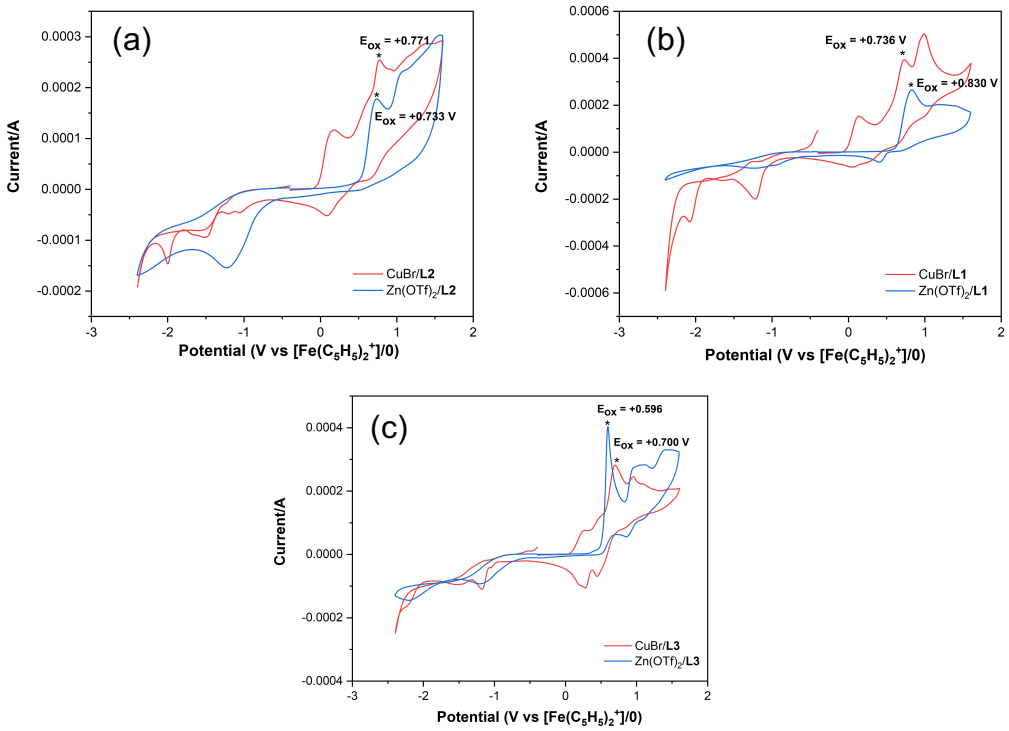


Figure S10 Overlaid CV data of CuBr/**Ln** and Zn(OTf)$_2$/**Ln** where **Ln** = **L1** (a), **L2** (b), and **L3** (c)

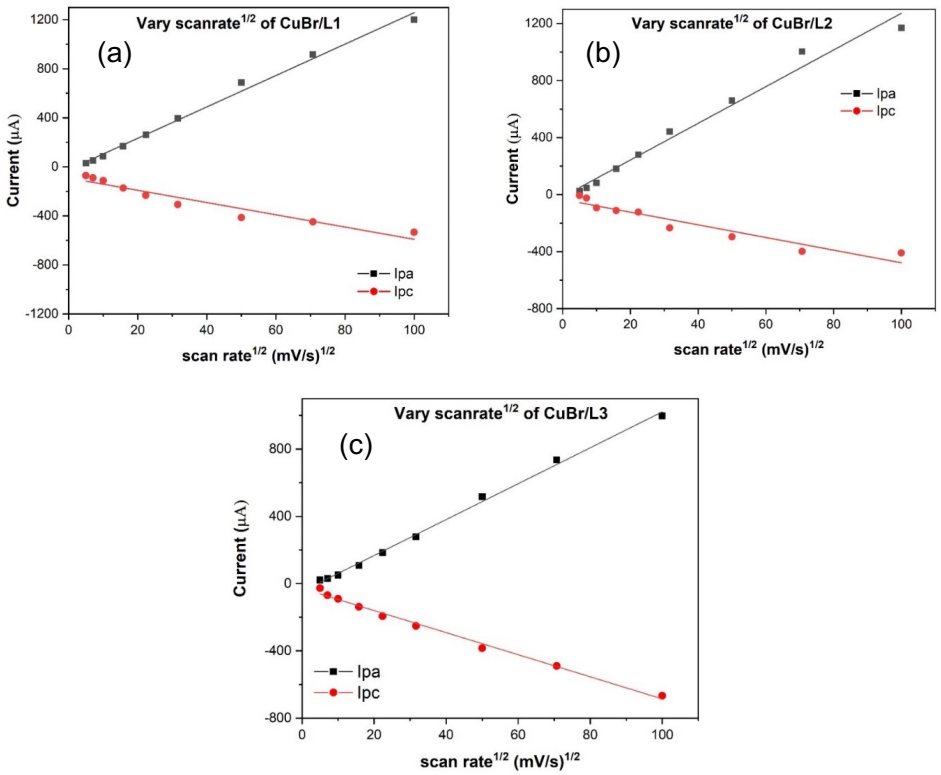


Figure S11 Square root scan rate *vs*. current of CuBr/**Ln** where **Ln** = **L1** (a), **L2** (b), **L3** (c)

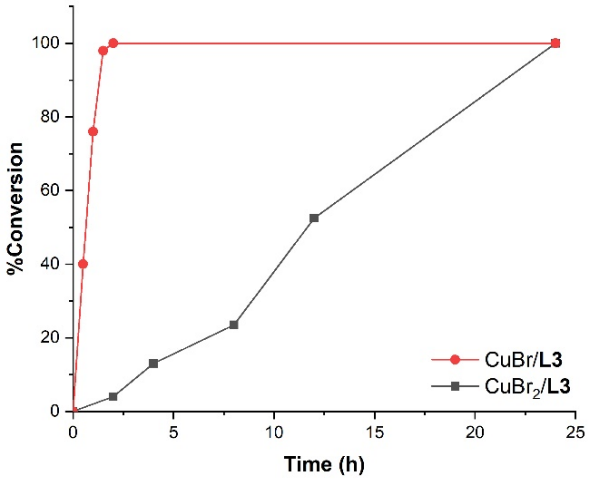


Figure S12 Oxidation profile of benzyl alcohol conversion to benzaldehyde by CuBr/**L3** and $CuBr_2$/**L3**

UV-Vis spectrophotometry titrations

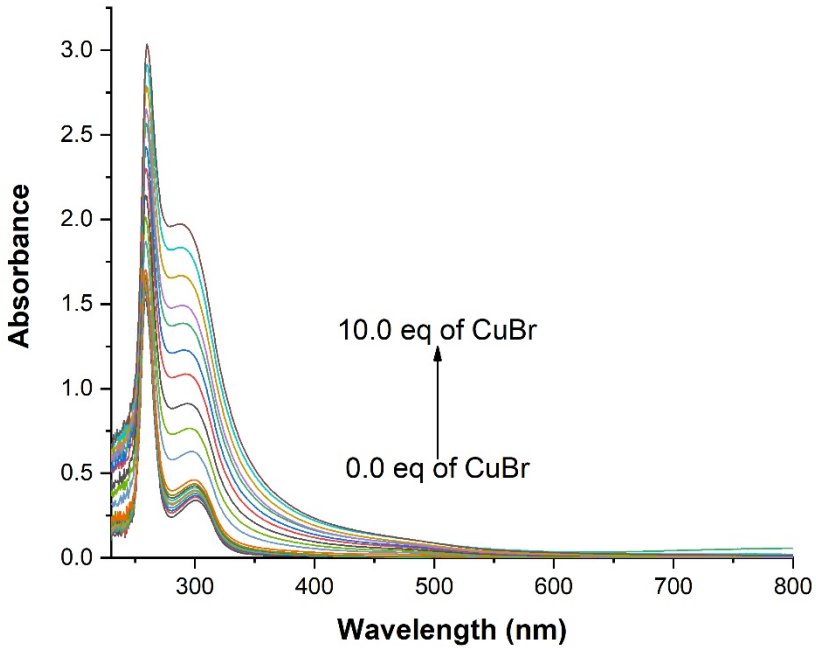


Figure S13 Absorbance spectra of CuBr at 0.0–10.0 equivalents in 1.0 x 10^{-4} M **L1** (aq.)

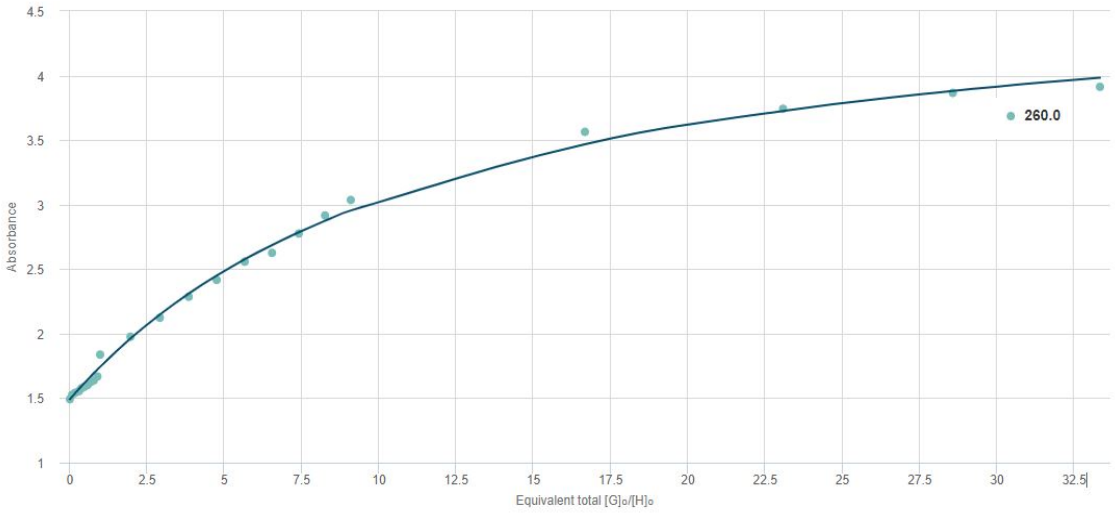


Figure S14 Binding isotherms from UV-Vis titrations of **L1** with CuBr. The solid symbols represent experimental data at wavelength of 260 nm and solid lines represent the fitted binding isotherm. The graph was generated from the online program "BindFit" using UV 1:1, the Nelder-Mead method.[7]

Table S1. Summary of BindFit analysis from UV-Vis titrations between **L1** and CuBr

Stoichiometry		**K**	**K error (%)**			**Covariance**
1:1		899.92	4.0972			3.1914e-3
Stoichiometry	**Mode**	**K_{11}**	**K_{12}**	**K_{11} error(%)**	**K_{12} error(%)**	**Covariance**
1:2	Full	539.85	303.73	3.4474	17.5155	1.8786e-3
	Non-Cooperative	507.17		3.2191		1.8902e-3
	Additive	486.97	-53.96	3.4938	-7.8090	1.9410e-3
	Statistical	1982.45		4.1783		2.9815e-3
Stoichiometry	**Mode**	**K_{11}**	**K_{12}**	**K_{11} error(%)**	**K_{12} error(%)**	**Covariance**
2:1	Full	416.01	-1914.52	5.8667	-3.3698	1.8762e-3
	Non-Cooperative	1843.60		8.3476		2.5508e-3
	Additive	1643.35	-1223.60	12.6660	-26.8204	2.3653e-3
	Statistical	826.25		3.9026		3.2947e-3

Result for (CuBr/L1) stoichiometry 1:1 ratio model:

http://app.supramolecular.org/bindfit/view/9adde80d-0685-4b8c-afa3-73c3fa8fcb35

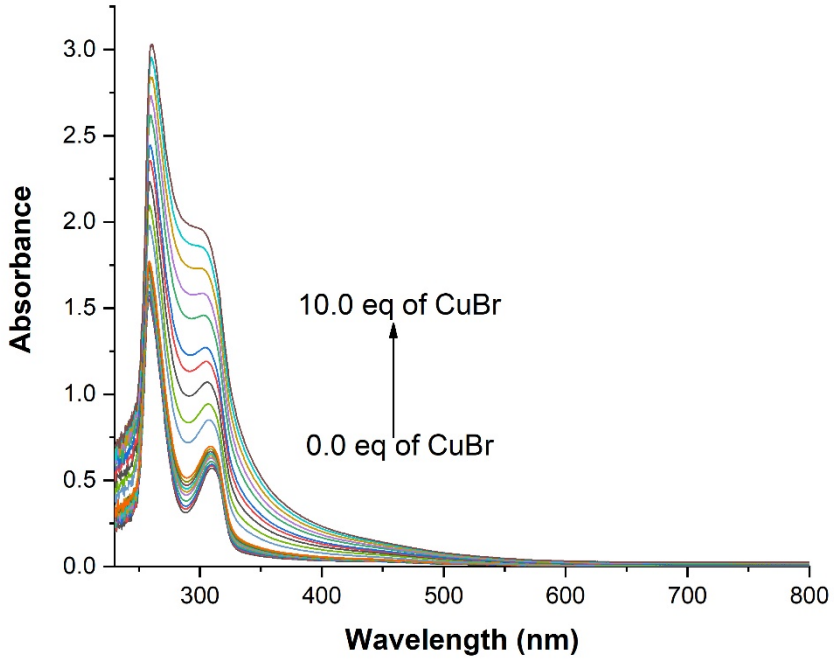


Figure S15 Absorbance spectra of CuBr at 0.0–10.0 equivalents in 1.0 x 10^{-4} M **L2** (aq.)

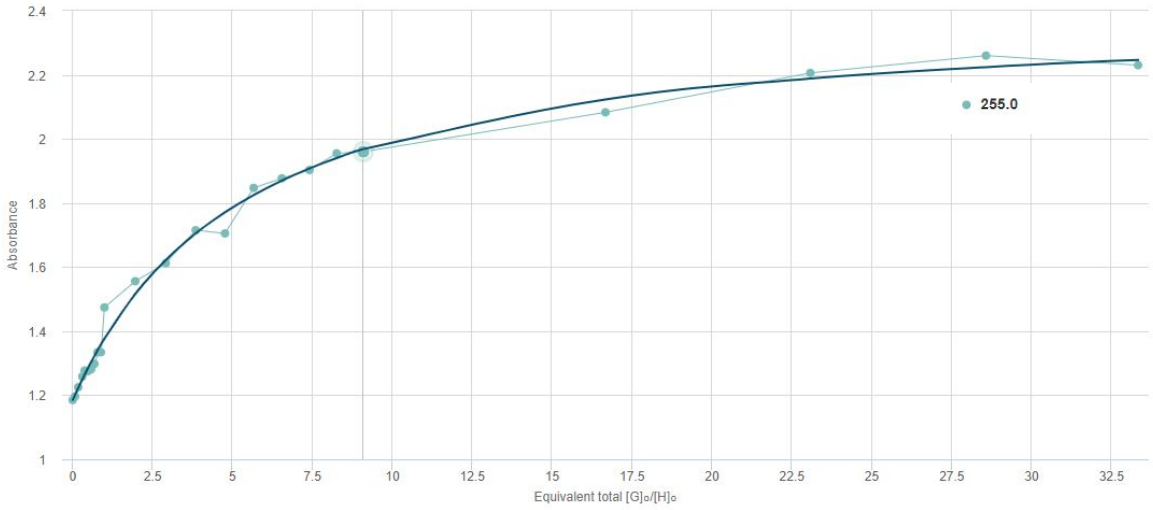


Figure S16 Binding isotherms from UV-Vis titrations of **L2** with CuBr. The solid symbols represent experimental data at wavelength of 255 nm and solid lines represent the fitted binding isotherm. The graph was generated from the online program "BindFit" using UV 2:1, the Nelder-Mead method.[7]

Table S2. Summary of BindFit analysis from UV-Vis titrations between **L2** and CuBr

Stoichiometry		**K**	**K error (%)**			**Covariance**
1:1		2217.56	7.5071			7.5329e-3
Stoichiometry	**Mode**	**K_{11}**	**K_{12}**	**K_{11} error(%)**	**K_{12} error(%)**	**Covariance**
1:2	Full					
	Non-Cooperative	3931.99		8.5868		7.9446e-3
	Additive	2682.90	31.98	9.8731	52.4564	7.2527e-3
	Statistical	5277.05		8.7400		8.1800e-3
Stoichiometry	**Mode**	**K_{11}**	**K_{12}**	**K_{11} error(%)**	**K_{12} error(%)**	**Covariance**
2:1	Full					
	Non-Cooperative	2009.46		7.1231		7.3474e-3
	Additive	548.53	8343.84	41.2815	43.4962	7.2121e-3
	Statistical	1870.05		6.4709		7.3537e-3

Result for (CuBr/L3) stoichiometry statistical model in 2:1 ratio:

http://app.supramolecular.org/bindfit/view/3ca9013e-0711-4f3e-a168-8a792dca3bb3

Result for (CuBr/L3) stoichiometry statistical model in 1:2 ratio:

http://app.supramolecular.org/bindfit/view/7b6d17c4-df89-4091-8f7a-50c4c938dd58

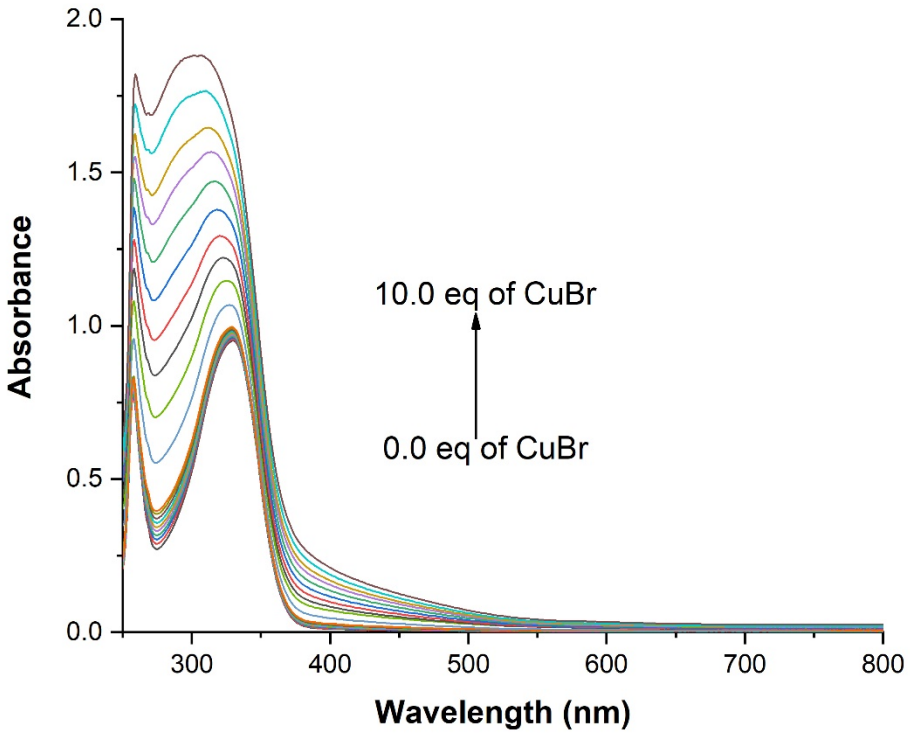


Figure S17 Absorbance spectra of CuBr at 0.0–10.0 equivalents in 1.0 x 10^{-4} M **L3** (aq.)

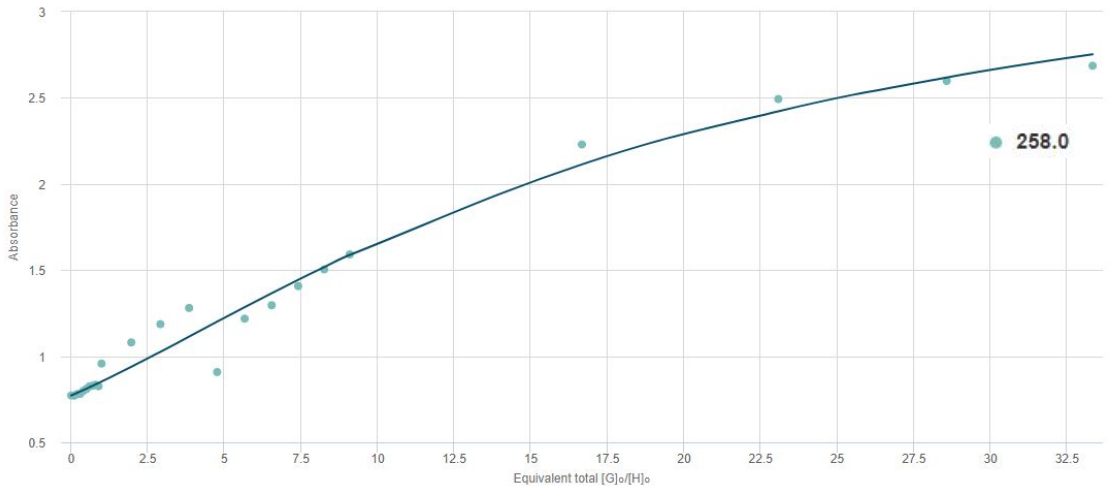


Figure S18 Binding isotherms from UV-Vis titrations of **L3** with CuBr. The solid symbols represent experimental data at wavelength of 258 nm and solid lines represent the fitted binding isotherm. The graph was generated from the online program "BindFit" using UV 2:1, the Nelder-Mead method.[7]

Table S3. Summary of BindFit analysis from UV-Vis titrations between **L3** and CuBr

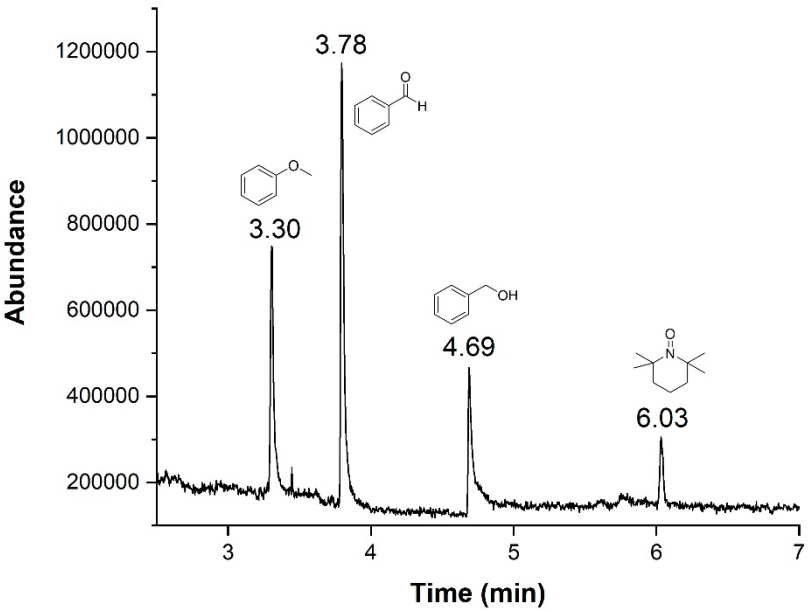
Stoichiometry		**K**	**K error (%)**			**Covariance**
1:1		238.98	8.5213			2.5578e-2
Stoichiometry	**Mode**	**K_{11}**	**K_{12}**	**K_{11} error(%)**	**K_{12} error(%)**	**Covariance**
1:2	Full	-195.38	-351.77	-9.9747	-15.1702	2.0046e-2
	Non-Cooperative	1592.77		9.3234		2.3750e-2
	Additive	571.66	719.71	40.4320	46.6436	2.2460e-2
	Statistical	496.16		8.6760		2.5535e-2
Stoichiometry	**Mode**	**K_{11}**	**K_{12}**	**K_{11} error(%)**	**K_{12} error(%)**	**Covariance**
2:1	Full	1140.51	-4978.31	15.4087	-3.9917	1.8825e-2
	Non-Cooperative	735.62		25.8192		2.3980e-2
	Additive	835.20	-1711.81	25.2889	-32.5196	2.3046e-2
	Statistical	232.03		8.3516		2.5599e-2

Result for (CuBr/L3) stoichiometry statistical model in 2:1 ratio:

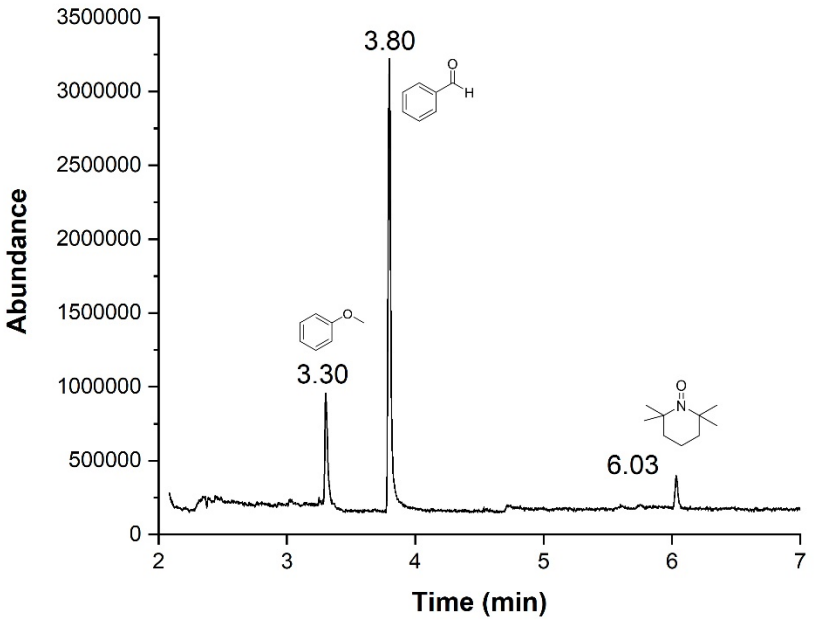
http://app.supramolecular.org/bindfit/view/daea4bc1-18e6-464f-a819-a5ee9ff60727

"BindFit v0.5 | Supramolecular," can be found at http://supramolecular.org.

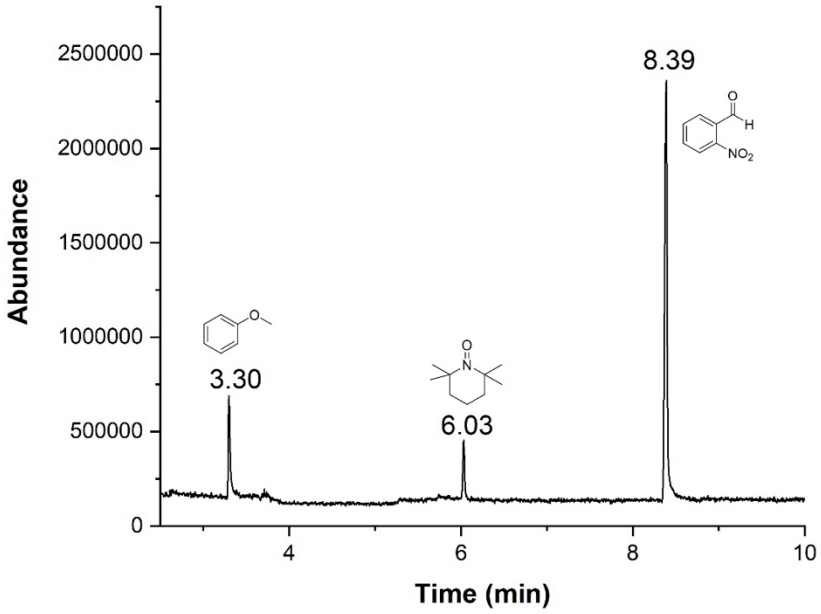
Table S4 Examples of GC-MS data from aerobic oxidation of various alcohols by CuBr/**L3**/NMI/TEMPO in CH_3CN



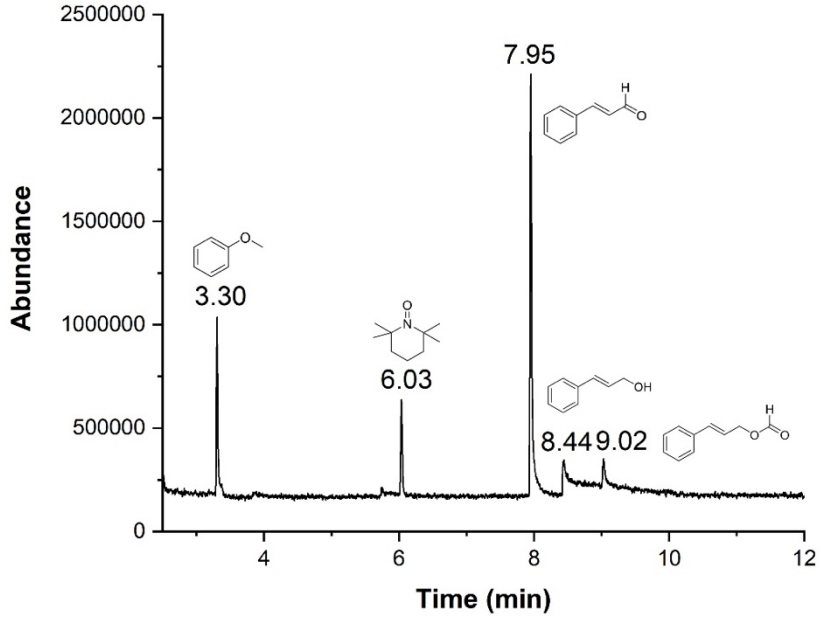
Catalytic conditions: Benzyl alcohol (1.0 mmol), 2.5 mol% CuBr / 1.25 mol% **L3** / 5 mol% TEMPO / 10 mol% NMI, anisole (0.10 mmol), ambient temperature, time = 30 min



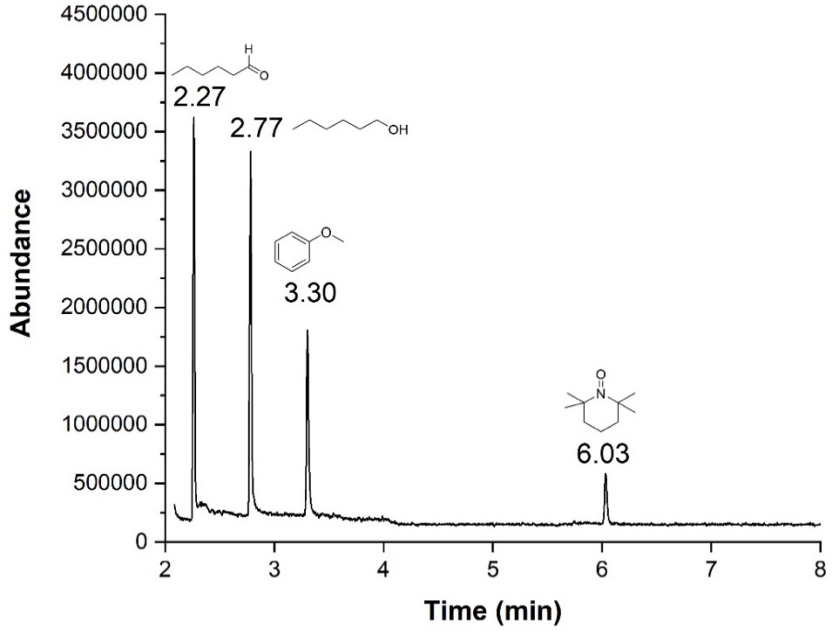
Catalytic conditions: Benzyl alcohol (1.0 mmol), 2.5 mol% CuBr / 1.25 mol% **L3** / 5 mol% TEMPO / 10 mol% NMI, anisole (0.10 mmol), ambient temperature, time = 90 min



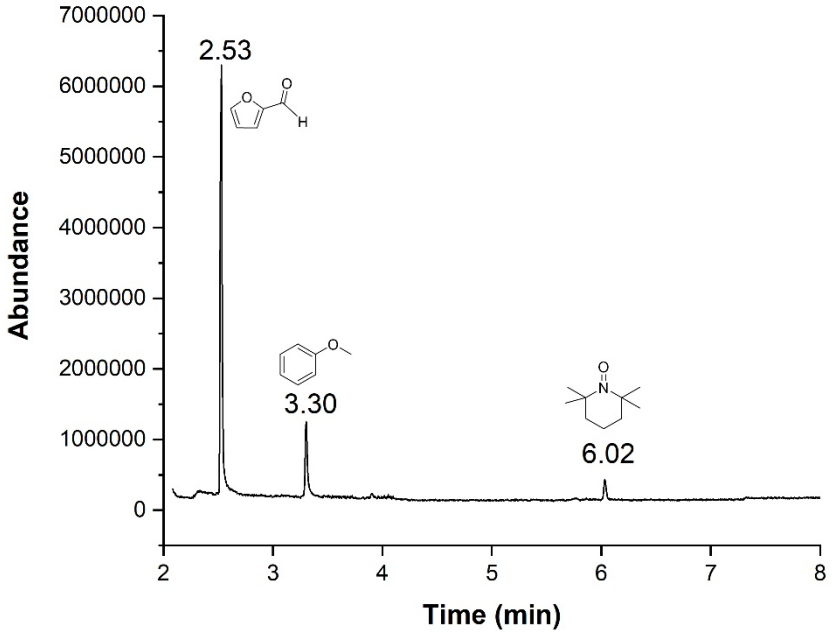
Catalytic conditions: 2-nitrobenzyl alcohol (1.0 mmol), 2.5 mol% CuBr / 1.25 mol% **L3** / 5 mol% TEMPO / 10 mol% NMI, anisole (0.10 mmol), ambient temperature, time = 2 h



Catalytic conditions: cinnamyl alcohol (1.0 mmol), 2.5 mol% CuBr / 1.25 mol% **L3** / 5 mol% TEMPO / 10 mol% NMI, anisole (0.10 mmol), ambient temperature, time = 2 h



Catalytic conditions: 1-hexanol (1.0 mmol), 2.5 mol% CuBr / 1.25 mol% **L3** / 5 mol% TEMPO / 10 mol% NMI, anisole (0.10 mmol), temperature = 60 °C, time = 24 h



Catalytic conditions: furfuryl alcohol (1.0 mmol), 2.5 mol% CuBr / 1.25 mol% **L3** / 5 mol% TEMPO / 10 mol% NMI, anisole (0.10 mmol), ambient temperature, time = 4 h

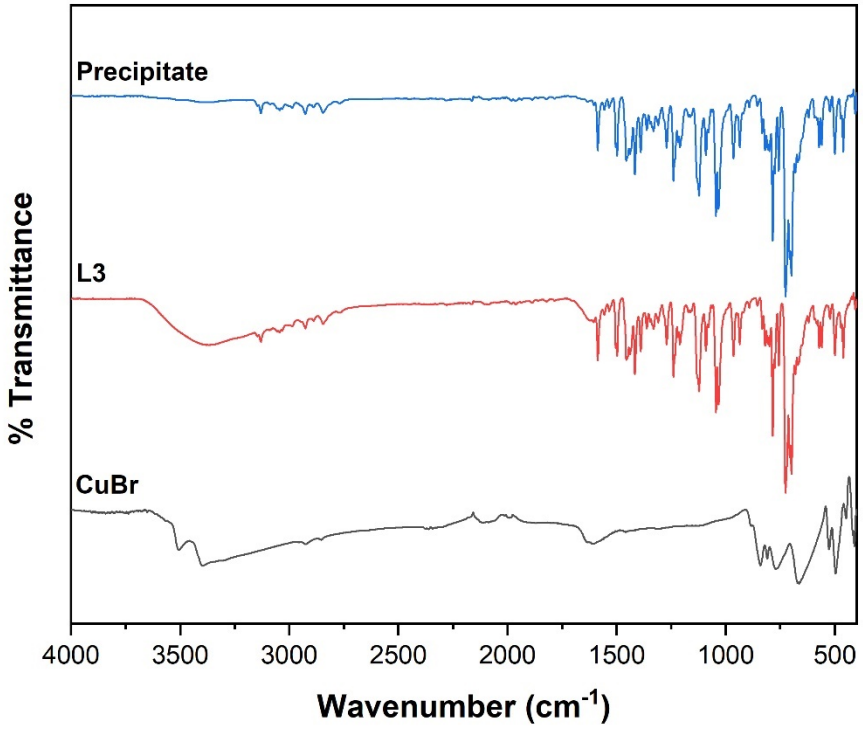


Figure S19 FT-IR spectra of CuBr, free ligand **L3,** and off-white solids

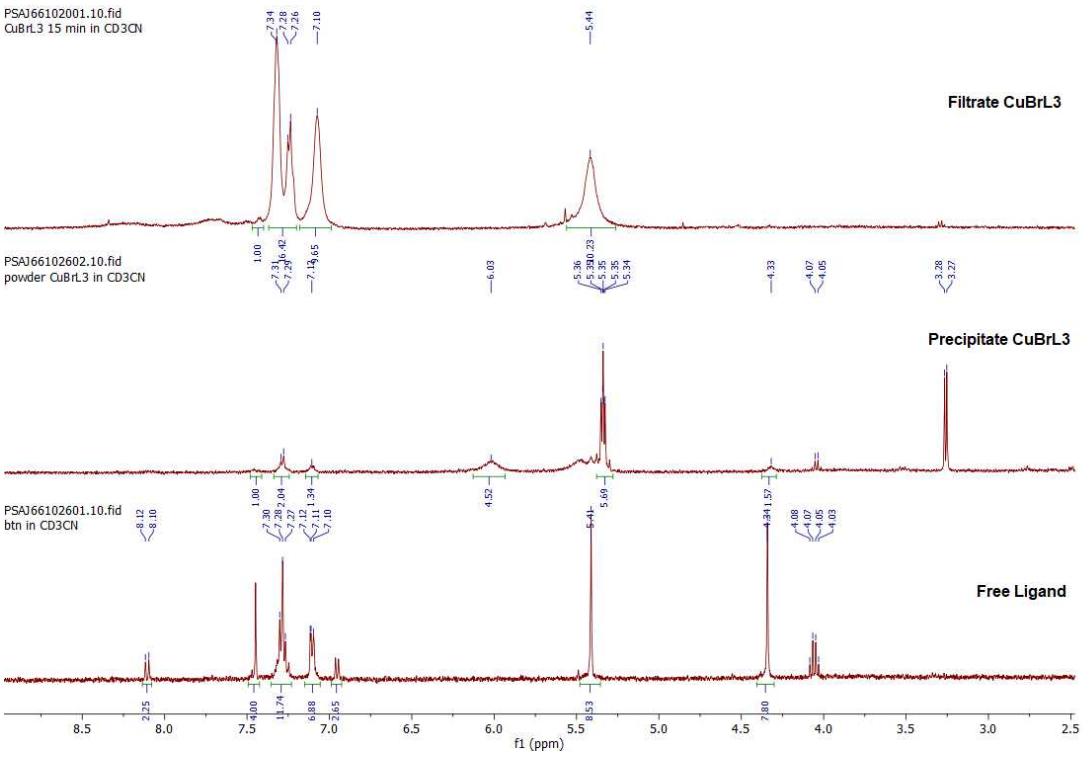


Figure S20 ^{1}H NMR of filtrate CuBr/**L3**, precipitate CuBr/**L3**, and **L3**

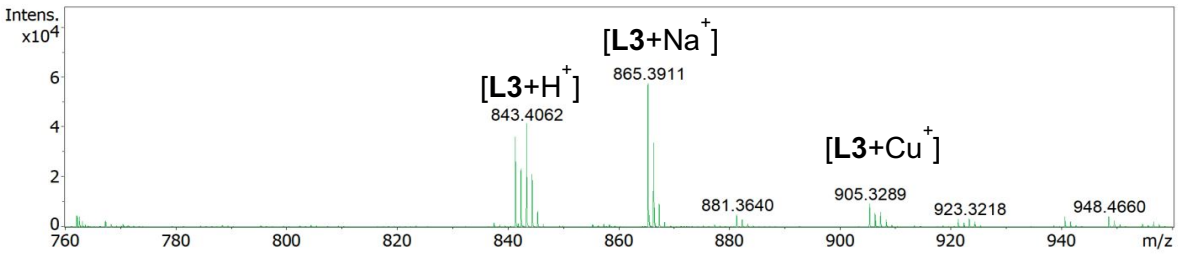


Figure S21 ESI-MS of precipitate CuBr/**L3**

Theoretical study on Cu(I)Br complexes of L1–L3

Computational details

CREST[1] program was used to explore the lowest-energy conformations of each intermediate. All geometry optimizations and frequency calculations were performed using Gaussian16.[2] The input geometries produced by CREST were optimized in the gas-phase using ωB97XD[3] functional and def2-SVP[4] basis set. Frequency calculations at the same level were performed to ensure that the optimized geometries corresponded to either energy minima with no imaginary frequency or transition states with one imaginary frequency. To take into account of the solvent effect, the single-point energy calculations were carried out with the SMD[5] continuum solvation model with the solvent parameters of dimethylsulfoxide (ε = 46.826) using ωB97XD functional and def2-TZVPP basis set. Finally, the quasi-harmonic approximation implemented in the GoodVibes[6] program was used to correct the free energies.

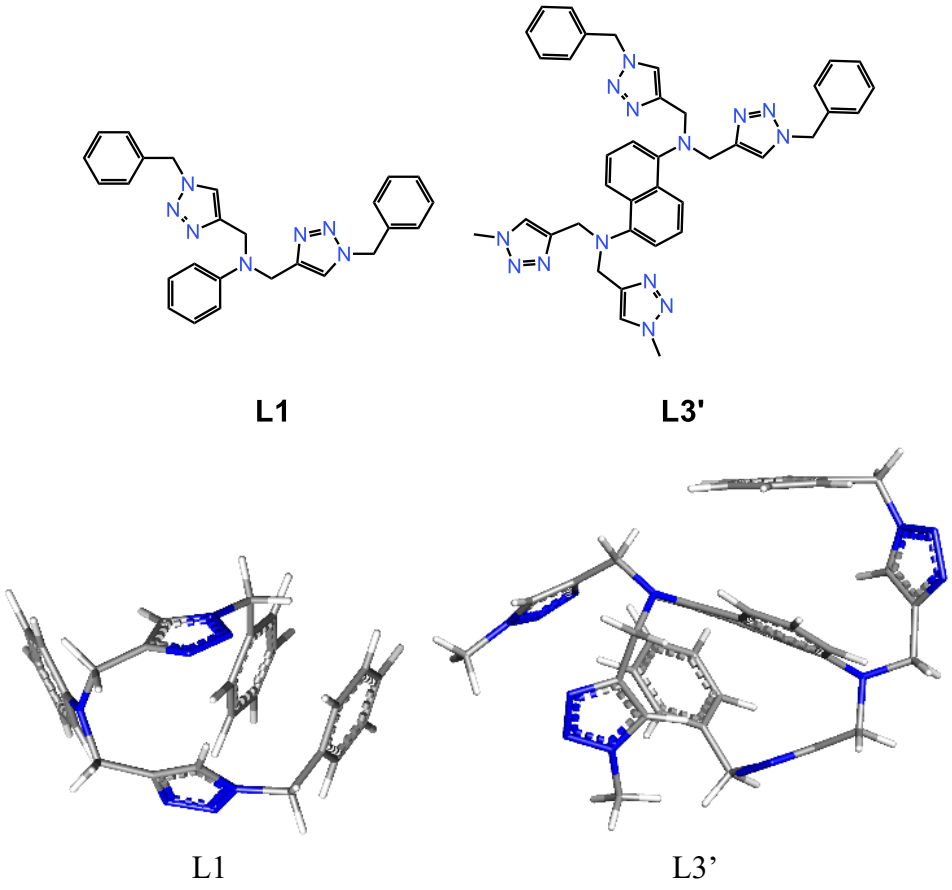


Figure S22 Optimized geometries of **L1** and **L3'**

References

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Cartesian Coordinates

L1

58

N	-0.707834	-1.495373	-2.332568
N	0.578510	-1.597273	-2.409307
N	0.994156	-2.285546	-1.348179
N	-0.553359	-1.856228	2.362341
N	0.479606	-1.101298	2.551633
N	0.105031	0.159711	2.339515
N	-3.178450	-1.345365	0.121134
C	-0.045951	-2.638143	-0.563201
C	-1.151132	-2.120410	-1.208752
C	-2.619431	-2.236797	-0.877691
C	-2.909996	-1.675523	1.512190

C	-1.617699	-1.088980	2.008038
C	-1.201925	0.225454	2.007776
C	2.412752	-2.550170	-1.152533
C	3.168979	-1.383740	-0.561432
C	3.603588	-0.341382	-1.385910
C	4.288684	0.743919	-0.848283
C	4.556304	0.791304	0.519498
C	4.130548	-0.246833	1.345903
C	3.428818	-1.325732	0.809538
C	1.078384	1.229142	2.290428
C	1.213248	1.835967	0.907383
C	1.805195	3.096374	0.774744
C	1.963020	3.675559	-0.481489
C	1.519954	3.004310	-1.621851
C	0.928346	1.750159	-1.497449
C	0.782222	1.167148	-0.239888
C	-3.492300	-0.024269	-0.213275
C	-3.127798	0.535927	-1.452639
C	-3.467576	1.849953	-1.767076
C	-4.165013	2.652341	-0.868366
C	-4.525084	2.109367	0.364233
C	-4.198578	0.797324	0.690247
H	0.071208	-3.176870	0.372898
H	-3.178604	-2.109422	-1.815835
H	-2.815423	-3.265127	-0.537834
H	-3.755527	-1.371773	2.145532
H	-2.838425	-2.767888	1.607288
H	-1.698167	1.155562	1.746770
H	2.819863	-2.817824	-2.136681
H	2.487701	-3.431118	-0.501927
H	3.379173	-0.373962	-2.454751
H	4.607407	1.561482	-1.497560
H	5.097154	1.641453	0.940787
H	4.342721	-0.219514	2.417411
H	3.072042	-2.120260	1.469104
H	2.028694	0.780575	2.611093
H	0.803479	2.002674	3.023348
H	2.143510	3.633341	1.665672
H	2.424380	4.661762	-0.569514
H	1.633365	3.462612	-2.606718
H	0.581710	1.202067	-2.375635
H	0.321185	0.180632	-0.165416
H	-2.536231	-0.034149	-2.168788
H	-3.158343	2.252964	-2.734350
H	-4.418891	3.683720	-1.119321
H	-5.076501	2.713224	1.089199
H	-4.506485	0.411820	1.662389

L3’
90

N	0.026991	-3.169295	1.781740
N	-1.051072	-3.461674	1.129680
N	-0.701632	-4.051765	-0.009532
N	6.258540	-0.361509	0.585296
N	6.443962	0.669316	-0.173255
N	5.473575	0.681635	-1.087894
N	3.127369	-2.158705	0.888385
C	0.640068	-4.145780	-0.100610
C	1.105631	-3.570912	1.064785
C	2.516660	-3.335174	1.504307
C	4.584682	-2.202941	0.899206
C	5.152738	-1.029556	0.170286
C	4.635309	-0.361784	-0.916763
C	-1.715643	-4.423930	-0.985312
C	-2.058831	-3.306503	-1.943267
C	-2.873401	-2.249698	-1.524430
C	-3.201038	-1.216360	-2.396885
C	-2.703647	-1.227349	-3.700623
C	-1.884697	-2.272022	-4.126404
C	-1.564591	-3.309398	-3.249619
C	5.260474	1.844544	-1.930600
C	4.057608	2.628119	-1.453571
C	2.882306	2.673615	-2.204614
C	1.761630	3.349274	-1.721408
C	1.809096	3.979035	-0.481033
C	2.978788	3.929175	0.277955
C	4.096535	3.256313	-0.203905
C	2.539901	-0.920187	1.308079
C	2.980509	-0.256463	2.431580
C	2.413210	0.979657	2.806217
C	1.358022	1.500230	2.099616
C	0.831130	0.820590	0.970387
C	1.487840	-0.359630	0.516008
C	1.117370	-0.919097	-0.736600
C	-0.312491	1.311721	0.245373
C	-0.642650	0.728419	-0.961079
C	0.102522	-0.360440	-1.467066
N	-1.059378	2.371646	0.808647
N	-4.043863	1.144263	2.258153
N	-4.647038	0.000296	2.255241
N	-3.723016	-0.945244	2.098771
N	-3.494039	2.087326	-1.459169
N	-4.756807	1.816060	-1.428245
N	-5.288999	2.473793	-0.399840
C	-2.487443	-0.404281	1.997058
C	-2.707446	0.955843	2.097195
C	-1.720900	2.091335	2.085422
C	-1.768562	3.291610	-0.073048
C	-3.180215	2.918709	-0.432382
C	-4.347649	3.186563	0.248777

C	-4.097418	-2.342529	2.125864
C	-6.649178	2.212262	0.011890
H	1.142683	-4.584530	-0.957426
H	2.527283	-3.274379	2.610693
H	3.124724	-4.207811	1.220146
H	5.030607	-2.221024	1.914569
H	4.890826	-3.144812	0.412991
H	3.736304	-0.500728	-1.509516
H	-2.598867	-4.730064	-0.408987
H	-1.344538	-5.304398	-1.526982
H	-3.246605	-2.230291	-0.499035
H	-3.833586	-0.392800	-2.061964
H	-2.955550	-0.411282	-4.380863
H	-1.494723	-2.283689	-5.146595
H	-0.929148	-4.132100	-3.590129
H	5.130043	1.514514	-2.971036
H	6.183951	2.435202	-1.867580
H	2.835712	2.170524	-3.174303
H	0.845462	3.368297	-2.315340
H	0.927896	4.492918	-0.092387
H	3.016112	4.410436	1.257388
H	5.006718	3.196509	0.398946
H	3.799997	-0.671098	3.022003
H	2.822710	1.522185	3.660841
H	0.940224	2.470565	2.368270
H	1.665555	-1.788498	-1.097121
H	-0.181063	-0.788638	-2.431027
H	-1.513949	1.075946	-1.517491
H	-1.588805	-1.006790	1.880669
H	-2.249817	3.000649	2.406197
H	-0.959393	1.889661	2.851486
H	-1.789062	4.277813	0.421560
H	-1.177538	3.405442	-0.991557
H	-4.562202	3.753433	1.148367
H	-3.215631	-2.940109	1.861224
H	-4.908219	-2.515727	1.405955
H	-7.125468	3.143982	0.341882
H	-6.646275	1.482326	0.834701
H	-4.445821	-2.617719	3.130724
H	-7.190072	1.805194	-0.849805

$[Cu(L1)Br]_2$

120

Cu	0.872391	0.755170	-1.498216
N	-0.935031	1.453508	-2.203353
N	-1.979183	0.806399	-1.802626
N	-3.004643	1.642598	-1.852554
N	2.661215	1.784327	-1.752672
N	3.650348	1.073886	-1.305812
N	4.547603	1.904102	-0.805573

N	0.626367	4.127337	-1.813936
C	-2.617400	2.860778	-2.295625
C	-1.268219	2.733268	-2.518701
C	-0.233797	3.741193	-2.915558
C	2.046484	4.223341	-2.058267
C	2.915034	3.104931	-1.550658
C	4.135852	3.188793	-0.921662
C	-4.248326	1.303766	-1.189127
C	-4.424618	2.123830	0.070176
C	-3.319429	2.415549	0.879447
C	-3.490658	3.127523	2.063436
C	-4.762867	3.548168	2.454967
C	-5.865057	3.265745	1.647837
C	-5.693298	2.562748	0.454560
C	5.698765	1.383142	-0.096750
C	5.413650	1.081828	1.360139
C	6.491462	0.826561	2.217432
C	6.268259	0.510344	3.554581
C	4.962399	0.452213	4.051185
C	3.890360	0.701524	3.199256
C	4.112544	1.010008	1.856398
C	0.093257	4.715931	-0.664007
C	0.835086	4.739197	0.530268
C	0.314701	5.322605	1.678893
C	-0.958715	5.891758	1.680390
C	-1.699595	5.878026	0.502085
C	-1.180478	5.310103	-0.658906
Br	0.465203	1.274837	1.022958
Cu	0.022350	-1.071057	0.236646
N	-1.805798	-1.528018	1.144806
N	-2.782000	-0.685889	1.234974
N	-3.671627	-1.191926	2.075970
N	1.437477	-2.437073	1.172494
N	2.569902	-1.936354	1.545575
N	3.486588	-2.880633	1.413415
N	-0.827175	-4.143519	0.558270
C	-3.274387	-2.404534	2.529983
C	-2.059293	-2.614813	1.926848
C	-1.157676	-3.811933	1.922805
C	0.505896	-4.588539	0.230375
C	1.603543	-3.731193	0.791106
C	2.937064	-4.029494	0.949451
C	-4.965037	-0.563425	2.225251
C	-5.933194	-0.942332	1.121425
C	-5.586774	-1.825798	0.095979
C	-6.501914	-2.122845	-0.915088
C	-7.768752	-1.545242	-0.910263
C	-8.122437	-0.668155	0.116803
C	-7.209792	-0.369690	1.124350
C	4.887665	-2.548056	1.556004

C	5.549346	-2.244123	0.226785
C	6.947259	-2.204605	0.158075
C	7.587162	-1.902363	-1.041049
C	6.833504	-1.643984	-2.189560
C	5.443136	-1.676742	-2.121898
C	4.800052	-1.968378	-0.918013
C	-1.882749	-4.373949	-0.344744
C	-1.769968	-3.980385	-1.688375
C	-2.825707	-4.175911	-2.570944
C	-4.024701	-4.748556	-2.140148
C	-4.152461	-5.122288	-0.805178
C	-3.092423	-4.943474	0.083665
Br	1.086593	-1.655902	-2.048696
H	-3.304277	3.698138	-2.366621
H	0.401574	3.282036	-3.684827
H	-0.734099	4.608877	-3.388261
H	2.202778	4.298191	-3.147073
H	2.432445	5.164926	-1.633618
H	4.719098	4.029362	-0.557548
H	-4.172389	0.234418	-0.947243
H	-5.090969	1.444370	-1.881311
H	-2.315805	2.074033	0.608955
H	-2.613769	3.349469	2.674768
H	-4.894754	4.105455	3.385368
H	-6.862245	3.602111	1.941611
H	-6.557975	2.340362	-0.176465
H	6.510243	2.118955	-0.190555
H	6.013134	0.471678	-0.623920
H	7.514262	0.870415	1.831914
H	7.116189	0.313947	4.214952
H	4.786926	0.207347	5.101225
H	2.858581	0.639927	3.550275
H	3.239925	1.161322	1.215765
H	1.801094	4.237112	0.577809
H	0.907816	5.303356	2.595927
H	-1.369761	6.334357	2.589851
H	-3.878304	-3.008822	3.199925
H	-0.230304	-3.562752	2.454287
H	-1.634332	-4.635757	2.490349
H	0.687767	-5.637100	0.547359
H	0.607534	-4.568803	-0.864231
H	3.523637	-4.920770	0.748517
H	-4.805641	0.524176	2.239643
H	-5.364911	-0.853136	3.207964
H	-4.597700	-2.289410	0.060449
H	-6.206080	-2.812829	-1.707905
H	-8.482507	-1.777792	-1.703473
H	-9.114850	-0.211929	0.131139
H	-7.484266	0.330187	1.918314
H	5.395337	-3.383062	2.060801

H	4.934538	-1.674013	2.221229
H	7.540097	-2.409609	1.054196
H	8.678525	-1.876385	-1.082979
H	7.334224	-1.413955	-3.132759
H	4.831515	-1.455726	-2.998594
H	3.706953	-1.946839	-0.897938
H	-0.867662	-3.463134	-2.023377
H	-2.714558	-3.848601	-3.607149
H	-4.851363	-4.896928	-2.838790
H	-3.213754	-5.257758	1.121471
H	-1.774299	5.350682	-1.570651
H	-2.698603	6.319649	0.477211
H	-5.084235	-5.565327	-0.445066

[Cu(L1)Br]
60

Cu	-0.247164	-1.050014	0.223974
N	1.076364	-0.593214	1.953544
N	2.140111	-1.307415	2.126744
N	3.157561	-0.476105	2.302404
N	-2.019547	-0.177279	0.610419
N	-3.070914	-0.798274	1.044572
N	-4.032733	0.100004	1.174160
N	0.067086	1.750351	0.289385
C	2.748696	0.814051	2.241615
C	1.394657	0.728312	2.028742
C	0.366986	1.766787	1.719001
C	-1.278990	2.124809	-0.080100
C	-2.289979	1.147848	0.448963
C	-3.602589	1.333316	0.817184
C	4.516259	-0.989328	2.237313
C	5.056497	-0.917760	0.823116
C	4.306896	-1.449147	-0.232387
C	4.787125	-1.377153	-1.536700
C	6.022319	-0.781586	-1.798693
C	6.771672	-0.249774	-0.750484
C	6.287219	-0.314238	0.556752
C	-5.371089	-0.316260	1.560713
C	-6.335152	-0.289733	0.396058
C	-7.551724	0.387599	0.493652
C	-8.441890	0.397750	-0.580942
C	-8.115205	-0.264394	-1.761786
C	-6.897753	-0.939759	-1.866031
C	-6.012360	-0.954802	-0.792550
C	1.121795	2.287649	-0.518098
C	2.084026	1.423546	-1.047455
C	3.160467	1.938791	-1.767317
C	3.270308	3.311590	-1.984912
C	2.299830	4.175089	-1.476610
C	1.234143	3.665962	-0.736608

Br	0.857667	-2.240703	-1.429533
H	3.432561	1.654491	2.309475
H	-0.552154	1.519931	2.270415
H	0.706799	2.762360	2.064462
H	-1.576701	3.143950	0.246632
H	-1.327179	2.119388	-1.180275
H	-4.244754	2.208647	0.839723
H	4.464332	-2.027206	2.593924
H	5.142290	-0.415192	2.934096
H	3.326944	-1.906394	-0.058713
H	4.172492	-1.784362	-2.342693
H	6.399301	-0.727341	-2.822641
H	7.736013	0.223276	-0.948889
H	6.875482	0.111678	1.374836
H	-5.719053	0.334374	2.375210
H	-5.255920	-1.332270	1.962655
H	-7.810429	0.912065	1.417773
H	-9.391763	0.929426	-0.494218
H	-8.809024	-0.254551	-2.604976
H	-6.636966	-1.460457	-2.789633
H	-5.059186	-1.484387	-0.876238
H	1.969807	0.345293	-0.908533
H	3.913284	1.252774	-2.161108
H	4.111607	3.710230	-2.556196
H	2.376693	5.251066	-1.649364
H	0.486455	4.346723	-0.320532

$[Cu(L1)_2]^+$
117

Cu	0.232812	-0.623058	0.224828
N	0.167680	-0.536144	3.517409
N	-1.217486	1.411995	1.863261
N	-2.022578	1.871958	0.963925
N	-3.220575	1.340898	1.178151
N	1.732679	0.368978	1.187860
N	2.666577	0.785454	0.382896
N	3.555501	1.434886	1.098811
C	2.090984	-3.570208	2.602914
C	1.132423	-4.323210	1.927324
C	-0.153589	-3.806517	1.799390
C	-0.483941	-2.559445	2.325952
C	0.481021	-1.791380	3.003420
C	1.778728	-2.321771	3.130952
C	-1.197672	-0.157293	3.802914
C	-1.889496	0.557831	2.675988
C	-3.197498	0.515795	2.249251
C	-4.330588	1.688920	0.309560
C	1.185944	0.466110	3.681147
C	2.024383	0.740415	2.460382
C	3.218665	1.428291	2.407351

C	4.775898	1.948396	0.478901
N	0.015915	0.677760	-2.305515
N	1.613324	-1.409568	-1.308321
N	2.511175	-2.268658	-0.936980
N	3.608056	-2.014990	-1.627653
N	-1.588938	-1.031143	-0.549832
N	-2.619486	-1.530742	0.058196
N	-3.598911	-1.612107	-0.821798
C	-2.247047	3.644095	-2.112197
C	-1.499318	4.499605	-1.311415
C	-0.258936	4.069697	-0.837790
C	0.225071	2.811428	-1.163486
C	-0.510899	1.951726	-1.992198
C	-1.760729	2.381154	-2.456227
C	1.379189	0.601987	-2.796893
C	2.126951	-0.579340	-2.249812
C	3.425313	-0.974990	-2.473582
C	4.852383	-2.671232	-1.264844
C	-0.871940	-0.322511	-2.848482
C	-1.891228	-0.793087	-1.855327
C	-3.201920	-1.167183	-2.036842
C	-4.869455	-2.220626	-0.451936
H	1.386019	-5.297509	1.507538
H	-0.921696	-4.374747	1.269754
H	-1.492840	-2.174389	2.177292
H	2.549992	-1.760910	3.661158
H	-1.196133	0.487785	4.697803
H	-1.771757	-1.051263	4.084672
H	-4.071020	-0.029590	2.592855
H	-3.886455	1.865567	-0.680868
H	1.873344	0.231970	4.517510
H	0.684766	1.406284	3.949813
H	3.826449	1.898375	3.174829
H	5.155501	2.737340	1.143720
H	-1.882346	5.487901	-1.050652
H	0.329259	4.716240	-0.182304
H	1.171029	2.463453	-0.749462
H	-2.367080	1.744878	-3.101706
H	1.408312	0.583791	-3.904661
H	1.919984	1.508151	-2.493631
H	4.208070	-0.594997	-3.121174
H	4.589788	-3.693533	-0.960441
H	5.482115	-2.733568	-2.161905
H	-1.381515	-0.003768	-3.778172
H	-0.260935	-1.196033	-3.119497
H	-3.852816	-1.171258	-2.906185
H	-5.680485	-1.538382	-0.744063
H	-3.222430	3.962228	-2.488274
H	3.103662	-3.961102	2.727358
H	-4.990113	0.812695	0.239669

H	-4.854399	-2.285136	0.644990
H	5.516836	1.136237	0.462467
C	-4.238099	-5.818708	-1.504667
C	-5.395377	-6.107841	-2.230265
C	-6.379910	-5.135055	-2.383750
C	-4.069212	-4.561740	-0.932477
C	-5.055561	-3.580486	-1.084272
C	-6.208352	-3.872549	-1.814736
H	-3.465170	-6.579932	-1.381771
H	-5.527992	-7.095252	-2.676761
H	-7.285913	-5.355953	-2.951336
H	-3.162211	-4.336463	-0.364544
H	-6.983735	-3.111785	-1.940266
C	5.580573	-1.115285	2.131353
C	6.899397	-0.682614	1.973465
C	7.545790	-0.868657	0.753077
C	4.912681	-1.734096	1.078325
C	5.565166	-1.942136	-0.143574
C	6.880113	-1.498569	-0.300831
H	5.068399	-0.976578	3.086184
H	7.424822	-0.205160	2.803224
H	8.576374	-0.533282	0.620976
H	3.876901	-2.061451	1.200818
H	7.400137	-1.657813	-1.249573
C	5.183481	1.898364	-2.001877
C	4.533156	2.477135	-0.911469
C	3.662340	3.550023	-1.126261
C	4.958356	2.376006	-3.293351
C	4.072558	3.431558	-3.502090
C	3.424916	4.020062	-2.414569
H	5.871296	1.064907	-1.833507
H	3.151981	4.014558	-0.278094
H	5.479208	1.923922	-4.140505
H	3.891621	3.803688	-4.512427
H	2.728939	4.846299	-2.571032
C	-6.486434	2.841453	0.949182
C	-5.102399	2.900948	0.777869
C	-4.430501	4.103878	1.024256
C	-7.197352	3.970451	1.357415
C	-6.524339	5.165006	1.602139
C	-5.139651	5.228448	1.436371
H	-7.020014	1.904957	0.762549
H	-3.346446	4.147781	0.890984
H	-8.279822	3.913504	1.488573
H	-7.078470	6.048935	1.924378
H	-4.609319	6.163507	1.628762

$[Cu(L3')Br]_2$
184
Cu	0.741279	2.224965	1.142153

N	1.011536	0.469000	2.199497
N	0.539220	-0.627311	1.702347
N	1.159543	-1.632048	2.304071
N	1.783174	3.834451	2.253965
N	1.173909	4.917054	1.875420
N	2.060369	5.894638	1.861553
N	3.818464	1.750959	3.098374
C	2.044302	-1.181410	3.221469
C	1.932087	0.187673	3.160069
C	2.691795	1.253933	3.878767
C	4.092733	3.159325	3.127735
C	3.092071	4.108657	2.505023
C	3.281139	5.446844	2.235388
C	0.980818	-2.979835	1.813937
C	1.665087	-3.231797	0.484509
C	2.162824	-2.201602	-0.317997
C	2.725059	-2.492128	-1.562241
C	2.786043	-3.804698	-2.021630
C	2.296199	-4.838584	-1.220942
C	1.744779	-4.552472	0.025469
C	1.687853	7.206808	1.373942
C	1.825286	7.349073	-0.126839
C	1.857045	8.632809	-0.685131
C	1.935597	8.799079	-2.065608
C	1.990516	7.680783	-2.902411
C	1.956120	6.403637	-2.348392
C	1.867871	6.235853	-0.966092
C	4.438828	0.918884	2.141485
C	4.412498	1.234826	0.801814
C	4.971195	0.361832	-0.155303
C	5.509870	-0.845967	0.216928
C	5.560026	-1.209185	1.590808
C	5.083501	-0.288754	2.570824
Br	1.781289	2.521471	-1.130661
C	5.285787	-0.571539	3.949989
C	6.119846	-2.460924	2.030045
C	6.247631	-2.714928	3.381835
C	5.861816	-1.752254	4.342557
N	6.550985	-3.389305	1.054164
N	8.882201	-5.797898	-0.185061
N	9.474756	-5.766587	-1.336810
N	9.508695	-4.495198	-1.742237
N	6.073246	-3.489924	-2.052371
N	6.471811	-4.077925	-3.132375
N	6.505597	-5.390926	-2.894107
C	8.929754	-3.685244	-0.832553
C	8.519798	-4.539990	0.167082
C	7.696411	-4.224153	1.380207
C	5.479859	-4.058745	0.318435
C	5.850482	-4.418095	-1.086842

C	6.119757	-5.654065	-1.627166
C	10.001994	-4.151114	-3.055397
C	7.042224	-6.306948	-3.873074
H	2.687504	-1.836100	3.802297
H	1.998445	2.087529	4.059292
H	3.000314	0.863919	4.867159
H	4.215257	3.476535	4.182191
H	5.070819	3.326794	2.653646
H	4.153038	6.092281	2.283486
H	-0.098826	-3.162527	1.722919
H	1.368602	-3.663056	2.582213
H	2.096829	-1.158822	-0.005704
H	3.117369	-1.675046	-2.169280
H	3.239777	-4.023511	-2.990136
H	2.353141	-5.873679	-1.565714
H	1.356740	-5.363942	0.647835
H	2.312226	7.947316	1.893699
H	0.646847	7.374601	1.683112
H	1.815534	9.510227	-0.033086
H	1.961027	9.805102	-2.490917
H	2.056377	7.810376	-3.985104
H	1.975363	5.511433	-2.977277
H	1.804060	5.217654	-0.574177
H	3.895145	2.134907	0.467347
H	4.921611	0.641226	-1.209782
H	5.897362	-1.528616	-0.540997
H	5.005180	0.180235	4.687476
H	6.025117	-1.958628	5.402946
H	6.660431	-3.667239	3.719533
H	8.792741	-2.619072	-0.983508
H	7.413026	-5.187284	1.851766
H	8.312677	-3.677427	2.108201
H	5.164095	-4.982170	0.845834
H	4.605986	-3.394438	0.296199
H	6.126712	-6.653177	-1.202970
H	10.501456	-5.036538	-3.464947
H	10.720748	-3.324116	-2.987786
H	8.024701	-6.671675	-3.537181
H	7.145093	-5.760727	-4.817686
H	9.160657	-3.856807	-3.700808
H	6.361658	-7.156855	-4.014164
Cu	-0.718118	2.232762	-1.124686
N	-1.020190	0.485281	-2.187757
N	-0.561456	-0.620081	-1.698161
N	-1.192207	-1.613094	-2.308380
N	-1.729119	3.857690	-2.244246
N	-1.094209	4.929838	-1.878390
N	-1.959618	5.926061	-1.865550
N	-3.803178	1.812034	-3.071966
C	-2.070282	-1.145380	-3.223747

C	-1.942242	0.221747	-3.151963
C	-2.690085	1.301715	-3.862634
C	-4.059323	3.224029	-3.093642
C	-3.033727	4.157605	-2.487753
C	-3.192340	5.501674	-2.227343
C	-1.028615	-2.966409	-1.828413
C	-1.714319	-3.220296	-0.500085
C	-2.204561	-2.190810	0.307927
C	-2.768302	-2.483712	1.550923
C	-2.838415	-3.798166	2.003569
C	-2.356528	-4.831327	1.197216
C	-1.803472	-4.542695	-0.047905
C	-1.555927	7.233226	-1.389543
C	-1.689181	7.391167	0.110057
C	-1.693183	8.679777	0.657876
C	-1.767478	8.858912	2.037002
C	-1.846020	7.748909	2.882896
C	-1.839169	6.466842	2.339266
C	-1.755035	6.285962	0.958374
C	-4.433578	0.982031	-2.119747
C	-4.397198	1.286907	-0.777704
C	-4.966007	0.415314	0.174662
C	-5.524781	-0.781118	-0.204851
C	-5.585610	-1.132770	-1.581277
C	-5.098507	-0.212096	-2.555966
Br	-1.749746	2.573218	1.144559
C	-5.310826	-0.480793	-3.936476
C	-6.166684	-2.372145	-2.028093
C	-6.303922	-2.613288	-3.381288
C	-5.906935	-1.649127	-4.335940
N	-6.608382	-3.301580	-1.057919
N	-8.965902	-5.688269	0.170724
N	-9.553114	-5.659306	1.325249
N	-9.569945	-4.390974	1.741224
N	-6.120143	-3.432626	2.045340
N	-6.521227	-4.022525	3.123387
N	-6.573853	-5.333319	2.876455
C	-8.984975	-3.580627	0.835771
C	-8.589650	-4.431997	-0.172628
C	-7.767482	-4.116329	-1.386563
C	-5.544923	-3.993466	-0.331942
C	-5.914633	-4.357139	1.072492
C	-6.197932	-5.593008	1.605835
C	-10.052458	-4.052155	3.059751
C	-7.118771	-6.248425	3.851681
H	-2.720188	-1.788116	-3.810420
H	-1.986000	2.125700	-4.045294
H	-3.010741	0.919420	-4.850180
H	-4.197823	3.546466	-4.144673
H	-5.025800	3.402814	-2.600390

H -4.050592 6.165251 -2.273966
H 0.048960 -3.162230 -1.739792
H -1.425018 -3.639429 -2.601296
H -2.131684 -1.147113 0.000420
H -3.155212 -1.667367 2.162373
H -3.293052 -4.018618 2.971281
H -2.420610 -5.867770 1.536632
H -1.421437 -5.353701 -0.674565
H -2.162591 7.984133 -1.915342
H -0.511362 7.373015 -1.700575
H -1.633285 9.550769 -0.001315
H -1.771150 9.868677 2.454103
H -1.908734 7.888705 3.964507
H -1.877310 5.580446 2.975462
H -1.713117 5.263432 0.574806
H -3.864770 2.176440 -0.438527
H -4.908744 0.685948 1.231063
H -5.920337 -1.463391 0.549247
H -5.021864 0.272415 -4.669242
H -6.077834 -1.844402 -5.397232
H -6.732910 -3.556289 -3.724859
H -8.834461 -2.517467 0.994889
H -7.500473 -5.078887 -1.868743
H -8.378988 -3.553461 -2.106222
H -5.246374 -4.917953 -0.867436
H -4.660500 -3.343335 -0.309053
H -6.220399 -6.589027 1.174958
H -10.566379 -4.932722 3.461821
H -10.756350 -3.211677 3.003356
H -8.109331 -6.594415 3.519673
H -7.206219 -5.708471 4.801441
H -9.203772 -3.779707 3.705178
H -6.451293 -7.110480 3.980989

[Cu(L3')Br]
92
Cu 3.306816 -1.253061 0.962981
N 2.301919 -3.031495 0.870291
N 1.514814 -3.251371 1.878395
N 0.351817 -3.647169 1.390106
N 4.656756 -1.011717 -0.642803
N 5.683770 -0.366421 -0.173102
N 6.077517 0.485026 -1.098621
N 2.161984 -1.761873 -2.160215
C 0.375645 -3.696265 0.038136
C 1.653262 -3.308137 -0.295645
C 2.307978 -3.113794 -1.627326
C 3.303517 -1.161968 -2.793883
C 4.379191 -0.581085 -1.904054
C 5.295060 0.403658 -2.200419

C	-0.786153	-3.744614	2.281885
C	-1.438555	-2.402377	2.559780
C	-0.770934	-1.193265	2.348669
C	-1.381713	0.012644	2.693104
C	-2.654532	0.022893	3.256006
C	-3.328427	-1.181697	3.461202
C	-2.725798	-2.386805	3.109688
C	7.066123	1.498763	-0.767899
C	6.408334	2.814436	-0.406968
C	6.915499	4.018477	-0.900561
C	6.315426	5.229055	-0.552889
C	5.199344	5.239567	0.282206
C	4.687553	4.037321	0.771884
C	5.290070	2.828903	0.433866
C	1.045337	-0.967908	-1.810971
C	1.192244	0.218007	-1.123625
C	0.063506	0.960879	-0.718621
C	-1.207603	0.498546	-0.952501
C	-1.404335	-0.719935	-1.658705
C	-0.269583	-1.422808	-2.160418
Br	2.717172	0.652599	2.179777
C	-0.463963	-2.538946	-3.020760
H	-0.488756	-3.960553	-0.564565
H	3.380011	-3.314654	-1.486377
H	1.922720	-3.881406	-2.323525
H	3.779247	-1.916621	-3.446508
H	2.953193	-0.364785	-3.467037
H	5.434973	1.042570	-3.067186
H	-0.413199	-4.187262	3.217063
H	-1.504752	-4.447989	1.838502
H	0.240207	-1.157271	1.937432
H	-0.837275	0.942323	2.519229
H	-3.130131	0.970986	3.513882
H	-4.333070	-1.182034	3.890170
H	-3.259173	-3.327946	3.273920
H	7.749138	1.614744	-1.620886
H	7.637689	1.090420	0.077279
H	7.785979	4.014610	-1.563173
H	6.718753	6.166209	-0.942967
H	4.725674	6.186909	0.549312
H	3.811774	4.021086	1.424222
H	4.864418	1.902091	0.833427
H	2.182854	0.570793	-0.833281
H	0.218565	1.888332	-0.164575
H	-2.066628	1.066831	-0.592796
C	-2.719358	-1.244590	-1.924737
C	-2.856508	-2.366401	-2.720564
C	-1.728371	-2.990602	-3.299255
N	-3.837300	-0.575840	-1.381875
H	0.404474	-3.007091	-3.483438

H	-1.872604	-3.840968	-3.969857
H	-3.848432	-2.776989	-2.915998
N	-7.192918	0.624423	-1.576865
N	-7.586254	1.843200	-1.381997
N	-6.552132	2.649284	-1.632893
N	-4.009816	1.735670	0.734440
N	-4.815591	2.603121	1.253487
N	-5.945359	1.969553	1.575116
C	-5.467556	1.938438	-2.002801
C	-5.890793	0.628322	-1.953732
C	-5.080485	-0.619995	-2.136519
C	-3.984503	-0.682940	0.069569
C	-4.612924	0.520070	0.701205
C	-5.865170	0.660861	1.252521
C	-6.645312	4.069689	-1.387214
C	-7.090785	2.700804	2.063999
H	-4.497886	2.386645	-2.195412
H	-5.724895	-1.479337	-1.860811
H	-4.823511	-0.735733	-3.199136
H	-4.589853	-1.574089	0.331905
H	-2.991259	-0.838139	0.511807
H	-6.692670	-0.030444	1.377682
H	-7.698933	4.304935	-1.198267
H	-6.296502	4.632153	-2.263102
H	-7.868762	2.731226	1.286362
H	-6.757668	3.716761	2.304902
H	-6.034060	4.333879	-0.511114
H	-7.491179	2.223662	2.968097

$[Cu(L3')_2]^+$
181

Cu	-1.249314	1.020687	-0.071462
N	-0.108499	2.548364	-0.937667
N	-0.544893	3.751469	-0.719010
N	0.056350	4.561653	-1.562204
N	-0.666854	-0.690693	-1.286265
N	-1.437638	-1.715215	-1.483805
N	-0.705091	-2.802537	-1.297017
N	2.323630	0.523922	-1.645397
C	0.935846	3.883514	-2.333838
C	0.830979	2.570388	-1.925840
C	1.511819	1.352499	-2.504700
C	1.660741	-0.174101	-0.555051
C	0.587071	-1.112564	-0.981098
C	0.570647	-2.486304	-0.989491
C	-0.222725	5.998490	-1.590439
C	-1.480545	6.392420	-0.855450
C	-1.440072	7.463084	0.038920
C	-2.593052	7.874461	0.709682
C	-3.795881	7.203950	0.502722

C	-3.846731	6.139212	-0.399959
C	-2.700883	5.745863	-1.083608
C	-1.337718	-4.107554	-1.254212
C	-2.077529	-4.359575	0.045694
C	-2.023486	-5.628694	0.630759
C	-2.736208	-5.906552	1.797194
C	-3.519665	-4.915639	2.390687
C	-3.584109	-3.648732	1.809853
C	-2.869529	-3.373065	0.645585
C	3.663970	0.860085	-1.351074
C	4.081787	2.140063	-1.063784
C	5.417123	2.390691	-0.665184
C	6.294833	1.352014	-0.478793
C	5.901012	0.012078	-0.755811
C	4.602886	-0.226618	-1.286731
N	-1.391640	-0.131589	1.659190
N	-0.693357	-1.224549	1.655327
N	-0.872073	-1.826006	2.808867
N	-0.721406	2.870397	2.220630
N	0.425926	3.462495	2.288883
N	0.199894	4.763944	2.436734
N	-3.447158	1.989510	2.208261
C	-1.740726	-1.134281	3.580849
C	-2.068626	-0.022978	2.831782
C	-2.926609	1.133446	3.261221
C	-3.174808	3.401692	2.365226
C	-1.715566	3.784757	2.326591
C	-1.127712	5.022766	2.466574
C	-0.254734	-3.120287	3.081192
C	1.083043	-3.313316	2.404267
C	1.389455	-4.565117	1.865677
C	2.634246	-4.802558	1.278315
C	3.577113	-3.780156	1.199032
C	3.270129	-2.521531	1.720410
C	2.040794	-2.293599	2.334904
C	1.309163	5.681961	2.636041
C	1.974665	6.173882	1.370652
C	2.067116	7.545231	1.115500
C	2.741265	8.017148	-0.011091
C	3.338615	7.115427	-0.889789
C	3.254388	5.744880	-0.637834
C	2.573308	5.272611	0.482737
C	-3.767458	1.487118	0.940662
C	-4.657323	0.363861	0.808522
C	-4.877837	-0.202107	-0.483432
C	-4.303556	0.418426	-1.625457
C	-3.559781	1.562887	-1.489134
C	-3.271582	2.097051	-0.208656
C	4.270228	-1.520237	-1.767437
C	-5.431080	-0.105901	1.905515

H	1.546065	4.363925	-3.092970
H	0.720209	0.718514	-2.936736
H	2.139236	1.686826	-3.343019
H	2.416345	-0.758327	-0.020991
H	1.236497	0.531703	0.187352
H	1.329758	-3.226336	-0.750203
H	-0.292656	6.281207	-2.652028
H	0.644135	6.521069	-1.163802
H	-0.493898	7.979989	0.214684
H	-2.548262	8.721262	1.398068
H	-4.698299	7.518283	1.031130
H	-4.788787	5.616797	-0.580147
H	-2.756847	4.916386	-1.791613
H	-0.552211	-4.859219	-1.402248
H	-2.030290	-4.186240	-2.106359
H	-1.423302	-6.413933	0.163677
H	-2.679184	-6.902354	2.242625
H	-4.080185	-5.132751	3.302862
H	-4.203898	-2.863786	2.249122
H	-2.936259	-2.379017	0.199596
H	3.361733	2.956870	-1.110061
H	5.734841	3.417880	-0.470064
H	7.320086	1.534803	-0.153405
H	-2.043653	-1.465224	4.569701
H	-2.300118	1.764285	3.908244
H	-3.721319	0.732341	3.914571
H	-3.596763	3.734160	3.330277
H	-3.728193	3.957279	1.595218
H	-1.532959	6.024291	2.572127
H	-0.149857	-3.189036	4.174617
H	-0.954653	-3.907294	2.764355
H	0.644529	-5.364337	1.904289
H	2.865014	-5.791332	0.876483
H	4.553134	-3.952581	0.742648
H	4.005412	-1.716768	1.641537
H	1.813739	-1.301746	2.732859
H	0.931310	6.529423	3.222487
H	2.040416	5.148384	3.259340
H	1.616576	8.257730	1.812074
H	2.808019	9.091157	-0.195707
H	3.879723	7.479969	-1.765331
H	3.735480	5.039995	-1.319528
H	2.504043	4.198631	0.679793
H	-4.513602	0.008959	-2.612314
H	-2.696715	3.021605	-0.131251
H	-3.164557	2.068061	-2.373358
C	6.790391	-1.099451	-0.568995
C	6.432628	-2.341129	-1.056839
C	5.186680	-2.538365	-1.688062
C	-6.357988	-1.101619	1.728588

C	-6.517828	-1.723681	0.473001
C	-5.778707	-1.317668	-0.620161
H	3.296247	-1.671691	-2.234076
H	4.948408	-3.523675	-2.094661
H	7.116483	-3.183188	-0.954196
H	-5.352320	0.389261	2.870912
H	-6.989529	-1.415028	2.562401
H	-7.273634	-2.502726	0.363182
N	9.467410	-2.799905	-2.484489
N	9.688263	-2.479554	-3.715151
N	9.777020	-1.151426	-3.783842
N	7.394262	-3.102665	1.993761
N	6.676591	-3.842390	2.771567
N	5.995799	-3.042179	3.587942
N	8.010932	-0.875596	0.113388
C	9.611566	-0.595633	-2.562108
C	9.416727	-1.674736	-1.726371
C	9.146415	-1.720136	-0.258034
C	7.865897	-0.670829	1.550023
C	7.182634	-1.792735	2.287672
C	6.270496	-1.743359	3.321305
C	10.020266	-0.503517	-5.052112
C	5.081506	-3.599544	4.558266
H	9.633596	0.476186	-2.389805
H	9.023214	-2.774223	0.043313
H	10.019045	-1.336161	0.294147
H	8.874372	-0.515812	1.965206
H	7.305479	0.257239	1.742977
H	5.815701	-0.920841	3.865875
H	10.083768	-1.291280	-5.811010
H	10.965578	0.055500	-5.025948
H	5.322400	-3.232726	5.564921
H	5.200634	-4.688224	4.526621
H	9.195946	0.178976	-5.300156
H	4.044948	-3.338898	4.300343
N	-9.387146	-1.588462	-1.207468
N	-10.135817	-0.540175	-1.127938
N	-9.587316	0.412608	-1.880510
N	-4.022918	-5.001113	-2.672652
N	-4.110757	-6.159545	-2.101798
N	-4.957376	-6.046236	-1.084289
N	-5.950450	-1.889720	-1.898577
C	-8.451832	-0.030847	-2.466231
C	-8.335329	-1.331891	-2.026506
C	-7.275387	-2.352479	-2.283607
C	-4.847387	-2.663641	-2.439192
C	-4.812893	-4.109535	-2.021428
C	-5.426739	-4.781884	-0.985671
C	-10.219368	1.707980	-1.988996
C	-5.300394	-7.199905	-0.284428

H	-7.837101	0.587237	-3.113637
H	-7.594068	-3.284873	-1.780689
H	-7.227836	-2.589869	-3.358754
H	-4.878229	-2.632669	-3.541387
H	-3.896332	-2.189967	-2.146089
H	-6.111834	-4.471329	-0.204207
H	-11.098131	1.695566	-1.334777
H	-10.536815	1.897967	-3.023315
H	-5.278465	-6.932280	0.779540
H	-4.552305	-7.975012	-0.484569
H	-9.530260	2.499023	-1.663838
H	-6.296870	-7.576885	-0.553748

$[(CuBr)_2(L3')]$

94

Cu	-2.697138	-0.765685	-0.767408
N	-1.584425	-2.383488	-0.434790
N	-0.588326	-2.670345	-1.217092
N	0.017832	-3.726677	-0.714085
N	-4.671970	-1.413396	0.082143
N	-5.600224	-1.071765	-0.757405
N	-6.668029	-0.737934	-0.059408
N	-2.949421	-2.015296	2.352507
C	-0.589990	-4.139429	0.421935
C	-1.640369	-3.266508	0.598406
C	-2.708569	-3.279041	1.653793
C	-4.331869	-1.680838	2.577930
C	-5.141586	-1.312273	1.354179
C	-6.441354	-0.862100	1.269696
C	1.104967	-4.380982	-1.452018
C	2.251736	-3.474435	-1.825898
C	2.090068	-2.494505	-2.812712
C	3.156136	-1.668929	-3.161259
C	4.394827	-1.817974	-2.539327
C	4.565250	-2.799144	-1.563836
C	3.498648	-3.623379	-1.209173
C	-7.801191	-0.119516	-0.729999
C	-7.751818	1.389846	-0.625116
C	-8.882974	2.111843	-0.239114
C	-8.834804	3.503829	-0.156011
C	-7.651457	4.178412	-0.450274
C	-6.518102	3.458498	-0.831422
C	-6.565589	2.070449	-0.923011
C	-1.997090	-0.984314	2.274853
C	-2.308805	0.285622	1.827049
C	-1.289951	1.234330	1.579016
C	0.029711	0.885755	1.697124
C	0.381451	-0.393940	2.202333
C	-0.638433	-1.288843	2.621977
Br	-2.870650	1.332295	-1.754799

C	-0.276449	-2.437843	3.375447
C	1.750473	-0.800250	2.320360
C	2.066289	-1.933315	3.041931
C	1.045270	-2.723132	3.619607
N	2.703221	-0.068621	1.581506
N	4.643315	2.490725	1.071373
N	4.631532	3.770534	1.250873
N	4.100745	3.997290	2.444140
N	3.229449	1.420282	-1.431041
N	2.651146	2.172864	-2.314462
N	1.365885	1.853285	-2.310044
C	3.757952	2.836557	3.052158
C	4.114904	1.856827	2.153031
C	3.940539	0.365653	2.206511
C	2.740788	-0.430423	0.164259
C	2.320106	0.601152	-0.837236
C	1.098933	0.876972	-1.413673
C	3.971826	5.351082	2.935609
C	0.446923	2.506563	-3.221118
H	-0.237760	-4.982660	1.007615
H	-3.645493	-3.571274	1.153334
H	-2.463239	-4.093799	2.358393
H	-4.824893	-2.535713	3.073244
H	-4.372551	-0.852131	3.300603
H	-7.189227	-0.613729	2.016736
H	0.653476	-4.826186	-2.351291
H	1.454959	-5.201793	-0.813313
H	1.117429	-2.363979	-3.290889
H	3.015316	-0.889864	-3.913559
H	5.226372	-1.148445	-2.768200
H	5.530292	-2.880192	-1.059530
H	3.635411	-4.384804	-0.435719
H	-8.726916	-0.519794	-0.294030
H	-7.741907	-0.450416	-1.776071
H	-9.812135	1.585859	-0.001225
H	-9.724646	4.060813	0.145289
H	-7.611718	5.267730	-0.380950
H	-5.582306	3.971208	-1.063648
H	-5.663583	1.526870	-1.224468
H	-3.337103	0.557638	1.585213
H	-1.573437	2.216528	1.198366
H	0.829737	1.574424	1.425857
H	-1.064522	-3.067806	3.790416
H	1.315209	-3.590061	4.227177
H	3.111152	-2.238497	3.136285
H	3.302989	2.797205	4.037451
H	4.821591	-0.095330	1.723625
H	3.936462	0.054255	3.260535
H	3.769857	-0.726486	-0.099223
H	2.114633	-1.321152	0.013016

H	0.096787	0.477514	-1.267788
H	4.301086	6.020974	2.133796
H	4.604454	5.500580	3.821050
H	-0.578721	2.241613	-2.930745
H	0.642263	2.174918	-4.249540
H	2.925081	5.565956	3.188421
H	0.588988	3.591977	-3.155636
Cu	5.121805	1.380373	-0.694800
Br	6.977443	-0.006402	-0.635547