

SUPPORTING INFORMATION

Synthesis, Characterization and Catalytic Activity of Copper(II) Complexes containing a Redox-Active Benzoxazole Iminosemiquinone Ligand

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Clarke, and Tim Storr^{*b}**

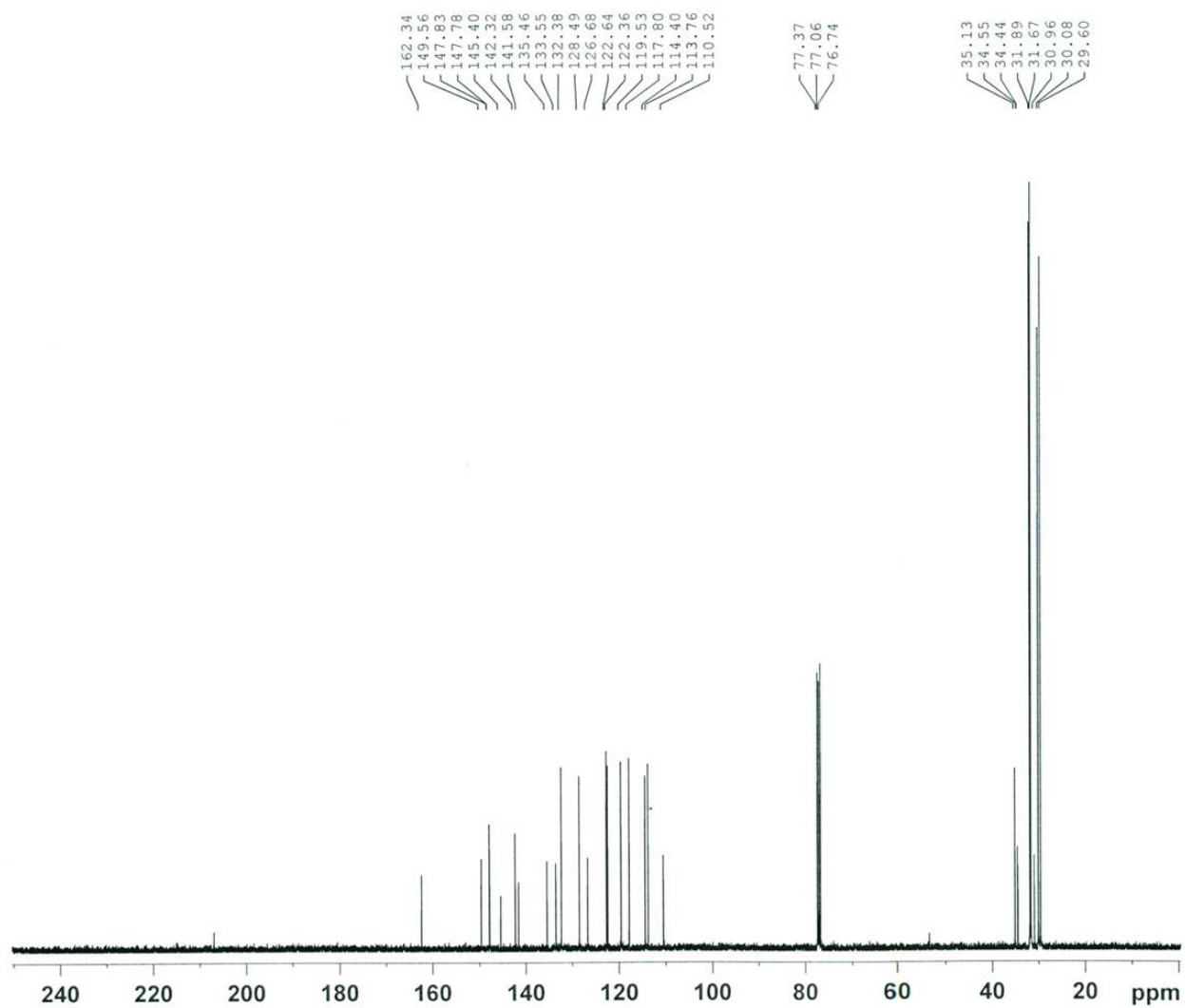


Figure S1. ^{13}C NMR titration of HL^{BAP} .

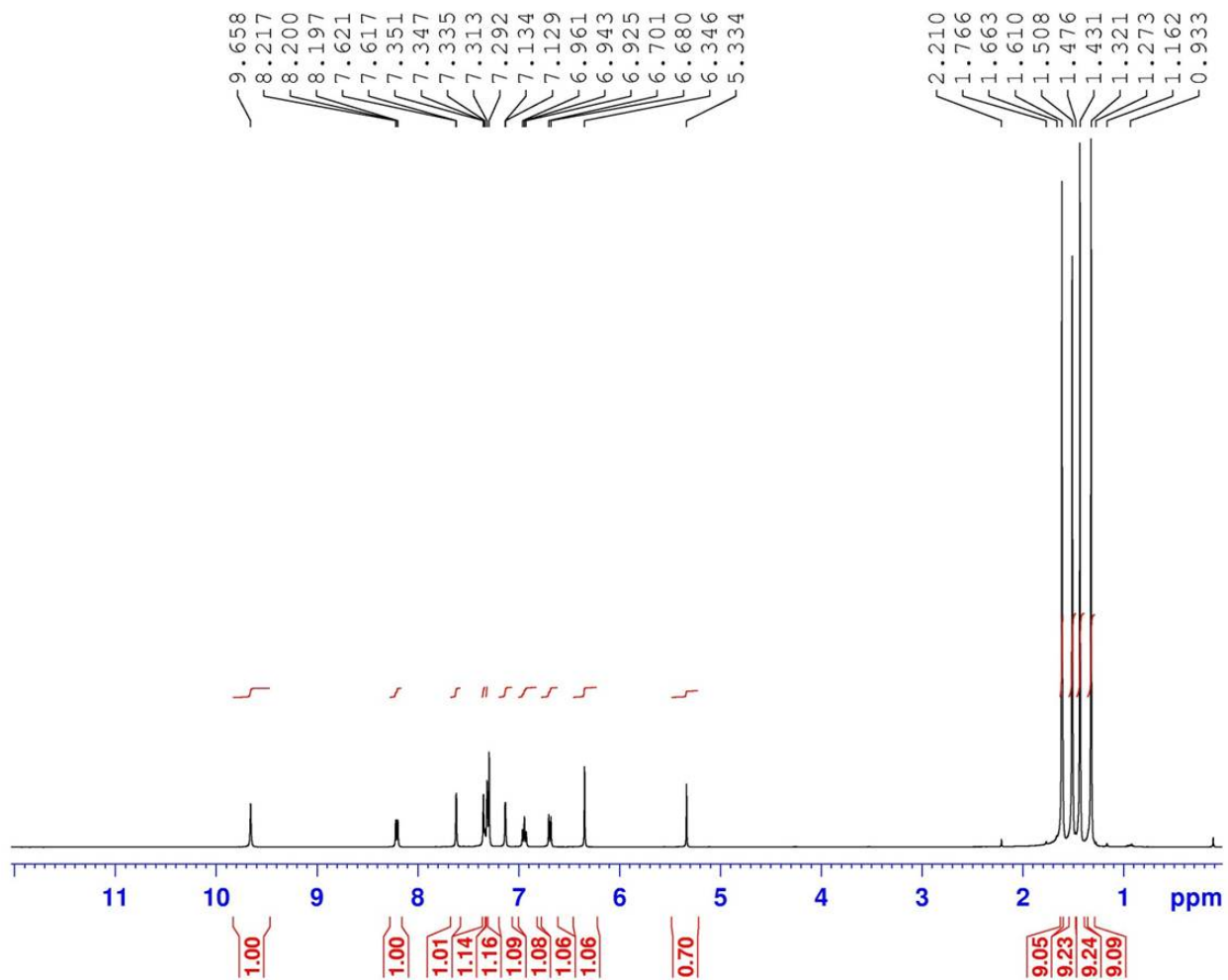


Figure S2. ¹H NMR titration of HL^{BAP}.

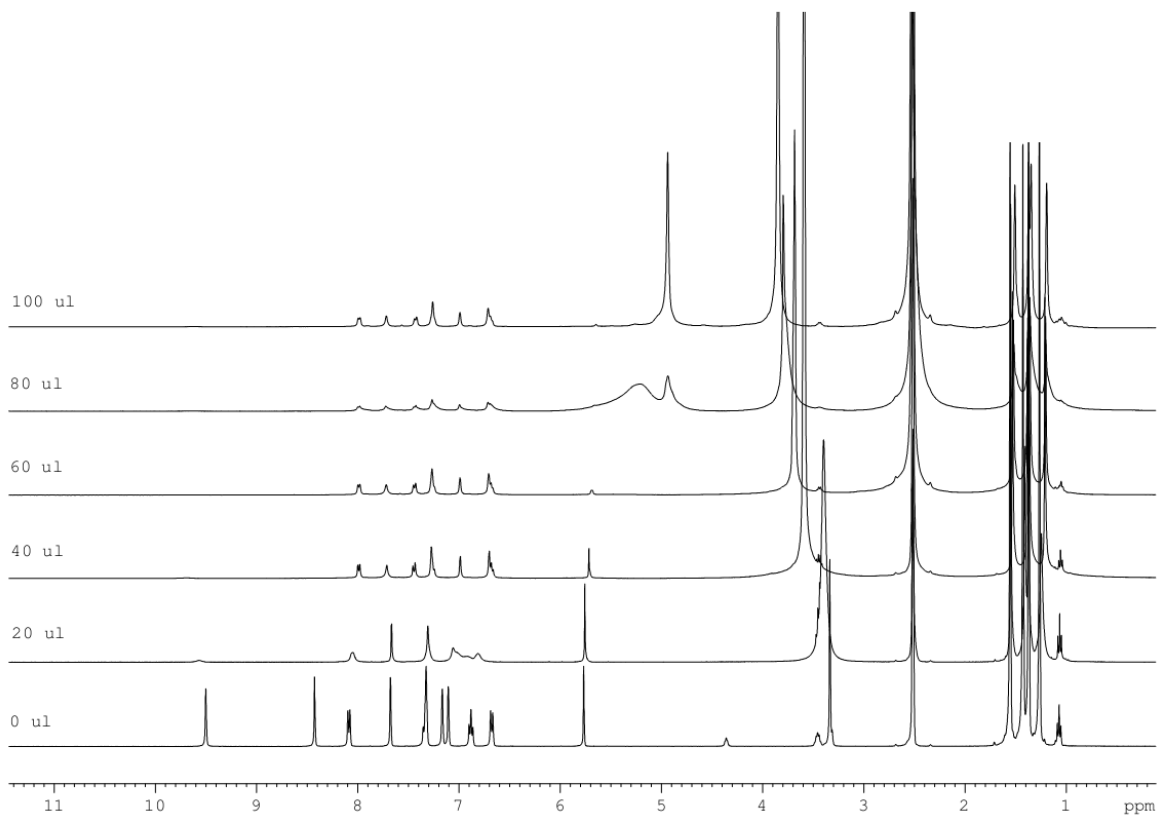


Figure S3. ¹H NMR titration of HL^{BAP} using NaOD.

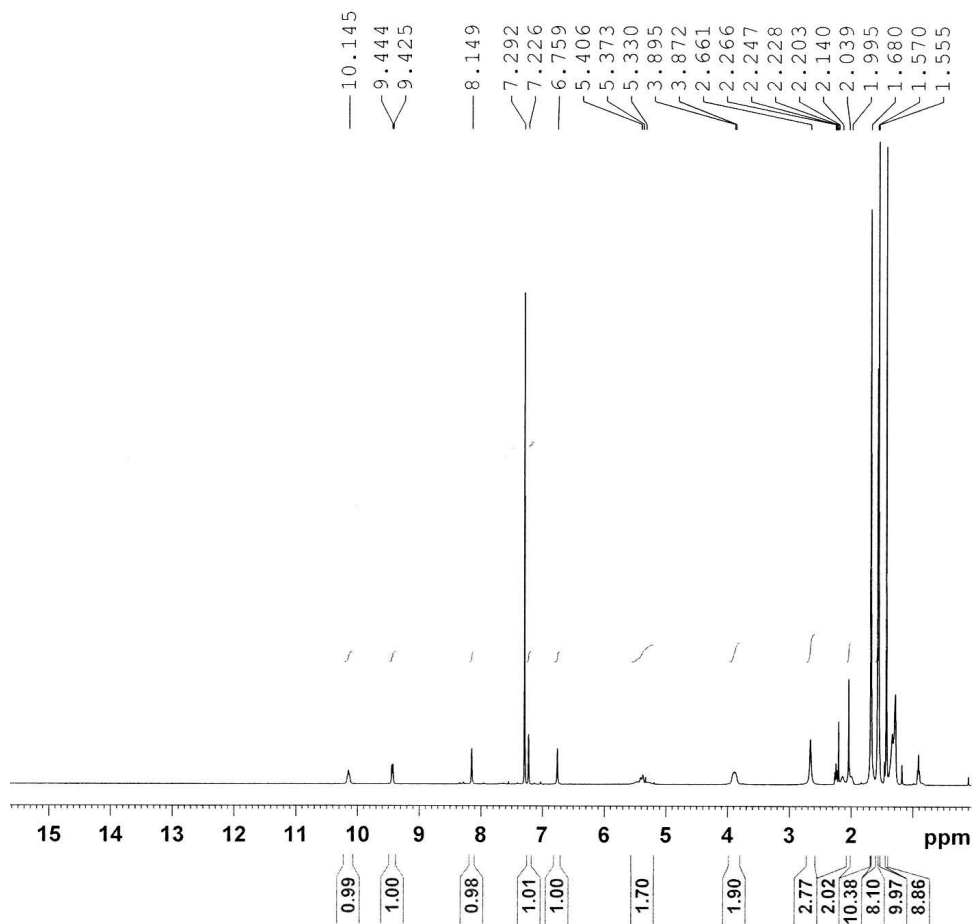


Figure S4. ^1H NMR spectrum of $\text{L}^{\text{BIS}}\text{Cu}^{\text{II}}\text{OAc}$.

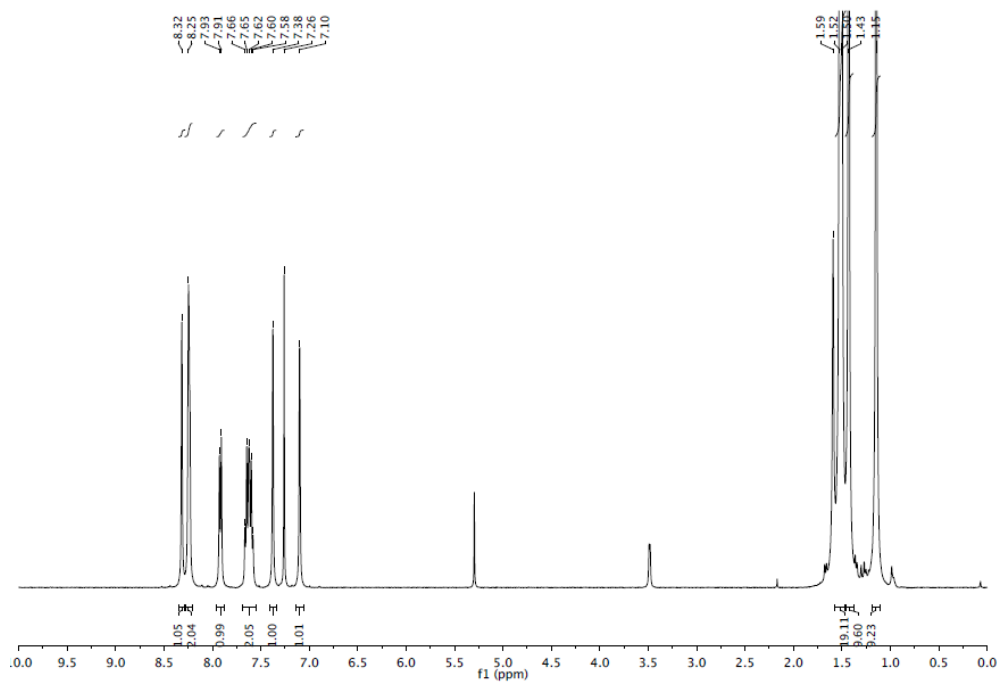


Figure S5. ^1H NMR spectrum of $\text{L}^{\text{BIS}}\text{Cu}^{\text{II}}\text{Cl}$.

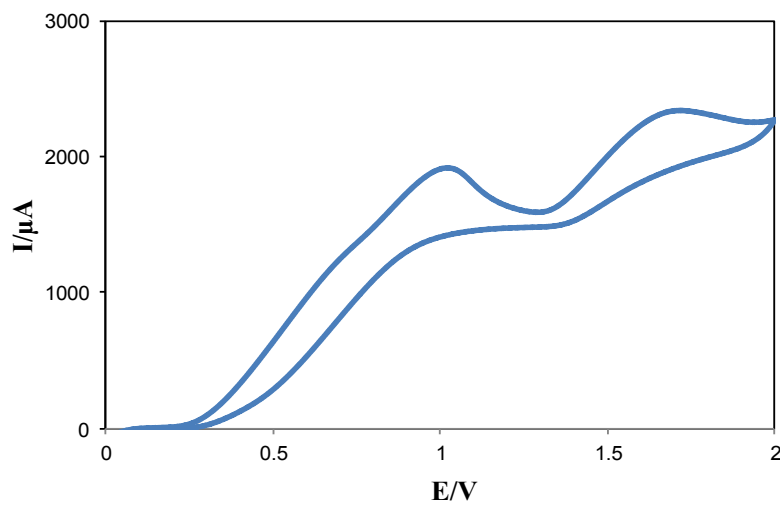


Figure S6. Cyclic voltammograms of HL^{BAP} . Conditions: 2mM, 0.1 M NBu_4ClO_4 , scan rate 50 mV/s, CH_2Cl_2 , 203 K.

Broken symmetry optimized coordinates for L^{BIS}Cu^{II}Cl (B3LYP, 6-31g*)

Cu	-0.27151100	-0.75578900	-1.03978600
Cl	0.68553800	-2.20058000	-2.41715500
O	-1.81244500	-1.78110300	-0.49378000
O	2.53426600	2.06284200	-0.07204400
N	1.27783900	0.25445100	-0.41814700
N	-1.44961800	0.77535600	-0.74257500
C	2.55388400	-0.17505500	-0.04066900
C	3.33130000	0.95766200	0.18321100
C	-2.82275300	-1.04661500	-0.19163700
C	1.31828500	1.56839700	-0.43092700
C	5.15420600	-0.37919100	0.75485800
C	0.64048400	3.84149900	-1.06262200
C	4.40435400	-1.56287000	0.53084100
C	-1.61395500	4.36292000	-1.70823900
C	-2.62671100	0.40375100	-0.18282500
C	-4.10732800	-1.59167400	0.17085300
C	-5.03361800	-0.70455200	0.67565700
C	3.07369900	-1.45871500	0.12689700
C	-1.99875200	3.05523400	-1.45108600
C	0.27941100	2.50250200	-0.81516200
C	-5.90530300	1.55196900	1.50346500
C	-3.44393100	-3.88631000	0.99413100
C	-4.37610000	-3.10009400	0.03865200
C	-3.60864600	1.23554800	0.41720300
C	-0.29166100	4.77137700	-1.49471700
C	-1.08034300	2.09372300	-0.97232900
C	4.66737400	0.92327700	0.59353200
C	-4.80460300	0.70202400	0.84877700
C	-5.50351200	3.03289300	1.63433500
C	-4.12107200	-3.54778200	-1.42209800
C	5.09005500	-2.92884200	0.72839300
C	-7.19338200	1.47660000	0.64747900
C	-5.83207800	-3.45598800	0.39605300
C	-6.20035000	1.00768600	2.92296500
C	4.82518800	3.05429000	1.92522100
C	5.49839300	2.19255600	0.82959800
C	5.58385300	3.00188900	-0.48720800
C	6.93129000	1.86410400	1.28750100
C	4.13166400	-4.10306100	0.45230200
C	6.28793500	-3.04774800	-0.24418100
C	5.59574700	-3.05129900	2.18549400
H	6.18417600	-0.49291000	1.06922200
H	1.67554900	4.13416200	-0.92544300
H	-2.34758100	5.06776300	-2.08994500
H	-5.99508500	-1.09082500	0.99002800
H	2.45569900	-2.31852400	-0.09296000
H	-3.01625800	2.74204500	-1.65330500
H	-3.64286900	-4.96147600	0.90522400
H	-2.39330400	-3.71006400	0.75662200
H	-3.62067800	-3.59642600	2.03717900
H	-3.39831000	2.28991900	0.53133600

H	0.00932000	5.79599900	-1.68876000
H	-6.31636200	3.59490000	2.10742900
H	-4.60948600	3.15935000	2.25531700
H	-5.31125000	3.49187300	0.65790800
H	-4.31738800	-4.62241100	-1.52043200
H	-4.78994700	-3.02033700	-2.11305400
H	-3.08931400	-3.35996200	-1.72519600
H	-7.99102500	2.06826700	1.11273700
H	-7.56018600	0.45047100	0.54277500
H	-7.01858700	1.87388400	-0.35891700
H	-5.98470200	-4.53102000	0.25197900
H	-6.55271600	-2.93180300	-0.24299100
H	-6.06979100	-3.23053200	1.44250000
H	-6.98720800	1.60434600	3.40010700
H	-6.53984900	-0.03289600	2.90281800
H	-5.30630900	1.05632100	3.55477500
H	5.40749300	3.96786400	2.09522300
H	4.76917500	2.50741700	2.87333500
H	3.81063800	3.35021400	1.64347700
H	6.17438900	3.91260900	-0.33107800
H	6.06722800	2.41519900	-1.27637800
H	4.59419600	3.29991200	-0.84560200
H	7.48502500	2.79596700	1.44641900
H	7.47696000	1.27988600	0.53809000
H	6.94153300	1.30862600	2.23211300
H	4.66136400	-5.05060800	0.60124500
H	3.27150000	-4.09595100	1.13135600
H	3.75414800	-4.09187200	-0.57572300
H	6.78502500	-4.01688800	-0.11577700
H	5.95451000	-2.97192000	-1.28504800
H	7.03637200	-2.26624900	-0.07318200
H	6.08642700	-4.02055100	2.33527900
H	4.76505800	-2.97839400	2.89675900
H	6.32184700	-2.27084000	2.43732700