Electronic Supplementary Material (ESI) for Dalton Transactions

A novel thermally stable hydroperoxo-copper (II) complex in Cu (N_2O_2) chromophore of a potential N_4O_2 donor Schiff base ligand: synthesis, structure and catalytic studies.

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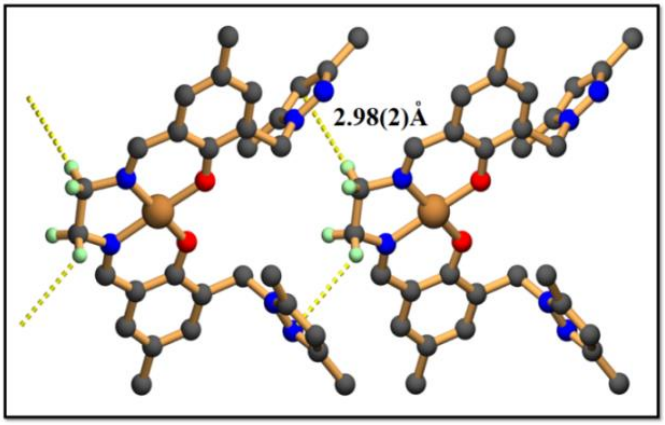

Fig. S1: CH-π interaction in Cu complex 1.

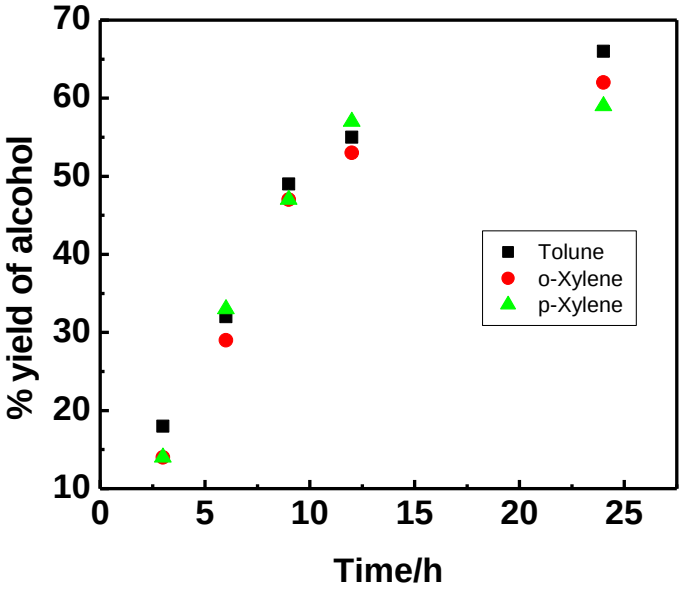

Fig. S2: plot of the % yield of alcohol with reaction time

Table S1 XYZ coordinates of complex **1**

At.No.	X	Y	Z
29	0.000073	-2.240976	0.000196
8	-1.407210	-0.913194	0.013594
7	-1.302727	-3.722791	-0.233801
7	-3.726428	2.539059	0.057352
7	-4.344401	3.056018	1.153406
6	-2.596930	-3.606597	-0.242296
1	-3.193293	-4.522106	-0.349772
6	-3.334383	-2.387362	-0.129274
6	-2.694002	-1.106051	-0.015302
6	-3.542649	0.047525	0.072100
6	-4.916608	-0.092747	0.058642
1	-5.529521	0.802169	0.141710
6	-5.560425	-1.354152	-0.048159
6	-4.755748	-2.470687	-0.141043
1	-5.210481	-3.457231	-0.226386
6	-7.069344	-1.441937	-0.054224
1	-7.500130	-1.019913	0.863232
1	-7.502920	-0.887016	-0.896739
1	-7.406455	-2.481553	-0.132195
6	-2.847418	1.391106	0.204121
1	-2.043559	1.462753	-0.534472
1	-2.372116	1.476434	1.186532
6	-4.098223	3.172145	-1.094675
6	-4.996670	4.158067	-0.714695
1	-5.488114	4.867939	-1.367336

6	-5.114047	4.045379	0.693818
6	-3.563141	2.800661	-2.443323
1	-4.030147	3.425675	-3.210093
1	-3.767385	1.751645	-2.691681
1	-2.477156	2.948801	-2.508663
6	-5.940912	4.868771	1.636749
1	-5.634582	5.922718	1.624346
1	-7.005634	4.835196	1.372799
1	-5.827307	4.492094	2.657826
6	-0.644861	-5.015195	-0.415611
1	-0.388895	-5.134908	-1.478000
1	-1.298757	-5.849526	-0.125849
8	1.407313	-0.913154	-0.013866
7	1.302972	-3.722605	0.234841
7	3.726288	2.539152	-0.057667
7	4.344462	3.057164	-1.153116
6	2.597175	-3.606399	0.242773
1	3.193586	-4.521856	0.350435
6	3.334573	-2.387200	0.128966
6	2.694122	-1.105941	0.014697
6	3.542717	0.047618	-0.073331
6	4.916692	-0.092632	-0.060295
1	5.529551	0.802279	-0.143834
6	5.560567	-1.353981	0.046705
6	4.755936	-2.470499	0.140274
1	5.210717	-3.457001	0.225840
6	7.069490	-1.441747	0.052307
1	7.499983	-1.019878	-0.865357
1	7.503328	-0.886675	0.894589

1	**7.406637**	**-2.481345**	**0.130354**
6	**2.847497**	**1.391181**	**-0.205641**
1	**2.042866**	**1.462502**	**0.532139**
1	**2.373238**	**1.476836**	**-1.188530**
6	**4.097732**	**3.171244**	**1.095011**
6	**4.996119**	**4.157640**	**0.716130**
1	**5.487289**	**4.867006**	**1.369529**
6	**5.113875**	**4.046209**	**-0.692449**
6	**3.562358**	**2.798466**	**2.443186**
1	**4.029200**	**3.422731**	**3.210665**
1	**3.766530**	**1.749204**	**2.690552**
1	**2.476357**	**2.946541**	**2.508422**
6	**5.940880**	**4.870540**	**-1.634435**
1	**5.634470**	**5.924452**	**-1.621108**
1	**7.005548**	**4.836790**	**-1.370290**
1	**5.827522**	**4.494814**	**-2.655890**
6	**0.645166**	**-5.014929**	**0.417386**
1	**0.389201**	**-5.134029**	**1.479843**
1	**1.299098**	**-5.849402**	**0.128113**

S^2 = 0.7531 (doublet ground state)

Table S2 XYZ coordinates of complex **2**

At. No.	**X**	**Y**	**Z**
29	**0.051099**	**-1.894372**	**0.587664**
8	**-1.548107**	**-0.636456**	**0.659573**
7	**-1.361672**	**-3.321254**	**-0.498073**
7	**-3.245820**	**2.738453**	**-0.026528**
7	**-4.102950**	**3.764792**	**0.219670**

6	-2.636921	-3.238938	-0.409505
1	-3.256936	-4.143414	-0.552171
6	-3.387403	-2.017954	-0.153595
6	-2.794668	-0.791974	0.330942
6	-3.692081	0.326819	0.478377
6	-5.047497	0.209576	0.200737
1	-5.677051	1.091630	0.324712
6	-5.631766	-0.996231	-0.233346
6	-4.777734	-2.080790	-0.392148
1	-5.190076	-3.033620	-0.728092
6	-7.116829	-1.094366	-0.504462
1	-7.713356	-0.892775	0.396913
1	-7.442189	-0.375174	-1.269455
1	-7.387654	-2.096514	-0.858760
6	-3.124148	1.650260	0.952014
1	-2.069954	1.512072	1.202054
1	-3.648282	2.017593	1.838293
6	-2.597073	2.877945	-1.217039
6	-3.059271	4.069612	-1.765106
1	-2.753082	4.503925	-2.708584
6	-3.993460	4.580276	-0.834072
6	-1.625500	1.871736	-1.752401
1	-1.000940	2.334373	-2.523526
1	-2.144986	1.017285	-2.204862
1	-0.972915	1.458192	-0.976722
6	-4.800357	5.844298	-0.901987
1	-4.157482	6.733316	-0.954974
1	-5.453817	5.861656	-1.784712
1	-5.429173	5.931017	-0.009813

6	-0.706404	-4.590723	-0.736900
1	-0.378965	-4.620402	-1.787899
1	-1.369742	-5.456392	-0.561125
8	1.401530	-0.622286	-0.315058
7	1.280822	-3.443274	0.078459
7	3.448713	2.483614	0.104123
7	4.614818	3.158335	-0.079365
6	2.469850	-3.381874	-0.412487
1	2.979252	-4.326605	-0.665155
6	3.218005	-2.179581	-0.694488
6	2.626898	-0.860160	-0.642223
6	3.494545	0.235998	-1.008359
6	4.811061	0.013795	-1.378633
1	5.425617	0.878038	-1.630018
6	5.387347	-1.276160	-1.427755
6	4.567107	-2.340989	-1.091065
1	4.969113	-3.354972	-1.125560
6	6.832412	-1.466755	-1.831621
1	7.036861	-1.057096	-2.831096
1	7.520496	-0.966203	-1.135548
1	7.100155	-2.530299	-1.850411
6	2.933483	1.645253	-0.984892
1	1.847931	1.594753	-0.889690
1	3.183481	2.177876	-1.907114
6	2.958067	2.627270	1.368610
6	3.858423	3.451473	2.033548
1	3.782658	3.788045	3.059778
6	4.868342	3.753563	1.089671
6	1.673547	2.012627	1.834120

1	**1.625843**	**2.041012**	**2.927147**
1	**1.564320**	**0.974496**	**1.506432**
1	**0.804382**	**2.564184**	**1.449885**
6	**6.088263**	**4.612088**	**1.256276**
1	**5.824288**	**5.651846**	**1.492727**
1	**6.731284**	**4.246719**	**2.068149**
1	**6.672540**	**4.610892**	**0.330205**
6	**0.550427**	**-4.695915**	**0.163484**
1	**0.237362**	**-4.828647**	**1.204677**
1	**1.168394**	**-5.553887**	**-0.151677**
8	**-0.157821**	**-2.589994**	**2.414575**
8	**-1.525330**	**-2.581035**	**2.866184**
1	**-1.788786**	**-1.663709**	**2.659386**

S^2 = 0.7548 (doublet ground state)