SUPPLEMENTARY INFORMATION

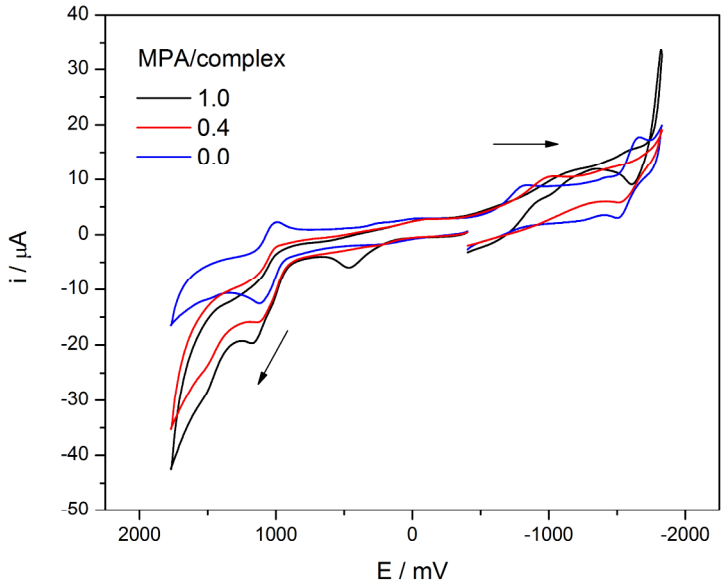


Figure S1. Eletrochemical changes during addition of MPA to solution of the complex **2** in CH_3CN. [complex] = 1 x 10^{-4} mol L^{-1}.

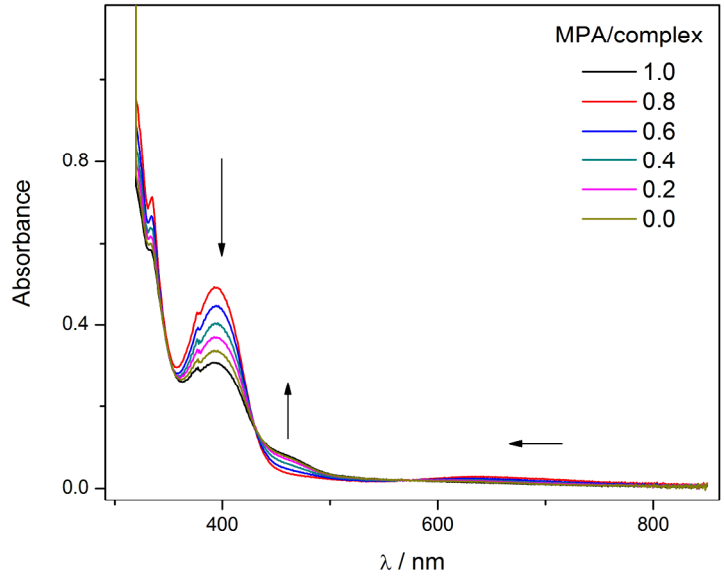
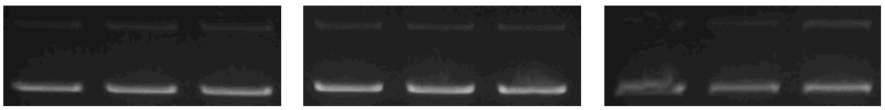
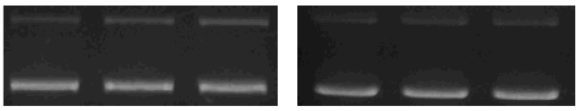


Figure S2. Spectral changes during addition of MPA to solution of the complex **2** in CH_3CN. [complex] = 1 x 10^{-4} mol L^{-1}. After the composition 1 : 1, no other change is observed with additional MPA.

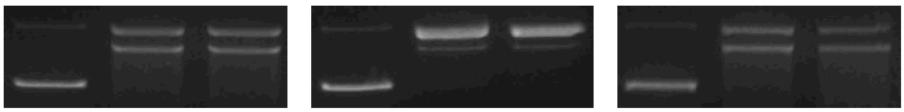


Lanes	1	2	3	4	5	6	7	8	9
F II (%)	-	-	-	-	-	1.2	-	2.1	3.6
F III (%)	-	-	-	-	-	-	-	-	-
F I (%)	100.0	100.0	100.0	100.0	100.0	98.8	100.0	97.9	96.4

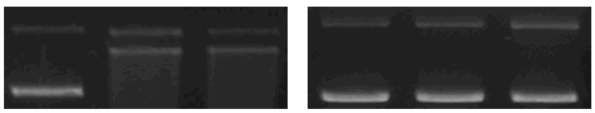


Lanes	10	11	12	13	14	15
F II (%)	-	4.3	7.0	-	-	-
F III (%)	-	-	-	-	-	-
F I (%)	100.0	95.7	93.0	100.0	100.0	100.0

Figure S3. DNA cleavage of complexes **1-5** in dark for 15 min at 37ºC. Lane 1: DNA control; lane 2: DNA + **2** (6.25 μmol L^{-1}); lane 3: DNA + **2** (12.50 μmol L^{-1}); lane 4: DNA control; lane 5: DNA + **3** (6.25 μmol L^{-1}); lane 6: DNA + **3** (12.50 μmol L^{-1}); lane 7: DNA control; lane 8: DNA + **4** (6.25 μmol L^{-1}); lane 9: DNA + **4** (12.50 μmol L^{-1}); lane 10: DNA control; lane 11: DNA + **1** (6.25 μmol L^{-1}); lane 12: DNA + **1** (12.50 μmol L^{-1}); lane 13: DNA control; lane 14: DNA + **5** (6.25 μmol L^{-1}); lane 15: DNA + **5** (12.50 μmol L^{-1}).



Lanes	1	2	3	4	5	6	7	8	9
F II (%)	-	55.6	46.4	-	87.8	90.0	-	38.5	50.3
F III (%)	-	44.4	53.6	-	10.9	10.0	-	61.5	49.7
F I (%)	100.0	-	-	100.0	1.9	-	100.0	-	-



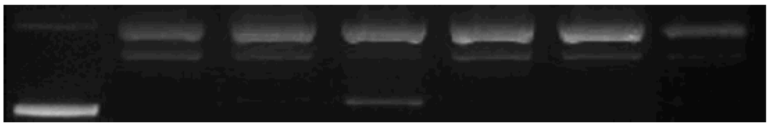
Lanes	10	11	12	13	14	15
F II (%)	-	43.6	39.5	-	-	4.9
F III (%)	-	56.4	60.5	-	-	-
F I (%)	100.0	-	-	100.0	100.0	95.1

Figure S4. DNA cleavage of complexes **1-5** in dark at 500 μmol L^{-1} of MPA for 15 min at 37ºC. Lane 1: DNA control; lane 2: DNA + **2** (6.25 μmol L^{-1}); lane 3: DNA + **2** (12.50 μmol L^{-1}); lane 4: DNA control; lane 5: DNA + **3** (6.25 μmol L^{-1}); lane 6: DNA + **3** (12.50 μmol L^{-1}); lane 7: DNA control; lane 8: DNA + **4** (6.25 μmol L^{-1}); lane 9: DNA + **4** (12.50 μmol L^{-1}); lane 10: DNA control; lane 11: DNA + **1** (6.25 μmol L^{-1}); lane 12: DNA + **1** (12.50 μmol L^{-1}); lane 13: DNA control; lane 14: DNA + **5** (6.25 μmol L^{-1}); lane 15: DNA + **5** (12.50 μmol L^{-1}).

A

1	2	3	4	5	6	7	Lanes
-	67.2	43.9	62.7	49.7	41.8	50.1	F II (%)
-	-	-	-	-	-	-	F III (%)
100.0	32.4	56.1	37.3	50.3	58.2	49.9	F I (%)

B



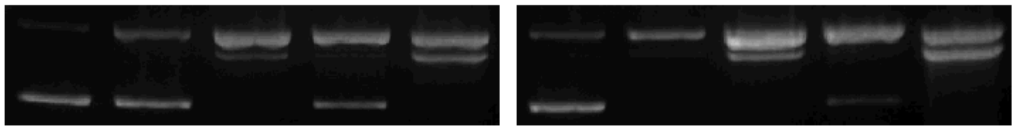
1	2	3	4	5	6	7	Lanes
-	78.3	82.4	73.4	89.0	93.0	87.8	F II (%)
-	21.7	9.7	-	7.7	7.0	12.2	F III (%)
100.0	-	7.8	26.6	3.3	-	-	F I (%)

Figure S5. Photocleavage of PBSK-II (25 μmol L^{-1} bp) of **3** in a Tris-HCl buffer (pH 7.2, NaCl 50 μmol L^{-1}) in CH_3CN/H_2O 25/75 at: (A) 37ºC (365 nm, 12.5 μmol L^{-1}, 15 min) and (B) 50ºC (635 nm, 50 μmol L^{-1}, 20 min). (A) Lane 1: DNA control; lane 2: DNA + **3**; lane 3: DNA + **3** + DMSO; lane 4: DNA + **3** + KI; lane 5: DNA + **3** + SOD; lane 6: DNA + **3** + NaN_3; lane 7: DNA + **3** + D_2O; (B) Lane 1: DNA control; lane 2: DNA + **3**; lane 3: DNA + **3** + DMSO; lane 4: DNA + **3** + KI; lane 5: DNA + **3** + SOD; lane 6: DNA + **3** + NaN_3; lane 7: DNA + **3** + D_2O.

Lanes	1	2	3	4	5	6	7
F II (%)	-	20.7	11.8	27.9	6.9	34.6	37.8
F III (%)	-	-	-	-	-	-	-
F I (%)	100.0	79.3	88.2	72.1	93.1	65.4	62.2

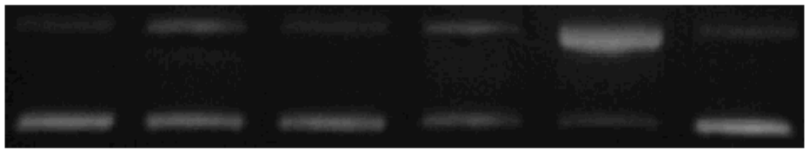
Lanes	1	2	3	4	5	6	7
F II (%)	-	70.2	3.7	22.8	-	36.0	67.8
F III (%)	-	-	-	-	-	-	-
F I (%)	100.0	29.8	96.3	77.2	100.0	64.0	32.2

Figure S6. Photocleavage of PBSK-II (25 μmol L^{-1} bp) of **4** in a Tris-HCl buffer (pH 7.2, NaCl 50 μmol L^{-1}) in CH_3CN/H_2O 25/75 at: (A) 37ºC (365 nm, 12.5 μmol L^{-1}, 15 min) and (B) 50ºC (635 nm, 50 μmol L^{-1}, 20 min). (A) Lane 1: DNA control; lane 2: DNA + **4**; lane 3: DNA + **4** + DMSO; lane 4: DNA + **4** + KI; lane 5: DNA + **4** + SOD; lane 6: DNA + **4** + NaN_3; lane 7: DNA + **4** + D_2O; (B) Lane 1: DNA control; lane 2: DNA + **4**; lane 3: DNA + **4** + DMSO; lane 4: DNA + **4** + KI; lane 5: DNA + **4** + SOD; lane 6: DNA + **4** + NaN_3; lane 7: DNA + **4** + D_2O.



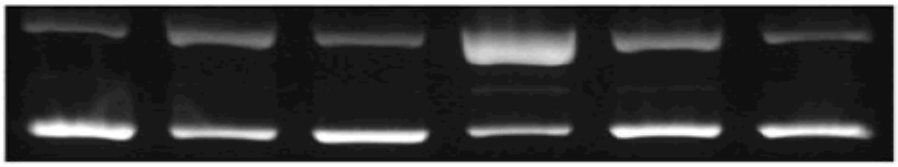
Lanes	1	2	3	4	5	6	7	8	9	10
F II (%)	-	19.8	88.8	52.5	75.9	-	90.4	94.2	64.6	61.7
F III (%)	-	-	11.2	2.0	24.1	-	9.6	5.8	1.1	38.3
F I (%)	100.0	80.2	-	45.5	-	100.0	-	-	34.3	-

Figure S7. DNA photocleavage under UV irradiation in Oxygen (lanes 1-5) and Argon (6-7) atmosphere. Lane 1: DNA control; lane 2: DNA + Fe(EDTA); lane 3: DNA + **2**; lane 4: DNA + **3**; lane 5: DNA + **4**; lane 6: DNA control; lane 7: DNA + Fe(EDTA); lane 8: DNA + **2**; lane 9: DNA + **3**; lane 10: DNA + **4**.



1	2	3	4	5	6	Lanes
-	21.8	1.8	27.8	88.5	4.9	F II (%)
-	-	-	-	-	-	F III (%)
100.0	78.2	98.2	72.2	11.5	95.1	F I (%)

Figure S8. DNA photocleavage under UV light (365 nm). [complex] = 5 $\mu molL^{-1}$ and 10 minutes of irradiation for **1**-**5**.



1	2	3	4	5	6	Lanes
-	19.6	6.7	65.2	17.0	4.1	F II (%)
-	-	-	-	-	-	F III (%)
100.0	80.4	93.3	34.8	83.0	95.9	F I (%)

Figure S9. DNA photocleavage under red light (635 nm). [complex] = 50 $\mu molL^{-1}$ and 20 minutes of irradiation for **1**-**5**.

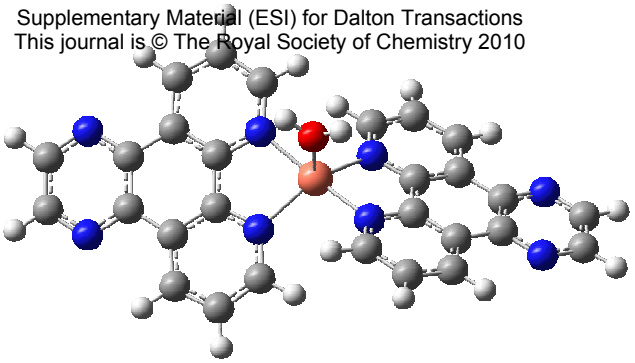


Figure S10. Calculated structure for the optimized complex $Cu(dpq)_2(H_2O)^{2+}$ **1.**

Table S1. Cartesian coordinates the optimized complex $Cu(dpq)_2(H_2O)^{2+}$ **1.**

	x	y	z
Cu	0.06133535	0.73249614	-0.00936802
C	4.05167154	1.44357331	2.60921162
N	-1.33506710	-0.05178529	1.33116865
C	-2.55181017	-0.23976333	0.73361165
C	-2.67624250	0.18992171	-0.64257835
N	-1.55256107	0.69363654	-1.23778951
C	-1.62705229	1.14235027	-2.50361218
C	-2.81966223	1.08748518	-3.24655375
C	-3.96334497	0.54707349	-2.66535944
C	-3.90895296	0.07927816	-1.33210688
C	-5.06358279	-0.48247947	-0.62983258
N	-6.23929875	-0.57734243	-1.29989587
C	-7.25608955	-1.12647231	-0.63659600
C	-7.12327241	-1.59306059	0.69724712
N	-5.97419047	-1.50998982	1.36677540
C	-4.92763663	-0.95716046	0.70360042
C	-3.65604381	-0.80877334	1.41346101
C	-3.46143570	-1.22651062	2.75048818
C	-2.21239483	-1.05892654	3.33823900
C	-1.17317273	-0.46494571	2.59886303
C	4.06371667	0.75170528	1.37599367
C	5.28060738	0.20665271	0.77256015
N	6.45140252	0.35175893	1.44210908
C	7.52926937	-0.18746263	0.87385579
C	7.46394720	-0.88091502	-0.36295580
N	6.32086507	-1.03477753	-1.03041659
C	5.21300975	-0.49565122	-0.46265385
C	3.94123330	-0.60732191	-1.17964986
C	3.80944224	-1.26175859	-2.42655868
C	2.55641243	-1.33322027	-3.02587414
C	1.44968848	-0.74163080	-2.38988881
N	1.55042213	-0.10630271	-1.21045539
C	2.77366456	-0.05637378	-0.59798670
C	2.83464324	0.60980481	0.68550415
C	1.66755446	1.75006748	2.36181649
C	2.85012644	1.95101513	3.09563240
O	-0.09080470	3.15469917	-0.18243968
H	4.98761675	1.57063723	3.15550934
H	-0.71449565	1.56338380	-2.92991102
H	-2.83050455	1.46629777	-4.26933325

H	-4.90403479	0.47826881	-3.21435649
H	-8.21099096	-1.20536946	-1.16440268
H	-7.97337926	-2.04047943	1.22006101
H	-4.29423051	-1.67423109	3.29503433
H	-2.02416383	-1.37653396	4.36467670
H	-0.18595606	-0.32338075	3.04162245
H	8.48042737	-0.07415678	1.40185668
H	8.36347285	-1.31466891	-0.80855902
H	4.69244803	-1.69977818	-2.89383172
H	2.41659216	-1.83609530	-3.98364368
H	0.45826168	-0.78589701	-2.84328629
H	0.71037018	2.13938212	2.71364792
H	2.80810606	2.49924065	4.03787059
H	-0.88772870	3.68102627	-0.37792940
H	0.64679853	3.79070196	-0.13980651
N	1.65697991	1.08516473	1.19242208

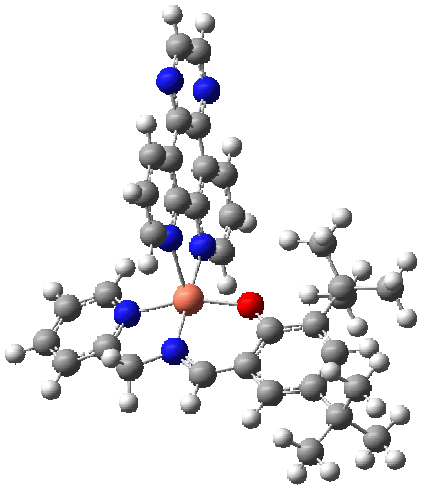


Figure S11. Calculated structure for the optimized complex $Cu(L_1)(dpq)^+$ **2.**

Table S2. Cartesian coordinates the optimized complex $Cu(L_1)(dpq)^+$ **2.**

	x	y	z
Cu	0.02887509	0.09123915	0.01133551
O	1.99806005	0.06433155	0.03472779
N	-0.45376790	2.38348259	-0.14534224
C	-0.43515991	2.79495812	-1.44055065
C	-0.12671784	1.79099140	-2.46107480
N	0.10539729	0.51001468	-2.05165565
C	0.42883942	-0.41731765	-2.96643007
H	0.62771587	-1.42247290	-2.58716609
C	0.51668073	-0.13401626	-4.34036683
H	0.78416236	-0.92701429	-5.04056676
C	0.26164375	1.16061112	-4.77715238
H	0.31462868	1.42980782	-5.83306631
C	-0.06716106	2.15840393	-3.83215611
C	-0.32207209	3.54664805	-4.22059867
N	-0.27501977	3.86875348	-5.53850932

C	-0.53377897	5.13876883	-5.85046301
H	-0.49496541	5.40890005	-6.91034154
C	-0.84454731	6.10707641	-4.86703525
H	-1.05249598	7.14389657	-5.14845912
N	-0.90041573	5.80839660	-3.56912327
C	-0.64529091	4.51787881	-3.23186273
C	-0.66843342	4.14432095	-1.81838003
C	-0.92919344	5.08048313	-0.79135494
H	-1.11334766	6.12208440	-1.05792110
C	-0.93710464	4.65233957	0.53044780
H	-1.12523509	5.34950520	1.34898393
C	-0.69444671	3.29227202	0.80569141
H	-0.68823893	2.92521722	1.83654986
N	-0.05971977	-0.43675221	1.90210169
C	0.97743589	-0.60138190	2.68994978
H	0.78085024	-0.97133236	3.71023950
C	2.35084559	-0.35434820	2.38960253
C	2.81066410	-0.00840386	1.06036114
C	4.23135685	0.22858870	0.87921794
C	5.05454074	0.09509527	1.99627513
H	6.12006347	0.27269192	1.85574153
C	4.62645646	-0.25300546	3.31087631
C	3.27121606	-0.47704800	3.47288286
H	2.86364162	-0.74190333	4.45053360
C	-1.38857962	-0.79411196	2.40705426
H	-1.79175554	0.03258991	3.02531480
H	-1.35170867	-1.68351603	3.06133431
C	-2.35381427	-1.04358093	1.26513950
N	-1.94033157	-0.67882381	0.02700868
C	-2.78405284	-0.85077361	-1.01821799
H	-2.40906725	-0.53994654	-1.99394517
C	-4.06079773	-1.39224365	-0.87716950
H	-4.70138266	-1.51296221	-1.75229743
C	-4.48837665	-1.77655069	0.40115922
H	-5.47879431	-2.21129678	0.55052796
C	-3.62407727	-1.59747605	1.48323673
H	-3.92504736	-1.88676825	2.49262858
C	4.81711214	0.59218215	-0.51098308
C	6.34953113	0.80707680	-0.46594956
H	6.70471702	1.06644932	-1.47434338
H	6.89302898	-0.09901594	-0.15697673
H	6.63860373	1.63349979	0.20148530
C	4.54846790	-0.56085380	-1.51765019
H	4.97249869	-0.30761232	-2.50248609
H	3.47532713	-0.74848100	-1.64276356
H	5.02402679	-1.49451615	-1.17996155
C	4.18531419	1.91495858	-1.02830834
H	4.60723409	2.17067079	-2.01345487
H	4.40739665	2.74767137	-0.34279996
H	3.09668758	1.83211059	-1.13054856
C	5.65683706	-0.35667922	4.45803627
C	4.99648841	-0.74577638	5.80042719
H	5.76433465	-0.80511408	6.58634748
H	4.50549289	-1.73005982	5.75081100
H	4.25332670	-0.00115308	6.12732432

C	6.36348554	1.01336596	4.64810086
H	7.10446016	0.94975198	5.46074090
H	5.63904718	1.80002287	4.90884978
H	6.89730738	1.33600745	3.74207162
C	6.71383316	-1.44029347	4.10860942
H	7.45437650	-1.52742621	4.91954498
H	7.26448389	-1.20291778	3.18664189
H	6.24203301	-2.42555801	3.97418676

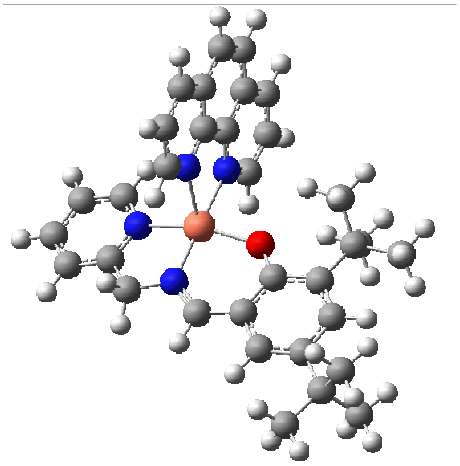


Figure S12. Calculated structure for the optimized complex $Cu(L_1)(phen)^+$ **3.**

Table S3. Cartesian coordinates the optimized complex $Cu(L_1)(phen)^+$ **3.**

	x	y	z
Cu	-0.00803450	0.05239331	0.01009406
O	1.96097531	0.06340178	0.02148407
N	-0.49425949	2.35209550	-0.18647465
C	-0.45043832	2.72731922	-1.49471829
C	-0.15530082	1.70828470	-2.48616521
N	0.05774012	0.42585327	-2.06350552
C	0.37045847	-0.51188109	-2.96710477
H	0.55208322	-1.51773274	-2.58086571
C	0.47157313	-0.24264682	-4.34698843
H	0.72931314	-1.04835252	-5.03616718
C	0.24194936	1.04931827	-4.79695472
H	0.31161343	1.29033522	-5.86097406
C	-0.07606923	2.07132940	-3.86638065
C	-0.31168117	3.43648446	-4.25454010
C	-0.59468410	4.39785083	-3.32082643
C	-0.66390366	4.07431344	-1.92118329
C	-0.92778742	5.03955021	-0.91500303
H	-1.09624676	6.08229239	-1.19632741
C	-0.96187331	4.64831941	0.41491624
H	-1.15438112	5.36790046	1.21276524
C	-0.73759265	3.28970657	0.73158490
H	-0.75219106	2.95519564	1.77348569
N	-0.07593006	-0.46431388	1.90337225
C	0.96869494	-0.60813102	2.68575023
H	0.78345062	-0.97134400	3.71053689

C	2.33654298	-0.34551517	2.37472630
C	2.78198270	0.00228975	1.04139754
C	4.19803773	0.25700710	0.84890297
C	5.03116645	0.13698811	1.96004501
H	6.09316963	0.32794702	1.81096943
C	4.61755358	-0.21326478	3.27873620
C	3.26668524	-0.45364090	3.45160200
H	2.86967848	-0.72119292	4.43287125
C	-1.39682315	-0.82912920	2.42378738
H	-1.79332296	-0.00931352	3.05527523
H	-1.34820287	-1.72445689	3.06928520
C	-2.37762407	-1.07122673	1.29385425
N	-1.97806350	-0.70604681	0.05130903
C	-2.83624294	-0.86961338	-0.98345793
H	-2.47215100	-0.55722311	-1.96275123
C	-4.11412874	-1.40407764	-0.82720564
H	-4.76694032	-1.51788990	-1.69421547
C	-4.52713465	-1.79005053	0.45543217
H	-5.51796931	-2.21970171	0.61643805
C	-3.64802201	-1.61885216	1.52671341
H	-3.93755552	-1.90899899	2.53921787
C	4.76826114	0.62630350	-0.54631148
C	6.29815173	0.86095657	-0.51346068
H	6.64227305	1.12303213	-1.52499358
H	6.85561403	-0.03748903	-0.20697181
H	6.58158647	1.69228080	0.15027681
C	4.50658670	-0.53101191	-1.54981940
H	4.91997203	-0.27332481	-2.53809549
H	3.43500647	-0.73225907	-1.66657178
H	4.99657149	-1.45824316	-1.21502113
C	4.11550725	1.94027654	-1.05988805
H	4.52646101	2.20049680	-2.04852927
H	4.33231328	2.77647131	-0.37692025
H	3.02737489	1.84365301	-1.15362069
C	5.65822615	-0.30128125	4.41798655
C	5.01341679	-0.69599667	5.76623546
H	5.78800687	-0.74368930	6.54633533
H	4.53478602	-1.68660802	5.72231216
H	4.26321543	0.03969041	6.09723953
C	6.34856062	1.07816478	4.59982032
H	7.09623040	1.02606992	5.40722150
H	5.61600204	1.85610561	4.86399883
H	6.87157613	1.40537412	3.68918036
C	6.72656093	-1.37168299	4.06256412
H	7.47451646	-1.44755378	4.86786765
H	7.26698266	-1.12881392	3.13594936
H	6.26673765	-2.36327279	3.93350361
H	-0.76540568	5.43237330	-3.62882134
H	-0.25295572	3.69535480	-5.31465411

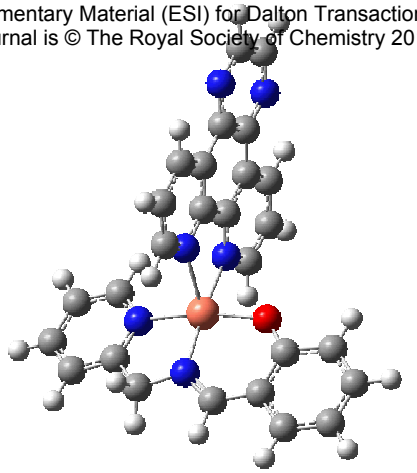


Figure S13. Calculated structure for the optimized complex $Cu(L_2)(dpq)^+$ **4.**

Table S4. Cartesian coordinates the optimized complex $Cu(L_2)(dpq)^+$ **4.**

	x	y	z
Cu	4.75955036	11.43180182	7.65873047
O	4.66923144	9.49250056	7.39779634
N	5.62986648	11.36721098	9.83658854
C	6.95668741	11.07108392	9.80916763
C	7.60196351	10.98140689	8.49768173
N	6.84289049	11.22203596	7.39021164
C	7.40752632	11.12150393	6.17746069
H	6.75358178	11.30114267	5.32062059
C	8.76267147	10.79885503	5.99352344
H	9.17047186	10.73024985	4.98361459
C	9.55554673	10.56659967	7.11077430
H	10.61198879	10.31106103	7.01989764
C	8.98120580	10.65617985	8.39867478
C	9.75394799	10.40159056	9.61485480
N	11.07026581	10.09221502	9.49250585
C	11.74140015	9.88808278	10.62596859
H	12.80208514	9.63358186	10.53763780
C	11.12403181	9.99096700	11.89515101
H	11.69654073	9.81781862	12.81168600
N	9.83489200	10.29952391	12.03473368
C	9.13526993	10.51504299	10.89088107
C	7.70921345	10.82466089	10.98844866
C	7.03579730	10.90295372	12.22931480
H	7.59405283	10.71921809	13.14823797
C	5.68034046	11.20571296	12.24729201
H	5.12765452	11.26792410	13.18654988
C	5.01787352	11.42871884	11.02429459
H	3.94880953	11.66055192	11.00600782
N	2.80286244	11.62629775	7.56056544
C	1.94581015	10.64929684	7.37794955
H	0.87909729	10.91677477	7.29427869
C	2.24184037	9.25795756	7.26874959
C	3.59725804	8.74752641	7.28530649
C	3.76710753	7.33427655	7.15618247
C	2.67849997	6.48763158	7.01514245
H	2.85051538	5.41181847	6.91773468
C	1.35250931	6.98740245	6.99476066
C	1.14978098	8.34882946	7.11806372

H	0.13281502	8.75294148	7.10466866
C	2.29545607	13.00054407	7.63556944
H	1.85351211	13.18673879	8.63396762
H	1.49048434	13.17565888	6.90010831
C	3.41204018	14.00160032	7.41913541
N	4.67593453	13.51309986	7.43162135
C	5.71133226	14.37372728	7.28655640
H	6.70880862	13.93248501	7.30970473
C	5.53223116	15.74567804	7.11740860
H	6.39925369	16.39786201	7.00207759
C	4.22581213	16.25339133	7.09425445
H	4.04515842	17.32172029	6.95585872
C	3.15524422	15.37004316	7.24866043
H	2.12487791	15.73296297	7.23641157
H	0.50698620	6.30661645	6.88368477
H	4.78771634	6.94633036	7.16678137

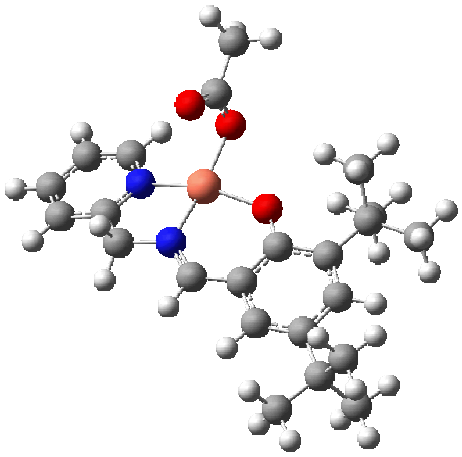


Figure S14. Calculated structure for the optimized complex Cu(L_1)(OAc) **5.**

Table S5. Cartesian coordinates the optimized complex Cu(L_1)(OAC) **5.**

	x	y	z
Cu	-0.63969856	1.09296216	1.69066786
O	1.26885539	1.24748033	2.11180246
O	-0.31006135	0.80746257	-0.25689703
O	-1.09078407	2.90127989	-0.03513102
N	-1.15864946	1.52054002	3.53043300
C	-0.33465804	1.76535488	4.51907263
C	1.09363845	1.80306776	4.46284702
C	-0.39233466	2.16392007	-2.24169696
C	1.83868509	1.53819073	3.24680088
C	3.29113376	1.59922974	3.32371573
C	3.86597001	1.90706643	4.55324743
C	3.15063773	2.16936319	5.76038434
C	1.77178386	2.10695732	5.68175390
C	-2.60148827	1.53316461	3.76791664
C	-0.63419406	1.97639289	-0.74657120
C	-3.30851829	0.67152963	2.73548654
N	-2.58078580	0.34925857	1.64177030

C	-3.14138030	-0.38562310	0.65732863
C	-4.46120551	-0.83467868	0.72676515
C	-5.22353138	-0.50540184	1.85575159
C	-4.64091146	0.25833322	2.87229261
H	-0.77344653	1.96189184	5.51328132
H	4.95419339	1.95461830	4.60227411
H	1.15294969	2.29557091	6.56217678
H	-2.98524814	2.56806861	3.66704540
H	-2.85961935	1.19473353	4.78786557
H	-2.49197980	-0.59796447	-0.19438003
H	-4.87806965	-1.43078204	-0.08730313
H	-6.25897674	-0.84223639	1.94470734
H	-5.20960767	0.53095634	3.76484847
H	0.67006540	2.40737653	-2.40211228
H	-1.00004604	2.99287676	-2.62554150
H	-0.60571321	1.24231768	-2.80152680
C	4.16059738	1.32752315	2.06887031
C	3.90429673	-0.11285710	1.54150391
C	3.83179945	2.36378556	0.95786903
C	5.67463011	1.44123858	2.36890641
H	4.14878138	-0.86097403	2.31267233
H	2.86055546	-0.25315469	1.23859121
H	4.54464618	-0.30945015	0.66625903
H	4.03222533	3.38926016	1.30768906
H	4.46583158	2.18063890	0.07497119
H	2.78370676	2.30368531	0.64558936
H	6.23884207	1.23757678	1.44606785
H	5.96185482	2.44861849	2.70808415
H	6.00985914	0.71079141	3.12239025
C	3.92199136	2.50247868	7.05802644
C	4.86414753	1.32273886	7.42396521
C	4.76615819	3.78919750	6.84922951
C	2.97448627	2.74192768	8.25551699
H	4.29035270	0.39779471	7.58954213
H	5.60065801	1.12026242	6.63263038
H	5.42335188	1.54710208	8.34688896
H	4.12190553	4.64628473	6.59969386
H	5.32551124	4.03855165	7.76582165
H	5.49886071	3.67444965	6.03666408
H	3.56445381	2.97150329	9.15632113
H	2.29666789	3.59183662	8.08186959
H	2.36422636	1.85329409	8.48235252