Supplementary Material

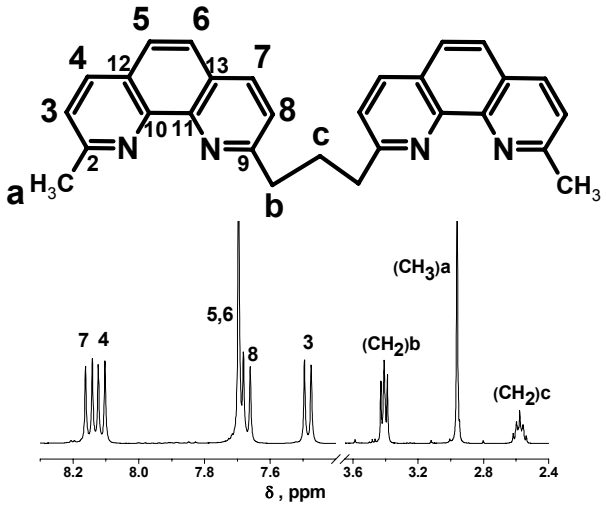

Figure S1. ^{1}H-NMR spectrum of 1,3-bis(9-methyl-1,10-henantrolin-2-yl)propane, mphenpr, in CD_3Cl.

(a) (b)

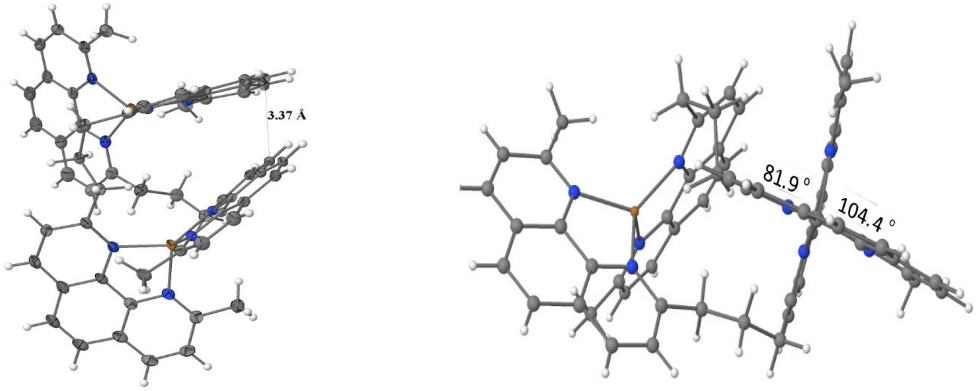

Figure S2. Interplanar distance and deviation from a parallel arrangement of the planes of two 9-methyl-1,10-phenanthrolin-2-yl (mphenoliyl).

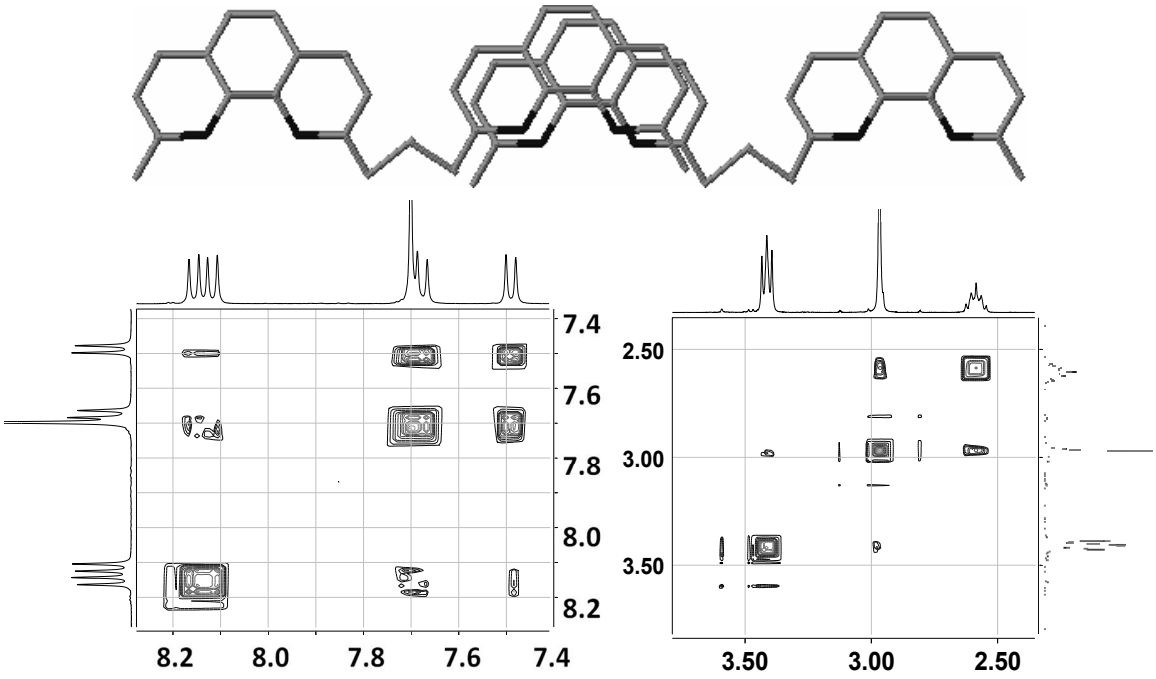

Figure S3. The NMR-based structure of $(mphenpr)_2$ (top). The NOESY spectrum in CD_3Cl (bottom) showing the correlation between protons of 1,10-phenanthroline groups in different chains of the dimer. In the left: H3-H8, H4-H7 and in the right: Ha-Hb, Ha-Hc protons. Proton labels are shown in Fig. S1.

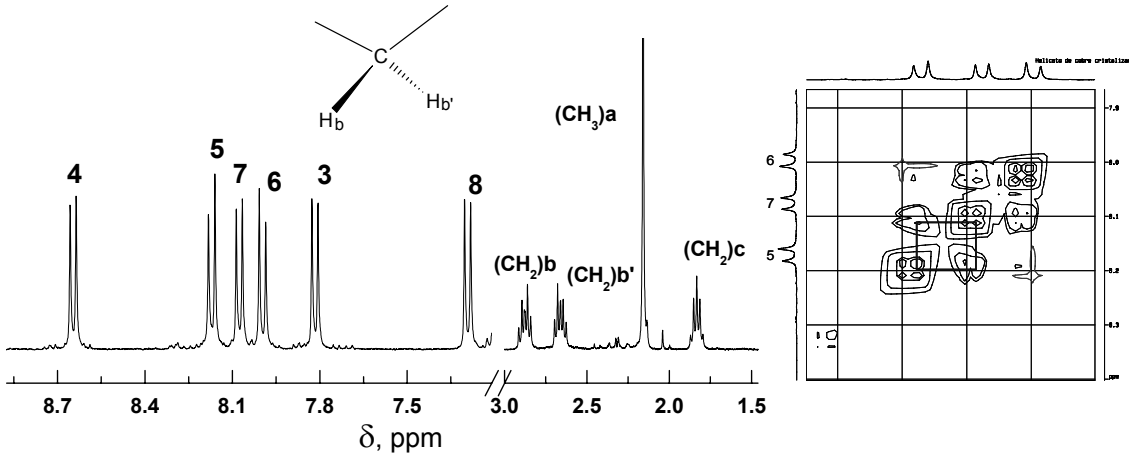

Figure S4. ^{1}H-NMR spectrum of $[Cu^I_2(mphenpr)_2]^{2+}$ in CH_3OD and NOE coupling of the aromatic protons 5-7 and 6-7.

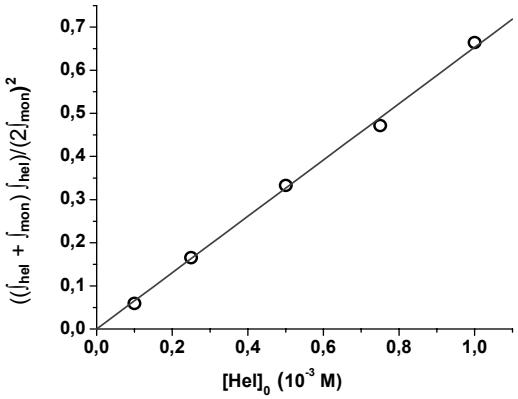

Figure S5. Plot of the eq.

$$\frac{(\int Hel + \int Mono)\int Hel}{(2\int Mono)^2} = \frac{[Hel]_0}{K}$$

where ∫ hel and ∫ mon are the respective integrations of the $[Cu^{I}_2(mphenpr)_2]^{2+}$ and $[Cu^{I}(mphenpr)]^{+}$ resonances and $[Hel]_0$ is the total concentration of helicate

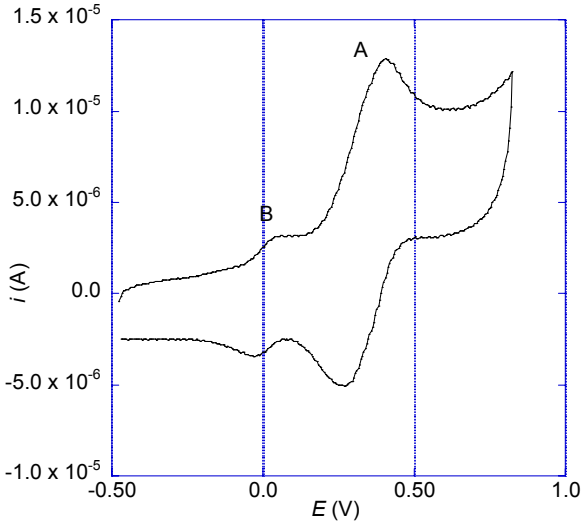

Figure S6. Cyclic voltammetry of a solution of 5 x 10^{-4} M $[Cu^{I}_2(mphenpr)_2]^{2+}$ in CH_3CN with 0.10 M tetraethyl ammonium perchlorate as supporting electrolyte showing the two-electron oxidation of the helicate dimer, $[Cu^{I}_2(mphenpr)_2]^{2+}$ (A) and the presence of the monomeric form, $[Cu^{I}(mphenpr)]^{+}$ (B) that increases in intensity with time.

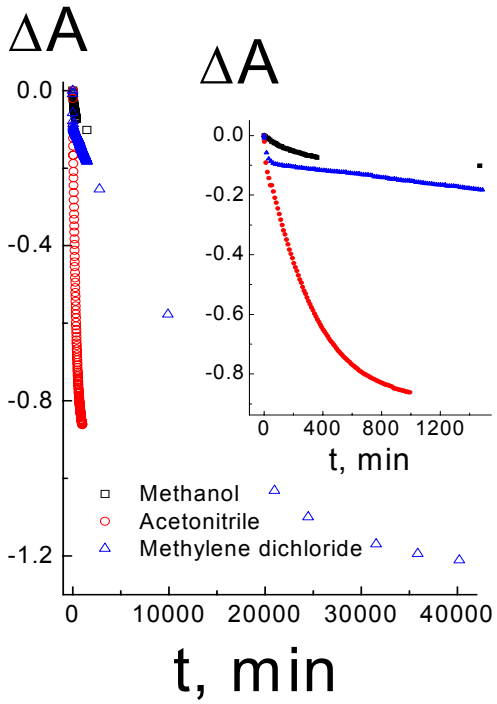

Figure S7**.** The solvent-dependent rate of the $[Cu^{I}_{2}(mphenpr)_{2}]^{2+}$ unfolding increased in the order $CH_3CN > CH_2Cl_2 > CH_3OH$. The inset shows the shorter-lived step of the process.

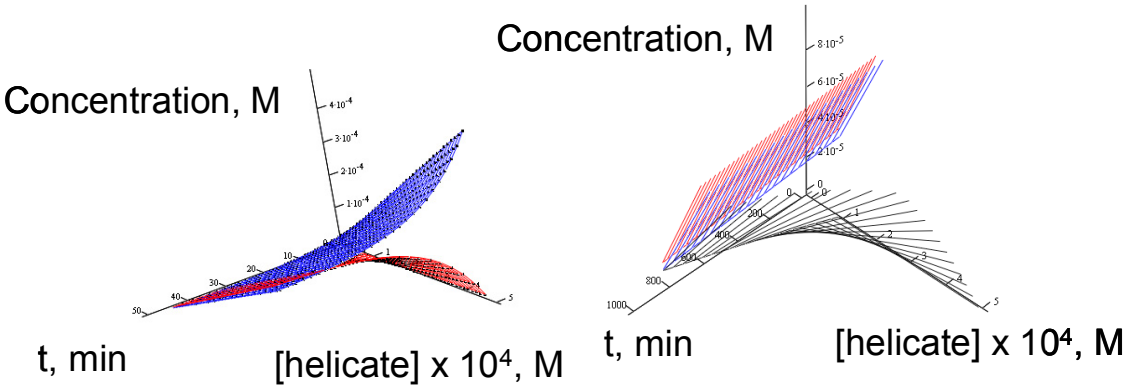

Figure S8. Calculated concentrations of the species, blue = $[Cu^{I}_{2}(mphenpr)_{2}]^{2+}$, red = [B], black = $[Cu^{I}(mphenpr)^{+}]$, as a function of time and the initial concentration of $[Cu^{I}_{2}(mphenpr)_{2}]^{2+}$.

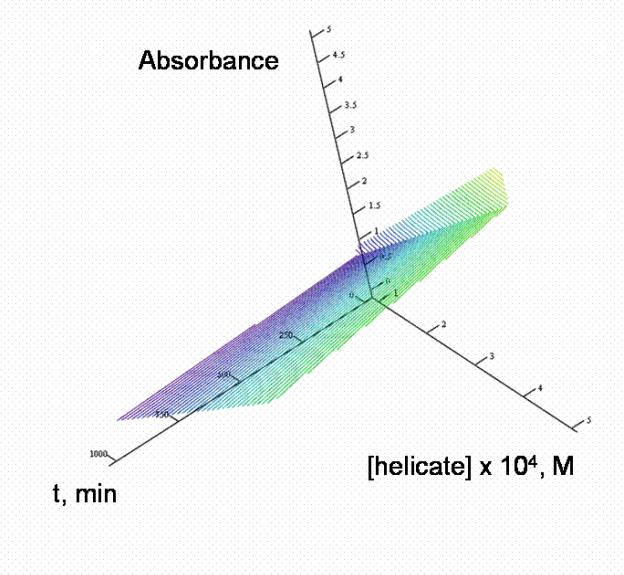

Figure S9. Absorbance change at λ_{obs} = 435 nm as a function of time and helicate concentration. Rate constants and extinction coefficients of the products and intermediates used in the calculation have been communicated in the text.

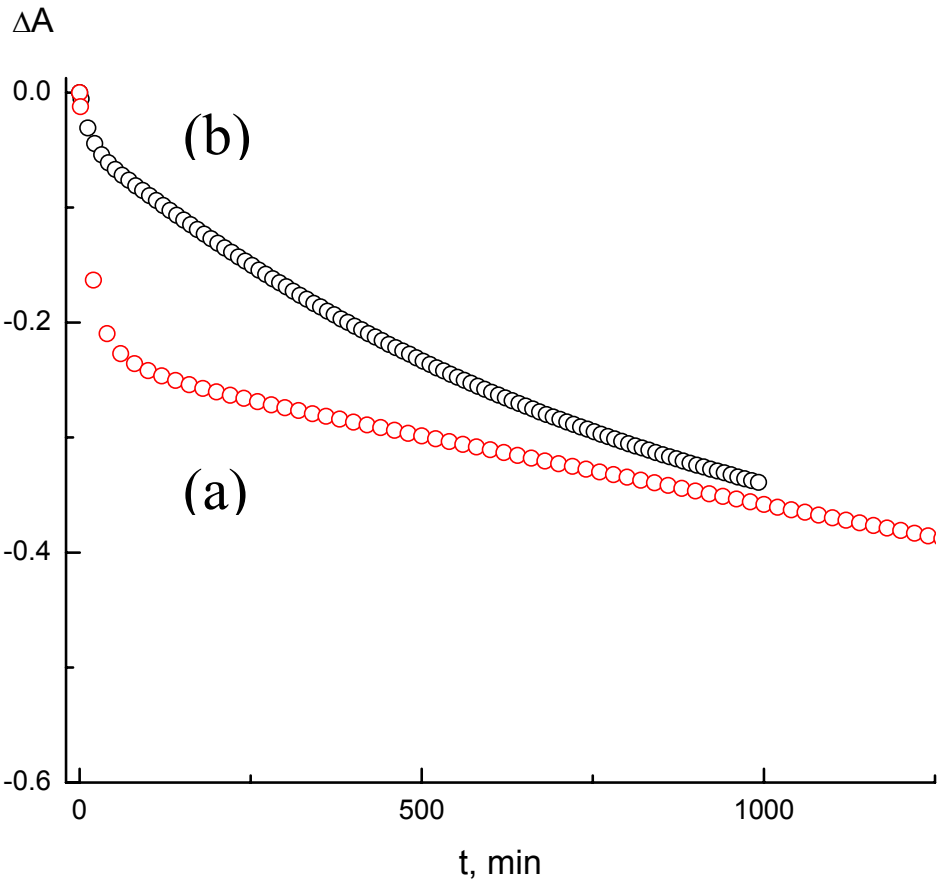

Figure S10. Oxidation of 1 x 10^{-4} M $[Cu^{I}_{2}(mphenpr)_{2}]^{2+}$ in CH_3CN containing 1.0 M CCl_4, i.e., 5 x 10^{-2} cc of CCl_4 in a 5 cc volume. In (a), the halocarbon was added 15 min after the dissolution of the complex in CH_3CN. The halocarbon was added in (b) with a delay equal to or less than 1 min after the dissolution of the complex. The 435 nm absorbance, A = 1.006, in (a) at the time of mixing, t = 0, was smaller than in (b) where A = 1.043. This difference in the absorbance at t = 0 is caused by a larger build up of the $\{[Cu^{I}_{2}(mphenpr)_{2}]^{2+}\}^*$ concentration in (a) than in (b) before the addition of CCl_4. ΔA is the difference between the absorbance at a time t and the absorbance at t = 0.

- Input coordinates and keywords of the reported calculations.

Figure 3. Geometry optimization of the $[Cu^{I}_{2}(mphenpr)_{2}]^{2+}$ helicate

opt NoSymm b3lyp/gen pseudo=read SCF=(MaxCycle=800)

2 1

N	13.512	6.436	16.140
N	13.237	8.655	14.644
N	9.239	12.187	16.143
N	9.703	13.868	18.189
N	11.193	5.839	13.607
N	10.137	6.958	15.826
N	12.360	11.487	18.172
N	12.565	13.314	16.179
Cu	11.979	7.120	14.974
Cu	10.943	12.580	17.199
C	13.629	5.310	16.836
C	14.836	4.964	17.469
C	15.908	5.805	17.428
C	15.790	7.034	16.749
C	16.843	8.003	16.680
C	16.670	9.165	16.014
C	15.447	9.448	15.312
C	15.252	10.597	14.537
C	14.082	10.744	13.832
C	13.099	9.738	13.875
C	14.404	8.506	15.351
C	14.568	7.296	16.102
C	12.407	4.447	16.957
C	11.883	9.829	12.986
C	10.829	10.845	13.457

C 10.153 10.409 14.758

C 9.027 11.316 15.156

C 7.775 11.244 14.492

C 6.761 12.091 14.839

C 6.971 13.038 15.864

C 5.973 13.974 16.292

C 6.216 14.834 17.303

C 7.467 14.819 18.006

C 7.746 15.632 19.120

C 8.955 15.526 19.747

C 9.939 14.634 19.255

C 8.476 13.935 17.588

C 8.226 13.038 16.499

C 11.282 14.531 19.904

C 11.759 5.264 12.541

C 11.096 4.264 11.809

C 9.841 3.860 12.186

C 9.200 4.475 13.273

C 7.881 4.131 13.722

C 7.331 4.726 14.797

C 8.059 5.716 15.543

C 7.568 6.320 16.713

C 8.369 7.182 17.414

C 9.674 7.479 16.964

C 9.354 6.072 15.134

C 9.923 5.461 13.966

C 13.143 5.712 12.159

C 10.620 8.309 17.787

C 10.005 9.541 18.446

C 10.876 10.133 19.556

C 12.257 10.577 19.145

C 13.382 10.067 19.813

C	14.630	10.505	19.485
C	14.785	11.440	18.449
C	16.058	11.909	17.996
C	16.168	12.754	16.954
C	15.000	13.255	16.294
C	15.051	14.099	15.171
C	13.887	14.512	14.589
C	12.643	14.128	15.130
C	13.725	12.859	16.742
C	13.614	11.906	17.812
C	11.367	14.647	14.543
H	17.795	7.799	17.170
H	17.472	9.902	16.008
H	17.156	13.059	16.609
H	14.905	4.136	17.930
H	16.724	5.564	17.852
H	15.922	11.269	14.500
H	13.936	11.527	13.312
H	11.792	4.841	17.608
H	12.669	3.550	17.256
H	11.965	4.384	16.086
H	11.460	8.934	12.935
H	12.175	10.076	12.073
H	11.262	11.724	13.593
H	10.142	10.951	12.752
H	9.805	9.488	14.650
H	10.827	10.392	15.483
H	7.640	10.602	13.804
H	5.922	12.045	14.394
H	5.128	13.988	15.858
H	5.548	15.461	17.553
H	7.097	16.252	19.432

H 9.136 16.052 20.517

H 11.286 13.776 20.529

H 11.474 15.357 20.392

H 11.966 14.390 19.217

H 11.516 3.868 11.055

H 9.404 3.163 11.708

H 7.386 3.472 13.251

H 6.452 4.487 15.068

H 6.687 6.130 17.016

H 8.043 7.585 18.211

H 13.307 6.607 12.522

H 13.220 5.736 11.182

H 13.801 5.086 12.524

H 11.364 8.603 17.206

H 11.005 7.734 18.495

H 9.125 9.296 18.827

H 9.854 10.233 17.755

H 10.401 10.913 19.941

H 10.968 9.458 20.273

H 13.273 9.415 20.496

H 15.390 10.180 19.954

H 16.844 11.618 18.442

H 15.888 14.380 14.819

H 13.916 15.062 13.814

H 10.612 14.124 14.888

H 11.401 14.566 13.568

H 11.252 15.587 14.792

Cu 0

LANL2DZ

****

C N H 0

6-31+G*

******

Cu 0

LANL2DZ

Figure3- Time dependent DFT of the $[Cu^{I}_{2}(mphenpr)_{2}]^{2+}$ helicate

NoSymm b3lyp/gen pseudo=read geom=checkpoint SCRF=(PCM, Solvent=Methanol) pop=(full,MK,ReadRadii) TD=(NStates=80)

2 1

Cu 0

LANL2DZ

****

C N H 0

6-31+G*

******

Cu 0

LANL2DZ

Cu 1.85

Figure 6.a- Geometry optimization of the $[Cu^{I}(mphenpr)_{2}]^{+}$ monometallic complex

opt b3lyp/gen pseudo=read

1 1

Cu	-4.897	5.278	4.586
N	-5.241	4.299	6.291
N	-4.619	6.843	5.775
N	-5.436	5.895	2.765
N	-3.860	3.884	3.577
C	-5.630	3.058	6.484
C	-5.781	2.499	7.770
C	-5.501	3.307	8.899
C	-5.153	4.641	8.703
C	-4.911	5.553	9.769
C	-4.614	6.820	9.531
C	-4.526	7.338	8.197
C	-4.233	8.687	7.854
C	-4.122	9.089	6.514
C	-4.317	8.110	5.483
C	-4.138	8.549	4.029
C	-5.486	9.078	3.481
C	-6.560	7.974	3.397
C	-6.174	6.911	2.382
C	-6.615	7.053	1.031
C	-6.305	6.072	0.128
C	-5.556	4.974	0.523
C	-5.180	3.891	-0.375
C	-4.387	2.903	-0.002
C	-3.871	2.872	1.372
C	-2.923	1.909	1.838
C	-2.446	2.024	3.147
C	-2.954	3.023	4.006
C	-5.027	5.109	7.370
C	-4.700	6.450	7.084
C	-5.100	4.918	1.839

C	-4.273	3.860	2.277
C	-5.942	2.162	5.306
C	-2.403	3.169	5.415
H	-6.104	1.474	7.879
H	-5.559	2.886	9.892
H	-4.968	5.214	10.793
H	-4.430	7.495	10.354
H	-4.092	9.423	8.631
H	-3.894	10.117	6.276
H	-3.389	9.339	3.977
H	-3.811	7.699	3.430
H	-5.862	9.864	4.136
H	-5.338	9.481	2.479
H	-6.672	7.500	4.372
H	-7.511	8.414	3.096
H	-7.183	7.923	0.737
H	-6.644	6.152	-0.894
H	-5.553	3.876	-1.389
H	-4.123	2.127	-0.706
H	-2.592	1.117	1.183
H	-1.685	1.347	3.506
H	-6.245	1.179	5.667
H	-6.751	2.599	4.721
H	-5.055	2.061	4.681
H	-1.672	2.382	5.603
H	-1.923	4.142	5.519
H	-3.218	3.087	6.135

Cu 0

LANL2DZ

****

C N H 0

6-31+G*

******

Cu 0

LANL2DZ

Figura 6a. Time dependent DFT the $[Cu^{I}(mphenpr)_2]^{+}$ monometallic complex

geom=checkpoint b3lyp/gen pseudo=read SCRF=(PCM, Solvent=Methanol) pop=(full,MK,ReadRadii) TD=(NStates=80)

1 1

Cu 0

LANL2DZ

****

C N H 0

6-31+G*

******

Cu 0

LANL2DZ

Cu 1.85

Figure 6.b. Geometry optimization of the $[Cu^{I}(mphenpr)_2]^{+}$ monometallic complex with a ClO_4^{-} specifically coordinated

opt b3lyp/gen pseudo=read

0 1

O	-0.105	6.369	5.053
O	-0.313	4.119	4.566
O	1.063	5.449	3.268
O	1.391	4.779	5.791
Cl	0.688	5.264	4.639
N	-1.085	8.974	2.015
N	-2.053	6.573	2.813
N	-3.064	8.538	5.343
N	-0.436	9.178	5.216
C	-0.732	10.209	1.635
C	-2.560	5.410	3.246
C	-4.357	8.179	5.372
C	0.890	9.363	5.164
C	-1.060	7.945	1.112
C	-1.562	6.674	1.539
C	-2.541	9.295	6.356
C	-1.148	9.625	6.296
C	-0.278	10.445	0.314
C	-0.600	8.110	-0.214
C	-1.557	5.584	0.638
C	-2.568	4.275	2.399
C	-3.181	5.334	4.616
C	-4.900	7.270	4.301
C	-5.190	8.603	6.435
C	-3.315	9.735	7.455
C	-0.554	10.353	7.350
C	1.552	10.070	6.198
C	-0.828	11.354	2.606
C	1.685	8.810	4.014
C	-0.190	9.411	-0.592
C	-0.593	6.985	-1.103
C	-1.047	5.766	-0.689

C	-2.075	4.357	1.116
C	-4.665	5.773	4.620
C	-4.681	9.368	7.462
C	-2.696	10.507	8.492
C	-1.363	10.799	8.445
C	0.842	10.578	7.264
Cu	-1.684	8.295	3.853
H	0.001	11.455	0.031
H	-2.972	3.343	2.778
H	-3.128	4.299	4.968
H	-2.604	5.936	5.325
H	-4.462	7.527	3.330
H	-5.978	7.440	4.213
H	-6.235	8.309	6.429
H	2.626	10.205	6.134
H	-1.302	12.215	2.121
H	-1.411	11.095	3.491
H	0.168	11.679	2.928
H	2.585	8.310	4.389
H	1.113	8.090	3.427
H	2.023	9.613	3.347
H	0.172	9.591	-1.599
H	-0.226	7.124	-2.115
H	-1.040	4.916	-1.364
H	-2.085	3.486	0.465
H	-5.225	5.179	3.889
H	-5.087	5.538	5.602
H	-5.321	9.688	8.280
H	-3.307	10.847	9.322
H	-0.894	11.367	9.243
H	1.348	11.133	8.049

Cu 0

LANL2DZ

****

C N H O Cl 0

6-31+G*

****

Cu 0

LANL2DZ

Figure 6b. Time dependent DFT of the $[Cu^{I}(mphenpr)_2]^+$ mono metallic complex with a ClO_4^- specifically coordinated

geom=checkpoint b3lyp/gen pseudo=read SCRF=(PCM, Solvent=Methanol) pop=(full,MK,ReadRadii) TD=(NStates=80)

0 1

Cu 0

LANL2DZ

****

C N H O Cl 0

6-31+G*

****

Cu 0

LANL2DZ

Cu 1.85

Figure 8.a. Geometry optimization of the $[Cu^{II}(mphenpr)Cl]^+$ structure

opt b3lyp/gen pseudo=read

1 2

Cu	9.565	3.461	5.680
Cl	9.445	3.202	8.009
N	7.822	4.432	5.791
N	10.228	5.390	5.038
N	11.220	2.320	5.726
N	9.043	2.005	4.202
C	6.494	2.437	6.332
H	7.308	2.088	6.750
H	6.361	2.007	5.463
H	5.724	2.255	6.909
C	6.630	3.921	6.137
C	5.531	4.773	6.344
H	4.692	4.402	6.593
C	5.656	6.116	6.193
H	4.900	6.675	6.326
C	6.865	6.669	5.849
C	7.959	5.786	5.635
C	7.109	8.078	5.717
H	6.394	8.688	5.856
C	8.315	8.547	5.406
H	8.446	9.486	5.345
C	9.418	7.671	5.161
C	9.228	6.295	5.272
C	10.691	8.116	4.812
H	10.866	9.047	4.755
C	11.666	7.240	4.558
H	12.529	7.551	4.312
C	11.416	5.844	4.653
C	12.508	4.884	4.362

H	13.055	5.225	3.610
H	12.121	4.014	4.090
C	13.418	4.683	5.625
H	14.222	4.169	5.364
H	13.718	5.569	5.950
C	12.697	3.942	6.777
H	13.286	3.909	7.573
H	11.872	4.432	7.024
C	12.352	2.558	6.355
C	13.303	1.519	6.570
H	14.130	1.711	6.999
C	13.021	0.251	6.156
H	13.625	-0.455	6.348
C	11.846	-0.010	5.449
C	10.956	1.067	5.241
C	11.467	-1.292	4.958
H	12.031	-2.037	5.131
C	10.324	-1.483	4.250
H	10.089	-2.354	3.952
C	9.476	-0.377	3.956
C	9.797	0.895	4.478
C	8.355	-0.461	3.134
H	8.065	-1.307	2.814
C	7.667	0.682	2.784
H	6.945	0.637	2.169
C	8.043	1.919	3.344
C	7.324	3.155	2.933
H	7.837	3.942	3.216
H	6.439	3.176	3.354
H	7.222	3.164	1.958

Cu 0

LANL2DZ

****

C N H Cl 0

6-31+G*

****

Cu 0

LANL2DZ

Figure 8.b. Geometry optimization of the $[Cu^{II}(mphenpr)]^{+2}$ structure

opt b3lyp/gen pseudo=read

2 2

Cu	-4.897	5.278	4.586
N	-5.241	4.299	6.291
N	-4.619	6.843	5.775
N	-5.436	5.895	2.765
N	-3.860	3.884	3.577
C	-5.630	3.058	6.484
C	-5.781	2.499	7.770
C	-5.501	3.307	8.899
C	-5.153	4.641	8.703
C	-4.911	5.553	9.769
C	-4.614	6.820	9.531
C	-4.526	7.338	8.197
C	-4.233	8.687	7.854
C	-4.122	9.089	6.514
C	-4.317	8.110	5.483
C	-4.138	8.549	4.029

C	-5.486	9.078	3.481
C	-6.560	7.974	3.397
C	-6.174	6.911	2.382
C	-6.615	7.053	1.031
C	-6.305	6.072	0.128
C	-5.556	4.974	0.523
C	-5.180	3.891	-0.375
C	-4.387	2.903	-0.002
C	-3.871	2.872	1.372
C	-2.923	1.909	1.838
C	-2.446	2.024	3.147
C	-2.954	3.023	4.006
C	-5.027	5.109	7.370
C	-4.700	6.450	7.084
C	-5.100	4.918	1.839
C	-4.273	3.860	2.277
C	-5.942	2.162	5.306
C	-2.403	3.169	5.415
H	-6.104	1.474	7.879
H	-5.559	2.886	9.892
H	-4.968	5.214	10.793
H	-4.430	7.495	10.354
H	-4.092	9.423	8.631
H	-3.894	10.117	6.276
H	-3.389	9.339	3.977
H	-3.811	7.699	3.430
H	-5.862	9.864	4.136
H	-5.338	9.481	2.479
H	-6.672	7.500	4.372
H	-7.511	8.414	3.096
H	-7.183	7.923	0.737
H	-6.644	6.152	-0.894

H -5.553 3.876 -1.389

H -4.123 2.127 -0.706

H -2.592 1.117 1.183

H -1.685 1.347 3.506

H -6.245 1.179 5.667

H -6.751 2.599 4.721

H -5.055 2.061 4.681

H -1.672 2.382 5.603

H -1.923 4.142 5.519

H -3.218 3.087 6.135

Cu 0

LANL2DZ

****

C N H 0

6-31+G*

******

Cu 0

LANL2DZ

Figure 8.b. Time dependent DFT of the $[Cu^{II}(mphenpr)]^{+2}$ structure

geom=checkpoint b3lyp/gen pseudo=read SCRF=(PCM, Solvent=Methanol) pop=(full,MK,ReadRadii) TD=(NStates=80)

2 2

Cu 0

LANL2DZ

****

C N H 0

6-31+G*

******

Cu 0

LANL2DZ

Cu 1.85

Figure 8.b. Geometry optimization of the $[Cu^{II}(mphenpr)(ClO_4)]^+$ (white) structure.

opt b3lyp/gen pseudo=read

1 2

8	0.083473	0.365164	2.090408
8	-1.520652	1.934548	2.947375
8	-2.266505	-0.368572	2.255569
8	-0.943055	-0.116603	4.255216
17	-1.190599	0.469720	2.909425
7	-1.123969	-1.430951	-1.309589
7	-1.455004	1.087203	-0.382788
7	1.860610	1.067729	-0.967708
7	1.645494	-1.263838	0.411566
6	-0.897265	-2.614766	-1.889515
6	-1.575051	2.325628	0.082426
6	1.929650	2.209582	-1.668632
6	1.455388	-2.332219	1.181603
6	-2.400675	-0.977239	-1.157342
6	-2.576337	0.350273	-0.654302
6	3.010599	0.447013	-0.561690
6	2.892780	-0.775318	0.186622

6	-1.978554	-3.438021	-2.280476
6	-3.529340	-1.754829	-1.510466
6	-3.881376	0.855444	-0.478448
6	-2.859066	2.888767	0.291555
6	-0.350847	3.151450	0.336034
6	0.660052	2.929816	-2.049884
6	3.185538	2.775973	-1.993988
6	4.295308	0.971660	-0.834631
6	4.051846	-1.408371	0.683792
6	2.576640	-3.011434	1.728139
6	0.514097	-3.075838	-2.135405
6	0.057734	-2.811059	1.467572
6	-3.276244	-3.025300	-2.073596
6	-4.841790	-1.223635	-1.305464
6	-5.008114	0.032999	-0.801763
6	-3.995636	2.175072	0.016706
6	0.128572	3.876283	-0.940108
6	4.352580	2.170333	-1.581888
6	5.458427	0.288528	-0.348608
6	5.340126	-0.853087	0.390635
6	3.855364	-2.571406	1.470746
29	0.205924	-0.090868	-0.476483
1	-1.767086	-4.396105	-2.743621
1	-2.908230	3.887666	0.702825
1	-0.598745	3.874251	1.118238
1	0.432215	2.521565	0.748424
1	-0.110618	2.198648	-2.314009
1	0.858197	3.529777	-2.944321
1	3.211178	3.698047	-2.564483
1	2.400948	-3.880774	2.353286
1	0.604241	-3.483863	-3.147387
1	1.232530	-2.262380	-2.026138

1	0.793435	-3.876249	-1.439203
1	-0.050846	-2.982693	2.542633
1	-0.699205	-2.065763	1.195206
1	-0.139437	-3.763441	0.956794
1	-4.111052	-3.660046	-2.359448
1	-5.699549	-1.837976	-1.562093
1	-6.003764	0.436123	-0.641724
1	-4.978439	2.603028	0.190259
1	-0.686534	4.469323	-1.373076
1	0.914834	4.587662	-0.657888
1	5.318161	2.605988	-1.823200
1	6.436076	0.706420	-0.569842
1	6.222045	-1.358128	0.773073
1	4.715618	-3.096250	1.876816

Cu 0

LANL2DZ

****

C N H O Cl 0

6-31+G*

****

Cu 0

LANL2DZ

Figure 10.a. Geometry optimization of the $[Cu^{I}Cu^{II}(CCl_3)(mphenpr)_2]^{2+}$ structure.

opt NoSymm b3lyp/gen pseudo=read SCF=(MaxCycle=800)

2 2

29	0.	0.	0.
29	-3.121	1.631	-6.226
7	2.287	0.	-0.349
7	0.293	-0.851	-2.1
7	0.096	2.218	0.514
6	-2.056	0.092	0.185
6	0.105	2.403	1.86
6	0.092	3.271	-0.304
6	0.017	1.243	2.731
6	-0.121	-1.079	2.957
6	3.284	0.316	0.489
6	2.532	0.02	-1.691
6	1.514	-0.48	-2.596
6	-0.574	-1.471	-2.915
17	-2.475	0.426	-0.762
17	-2.439	-0.892	0.469
17	-2.242	0.82	0.974
6	0.183	4.59	0.201
6	-0.051	1.44	4.135
6	-0.212	-0.959	4.363
6	-0.155	-2.429	2.292
6	-0.057	3.003	-1.79
6	4.538	0.777	0.018
6	3.779	0.436	-2.233
6	1.848	-0.622	-3.972
6	-0.259	-1.733	-4.272
6	3.113	0.152	1.974
6	-1.921	-1.915	-2.405
6	0.153	3.696	2.445
6	0.117	3.851	3.869

6	0.009	2.764	4.683
6	-0.169	0.289	4.946
6	-1.067	3.942	-2.489
6	0.221	4.798	1.562
6	4.778	0.858	-1.33
6	4.03	0.372	-3.64
6	3.102	-0.158	-4.48
6	0.919	-1.278	-4.806
6	-3.115	-1.044	-2.874
6	-1.652	3.395	-3.803
6	-3.552	-1.209	-4.347
6	-0.706	3.145	-4.96
6	-4.833	-0.453	-4.616
6	0.573	3.741	-5.037
7	-1.158	2.353	-5.941
7	-4.768	0.715	-5.264
6	-6.062	-0.971	-4.146
7	0.	0.	2.18
6	1.392	3.479	-6.115
6	-0.366	2.093	-7.018
6	-5.916	1.43	-5.46
6	-7.226	-0.26	-4.331
6	0.944	2.625	-7.145
6	-0.888	1.251	-8.075
7	-2.163	0.794	-7.965
7	-4.628	3.088	-6.641
6	-5.839	2.684	-6.173
6	-7.181	0.985	-4.998
6	1.746	2.3	-8.289
6	-0.066	0.952	-9.192

6	-2.679	0.032	-8.933
6	-4.546	4.238	-7.3
6	-7.012	3.454	-6.378
6	-8.35	1.785	-5.224
6	1.262	1.488	-9.271
6	-0.623	0.133	-10.2
6	-1.917	-0.323	-10.071
6	-4.105	-0.425	-8.782
6	-5.648	5.089	-7.554
6	-6.881	4.672	-7.081
6	-8.27	2.975	-5.883
6	-5.456	6.379	-8.31
1	-3.71	-2.274	-4.565
1	-0.305	-1.853	4.97
1	-1.9	-1.925	-1.316
1	-2.092	-2.95	-2.732
1	2.681	1.051	2.428
1	4.086	-0.015	2.444
1	2.465	-0.691	2.206
1	0.208	5.432	-0.483
1	5.305	1.041	0.738
1	-0.961	-2.297	-4.876
1	0.906	4.406	-4.249
1	-6.075	-1.932	-3.64
1	-0.384	1.965	-1.904
1	0.926	3.07	-2.277
1	0.012	-3.234	3.012
1	-1.915	4.112	-1.816
1	-0.621	4.93	-2.658
1	5.738	1.199	-1.709

1	2.379	3.929	-6.183
1	-8.177	-0.645	-3.975
1	4.993	0.713	-4.011
1	3.301	-0.261	-5.542
1	1.162	-1.445	-5.852
1	0.281	5.804	1.968
1	0.162	4.853	4.285
1	-0.033	2.881	5.762
1	-0.226	0.399	6.026
1	-3.966	-1.289	-2.227
1	-2.893	0.015	-2.699
1	-1.13	-2.597	1.819
1	0.607	-2.498	1.507
1	-2.184	2.456	-3.604
1	-2.425	4.095	-4.152
1	2.744	2.721	-8.361
1	-9.305	1.42	-4.857
1	-3.556	4.513	-7.659
1	-2.779	-0.839	-5.028
1	-4.246	-0.942	-7.827
1	-4.783	0.436	-8.787
1	-4.398	-1.098	-9.591
1	1.869	1.247	-10.139
1	-0.028	-0.123	-11.073
1	-2.364	-0.946	-10.838
1	-7.765	5.281	-7.252
1	-9.159	3.576	-6.05
1	-6.41	6.885	-8.477
1	-4.992	6.202	-9.287
1	-4.803	7.067	-7.76

Cu 0

LANL2DZ

****

C N H Cl 0

6-31+G*

******

Cu 0

LANL2DZ

Figure 10.b. Geometry optimization of the $[Cu^{I}Cu^{II}(CCl_3)(mphenpr)_2]^{2+}$ structure

opt=loose NoSymm b3lyp/gen pseudo=read SCF=(MaxCycle=800)

2 2			
29	0.00000	0.00000	0.00000
29	-5.24600	-5.04000	-0.69400
7	1.94900	0.00000	-0.93700
7	0.37400	-2.21000	-0.52200
7	-2.11700	-0.08700	0.52100
6	-0.40800	1.93500	-0.62500
6	-2.34400	0.32100	1.79900
6	-3.12800	-0.16400	-0.35400
6	-1.23500	0.37000	2.73300
6	1.02000	-0.02300	3.15600
6	2.80900	1.01900	-1.01900
6	2.07700	-1.05700	-1.78900
6	1.24400	-2.22100	-1.57300
6	-0.28400	-3.32900	-0.21200
17	-1.43900	2.00700	-0.97200

17	-0.26000	2.55300	0.26500
17	0.29100	2.20000	-1.41900
6	-4.44200	0.18200	0.03100
6	-1.47900	0.77900	4.06900
6	0.85700	0.37100	4.50800
6	2.36500	-0.49400	2.67100
6	-2.77300	-0.59000	-1.77000
6	3.80100	1.06100	-2.03100
6	3.04000	-1.08000	-2.82900
6	1.41800	-3.35300	-2.41200
6	-0.16500	-4.49900	-1.00400
6	2.74800	2.13400	-0.01000
6	-1.12100	-3.38500	1.04800
6	-3.63900	0.69300	2.25100
6	-3.83900	1.12300	3.60300
6	-2.79700	1.16400	4.48000
6	-0.37700	0.78000	4.95600
6	-3.93300	-0.86100	-2.74500
6	-4.69200	0.61300	1.31700
6	3.89900	0.03700	-2.94200
6	3.14200	-2.21900	-3.69200
6	2.35900	-3.31600	-3.49100
6	0.65800	-4.50400	-2.10600
6	-2.63900	-3.55300	0.81200
6	-4.64700	-2.22100	-2.58300
6	-3.36300	-4.03200	2.08800
6	-3.90200	-3.44000	-3.09800
6	-4.84100	-3.70800	2.16800
6	-3.17200	-3.39600	-4.31000
7	-4.01800	-4.58000	-2.40700
7	-5.65300	-4.03800	1.15600
6	-5.34000	-3.08100	3.33500

7	0.00000	0.00000	2.29700
6	-2.55300	-4.53100	-4.78500
6	-3.41800	-5.71400	-2.86900
6	-6.98900	-3.77200	1.26000
6	-6.68400	-2.80500	3.45300
6	-2.65400	-5.74000	-4.06300
6	-3.57800	-6.93900	-2.11100
7	-4.34400	-6.91000	-0.98600
7	-7.32000	-4.76400	-0.91200
6	-7.86400	-4.15200	0.17200
6	-7.55900	-3.14900	2.40100
6	-2.03300	-6.95800	-4.49700
6	-2.94900	-8.12500	-2.57000
6	-4.52200	-8.03000	-0.27600
6	-8.11400	-5.12800	-1.91300
6	-9.25500	-3.89300	0.25800
6	-8.97100	-2.89800	2.45600
6	-2.17100	-8.10500	-3.77500
6	-3.13900	-9.29600	-1.80300
6	-3.91700	-9.24800	-0.66600
6	-5.40900	-7.96300	0.93700
6	-9.51300	-4.91900	-1.93200
6	-10.06600	-4.29400	-0.82700
6	-9.78800	-3.25400	1.42700
6	-10.33500	-5.37300	-3.11100
1	-2.88000	-3.58900	2.96600
1	1.71200	0.34700	5.17600
1	-0.93000	-2.48800	1.64200
1	-0.75900	-4.24100	1.63400
1	2.47700	3.08400	-0.48600
1	3.73500	2.27500	0.44500
1	2.02200	1.92300	0.77500

1	-5.25400	0.12100	-0.68300
1	4.47500	1.91100	-2.07100
1	-0.71500	-5.39000	-0.72000
1	-3.11100	-2.47200	-4.87300
1	-4.65300	-2.82900	4.13600
1	-2.12100	-1.47000	-1.70900
1	-2.14300	0.20700	-2.18800
1	3.10800	0.31000	2.73600
1	-4.68000	-0.06300	-2.67200
1	-3.54100	-0.77000	-3.76300
1	4.64700	0.06300	-3.73000
1	-1.99500	-4.50800	-5.71800
1	-7.07900	-2.33100	4.34800
1	3.87400	-2.19800	-4.49400
1	2.45500	-4.19000	-4.12900
1	0.75900	-5.39400	-2.72200
1	-5.69700	0.89600	1.61800
1	-4.83700	1.41800	3.91200
1	-2.94700	1.49000	5.50500
1	-0.51900	1.09400	5.98700
1	-3.05700	-2.59800	0.48900
1	-2.82200	-4.26300	0.00000
1	2.73200	-1.31500	3.29800
1	2.30800	-0.83700	1.63700
1	-4.91000	-2.40300	-1.53500
1	-5.60100	-2.17300	-3.12800
1	-1.46000	-6.95000	-5.42000
1	-9.37600	-2.42100	3.34400
1	-7.62800	-5.61600	-2.75500
1	-3.23100	-5.11800	2.18900
1	-5.21700	-7.05100	1.51100
1	-6.46400	-7.94200	0.63500

1	-5.26400	-8.83000	1.58700
1	-1.70600	-9.02900	-4.10700
1	-2.67500	-10.22600	-2.11800
1	-4.07900	-10.13700	-0.06600
1	-11.13700	-4.10800	-0.78400
1	-10.85600	-3.06500	1.47600
1	-11.38900	-5.11400	-2.98400
1	-10.27000	-6.46000	-3.24300
1	-9.98400	-4.91200	-4.04200

Cu 0

LANL2DZ

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C N H Cl 0

6-31+G*

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Cu 0

LANL2DZ

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