Supporting Information

Catalytic performance of a dicopper-oxo complex for methane hydroxylation

Yuta Hori,[†] Yoshihito Shiota,[†*] Tomokazu Tsuji,[‡] Masahito Kodera,[‡] and Kazunari Yoshizawa[†*]

[†] Institute for Materials Chemistry and Engineering and IRCCS, Kyushu University, Fukuoka 819-0395, Japan

[‡] Department of Molecular Chemistry and Biochemistry, Doshisha University, Kyotanabe Kyoto 610-0321, Japan

* To whom all correspondence should be addressed (e-mail: shiota@ms.ifoc.kyushu-u.ac.jp, kazunari@ms.ifoc.kyushu-u.ac.jp).

Table of Contents:

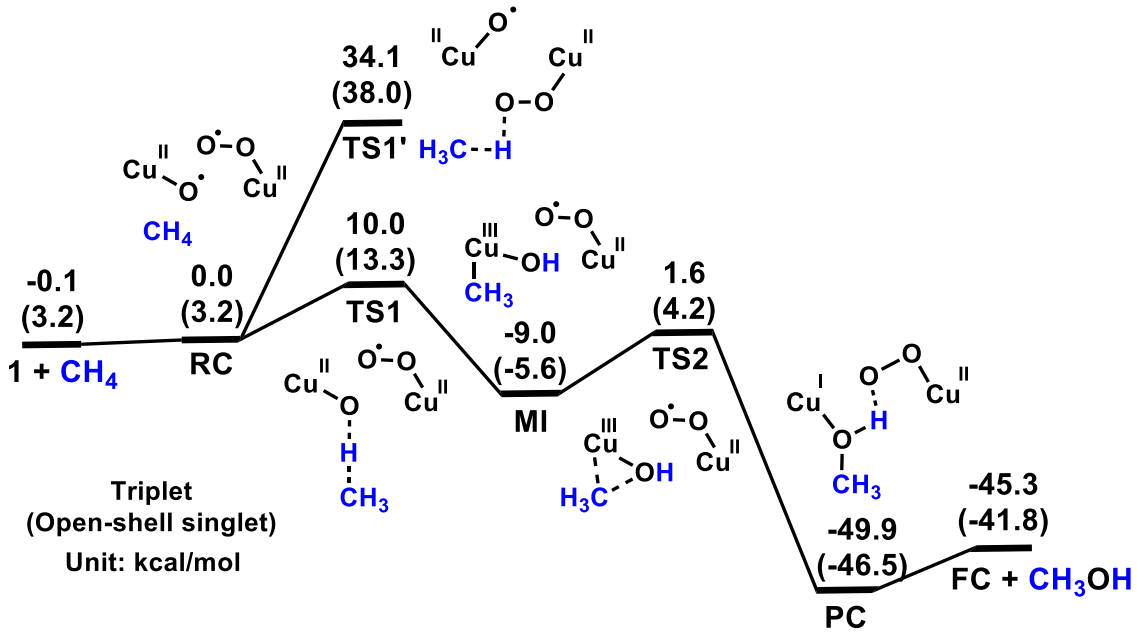

Figure S1. Computed energy diagram including the solvent effect of water for the methane hydroxylation catalyzed by **1**. Relative energies respect to reactant complex (**RC**), measured from **1** and methane in the triplet and open-shell singlet states, are in kcal/mol. The implicit solvent effect of water (dielectric constant = 78.39) was predicted by using the polarized continuum model (SCRF = PCM) implemented with the Gaussian 09 package.

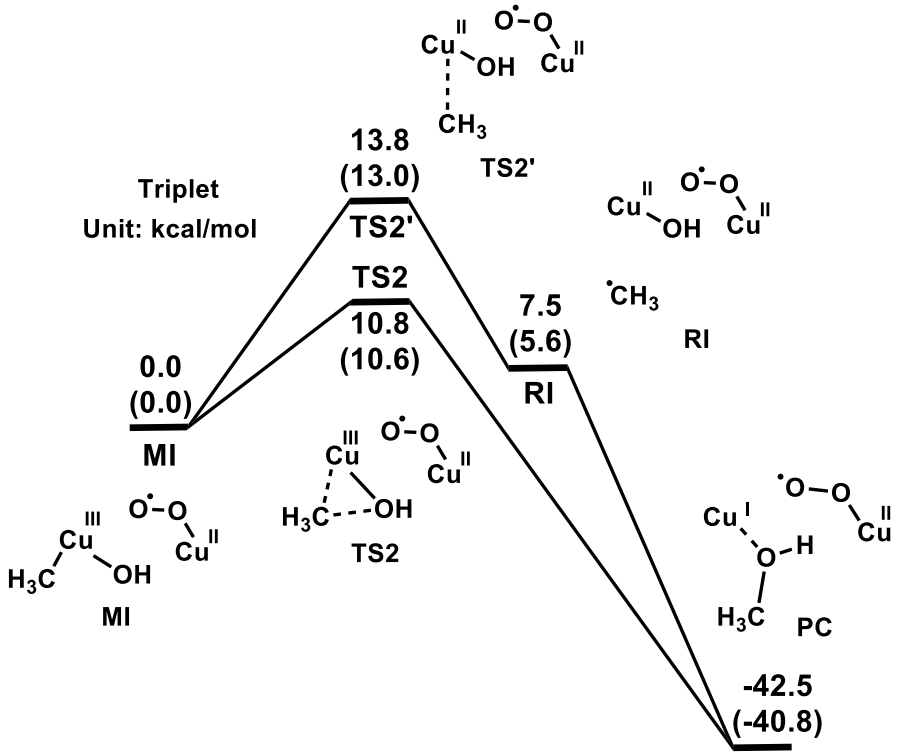

Figure S2. Computed energy diagrams for methyl intermediate (**MI**) to product complex (**PC**) with another pathway via radical intermediate (**RI**) in the triplet state. Relative energies respect to **MI** are in kcal/mol. The parenthesis values are energies including the solvent effect of water.

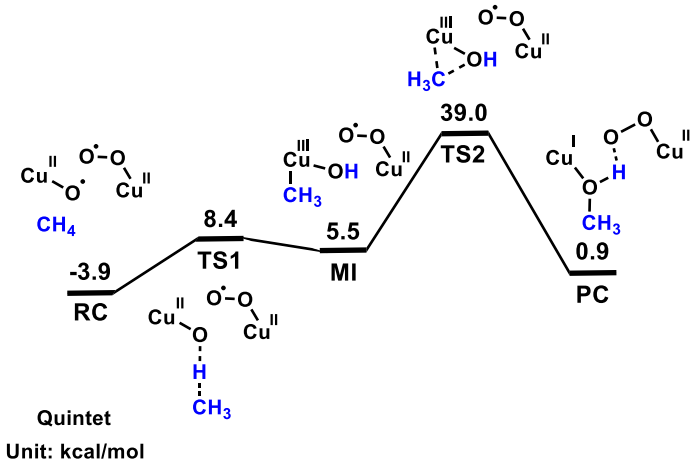

Figure S3. Computed energy diagram for the methane hydroxylation catalyzed by **1** in the quintet state. Relative energies respect to reactant complex (**RC**) measured from **1** and methane are in kcal/mol. The energy of **TS2** was calculated by using the obtained structure in the triplet state.

Table S1. Cartesian coordinates of **B** in the triplet state.

		angstrom	
Atom	x	y	z
Cu	-2.267315	0.206294	0.056911
Cu	2.267072	0.207095	-0.054583
O	-0.467405	0.792436	0.498550
O	0.467151	0.802419	-0.484008
N	-2.463424	0.148195	-2.095579
N	-3.088680	1.973409	0.985503
N	-2.473433	-1.768967	0.934536
N	-4.423254	-0.121149	-0.172285
N	3.088266	1.977473	-0.976505
N	2.467710	0.136072	2.097768
N	2.469398	-1.763975	-0.943216
N	4.423332	-0.123932	0.168570
C	-1.574494	0.594592	-3.000552
H	-0.615773	0.911981	-2.596183
C	-1.850594	0.647074	-4.370429
H	-1.099585	1.016628	-5.063058
C	-3.108586	0.223019	-4.816184
H	-3.364352	0.255255	-5.872747
C	-4.037316	-0.237915	-3.874248
H	-5.025454	-0.571840	-4.181412
C	-3.675436	-0.265530	-2.523238
C	-4.610183	-0.818944	-1.459760
H	-5.652909	-0.773863	-1.805552
H	-4.366907	-1.877541	-1.309350
C	-2.405273	2.850609	1.739384
H	-1.336749	2.664649	1.823650
C	-3.013601	3.942550	2.365165
H	-2.420320	4.627465	2.964400
C	-4.393247	4.123363	2.200076
H	-4.905103	4.956350	2.676408

C	-5.104181	3.212997	1.408134
H	-6.174360	3.325018	1.251325
C	-4.411735	2.154818	0.809707
C	-5.094454	1.193304	-0.147921
H	-6.163735	1.102520	0.093375
H	-5.027547	1.621661	-1.155591
C	-1.529144	-2.709443	1.174249
C	-1.859841	-3.938543	1.768600
H	-1.078204	-4.668766	1.957647
C	-3.187046	-4.213078	2.106159
H	-3.459489	-5.160474	2.565312
C	-4.159954	-3.248186	1.828482
H	-5.207442	-3.423423	2.059226
C	-3.761293	-2.040958	1.248401
C	-4.785502	-0.949438	0.991324
H	-5.786226	-1.394038	0.885068
H	-4.817366	-0.291913	1.869172
C	2.404181	2.859192	-1.724501
H	1.335170	2.675255	-1.806960
C	3.012357	3.953421	-2.346403
H	2.418488	4.641948	-2.940898
C	4.392582	4.131849	-2.183590
H	4.904320	4.966555	-2.657028
C	5.104209	3.216901	-1.397588
H	6.174836	3.327017	-1.242512
C	4.411913	2.156604	-0.802733
C	5.095634	1.190010	0.149017
H	6.164375	1.099448	-0.094756
H	5.031013	1.613734	1.158794
C	1.580890	0.577846	3.007084
H	0.621098	0.897023	2.606704
C	1.860244	0.623484	4.376556
H	1.110829	0.989477	5.072795

C	3.119322	0.197357	4.817222
H	3.377593	0.224386	5.873321
C	4.045817	-0.258857	3.870798
H	5.034699	-0.594261	4.173933
C	3.680683	-0.279776	2.520540
C	4.612814	-0.828143	1.452186
H	5.656345	-0.785183	1.795820
H	4.368799	-1.885895	1.297099
C	1.523777	-2.702346	-1.185764
C	1.852307	-3.929545	-1.785255
H	1.069514	-4.657978	-1.976442
C	3.178804	-4.204451	-2.125176
H	3.449627	-5.150389	-2.588275
C	4.153140	-3.241737	-1.844886
H	5.200155	-3.417273	-2.077533
C	3.756583	-2.036285	-1.259713
C	4.782345	-0.946947	-0.999769
H	5.782893	-1.392943	-0.897802
H	4.812883	-0.285328	-1.874580
C	0.094282	-2.427938	-0.776971
H	-0.539258	-3.199939	-1.225619
H	-0.220622	-1.460330	-1.175391
C	-0.098844	-2.435271	0.767884
H	0.532430	-3.213494	1.208892
H	0.219070	-1.472488	1.175623

Table S2. Cartesian coordinates of **B** in the singlet state.

		angstrom	
Atom	x	y	z
Cu	-2.245956	0.222482	0.057039
Cu	2.245977	0.223207	-0.054938
O	-0.459550	0.726427	0.524154
O	0.459657	0.735516	-0.513408
N	-2.429248	0.139235	-2.089276
N	-3.033617	1.982912	0.966151
N	-2.468889	-1.780821	0.932808
N	-4.384651	-0.103308	-0.169690
N	3.034704	1.985238	-0.959510
N	2.432427	0.129856	2.090817
N	2.464680	-1.777458	-0.939278
N	4.384681	-0.106896	0.166973
C	-1.529281	0.568951	-2.991036
H	-0.571327	0.878621	-2.578770
C	-1.796816	0.610088	-4.363064
H	-1.038132	0.965661	-5.054633
C	-3.055550	0.192665	-4.813065
H	-3.303810	0.216682	-5.871647
C	-3.994982	-0.251642	-3.873494
H	-4.983542	-0.580850	-4.184304
C	-3.641707	-0.268823	-2.520321
C	-4.583085	-0.805387	-1.455209
H	-5.625965	-0.746899	-1.797558
H	-4.353580	-1.866134	-1.299683
C	-2.330914	2.855909	1.706982
H	-1.264937	2.652060	1.779228
C	-2.922411	3.959721	2.327962
H	-2.316780	4.642459	2.917220
C	-4.300975	4.156213	2.171479
H	-4.798652	4.999238	2.645192

C	-5.030206	3.249651	1.391439
H	-6.099848	3.374795	1.241353
C	-4.355589	2.178538	0.796612
C	-5.049788	1.216827	-0.151368
H	-6.118005	1.131482	0.095019
H	-4.984777	1.638134	-1.162076
C	-1.535865	-2.732342	1.170906
C	-1.883048	-3.957528	1.765113
H	-1.111084	-4.698308	1.953039
C	-3.213255	-4.214501	2.104434
H	-3.497481	-5.158732	2.563002
C	-4.174205	-3.236137	1.830606
H	-5.223365	-3.397109	2.064214
C	-3.758508	-2.034929	1.250392
C	-4.763376	-0.925584	0.995514
H	-5.772162	-1.349970	0.885737
H	-4.784310	-0.267048	1.872900
C	2.332087	2.861976	-1.696010
H	1.265548	2.660532	-1.766682
C	2.924275	3.966856	-2.314413
H	2.318666	4.652606	-2.900186
C	4.303451	4.160536	-2.159844
H	4.801646	5.004334	-2.631628
C	5.032581	3.250191	-1.384137
H	6.102677	3.373126	-1.235484
C	4.357303	2.178174	-0.791685
C	5.051589	1.212374	0.152038
H	6.119333	1.126419	-0.096190
H	4.988605	1.630430	1.164225
C	1.534186	0.556669	2.995687
H	0.575566	0.868072	2.586287
C	1.804147	0.592756	4.367386
H	1.046802	0.946124	5.061550

C	3.063501	0.173257	4.813696
H	3.313621	0.193421	5.871921
C	4.001091	-0.268115	3.870906
H	4.990045	-0.598870	4.178803
C	3.645419	-0.280312	2.518305
C	4.584590	-0.813719	1.449683
H	5.628090	-0.757333	1.790492
H	4.353957	-1.873716	1.290758
C	1.529990	-2.726757	-1.179498
C	1.874676	-3.950871	-1.777384
H	1.101295	-4.689758	-1.966961
C	3.204219	-4.209146	-2.118234
H	3.486594	-5.152561	-2.579618
C	4.166945	-3.233062	-1.842426
H	5.215663	-3.395064	-2.077306
C	3.753640	-2.032773	-1.258624
C	4.760417	-0.925675	-1.001664
H	5.768814	-1.351770	-0.894978
H	4.780786	-0.264212	-1.876855
C	0.096429	-2.466690	-0.775193
H	-0.528400	-3.244104	-1.227115
H	-0.220492	-1.498240	-1.169130
C	-0.101463	-2.473658	0.768475
H	0.520621	-3.257503	1.212993
H	0.219199	-1.510068	1.171339

Table S3. Cartesian coordinates of **C** in the triplet state.

		angstrom	
Atom	x	y	z
Cu	3.475572	-0.048009	-0.517098
Cu	-3.421626	0.016250	-0.456412
O	2.159847	-0.767095	-1.674923
O	-2.149788	0.533996	-1.760545
O	1.317568	0.176614	-2.375194
H	1.550895	-0.001508	-3.303860
O	-1.440181	-0.556884	-2.359660
N	3.481641	2.060077	-0.674686
N	4.930704	-1.321576	-1.312961
N	2.639148	-0.635829	1.528085
N	5.111456	0.386968	0.781944
N	-4.954013	1.065769	-1.468782
N	-3.541948	-2.112958	-0.376313
N	-2.579844	0.860925	1.449062
N	-5.079076	-0.234208	0.919611
C	2.840908	2.804363	-1.595395
H	2.134876	2.266968	-2.222118
C	3.053539	4.179344	-1.732461
H	2.512761	4.736403	-2.492197
C	3.974530	4.804328	-0.883535
H	4.175106	5.869844	-0.968341
C	4.638450	4.031275	0.078091
H	5.359390	4.481178	0.756350
C	4.359357	2.663960	0.157366
C	4.969305	1.788282	1.236364
H	5.928208	2.202630	1.576760
H	4.291891	1.791482	2.098314
C	4.712426	-2.352843	-2.147245
H	3.674697	-2.521096	-2.424934
C	5.753626	-3.150540	-2.630783

H	5.536930	-3.975657	-3.303161
C	7.063656	-2.860989	-2.227656
H	7.897527	-3.462296	-2.582355
C	7.286146	-1.786135	-1.355934
H	8.289774	-1.534331	-1.022295
C	6.189895	-1.035579	-0.923439
C	6.332871	0.188148	-0.036991
H	7.232116	0.113322	0.590482
H	6.454077	1.070360	-0.677742
C	1.365092	-0.880532	1.918613
C	1.077827	-1.288502	3.232503
H	0.049278	-1.497265	3.513162
C	2.113317	-1.425284	4.160252
H	1.907164	-1.738495	5.181168
C	3.423183	-1.151099	3.751555
H	4.258751	-1.243746	4.440622
C	3.638644	-0.770779	2.423539
C	5.053927	-0.572213	1.908543
H	5.718703	-0.264292	2.728081
H	5.421859	-1.537575	1.541158
C	-4.763130	1.885204	-2.515607
H	-3.733694	1.969406	-2.857984
C	-5.819952	2.566314	-3.128024
H	-5.627092	3.219724	-3.974101
C	-7.115323	2.383827	-2.626805
H	-7.960459	2.901094	-3.075176
C	-7.309628	1.521672	-1.538822
H	-8.302554	1.350932	-1.129822
C	-6.198671	0.872905	-0.992258
C	-6.321368	-0.158207	0.116942
H	-7.199303	0.047460	0.746042
H	-6.478833	-1.138842	-0.348560
C	-3.009804	-2.975747	-1.261491

H	-2.348146	-2.533491	-2.002098
C	-3.290245	-4.346330	-1.234064
H	-2.841162	-5.003962	-1.972959
C	-4.161579	-4.835482	-0.254141
H	-4.409756	-5.893398	-0.208206
C	-4.721822	-3.934684	0.661946
H	-5.410646	-4.275330	1.431193
C	-4.384599	-2.581290	0.569778
C	-4.910608	-1.556339	1.560506
H	-5.844961	-1.909561	2.019511
H	-4.176725	-1.445072	2.367727
C	-1.296822	1.144749	1.777363
C	-0.978557	1.742679	3.008064
H	0.057763	1.976300	3.235787
C	-1.994899	2.034415	3.921574
H	-1.766522	2.497136	4.878987
C	-3.314062	1.717551	3.581668
H	-4.135783	1.923462	4.262717
C	-3.561600	1.141242	2.331507
C	-4.989742	0.877912	1.885889
H	-5.633159	0.707650	2.761738
H	-5.360720	1.781203	1.385945
C	-0.226048	0.785152	0.775194
H	0.625715	1.465095	0.885240
H	-0.646329	0.925246	-0.224159
C	0.270535	-0.691728	0.895389
H	-0.578433	-1.339571	1.137683
H	0.663954	-0.998714	-0.076025
H	-0.500308	-0.312993	-2.207911

Table S4. Cartesian coordinates of **C** in the singlet state.

		angstrom	
Atom	x	y	z
Cu	-3.475647	-0.047586	0.517252
Cu	3.421708	0.016283	0.456552
O	-2.160132	-0.765813	1.675839
O	2.149904	0.534079	1.760647
O	-1.317619	0.178518	2.374983
H	-1.550717	0.001312	3.303886
O	1.439210	-0.556460	2.358993
N	-3.481531	2.060725	0.672987
N	-4.930904	-1.320287	1.314005
N	-2.639034	-0.637346	-1.527445
N	-5.111247	0.386417	-0.782427
N	4.953640	1.067504	1.467951
N	3.542499	-2.112816	0.377748
N	2.579691	0.859699	-1.449532
N	5.079247	-0.234496	-0.919307
C	-2.841059	2.805809	1.593218
H	-2.135186	2.268949	2.220569
C	-3.053710	4.180913	1.729041
H	-2.513146	4.738614	2.488457
C	-3.974438	4.805178	0.879305
H	-4.175006	5.870774	0.963109
C	-4.638106	4.031290	-0.081825
H	-5.358849	4.480610	-0.760680
C	-4.359034	2.663896	-0.159816
C	-4.968808	1.787283	-1.238140
H	-5.927576	2.201432	-1.579165
H	-4.291181	1.789535	-2.099923
C	-4.712823	-2.350933	2.149104
H	-3.675140	-2.519079	2.427036
C	-5.754162	-3.148144	2.633154

H	-5.537617	-3.972764	3.306188
C	-7.064114	-2.858760	2.229669
H	-7.898091	-3.459693	2.584750
C	-7.286398	-1.784553	1.357087
H	-8.289968	-1.532911	1.023153
C	-6.190030	-1.034454	0.924115
C	-6.332746	0.188551	0.036633
H	-7.231989	0.113363	-0.590801
H	-6.453790	1.071336	0.676623
C	-1.364984	-0.882616	-1.917652
C	-1.077698	-1.292004	-3.231090
H	-0.049166	-1.501223	-3.511472
C	-2.113154	-1.429596	-4.158765
H	-1.906981	-1.743894	-5.179342
C	-3.422999	-1.154794	-3.750436
H	-4.258543	-1.248028	-4.439454
C	-3.638488	-0.773087	-2.422817
C	-5.053792	-0.573803	-1.908128
H	-5.718440	-0.266523	-2.728012
H	-5.421922	-1.538772	-1.539910
C	4.762450	1.887740	2.514099
H	3.732991	1.971919	2.856397
C	5.819032	2.569657	3.126025
H	5.625936	3.223698	3.971560
C	7.114492	2.387130	2.625042
H	7.959446	2.905007	3.073050
C	7.309119	1.524137	1.537787
H	8.302121	1.353344	1.128996
C	6.198380	0.874600	0.991677
C	6.321474	-0.157413	-0.116647
H	7.199374	0.048011	-0.745876
H	6.479240	-1.137601	0.349697
C	3.010385	-2.975134	1.263406

H	2.348391	-2.532584	2.003533
C	3.291243	-4.345652	1.237005
H	2.842199	-5.002893	1.976270
C	4.162918	-4.835239	0.257604
H	4.411407	-5.893116	0.212459
C	4.723081	-3.934930	-0.659015
H	5.412134	-4.275933	-1.427898
C	4.385473	-2.581569	-0.567861
C	4.911327	-1.557164	-1.559242
H	5.845874	-1.910422	-2.017825
H	4.177550	-1.446749	-2.366679
C	1.296608	1.143007	-1.778003
C	0.978154	1.739833	-3.009191
H	-0.058218	1.973082	-3.237061
C	1.994391	2.030975	-3.923009
H	1.765873	2.492815	-4.880812
C	3.313639	1.714670	-3.582892
H	4.135287	1.920178	-4.264150
C	3.561355	1.139489	-2.332244
C	4.989569	0.876883	-1.886432
H	5.633048	0.706169	-2.762147
H	5.360277	1.780654	-1.387156
C	0.225993	0.784054	-0.775428
H	-0.625843	1.463847	-0.885868
H	0.646380	0.924920	0.223768
C	-0.270473	-0.692943	-0.894541
H	0.578578	-1.340863	-1.136325
H	-0.663879	-0.999277	0.077079
H	0.499546	-0.311694	2.207339

Table S5. Cartesian coordinates of **1** in the triplet state.

		angstrom	
Atom	x	y	z
Cu	3.038054	-0.291325	0.053192
Cu	-3.020046	-0.301357	-0.056465
O	1.470567	-0.850721	0.846989
O	-1.522085	-0.990047	-1.107346
O	-1.229678	-2.218754	-0.872420
N	2.813677	-1.102307	-1.889452
N	4.343754	-1.181105	1.432237
N	2.829460	1.878368	0.079435
N	4.901907	0.267649	-0.788469
N	-4.493278	-1.374298	-1.128719
N	-2.494163	-0.794387	1.926860
N	-2.852352	1.881395	-0.393866
N	-4.796578	0.386365	0.950863
C	1.885319	-1.999327	-2.262199
H	1.115544	-2.227480	-1.528148
C	1.901599	-2.598307	-3.526791
H	1.135870	-3.322041	-3.790821
C	2.920656	-2.252200	-4.422636
H	2.969256	-2.706849	-5.409467
C	3.884523	-1.312526	-4.028925
H	4.688675	-1.020532	-4.699999
C	3.790593	-0.754527	-2.751644
C	4.732255	0.332392	-2.262354
H	5.699504	0.278462	-2.780065
H	4.288420	1.305537	-2.504015
C	4.003673	-1.635521	2.649694
H	2.949696	-1.544899	2.902948
C	4.944894	-2.187382	3.523912
H	4.635021	-2.546555	4.501094
C	6.282442	-2.257121	3.112021

H	7.042055	-2.674723	3.768787
C	6.632053	-1.776843	1.842256
H	7.660926	-1.815076	1.492898
C	5.627034	-1.249834	1.026800
C	5.883062	-0.775672	-0.392722
H	6.916154	-0.419830	-0.508333
H	5.754014	-1.628288	-1.070425
C	1.720921	2.626608	0.274373
C	1.806043	4.029286	0.345057
H	0.906999	4.609307	0.534717
C	3.038933	4.661625	0.178354
H	3.118468	5.745170	0.227243
C	4.174379	3.875123	-0.052412
H	5.153144	4.326833	-0.191606
C	4.026070	2.487529	-0.078365
C	5.242324	1.585339	-0.203456
H	6.033502	2.087345	-0.777698
H	5.638558	1.408602	0.803799
C	-4.345917	-2.005423	-2.307272
H	-3.352108	-1.977011	-2.746572
C	-5.398692	-2.668441	-2.943837
H	-5.230748	-3.165980	-3.894674
C	-6.657693	-2.668106	-2.330415
H	-7.502612	-3.169116	-2.797054
C	-6.812925	-2.006606	-1.105543
H	-7.775593	-1.984031	-0.600623
C	-5.704224	-1.376177	-0.532693
C	-5.779484	-0.710549	0.831741
H	-6.804073	-0.366496	1.035032
H	-5.533901	-1.462455	1.591998
C	-1.495177	-1.604800	2.318768
H	-0.801165	-1.925579	1.546273
C	-1.340105	-2.009462	3.649000

H	-0.521240	-2.670274	3.918110
C	-2.259582	-1.558408	4.602207
H	-2.178037	-1.864068	5.642815
C	-3.294450	-0.706012	4.193075
H	-4.026549	-0.333144	4.905314
C	-3.373272	-0.339323	2.847064
C	-4.414298	0.653287	2.352643
H	-5.286983	0.659189	3.021125
H	-3.971970	1.656010	2.393417
C	-1.803680	2.639721	-0.793685
C	-1.949591	4.019072	-1.022409
H	-1.099371	4.593539	-1.379699
C	-3.181772	4.636106	-0.798062
H	-3.310369	5.702382	-0.969053
C	-4.247187	3.852772	-0.343865
H	-5.221676	4.290725	-0.143886
C	-4.044224	2.481037	-0.168700
C	-5.218869	1.597783	0.224595
H	-5.949087	2.185549	0.800157
H	-5.723503	1.275836	-0.694662
C	-0.443964	1.995102	-0.957707
H	0.113352	2.568807	-1.705005
H	-0.553202	0.980935	-1.343823
C	0.376997	1.940006	0.384573
H	-0.190597	2.427270	1.184945
H	0.521993	0.893786	0.677199

Table S6. Cartesian coordinates of **1** in the singlet state.

		angstrom	
Atom	x	y	z
Cu	3.023843	-0.285069	0.063171
Cu	-3.019505	-0.291910	-0.042503
O	1.465160	-0.775950	0.915921
O	-1.527935	-0.967820	-1.064914
O	-1.279230	-2.220571	-0.817918
N	2.728189	-1.148839	-1.844589
N	4.340618	-1.152424	1.447392
N	2.875594	1.892833	0.025046
N	4.881711	0.194062	-0.840466
N	-4.481039	-1.355290	-1.126301
N	-2.489827	-0.774333	1.941443
N	-2.827128	1.890190	-0.375686
N	-4.775239	0.395997	0.944189
C	1.762584	-2.026704	-2.165285
H	0.997413	-2.202804	-1.412267
C	1.732982	-2.670639	-3.407592
H	0.937178	-3.376125	-3.628420
C	2.743697	-2.393057	-4.335570
H	2.756870	-2.885069	-5.305462
C	3.745705	-1.471788	-3.996514
H	4.544443	-1.230471	-4.693710
C	3.696555	-0.864790	-2.739485
C	4.680293	0.210221	-2.311620
H	5.633440	0.109248	-2.848174
H	4.258847	1.186686	-2.578786
C	4.019284	-1.549029	2.689921
H	2.974940	-1.419113	2.965100
C	4.967036	-2.092198	3.562478
H	4.672417	-2.403794	4.560496
C	6.291348	-2.215536	3.121442

H	7.055720	-2.628220	3.775799
C	6.621641	-1.795401	1.825478
H	7.639938	-1.876180	1.453151
C	5.610931	-1.272677	1.014189
C	5.843849	-0.860556	-0.428433
H	6.883088	-0.538614	-0.582468
H	5.674824	-1.734349	-1.069491
C	1.794113	2.679027	0.222324
C	1.918058	4.080560	0.227610
H	1.041748	4.693233	0.421045
C	3.160732	4.671255	-0.006106
H	3.269749	5.753333	-0.007985
C	4.267399	3.844637	-0.235383
H	5.252972	4.262769	-0.423007
C	4.082094	2.461707	-0.195020
C	5.270625	1.522390	-0.313171
H	6.061329	1.980410	-0.923612
H	5.685054	1.372464	0.691109
C	-4.322153	-1.984754	-2.303824
H	-3.324774	-1.951838	-2.734206
C	-5.370152	-2.650784	-2.945283
H	-5.196124	-3.147751	-3.895303
C	-6.632241	-2.655314	-2.338044
H	-7.472612	-3.159380	-2.809594
C	-6.797641	-1.995777	-1.113055
H	-7.762994	-1.978091	-0.613163
C	-5.694012	-1.361802	-0.535433
C	-5.768605	-0.695923	0.827901
H	-6.788721	-0.339750	1.030470
H	-5.528773	-1.447136	1.590503
C	-1.488953	-1.580852	2.335508
H	-0.795997	-1.902806	1.562988
C	-1.334817	-1.978169	3.668223

H	-0.514716	-2.635676	3.941499
C	-2.256079	-1.524641	4.618480
H	-2.174390	-1.825512	5.660474
C	-3.292929	-0.675823	4.205800
H	-4.025796	-0.300933	4.916143
C	-3.370385	-0.316399	2.858229
C	-4.408085	0.671868	2.351623
H	-5.290169	0.678258	3.006850
H	-3.969258	1.675973	2.391462
C	-1.771024	2.643099	-0.764615
C	-1.912548	4.023071	-0.997032
H	-1.057101	4.594773	-1.346292
C	-3.144744	4.643957	-0.787404
H	-3.268181	5.710310	-0.961699
C	-4.218591	3.864639	-0.344337
H	-5.194062	4.305775	-0.156594
C	-4.020174	2.493562	-0.165639
C	-5.197007	1.608719	0.213662
H	-5.933822	2.189992	0.786529
H	-5.692785	1.285136	-0.709632
C	-0.409493	1.998197	-0.915423
H	0.127302	2.531591	-1.706757
H	-0.515915	0.960862	-1.235190
C	0.437036	2.036533	0.411613
H	-0.101863	2.604706	1.177670
H	0.562896	1.014848	0.787960

Table S7. Cartesian coordinates of **RC** in the triplet state.

		angstrom	
Atom	x	y	z
Cu	3.004073	0.281953	-0.150400
Cu	-3.058634	0.303098	-0.127075
O	1.455751	0.101743	-1.136609
O	-1.573224	1.523344	0.215794
O	-1.315912	2.320507	-0.759245
C	1.663498	-3.631195	-2.424358
H	2.701385	-3.892422	-2.195089
H	1.505865	-3.702473	-3.504752
H	0.997666	-4.338047	-1.919927
H	1.452654	-2.611818	-2.084427
N	2.719250	2.195644	0.727414
N	4.337170	0.051637	-1.752823
N	2.805993	-1.318003	1.316977
N	4.845810	0.491984	0.873000
N	-4.552143	1.799194	-0.029797
N	-2.501311	-0.612978	-1.943851
N	-2.899959	-1.109859	1.574440
N	-4.814580	-0.894775	-0.458289
C	1.775272	3.086838	0.381850
H	1.021152	2.740206	-0.320979
C	1.755493	4.384526	0.905161
H	0.977382	5.077780	0.598933
C	2.755277	4.760554	1.810491
H	2.776355	5.764799	2.227584
C	3.735356	3.824412	2.171232
H	4.524867	4.082271	2.872957
C	3.676776	2.546469	1.609739
C	4.637911	1.436816	1.999814
H	5.590901	1.848298	2.358918
H	4.193895	0.873889	2.829237

C	4.027289	-0.431901	-2.967503
H	2.985497	-0.709409	-3.108487
C	4.984469	-0.568414	-3.977111
H	4.697431	-0.961105	-4.948316
C	6.307304	-0.197224	-3.702257
H	7.078869	-0.295957	-4.462306
C	6.626380	0.299074	-2.430826
H	7.643244	0.594157	-2.183729
C	5.606461	0.414938	-1.482563
C	5.830561	1.017644	-0.107471
H	6.862290	0.850152	0.231333
H	5.683080	2.102096	-0.178350
C	1.707291	-2.016898	1.678019
C	1.805692	-3.086635	2.587063
H	0.915601	-3.657434	2.837331
C	3.040314	-3.411528	3.150313
H	3.129670	-4.234631	3.855504
C	4.165107	-2.659263	2.789128
H	5.145096	-2.875930	3.206273
C	4.004767	-1.632845	1.857424
C	5.210220	-0.866009	1.339745
H	5.998449	-0.829415	2.104648
H	5.618390	-1.413002	0.481254
C	-4.427616	3.047492	0.454872
H	-3.441548	3.326260	0.817419
C	-5.493613	3.950457	0.493985
H	-5.344178	4.949416	0.893484
C	-6.741479	3.533262	0.014273
H	-7.596125	4.205489	0.032717
C	-6.872747	2.231854	-0.486752
H	-7.826177	1.872805	-0.866598
C	-5.752133	1.395876	-0.497763
C	-5.799962	0.001178	-1.099562

H	-6.819989	-0.406246	-1.045041
H	-5.538482	0.078523	-2.162189
C	-1.503421	-0.237490	-2.763090
H	-0.818464	0.513875	-2.379143
C	-1.338360	-0.786163	-4.039386
H	-0.521146	-0.446571	-4.669000
C	-2.245574	-1.756236	-4.478386
H	-2.156456	-2.193911	-5.470067
C	-3.278219	-2.154803	-3.618121
H	-4.000791	-2.908074	-3.922608
C	-3.368000	-1.565046	-2.354762
C	-4.407799	-2.009955	-1.338054
H	-5.269228	-2.468360	-1.844054
H	-3.954500	-2.784118	-0.707298
C	-1.863258	-1.400493	2.396470
C	-2.017544	-2.291176	3.473282
H	-1.178705	-2.473240	4.139483
C	-3.243286	-2.925325	3.683483
H	-3.377442	-3.618371	4.510778
C	-4.295200	-2.651763	2.803973
H	-5.264486	-3.129390	2.921125
C	-4.086281	-1.729513	1.774913
C	-5.251437	-1.339160	0.877818
H	-5.969002	-2.170558	0.817594
H	-5.775464	-0.500207	1.352058
C	-0.506164	-0.784998	2.127953
H	0.021914	-0.706611	3.083512
H	-0.622395	0.227225	1.738835
C	0.359167	-1.622010	1.114075
H	-0.176017	-2.538588	0.842746
H	0.501584	-1.044559	0.193732

Table S8. Cartesian coordinates of **RC** in the singlet state.

		angstrom	
Atom	x	y	z
Cu	2.992937	-0.281461	0.147699
Cu	-3.052559	-0.295968	0.125046
O	1.459328	-0.062659	1.148705
O	-1.566201	-1.472852	-0.232891
O	-1.348381	-2.307047	0.741715
C	1.567407	3.621860	2.538455
H	0.734670	4.247973	2.203633
H	1.585715	3.609995	3.632511
H	1.443752	2.602887	2.156932
H	2.505748	4.047062	2.169078
N	2.646761	-2.174595	-0.745939
N	4.340825	-0.087030	1.743221
N	2.836812	1.338129	-1.308938
N	4.824547	-0.535696	-0.885221
N	-4.528989	-1.795366	-0.026297
N	-2.496875	0.586984	1.954942
N	-2.876240	1.159168	-1.541741
N	-4.794804	0.873795	0.466533
C	1.675669	-3.037959	-0.404345
H	0.927320	-2.673383	0.295683
C	1.619408	-4.333218	-0.931728
H	0.819840	-5.002881	-0.628401
C	2.609282	-4.736849	-1.835563
H	2.602015	-5.740448	-2.254726
C	3.616894	-3.828702	-2.192989
H	4.399595	-4.107510	-2.894336
C	3.594505	-2.551190	-1.628630
C	4.586246	-1.468281	-2.016105
H	5.525971	-1.904944	-2.380455
H	4.155917	-0.888091	-2.840816

C	4.051546	0.405124	2.959534
H	3.019026	0.712799	3.106228
C	5.017563	0.513735	3.964125
H	4.747211	0.914560	4.936790
C	6.327558	0.104215	3.682351
H	7.105674	0.180449	4.438295
C	6.625352	-0.400968	2.409276
H	7.631933	-0.725255	2.156772
C	5.597610	-0.486845	1.466278
C	5.796903	-1.093951	0.089362
H	6.831917	-0.957982	-0.253581
H	5.615663	-2.173372	0.158940
C	1.758750	2.072990	-1.660721
C	1.885155	3.142312	-2.566656
H	1.012108	3.741999	-2.809280
C	3.125958	3.430353	-3.136606
H	3.236708	4.252610	-3.839747
C	4.228674	2.642518	-2.784034
H	5.212743	2.830363	-3.205535
C	4.041526	1.617958	-1.854987
C	5.226194	0.813327	-1.346775
H	6.009345	0.757574	-2.115764
H	5.654622	1.344114	-0.487933
C	-4.387400	-3.029701	-0.540154
H	-3.396386	-3.286590	-0.904850
C	-5.444588	-3.941826	-0.602403
H	-5.284431	-4.929732	-1.024536
C	-6.697623	-3.549068	-0.115321
H	-7.544793	-4.229983	-0.151506
C	-6.844878	-2.261600	0.417213
H	-7.802705	-1.922644	0.804283
C	-5.732965	-1.415382	0.449669
C	-5.786835	-0.036326	1.083958

H	-6.804351	0.376342	1.030366
H	-5.531478	-0.136390	2.146065
C	-1.494007	0.201781	2.763214
H	-0.806287	-0.537614	2.361922
C	-1.330561	0.729207	4.048779
H	-0.509392	0.384513	4.670335
C	-2.243310	1.684906	4.507290
H	-2.154320	2.105030	5.506535
C	-3.281099	2.093179	3.657327
H	-4.007348	2.836429	3.977229
C	-3.368772	1.525618	2.384212
C	-4.408324	1.978998	1.372582
H	-5.281316	2.412298	1.879892
H	-3.962964	2.771537	0.759622
C	-1.832694	1.476083	-2.344475
C	-1.984144	2.393436	-3.399941
H	-1.140005	2.598789	-4.052554
C	-3.211903	3.023852	-3.606792
H	-3.342426	3.736702	-4.417682
C	-4.272041	2.720316	-2.746272
H	-5.243745	3.193235	-2.862378
C	-4.065445	1.774261	-1.739546
C	-5.231960	1.347041	-0.862862
H	-5.959981	2.166836	-0.781058
H	-5.742879	0.513487	-1.360009
C	-0.473083	0.863706	-2.080878
H	0.044220	0.774197	-3.041571
H	-0.583189	-0.142759	-1.675013
C	0.401505	1.719884	-1.090753
H	-0.117961	2.655169	-0.855205
H	0.528649	1.172060	-0.150460

Table S9. Cartesian coordinates of **TS1** in the triplet state.

		angstrom	
Atom	x	y	z
Cu	3.102528	-0.263330	0.090818
Cu	-3.073714	-0.314338	-0.086349
O	1.681026	-0.929342	1.091155
O	-1.532191	-0.969121	-1.092467
O	-1.280137	-2.214990	-0.899039
C	1.741748	0.068310	3.394855
H	0.982100	0.852020	3.405360
H	1.511395	-0.750807	4.078937
H	1.689802	-0.451140	2.216190
H	2.752712	0.458412	3.528575
N	2.655716	-0.971617	-1.884646
N	4.626179	-1.330112	1.060676
N	2.724828	1.926535	0.105108
N	4.789858	0.480123	-0.963284
N	-4.508356	-1.363494	-1.237108
N	-2.600217	-0.901270	1.888514
N	-2.936853	1.872963	-0.378255
N	-4.880941	0.310675	0.900963
C	1.776136	-1.931691	-2.214250
H	1.129355	-2.288680	-1.416875
C	1.682932	-2.443366	-3.513551
H	0.960105	-3.223173	-3.735436
C	2.540781	-1.938190	-4.497647
H	2.504399	-2.320279	-5.515300
C	3.456370	-0.934043	-4.150915
H	4.138701	-0.519833	-4.889291
C	3.477936	-0.473810	-2.831661
C	4.386644	0.657996	-2.381564
H	5.262336	0.741884	-3.039310
H	3.830415	1.598873	-2.457159

C	4.474098	-2.055895	2.181562
H	3.456598	-2.126936	2.555321
C	5.549683	-2.691225	2.808041
H	5.385741	-3.272192	3.711075
C	6.827202	-2.556648	2.248553
H	7.688779	-3.028830	2.714881
C	6.979428	-1.808781	1.073606
H	7.953777	-1.693824	0.604956
C	5.847519	-1.219851	0.502687
C	5.892064	-0.505037	-0.834389
H	6.871422	-0.035259	-0.999542
H	5.758783	-1.259128	-1.619382
C	1.590067	2.615475	0.365346
C	1.625280	4.008427	0.561756
H	0.706048	4.534966	0.804008
C	2.832850	4.698976	0.446464
H	2.874312	5.775510	0.595549
C	3.990714	3.980754	0.123847
H	4.948473	4.480577	0.003675
C	3.891304	2.596430	-0.026055
C	5.129648	1.761368	-0.304057
H	5.851689	2.340663	-0.897734
H	5.615448	1.522228	0.650280
C	-4.325614	-1.945133	-2.435820
H	-3.321888	-1.888484	-2.849200
C	-5.354951	-2.593272	-3.123904
H	-5.158604	-3.050067	-4.089639
C	-6.628125	-2.631405	-2.541678
H	-7.455684	-3.122433	-3.048314
C	-6.820312	-2.021210	-1.295572
H	-7.795025	-2.029165	-0.813817
C	-5.733024	-1.402118	-0.671456
C	-5.848710	-0.791583	0.715617

H	-6.881364	-0.465339	0.906740
H	-5.614355	-1.570010	1.452268
C	-1.619837	-1.738468	2.271151
H	-0.905476	-2.032104	1.506359
C	-1.511287	-2.212861	3.582803
H	-0.707462	-2.895618	3.842517
C	-2.458038	-1.803036	4.527958
H	-2.412529	-2.162471	5.553464
C	-3.474012	-0.923402	4.129393
H	-4.227670	-0.582876	4.835288
C	-3.507542	-0.489055	2.801655
C	-4.533630	0.525292	2.320927
H	-5.422636	0.507357	2.967365
H	-4.091833	1.525210	2.409073
C	-1.895874	2.655397	-0.753136
C	-2.054142	4.041529	-0.926334
H	-1.209209	4.636375	-1.262096
C	-3.290383	4.639083	-0.674234
H	-3.427767	5.710446	-0.800863
C	-4.349145	3.828971	-0.252540
H	-5.327648	4.250017	-0.036574
C	-4.134382	2.453276	-0.132058
C	-5.304384	1.545495	0.215477
H	-6.047148	2.104354	0.803434
H	-5.794731	1.254110	-0.721512
C	-0.533785	2.027351	-0.950382
H	0.028329	2.654560	-1.649389
H	-0.640320	1.044522	-1.411683
C	0.272405	1.871318	0.393718
H	-0.326988	2.264784	1.222531
H	0.465139	0.812930	0.589447

Table S10. Cartesian coordinates of **TS1** in the singlet state.

		angstrom	
Atom	x	y	z
Cu	3.075718	-0.257489	0.094895
Cu	-3.058162	-0.309303	-0.077278
O	1.660393	-0.876150	1.135365
O	-1.516136	-0.933843	-1.056271
O	-1.299580	-2.202845	-0.864935
C	1.780701	0.182400	3.409460
H	1.525725	-0.609563	4.116384
H	2.806640	0.537387	3.525612
H	1.699726	-0.366193	2.244696
H	1.050868	0.994013	3.404789
N	2.598302	-0.979624	-1.871783
N	4.588398	-1.339101	1.064934
N	2.731257	1.936855	0.073900
N	4.768535	0.442054	-0.982593
N	-4.471764	-1.380462	-1.221802
N	-2.559867	-0.865087	1.899124
N	-2.936798	1.877199	-0.384736
N	-4.849519	0.295237	0.897903
C	1.694971	-1.923119	-2.185485
H	1.034887	-2.250418	-1.386299
C	1.588659	-2.453148	-3.476691
H	0.845863	-3.217885	-3.684493
C	2.457097	-1.985629	-4.469566
H	2.410865	-2.383579	-5.480742
C	3.395715	-0.996793	-4.140213
H	4.085904	-0.609629	-4.885943
C	3.429172	-0.515720	-2.828912
C	4.360082	0.606056	-2.400863
H	5.233301	0.665671	-3.064545
H	3.819300	1.554970	-2.487115

C	4.430763	-2.047328	2.196225
H	3.413897	-2.096711	2.575406
C	5.499746	-2.690709	2.825780
H	5.331678	-3.257216	3.737206
C	6.776372	-2.582824	2.258450
H	7.633058	-3.061775	2.726898
C	6.934120	-1.852796	1.073065
H	7.907785	-1.758596	0.598415
C	5.808349	-1.254492	0.499728
C	5.856291	-0.557850	-0.846588
H	6.841781	-0.105413	-1.023374
H	5.707002	-1.320041	-1.620832
C	1.607968	2.647522	0.324339
C	1.664001	4.044251	0.486810
H	0.753681	4.589667	0.721094
C	2.880370	4.714777	0.349019
H	2.937633	5.793902	0.471832
C	4.026390	3.972598	0.038451
H	4.990525	4.455631	-0.098115
C	3.906500	2.586767	-0.078599
C	5.130840	1.727305	-0.343666
H	5.861714	2.285318	-0.946857
H	5.613344	1.494928	0.614053
C	-4.275712	-1.968293	-2.414997
H	-3.272328	-1.895496	-2.826125
C	-5.293570	-2.642089	-3.095605
H	-5.089537	-3.104102	-4.057227
C	-6.565276	-2.700169	-2.511595
H	-7.383067	-3.212131	-3.013356
C	-6.769716	-2.083931	-1.270102
H	-7.743548	-2.108237	-0.787181
C	-5.693998	-1.438500	-0.653609
C	-5.810727	-0.819084	0.728416

H	-6.843367	-0.496392	0.923147
H	-5.564908	-1.587903	1.471239
C	-1.561413	-1.679911	2.282785
H	-0.842958	-1.962758	1.517995
C	-1.441376	-2.141167	3.598393
H	-0.623944	-2.806254	3.861267
C	-2.393105	-1.742406	4.543117
H	-2.337692	-2.093476	5.571042
C	-3.426805	-0.884039	4.142389
H	-4.183688	-0.551406	4.848556
C	-3.471324	-0.461746	2.811628
C	-4.511270	0.531338	2.319819
H	-5.404763	0.505514	2.958975
H	-4.086351	1.539174	2.398375
C	-1.903195	2.667236	-0.763090
C	-2.077687	4.051082	-0.942353
H	-1.239100	4.653826	-1.279830
C	-3.320565	4.636227	-0.694775
H	-3.469099	5.705468	-0.826635
C	-4.372239	3.816988	-0.271474
H	-5.355811	4.228425	-0.060148
C	-4.141161	2.445155	-0.143962
C	-5.296567	1.520670	0.204392
H	-6.049550	2.065280	0.791896
H	-5.780767	1.214926	-0.731047
C	-0.534607	2.053407	-0.959702
H	0.015366	2.680954	-1.668041
H	-0.630567	1.062900	-1.407287
C	0.279507	1.924187	0.382438
H	-0.306464	2.351385	1.204238
H	0.456833	0.868653	0.606156

Table S11. Cartesian coordinates of **TS1'** in the triplet state.

		angstrom	
Atom	x	y	z
Cu	3.199910	-0.265533	0.140990
Cu	-3.090396	-0.248632	0.086555
O	1.725730	-0.657487	1.162727
O	-1.824821	-1.283046	-0.891504
O	-1.248192	-2.326693	-0.158635
C	-2.451333	-4.600581	-0.560555
H	-2.399231	-4.731424	-1.640895
H	-1.770843	-5.216174	0.026724
H	-1.815784	-3.231504	-0.368683
H	-3.446763	-4.464086	-0.140173
N	2.783503	-1.389772	-1.590315
N	4.614216	-0.848473	1.563495
N	2.965799	1.845929	-0.299864
N	5.001996	0.098302	-0.952122
N	-4.750322	-1.228696	-0.755389
N	-2.466474	-0.248427	2.093660
N	-2.691552	1.828832	-0.685976
N	-4.711726	0.874156	0.941755
C	1.787134	-2.282667	-1.717052
H	1.060379	-2.312808	-0.907117
C	1.681100	-3.113964	-2.837867
H	0.861455	-3.823201	-2.906779
C	2.647130	-3.014236	-3.846282
H	2.601715	-3.655326	-4.723741
C	3.678086	-2.073281	-3.711227
H	4.440526	-1.964287	-4.478794
C	3.704802	-1.270255	-2.568291
C	4.717314	-0.150732	-2.386351
H	5.636870	-0.358569	-2.950293
H	4.283931	0.765863	-2.803883

C	4.368951	-1.038631	2.870717
H	3.335220	-0.893013	3.176262
C	5.376882	-1.401344	3.769005
H	5.142140	-1.548174	4.819364
C	6.681335	-1.562094	3.283444
H	7.491255	-1.838173	3.954687
C	6.931930	-1.357659	1.919463
H	7.932957	-1.472794	1.511015
C	5.865324	-1.006268	1.087488
C	6.016954	-0.840805	-0.414867
H	7.037789	-0.524762	-0.671782
H	5.850393	-1.816879	-0.887049
C	1.852763	2.607084	-0.198755
C	1.911574	3.993856	-0.424852
H	1.013707	4.593070	-0.302745
C	3.120635	4.586521	-0.795702
H	3.180798	5.657378	-0.976014
C	4.256111	3.778738	-0.933327
H	5.214224	4.199651	-1.227057
C	4.136728	2.414353	-0.660425
C	5.359200	1.509777	-0.682206
H	6.098245	1.885602	-1.403914
H	5.828607	1.549762	0.308319
C	-4.735436	-2.030498	-1.833235
H	-3.763121	-2.166739	-2.301469
C	-5.892080	-2.647664	-2.319076
H	-5.840205	-3.285851	-3.196614
C	-7.103465	-2.418452	-1.653391
H	-8.023496	-2.880937	-2.003253
C	-7.116267	-1.574535	-0.534312
H	-8.040188	-1.367723	0.000218
C	-5.914416	-0.997209	-0.115176
C	-5.816294	-0.098219	1.105456

H	-6.776913	0.401702	1.296183
H	-5.589525	-0.716904	1.982801
C	-1.475857	-0.988250	2.625407
H	-0.880304	-1.561361	1.920351
C	-1.224983	-1.019597	4.001084
H	-0.413630	-1.631556	4.384114
C	-2.039835	-0.266163	4.853115
H	-1.884775	-0.280827	5.929566
C	-3.063623	0.511904	4.295709
H	-3.712697	1.116525	4.924574
C	-3.236636	0.505140	2.909041
C	-4.245402	1.420447	2.234314
H	-5.084443	1.635419	2.910605
H	-3.744964	2.374689	2.031709
C	-1.578353	2.345297	-1.256880
C	-1.602206	3.607241	-1.875958
H	-0.706504	3.979369	-2.365673
C	-2.775237	4.365982	-1.860178
H	-2.810705	5.344644	-2.333325
C	-3.902853	3.847110	-1.214607
H	-4.830388	4.411559	-1.161152
C	-3.819675	2.568878	-0.654623
C	-5.053507	1.933830	-0.031511
H	-5.685709	2.710047	0.423726
H	-5.642637	1.474598	-0.833950
C	-0.293826	1.553809	-1.158248
H	0.305624	1.737032	-2.056225
H	-0.531375	0.487774	-1.127876
C	0.541628	1.927345	0.124296
H	-0.044885	2.588452	0.771207
H	0.741767	1.010336	0.689298

Table S12. Cartesian coordinates of **TS1'** in the singlet state.

		angstrom	
Atom	x	y	z
Cu	3.196643	-0.262340	0.140519
Cu	-3.086048	-0.250229	0.088018
O	1.709103	-0.626204	1.167329
O	-1.822443	-1.286754	-0.890832
O	-1.243321	-2.327522	-0.155719
C	-2.450299	-4.603071	-0.538916
H	-2.402317	-4.741685	-1.618467
H	-1.767925	-5.214659	0.050345
H	-1.812797	-3.232410	-0.358215
H	-3.444041	-4.462861	-0.115799
N	2.778117	-1.396020	-1.588812
N	4.608648	-0.846139	1.565211
N	2.961303	1.849675	-0.313472
N	4.987252	0.093407	-0.948052
N	-4.745959	-1.235861	-0.747086
N	-2.448560	-0.233659	2.089320
N	-2.695679	1.826472	-0.691208
N	-4.708236	0.870573	0.945412
C	1.782645	-2.290111	-1.711143
H	1.056787	-2.317966	-0.900230
C	1.677081	-3.124577	-2.829865
H	0.858344	-3.835082	-2.896474
C	2.642068	-3.026163	-3.839443
H	2.596473	-3.669722	-4.715084
C	3.672206	-2.083405	-3.708553
H	4.433500	-1.975443	-4.477397
C	3.698134	-1.277847	-2.567609
C	4.706232	-0.155402	-2.384868
H	5.629019	-0.359330	-2.944558
H	4.271035	0.760403	-2.801930

C	4.361931	-1.031642	2.872689
H	3.328937	-0.878820	3.177447
C	5.368860	-1.397392	3.770994
H	5.134298	-1.540915	4.821847
C	6.672353	-1.565170	3.285016
H	7.481137	-1.843605	3.956657
C	6.924120	-1.364549	1.920507
H	7.924626	-1.484866	1.512291
C	5.858462	-1.010118	1.088881
C	6.005333	-0.846707	-0.413657
H	7.023998	-0.528977	-0.676116
H	5.836718	-1.822659	-0.885164
C	1.848649	2.610771	-0.214801
C	1.909360	3.997108	-0.443934
H	1.012103	4.597846	-0.324729
C	3.120035	4.587509	-0.813569
H	3.181436	5.657906	-0.996211
C	4.256040	3.779084	-0.946117
H	5.215283	4.199163	-1.237364
C	4.133703	2.415611	-0.670795
C	5.352032	1.505785	-0.683174
H	6.095738	1.871167	-1.405145
H	5.818257	1.547367	0.308694
C	-4.732029	-2.039782	-1.823355
H	-3.760643	-2.174417	-2.293976
C	-5.888416	-2.661024	-2.304590
H	-5.837381	-3.300807	-3.181016
C	-7.098466	-2.433806	-1.635798
H	-8.018259	-2.899474	-1.982048
C	-7.110272	-1.587766	-0.518318
H	-8.033154	-1.382434	0.018569
C	-5.908772	-1.006324	-0.103873
C	-5.809405	-0.104592	1.114596

H	-6.770918	0.392842	1.307404
H	-5.577948	-0.720805	1.992478
C	-1.446702	-0.961121	2.616969
H	-0.846633	-1.527555	1.910558
C	-1.188270	-0.986204	3.991467
H	-0.367521	-1.587634	4.371040
C	-2.006886	-0.240323	4.846264
H	-1.846149	-0.251120	5.921936
C	-3.041398	0.526373	4.292627
H	-3.692945	1.126205	4.923519
C	-3.221367	0.514852	2.907014
C	-4.240075	1.421455	2.235426
H	-5.077700	1.631367	2.915023
H	-3.747377	2.379039	2.029624
C	-1.584954	2.344580	-1.265170
C	-1.612669	3.606304	-1.884565
H	-0.718959	3.979979	-2.376771
C	-2.787112	4.362821	-1.865978
H	-2.825641	5.341243	-2.339389
C	-3.912125	3.842160	-1.217234
H	-4.840500	4.405009	-1.161547
C	-3.825069	2.564321	-0.656909
C	-5.055620	1.926874	-0.029632
H	-5.689232	2.702179	0.425191
H	-5.645031	1.463895	-0.829709
C	-0.299088	1.554858	-1.169409
H	0.297784	1.738245	-2.069126
H	-0.535203	0.488512	-1.137528
C	0.538940	1.929646	0.110864
H	-0.046811	2.589696	0.759619
H	0.742315	1.012283	0.676545

Table S13. Cartesian coordinates of **MI** in the triplet state.

		angstrom	
Atom	x	y	z
Cu	3.646077	0.006685	0.928813
Cu	-3.730652	-0.471679	0.350236
O	2.426289	-1.093818	1.705910
O	-2.324879	-1.588310	1.173977
O	-1.695355	-1.161614	2.198910
C	3.547533	1.071916	2.555971
H	2.527735	1.445729	2.639486
H	3.842176	0.430125	3.386321
H	2.294049	-0.968468	2.655450
H	4.269725	1.876707	2.410319
N	3.814755	-1.212888	-0.667566
N	5.975023	-0.863862	1.462792
N	2.138198	1.760243	-0.308313
N	4.934069	1.258676	-0.191711
N	-5.093293	-2.089015	0.351235
N	-4.017497	1.159621	1.668825
N	-2.851844	0.085644	-1.639497
N	-5.445024	0.470835	-0.596007
C	3.333557	-2.466136	-0.692604
H	2.709381	-2.736485	0.156953
C	3.636415	-3.348168	-1.732758
H	3.233736	-4.356926	-1.722867
C	4.479174	-2.907047	-2.762839
H	4.748916	-3.572655	-3.579654
C	4.978521	-1.598985	-2.723923
H	5.636563	-1.227298	-3.505514
C	4.614631	-0.775030	-1.653759
C	5.019619	0.679028	-1.576530
H	6.027993	0.821822	-1.982794
H	4.334313	1.243917	-2.217911

C	6.421485	-2.041483	1.918952
H	5.689241	-2.675732	2.417305
C	7.753372	-2.457981	1.781137
H	8.069460	-3.418147	2.179658
C	8.650143	-1.610046	1.120956
H	9.690883	-1.896480	0.988587
C	8.182786	-0.381396	0.631834
H	8.852021	0.305166	0.118377
C	6.838111	-0.049567	0.834347
C	6.290396	1.309060	0.440511
H	6.202559	1.914597	1.349644
H	6.993407	1.826591	-0.225811
C	0.811933	1.865988	-0.525744
C	0.267869	2.996510	-1.162974
H	-0.806556	3.072371	-1.307006
C	1.118617	4.018783	-1.593861
H	0.720030	4.899362	-2.092478
C	2.494132	3.897622	-1.361491
H	3.186279	4.677862	-1.668789
C	2.952533	2.752732	-0.697247
C	4.414729	2.653939	-0.287752
H	5.035624	3.237962	-0.981678
H	4.523353	3.119159	0.698207
C	-4.810268	-3.384971	0.572356
H	-3.772404	-3.616537	0.801501
C	-5.783269	-4.387311	0.522199
H	-5.507771	-5.420736	0.711970
C	-7.101949	-4.024020	0.221326
H	-7.885946	-4.775751	0.167421
C	-7.395940	-2.674182	-0.011483
H	-8.408651	-2.355379	-0.246083
C	-6.364677	-1.733638	0.070845
C	-6.629282	-0.243288	-0.075270

H	-7.518526	-0.072061	-0.699395
H	-6.851625	0.159755	0.920594
C	-3.518433	1.290796	2.911654
H	-2.787204	0.542690	3.208989
C	-3.906657	2.318496	3.776985
H	-3.477425	2.377530	4.773122
C	-4.858018	3.244282	3.333345
H	-5.192387	4.051902	3.980441
C	-5.381942	3.105873	2.041313
H	-6.127636	3.801527	1.664093
C	-4.934457	2.054051	1.236328
C	-5.415923	1.890432	-0.196461
H	-6.393341	2.376827	-0.327512
H	-4.708755	2.408166	-0.856208
C	-1.562111	0.149648	-2.053526
C	-1.232420	0.606646	-3.340828
H	-0.189972	0.632537	-3.644931
C	-2.241475	1.015357	-4.214882
H	-2.002698	1.372744	-5.213905
C	-3.568311	0.950257	-3.778722
H	-4.388207	1.250782	-4.425819
C	-3.829293	0.470278	-2.491576
C	-5.269993	0.277877	-2.045601
H	-5.932967	0.933776	-2.628956
H	-5.556345	-0.755113	-2.279162
C	-0.475090	-0.304890	-1.105532
H	0.408955	-0.589301	-1.685979
H	-0.822175	-1.200361	-0.583880
C	-0.057282	0.731756	-0.021867
H	-0.959664	1.141027	0.446864
H	0.504814	0.187673	0.742957

Table S14. Cartesian coordinates of **MI** in the singlet state.

		angstrom	
Atom	x	y	z
Cu	3.715020	0.124981	0.970730
Cu	-3.718752	-0.480810	0.335711
O	2.493526	-0.796448	1.949697
O	-2.301861	-1.581203	1.080848
O	-1.653785	-1.142952	2.108667
C	3.840599	1.348816	2.479845
H	2.875768	1.846573	2.575174
H	4.111016	0.762563	3.357804
H	2.414594	-0.536152	2.877391
H	4.640437	2.042904	2.217200
N	3.645314	-1.248240	-0.502262
N	5.995259	-0.868680	1.387802
N	2.235881	1.841793	-0.352660
N	4.967216	1.168442	-0.379330
N	-4.988065	-2.151354	0.136934
N	-4.095104	1.019176	1.774235
N	-2.806330	0.272117	-1.588502
N	-5.427533	0.456350	-0.569011
C	3.098032	-2.464832	-0.355144
H	2.556475	-2.616910	0.576675
C	3.236882	-3.454142	-1.332286
H	2.785338	-4.430681	-1.182911
C	3.982346	-3.161067	-2.482806
H	4.124970	-3.913157	-3.255491
C	4.551230	-1.888481	-2.623413
H	5.137043	-1.631062	-3.502369
C	4.352547	-0.950929	-1.604870
C	4.834132	0.477832	-1.708382
H	5.782862	0.529570	-2.255990
H	4.092971	1.029626	-2.295881

C	6.383551	-2.025772	1.939732
H	5.656983	-2.522601	2.581616
C	7.650711	-2.585945	1.723788
H	7.923666	-3.521207	2.204852
C	8.540423	-1.912026	0.879152
H	9.531271	-2.314199	0.681188
C	8.132029	-0.705935	0.291040
H	8.798792	-0.152014	-0.365876
C	6.851919	-0.220826	0.582515
C	6.388619	1.137252	0.089643
H	6.469354	1.840404	0.926277
H	7.052522	1.503288	-0.704761
C	0.902927	2.039914	-0.428988
C	0.375079	3.242625	-0.929646
H	-0.700983	3.391900	-0.958395
C	1.246076	4.241852	-1.378087
H	0.859331	5.178835	-1.772399
C	2.625407	4.021431	-1.302051
H	3.334043	4.777543	-1.631906
C	3.070636	2.806391	-0.763251
C	4.561646	2.594280	-0.537040
H	5.130244	3.057049	-1.356656
H	4.846443	3.126346	0.377293
C	-4.638628	-3.445307	0.241850
H	-3.593978	-3.640439	0.473883
C	-5.557925	-4.484916	0.073725
H	-5.233459	-5.516982	0.170712
C	-6.888230	-4.160524	-0.221021
H	-7.630569	-4.942376	-0.363679
C	-7.250000	-2.811156	-0.330898
H	-8.274000	-2.523579	-0.556493
C	-6.270215	-1.833274	-0.137073
C	-6.597109	-0.349123	-0.148745

H	-7.474477	-0.151585	-0.781131
H	-6.859997	-0.049255	0.873192
C	-3.621099	1.064550	3.032884
H	-2.856346	0.329926	3.273522
C	-4.073411	1.995932	3.973143
H	-3.663133	1.990439	4.978921
C	-5.060969	2.910900	3.590501
H	-5.443942	3.643615	4.297095
C	-5.556261	2.861744	2.280420
H	-6.326431	3.553563	1.948139
C	-5.044970	1.904836	1.399589
C	-5.483227	1.840375	-0.053394
H	-6.482196	2.282528	-0.174508
H	-4.787911	2.444939	-0.648378
C	-1.512175	0.414220	-1.967058
C	-1.177157	0.997850	-3.201615
H	-0.131331	1.084052	-3.481822
C	-2.183725	1.452910	-4.054645
H	-1.939648	1.908849	-5.011375
C	-3.515786	1.302275	-3.655778
H	-4.333660	1.631942	-4.291173
C	-3.781053	0.696884	-2.424163
C	-5.218532	0.403174	-2.029003
H	-5.901966	1.081053	-2.560300
H	-5.455015	-0.615359	-2.360182
C	-0.425748	-0.087165	-1.042404
H	0.450293	-0.362558	-1.639690
H	-0.780564	-0.992406	-0.545112
C	0.016878	0.915257	0.065340
H	-0.873592	1.328440	0.552190
H	0.574819	0.343933	0.813976

Table S15. Cartesian coordinates of **TS2** in the triplet state.

		angstrom	
Atom	x	y	z
Cu	3.332554	-0.990067	0.088519
Cu	-3.326873	-0.484182	-0.015617
O	1.837983	-2.047250	-0.266064
O	-1.494639	-1.075201	-0.289249
O	-0.706784	-1.170514	0.734526
C	2.536310	-2.204994	1.573074
H	1.523196	-2.142251	1.956580
H	2.883981	-3.221769	1.423679
H	0.991821	-1.649792	0.021246
H	3.218543	-1.608871	2.198087
N	3.564119	0.360407	-1.516151
N	5.284667	-2.105309	-0.006827
N	1.880900	1.868123	1.279287
N	4.754508	0.437356	1.004526
N	-4.061709	-2.082001	-1.177645
N	-3.632619	-0.442975	2.076495
N	-3.269649	1.526002	-0.959912
N	-5.399986	-0.021998	0.018235
C	2.815636	0.356193	-2.630622
H	2.094387	-0.456236	-2.711322
C	2.953273	1.320473	-3.632197
H	2.340285	1.270888	-4.527875
C	3.902307	2.336828	-3.449385
H	4.040921	3.107559	-4.204315
C	4.673362	2.343640	-2.281642
H	5.419419	3.116075	-2.109944
C	4.479548	1.326239	-1.338368
C	5.372131	1.199039	-0.114929
H	6.269899	0.658168	-0.435816
H	5.707028	2.190489	0.215845

C	5.603477	-3.174940	-0.753880
H	4.814911	-3.569130	-1.392690
C	6.870501	-3.768247	-0.728359
H	7.079435	-4.634432	-1.349944
C	7.847790	-3.214752	0.108501
H	8.846418	-3.642934	0.154248
C	7.519294	-2.094236	0.882796
H	8.254058	-1.635434	1.540293
C	6.222191	-1.574172	0.799853
C	5.780413	-0.406508	1.667825
H	5.339001	-0.805308	2.591100
H	6.656036	0.186679	1.971680
C	0.926145	2.742704	0.920607
C	1.188813	4.120566	0.774972
H	0.385118	4.802462	0.506463
C	2.475571	4.600416	1.016478
H	2.701669	5.660832	0.931044
C	3.463747	3.686881	1.404953
H	4.469233	4.026317	1.641498
C	3.123491	2.332215	1.521098
C	4.151155	1.338358	2.033101
H	4.952095	1.895444	2.542512
H	3.664146	0.698916	2.777555
C	-3.351874	-2.911005	-1.963580
H	-2.276579	-2.749078	-1.983434
C	-3.949398	-3.929625	-2.711024
H	-3.336766	-4.578064	-3.330703
C	-5.339809	-4.084107	-2.640552
H	-5.840714	-4.862019	-3.212045
C	-6.078287	-3.217795	-1.823648
H	-7.158902	-3.308866	-1.745396
C	-5.400874	-2.231750	-1.100814
C	-6.117042	-1.310108	-0.128434

H	-7.161049	-1.158170	-0.436694
H	-6.136733	-1.796522	0.854508
C	-2.825156	-0.937887	3.032271
H	-1.857783	-1.297461	2.691304
C	-3.194495	-0.985967	4.379766
H	-2.507754	-1.396339	5.114551
C	-4.457548	-0.506965	4.747085
H	-4.783050	-0.535197	5.784361
C	-5.300735	0.004188	3.751883
H	-6.290226	0.381816	3.997704
C	-4.850836	0.025225	2.428831
C	-5.682617	0.634130	1.313854
H	-6.751805	0.596555	1.564076
H	-5.409494	1.692079	1.220318
C	-2.251678	2.395095	-1.169821
C	-2.489692	3.671184	-1.714542
H	-1.650486	4.339598	-1.884883
C	-3.787986	4.066929	-2.034708
H	-3.984118	5.051877	-2.451894
C	-4.833170	3.164438	-1.809743
H	-5.861507	3.424203	-2.046775
C	-4.529024	1.907632	-1.284175
C	-5.630415	0.873133	-1.134558
H	-6.609372	1.368699	-1.070637
H	-5.640923	0.252205	-2.038628
C	-0.831057	2.012215	-0.811718
H	-0.165528	2.633597	-1.419001
H	-0.641661	0.972411	-1.087508
C	-0.485428	2.227404	0.699256
H	-1.182426	2.959197	1.124649
H	-0.611771	1.289112	1.245222

Table S16. Cartesian coordinates of **TS2** in the singlet state.

		angstrom	
Atom	x	y	z
Cu	3.302132	-0.985671	0.098073
Cu	-3.308645	-0.482291	-0.018702
O	1.806283	-2.039754	-0.249350
O	-1.481027	-1.044452	-0.299520
O	-0.699734	-1.155547	0.741423
C	2.510982	-2.190319	1.589476
H	1.499997	-2.116892	1.976616
H	2.849508	-3.210787	1.444296
H	0.958510	-1.645047	0.044713
H	3.201031	-1.598007	2.209956
N	3.533123	0.357591	-1.513418
N	5.252753	-2.110389	-0.005873
N	1.877862	1.882121	1.276233
N	4.739294	0.438315	0.999188
N	-4.030931	-2.094926	-1.159335
N	-3.608385	-0.425505	2.075856
N	-3.258463	1.521855	-0.972671
N	-5.367261	-0.033700	0.015206
C	2.776996	0.352818	-2.622596
H	2.051121	-0.456305	-2.694654
C	2.912758	1.312661	-3.628760
H	2.293586	1.262764	-4.520174
C	3.868005	2.324993	-3.456170
H	4.005396	3.092155	-4.214962
C	4.646877	2.332460	-2.293625
H	5.397788	3.101912	-2.129819
C	4.454312	1.319508	-1.345287
C	5.353836	1.192541	-0.126896
H	6.246826	0.645864	-0.451218
H	5.695692	2.183628	0.197902

C	5.562597	-3.184290	-0.750378
H	4.768644	-3.577216	-1.383293
C	6.827011	-3.783423	-0.729326
H	7.028666	-4.652974	-1.348620
C	7.811304	-3.231222	0.100160
H	8.808194	-3.663816	0.142237
C	7.492084	-2.106271	0.871888
H	8.232415	-1.648359	1.523745
C	6.196879	-1.580629	0.793755
C	5.765016	-0.407812	1.659729
H	5.326821	-0.801302	2.586809
H	6.644973	0.182553	1.956605
C	0.925190	2.758622	0.917236
C	1.190567	4.136072	0.772645
H	0.388466	4.819779	0.503918
C	2.478364	4.613046	1.014626
H	2.706747	5.673015	0.929646
C	3.464812	3.697170	1.402035
H	4.471336	4.034144	1.637681
C	3.121457	2.343218	1.517777
C	4.147056	1.346337	2.027840
H	4.953843	1.901326	2.530309
H	3.661179	0.712192	2.777583
C	-3.312499	-2.927255	-1.933745
H	-2.239072	-2.754033	-1.954883
C	-3.902541	-3.961390	-2.665851
H	-3.285074	-4.613110	-3.277212
C	-5.291452	-4.127552	-2.591187
H	-5.785601	-4.918035	-3.151207
C	-6.037914	-3.257532	-1.785088
H	-7.117416	-3.358361	-1.703777
C	-5.368258	-2.255696	-1.077562
C	-6.084828	-1.325864	-0.114509

H	-7.128919	-1.175095	-0.421923
H	-6.101837	-1.800043	0.874316
C	-2.797234	-0.909898	3.034171
H	-1.830732	-1.270088	2.691905
C	-3.164923	-0.944100	4.382714
H	-2.476267	-1.345637	5.120575
C	-4.427816	-0.463021	4.747665
H	-4.750943	-0.480907	5.785918
C	-5.274438	0.036793	3.749300
H	-6.263900	0.415548	3.993442
C	-4.826479	0.044338	2.425791
C	-5.657019	0.638722	1.303303
H	-6.727279	0.599105	1.547236
H	-5.387243	1.696175	1.196940
C	-2.244333	2.394591	-1.186293
C	-2.489756	3.663734	-1.744443
H	-1.654548	4.336471	-1.917236
C	-3.789210	4.047325	-2.074389
H	-3.989879	5.026889	-2.501963
C	-4.829995	3.140232	-1.845747
H	-5.858868	3.390697	-2.090324
C	-4.518699	1.891544	-1.306232
C	-5.609366	0.848025	-1.148216
H	-6.593882	1.331871	-1.084925
H	-5.614716	0.217534	-2.045568
C	-0.822972	2.023609	-0.819882
H	-0.159495	2.648603	-1.425686
H	-0.625456	0.983793	-1.089819
C	-0.486380	2.245082	0.692041
H	-1.184182	2.980071	1.110759
H	-0.616607	1.308314	1.239868

Table S17. Cartesian coordinates of **PC** in the triplet state.

		angstrom	
Atom	x	y	z
Cu	-3.462328	-0.016399	-0.245619
Cu	3.462410	0.075682	-0.402032
O	-0.993643	2.635236	-2.026968
O	2.095356	0.561519	-1.718240
O	1.814286	1.804065	-1.915178
C	-0.891281	4.062824	-2.026730
H	-0.665959	4.459201	-3.026723
H	-1.860207	4.458844	-1.706946
H	-0.129649	2.276006	-2.290070
H	-0.127037	4.420971	-1.321384
N	-3.726716	-2.000248	-0.766978
N	-4.682395	1.289240	-1.243785
N	-2.718880	0.481829	1.606043
N	-5.339397	-0.409250	0.915547
N	4.647295	-0.879206	-1.857855
N	4.074134	1.891892	0.480933
N	2.295642	-1.322706	0.940510
N	5.040336	-0.655982	0.845452
C	-3.171100	-2.661750	-1.800726
H	-2.385575	-2.137500	-2.341108
C	-3.566783	-3.943704	-2.192540
H	-3.085561	-4.425260	-3.039181
C	-4.596772	-4.569767	-1.480749
H	-4.942652	-5.562696	-1.758203
C	-5.183234	-3.884310	-0.409445
H	-5.992571	-4.333145	0.161558
C	-4.722487	-2.605917	-0.075005
C	-5.300925	-1.858652	1.125578
H	-6.286990	-2.280666	1.375081
H	-4.648586	-2.053435	1.986808

C	-4.305896	2.244873	-2.118106
H	-3.246362	2.275631	-2.365660
C	-5.208093	3.156325	-2.674430
H	-4.855991	3.902018	-3.381771
C	-6.553851	3.086774	-2.294921
H	-7.283743	3.784892	-2.698168
C	-6.943094	2.100522	-1.380708
H	-7.979101	2.015481	-1.061020
C	-5.984669	1.209685	-0.884423
C	-6.409069	0.055991	0.025356
H	-7.319248	0.341306	0.574801
H	-6.689924	-0.782310	-0.624801
C	-1.427725	0.691165	1.958436
C	-1.062229	0.898451	3.296748
H	-0.019789	1.075175	3.547041
C	-2.045193	0.884421	4.291035
H	-1.783066	1.039895	5.334987
C	-3.376220	0.675870	3.915134
H	-4.172669	0.671464	4.654818
C	-3.678602	0.490827	2.561752
C	-5.139364	0.400036	2.118263
H	-5.753978	0.061596	2.967201
H	-5.463060	1.422665	1.885083
C	4.292875	-1.201902	-3.114459
H	3.286030	-0.921646	-3.415598
C	5.160345	-1.853599	-3.995359
H	4.832251	-2.091011	-5.003237
C	6.444036	-2.187458	-3.545370
H	7.145641	-2.698675	-4.200356
C	6.811095	-1.854173	-2.234841
H	7.799412	-2.097502	-1.852485
C	5.885786	-1.192679	-1.422284
C	6.239330	-0.718924	-0.022147

H	7.022186	-1.355371	0.414216
H	6.651325	0.294899	-0.098278
C	3.787881	3.137673	0.059215
H	3.074219	3.204144	-0.757957
C	4.369261	4.276871	0.623889
H	4.107480	5.260854	0.245499
C	5.291944	4.114451	1.663857
H	5.771334	4.976411	2.122036
C	5.596684	2.817687	2.098063
H	6.313943	2.650343	2.897848
C	4.964086	1.731881	1.486392
C	5.199411	0.307143	1.955818
H	6.184157	0.217874	2.435606
H	4.447476	0.066312	2.717191
C	0.965906	-1.446882	1.172835
C	0.479761	-2.285163	2.192297
H	-0.592698	-2.368023	2.343308
C	1.370990	-3.005017	2.987742
H	1.010596	-3.653747	3.782652
C	2.741455	-2.883043	2.732146
H	3.472973	-3.437104	3.314489
C	3.157526	-2.043635	1.695939
C	4.627000	-1.993384	1.314983
H	5.247660	-2.335635	2.155201
H	4.785319	-2.698039	0.489543
C	-0.003207	-0.682686	0.299518
H	-0.912639	-1.281056	0.171604
H	0.442243	-0.549728	-0.687951
C	-0.404159	0.720184	0.844428
H	0.492862	1.247634	1.187771
H	-0.819055	1.298153	0.009384

Table S18. Cartesian coordinates of **PC** in the singlet state.

		angstrom	
Atom	x	y	z
Cu	-3.528361	0.497714	0.854671
Cu	3.007015	0.109080	0.284657
O	-2.087549	-0.396223	2.072091
O	1.095699	0.205800	0.590849
O	0.685941	-0.323222	1.716790
N	-2.998354	2.218306	-0.106497
N	-5.481042	0.000562	1.235667
N	-1.710686	-1.729790	-1.881726
N	-4.208803	-0.033828	-1.313711
N	3.471133	1.757145	1.511423
N	3.543497	-1.826575	0.978003
N	3.046247	0.331766	-1.909210
N	5.085178	0.190035	-0.025111
C	-2.691427	3.377008	0.512794
H	-2.605027	3.332011	1.596404
C	-2.505552	4.582342	-0.166754
H	-2.271590	5.487703	0.386387
C	-2.652329	4.589879	-1.560340
H	-2.531729	5.509598	-2.128077
C	-2.976430	3.392077	-2.205877
H	-3.114792	3.361436	-3.284068
C	-3.137717	2.220939	-1.452437
C	-3.428926	0.898279	-2.144711
H	-3.923606	1.102503	-3.109539
H	-2.476148	0.403838	-2.363087
C	-6.036968	-0.312933	2.421355
H	-5.393882	-0.223314	3.294381
C	-7.367491	-0.719583	2.559164
H	-7.763467	-0.956185	3.542724
C	-8.158684	-0.810679	1.408158

H	-9.196971	-1.127992	1.469974
C	-7.586146	-0.481501	0.172500
H	-8.171222	-0.530638	-0.742638
C	-6.249411	-0.072757	0.123056
C	-5.613845	0.403049	-1.174631
H	-6.232085	0.090929	-2.030598
H	-5.626477	1.499927	-1.156551
C	-0.602509	-2.444537	-1.638867
C	-0.642199	-3.689054	-0.982467
H	0.274964	-4.251655	-0.822332
C	-1.874920	-4.193702	-0.566247
H	-1.941420	-5.158494	-0.067957
C	-3.028620	-3.436904	-0.810010
H	-4.006211	-3.799553	-0.502970
C	-2.902917	-2.210050	-1.476724
C	-4.152797	-1.421656	-1.835012
H	-4.270036	-1.422183	-2.932738
H	-5.011929	-1.958889	-1.423921
C	2.615537	2.654879	2.031553
H	1.563265	2.499291	1.807654
C	3.043158	3.727991	2.817857
H	2.317531	4.428189	3.221513
C	4.414524	3.874203	3.063649
H	4.784623	4.700072	3.666639
C	5.305136	2.941125	2.516919
H	6.375866	3.024529	2.686187
C	4.792666	1.890685	1.750618
C	5.679016	0.790519	1.194357
H	6.693227	1.166658	1.001972
H	5.762900	0.000933	1.950651
C	2.815327	-2.658899	1.744355
H	1.814531	-2.315556	1.994210
C	3.315186	-3.877990	2.211855

H	2.692209	-4.517234	2.830946
C	4.626237	-4.238889	1.877130
H	5.051401	-5.175982	2.229020
C	5.388772	-3.365347	1.090631
H	6.413706	-3.607058	0.820123
C	4.809933	-2.169759	0.655991
C	5.551017	-1.199993	-0.247039
H	6.636630	-1.288396	-0.104409
H	5.337395	-1.461826	-1.290016
C	2.100582	0.092649	-2.851523
C	2.382587	0.266982	-4.218386
H	1.601104	0.074833	-4.948084
C	3.652432	0.676273	-4.625324
H	3.883754	0.808749	-5.679609
C	4.625808	0.907240	-3.646296
H	5.630633	1.222289	-3.914932
C	4.278250	0.730791	-2.306539
C	5.282564	1.049215	-1.214763
H	6.307400	0.965656	-1.602217
H	5.138652	2.089522	-0.898872
C	0.735064	-0.392637	-2.426514
H	0.019735	-0.178834	-3.224809
H	0.401460	0.143399	-1.535254
C	0.729620	-1.908079	-2.139940
H	0.997916	-2.452233	-3.057124
H	1.505702	-2.151386	-1.404061
C	-2.247975	-1.635178	2.780634
H	-1.638663	-1.639607	3.693134
H	-3.300403	-1.721986	3.060927
H	-1.132819	-0.278253	1.868267
H	-1.979331	-2.492030	2.149473

Table S19. Cartesian coordinates of **FC** in the triplet state.

		angstrom	
Atom	x	y	z
Cu	3.512540	0.013699	-0.415320
Cu	-3.398466	0.007788	-0.514935
O	-2.041328	0.182524	-1.931550
O	-1.343858	-0.837475	-2.265849
N	3.884966	2.041315	-0.390273
N	4.657717	-1.105367	-1.704672
N	2.707546	-0.902375	1.246695
N	5.377318	-0.033082	0.810189
N	-4.706699	1.302903	-1.538736
N	-3.774960	-2.063558	-0.376815
N	-2.397190	0.899535	1.303524
N	-5.057303	0.039353	0.877124
C	3.371778	2.988386	-1.199743
H	2.566224	2.673204	-1.859505
C	3.832522	4.307601	-1.224000
H	3.382472	5.027040	-1.902277
C	4.885064	4.661642	-0.371696
H	5.281239	5.674317	-0.366232
C	5.426513	3.680134	0.467788
H	6.250140	3.914795	1.137893
C	4.900894	2.383533	0.439476
C	5.426087	1.311399	1.393282
H	6.434720	1.591194	1.734866
H	4.782739	1.312288	2.282771
C	4.248662	-1.815222	-2.774742
H	3.201514	-1.711483	-3.050086
C	5.096175	-2.646144	-3.511619
H	4.710793	-3.191178	-4.368620
C	6.433423	-2.756713	-3.112107
H	7.125093	-3.398807	-3.652276

C	6.862952	-2.024697	-1.998900
H	7.894088	-2.084501	-1.658712
C	5.954421	-1.201212	-1.324207
C	6.429079	-0.314889	-0.173055
H	7.326108	-0.760030	0.283954
H	6.743487	0.642126	-0.608544
C	1.400054	-1.112181	1.529516
C	0.998770	-1.674884	2.750163
H	-0.056665	-1.847839	2.941381
C	1.964092	-2.013140	3.703106
H	1.675201	-2.447921	4.657130
C	3.311632	-1.787860	3.403213
H	4.093470	-2.044868	4.113353
C	3.648471	-1.243484	2.159395
C	5.119741	-1.114359	1.763323
H	5.732897	-1.033245	2.674369
H	5.404030	-2.057995	1.279886
C	-4.403509	2.106716	-2.573305
H	-3.376822	2.061846	-2.929806
C	-5.344325	2.949201	-3.171949
H	-5.054811	3.578300	-4.008781
C	-6.650343	2.958756	-2.666046
H	-7.409140	3.604438	-3.101901
C	-6.964911	2.123075	-1.586500
H	-7.968843	2.103504	-1.169439
C	-5.966383	1.301940	-1.054046
C	-6.257856	0.302415	0.053861
H	-7.105161	0.644575	0.665687
H	-6.559133	-0.644084	-0.412018
C	-3.339679	-3.018408	-1.219478
H	-2.599696	-2.703599	-1.951456
C	-3.798101	-4.338254	-1.166325
H	-3.418185	-5.071261	-1.872251

C	-4.753564	-4.677538	-0.201270
H	-5.141372	-5.691414	-0.134869
C	-5.209830	-3.683536	0.674517
H	-5.954926	-3.907752	1.433997
C	-4.693821	-2.389393	0.560095
C	-5.094660	-1.286319	1.525825
H	-6.079462	-1.501559	1.964414
H	-4.371744	-1.275162	2.350768
C	-1.087361	1.071717	1.605856
C	-0.683783	1.540312	2.867563
H	0.374389	1.678350	3.070932
C	-1.642210	1.832068	3.839805
H	-1.347508	2.193088	4.822395
C	-2.992221	1.659158	3.518465
H	-3.774221	1.886177	4.238335
C	-3.325542	1.203462	2.239256
C	-4.787027	1.133034	1.827604
H	-5.425472	1.064280	2.720401
H	-5.037244	2.076456	1.326809
C	-0.056647	0.771579	0.540243
H	0.825270	1.399858	0.706445
H	-0.473961	1.043892	-0.431523
C	0.394547	-0.718130	0.470530
H	-0.483877	-1.369285	0.529551
H	0.849325	-0.880908	-0.513074

Table S20. Cartesian coordinates of **FC** in the singlet state.

		angstrom	
Atom	x	y	z
Cu	3.484174	-0.000491	-0.396627
Cu	-3.380037	0.002983	-0.509436
O	-1.999032	0.246222	-1.853582
O	-1.256551	-0.766105	-2.170831
N	3.924311	2.006698	-0.590582
N	4.572901	-1.263612	-1.596467
N	2.690710	-0.719528	1.361768
N	5.372963	0.018344	0.794535
N	-4.731704	1.189615	-1.593861
N	-3.620717	-2.083686	-0.321397
N	-2.470862	0.992064	1.310958
N	-5.048484	-0.032670	0.832176
C	3.427672	2.881826	-1.486487
H	2.600891	2.527537	-2.098351
C	3.930152	4.175398	-1.653210
H	3.491620	4.836133	-2.395713
C	5.007753	4.579702	-0.856427
H	5.435985	5.573791	-0.960982
C	5.531720	3.672299	0.072719
H	6.373219	3.947134	0.704234
C	4.964351	2.398201	0.185499
C	5.469190	1.412706	1.237967
H	6.489956	1.693845	1.540289
H	4.835873	1.522848	2.127810
C	4.123533	-2.052047	-2.592785
H	3.074365	-1.942066	-2.857943
C	4.933645	-2.967703	-3.268833
H	4.517034	-3.573433	-4.068549
C	6.275014	-3.081489	-2.884007
H	6.938501	-3.787458	-3.377847

C	6.745797	-2.268171	-1.846520
H	7.781458	-2.327613	-1.520270
C	5.873565	-1.362694	-1.231488
C	6.396592	-0.391099	-0.173545
H	7.286157	-0.823150	0.309827
H	6.735685	0.509333	-0.701391
C	1.383388	-0.866601	1.681766
C	0.989262	-1.304402	2.955087
H	-0.066853	-1.429754	3.177353
C	1.962136	-1.579983	3.920333
H	1.679052	-1.917415	4.914659
C	3.309782	-1.420184	3.580734
H	4.097097	-1.632151	4.299651
C	3.638664	-1.001923	2.287145
C	5.105574	-0.952416	1.857341
H	5.736892	-0.794609	2.745703
H	5.357678	-1.947888	1.469518
C	-4.447903	1.985004	-2.640105
H	-3.409059	1.998340	-2.962067
C	-5.425234	2.745707	-3.288150
H	-5.153194	3.372674	-4.132386
C	-6.744381	2.677591	-2.822197
H	-7.530708	3.258721	-3.298266
C	-7.037498	1.849137	-1.730588
H	-8.050888	1.770887	-1.344519
C	-6.002620	1.113238	-1.146781
C	-6.250290	0.123079	-0.021152
H	-7.129755	0.418605	0.568476
H	-6.472858	-0.854090	-0.467284
C	-3.105486	-3.029120	-1.128893
H	-2.375722	-2.680043	-1.855523
C	-3.474711	-4.374991	-1.040775
H	-3.033908	-5.101236	-1.717684

C	-4.421064	-4.750360	-0.080143
H	-4.739524	-5.786181	0.011607
C	-4.960216	-3.765070	0.758077
H	-5.701303	-4.017552	1.512564
C	-4.531645	-2.443133	0.610410
C	-5.020643	-1.336962	1.529420
H	-6.001657	-1.593276	1.953124
H	-4.319481	-1.251463	2.368482
C	-1.181128	1.253988	1.635776
C	-0.842758	1.816524	2.877990
H	0.199169	2.028333	3.100613
C	-1.844519	2.105771	3.806841
H	-1.599132	2.539144	4.773607
C	-3.172700	1.833249	3.463936
H	-3.986394	2.051316	4.150728
C	-3.441040	1.289243	2.204142
C	-4.881681	1.106483	1.757174
H	-5.540551	1.014867	2.632352
H	-5.183361	2.014805	1.221457
C	-0.107299	0.946006	0.616558
H	0.755122	1.597346	0.794021
H	-0.496879	1.179236	-0.376621
C	0.371037	-0.537570	0.607428
H	-0.496518	-1.200453	0.694172
H	0.826777	-0.734273	-0.369179

Table S21. Cartesian coordinates of **RI** in the triplet state.

		angstrom	
Atom	x	y	z
Cu	3.652055	0.028581	-0.598255
Cu	-3.538390	-0.064181	-0.507288
O	2.307479	0.049742	-1.879876
O	-2.259765	-0.030053	-2.016967
O	-1.696094	-1.106329	-2.400564
H	2.661578	0.065620	-2.780929
N	4.013961	2.092594	-0.519483
N	4.894654	-1.431716	-1.419215
N	2.571937	-0.701263	1.250885
N	5.236494	0.056789	0.829399
N	-4.968771	1.017087	-1.632086
N	-3.839906	-2.110930	-0.063937
N	-2.496399	1.102528	1.102758
N	-5.139986	0.105998	0.958849
C	3.530683	2.983535	-1.401528
H	2.788796	2.594446	-2.095633
C	3.953058	4.316323	-1.417346
H	3.541550	5.008291	-2.146698
C	4.918899	4.724140	-0.487538
H	5.280979	5.749643	-0.479708
C	5.417597	3.790822	0.432043
H	6.166612	4.074802	1.167359
C	4.930485	2.481117	0.388206
C	5.332992	1.422834	1.400942
H	6.336794	1.622898	1.800047
H	4.634417	1.479795	2.244515
C	4.548959	-2.344367	-2.343057
H	3.515751	-2.307681	-2.681306
C	5.458427	-3.285292	-2.834715
H	5.142579	-4.006494	-3.583056

C	6.768529	-3.273419	-2.338105
H	7.501848	-3.992720	-2.695216
C	7.121779	-2.325301	-1.367883
H	8.128512	-2.292040	-0.958592
C	6.153621	-1.414562	-0.936385
C	6.453692	-0.307374	0.059447
H	7.280746	-0.595175	0.723702
H	6.776232	0.582166	-0.495875
C	1.246311	-0.834975	1.489289
C	0.780488	-1.239735	2.753508
H	-0.287666	-1.355511	2.914279
C	1.688545	-1.496862	3.782351
H	1.342115	-1.806321	4.765795
C	3.057023	-1.359243	3.521529
H	3.799539	-1.563436	4.288695
C	3.451669	-0.973287	2.237605
C	4.925624	-0.954313	1.866306
H	5.545704	-0.811719	2.762251
H	5.177153	-1.938930	1.454511
C	-4.757660	1.677303	-2.784420
H	-3.750078	1.621953	-3.190655
C	-5.765466	2.391731	-3.438547
H	-5.548234	2.907076	-4.369739
C	-7.042088	2.424474	-2.863641
H	-7.850932	2.973980	-3.339568
C	-7.261083	1.738563	-1.661844
H	-8.239512	1.741066	-1.187566
C	-6.199688	1.038763	-1.079655
C	-6.388292	0.198802	0.174237
H	-7.222159	0.590974	0.774896
H	-6.664675	-0.816581	-0.135982
C	-3.416996	-3.162948	-0.788685
H	-2.739985	-2.931209	-1.607637

C	-3.814821	-4.475948	-0.517992
H	-3.447878	-5.289984	-1.136607
C	-4.694760	-4.703629	0.546375
H	-5.035257	-5.709348	0.781665
C	-5.138961	-3.608643	1.299128
H	-5.827770	-3.744449	2.129406
C	-4.686239	-2.328062	0.967635
C	-5.080126	-1.110898	1.789631
H	-6.026710	-1.298654	2.316937
H	-4.312214	-0.953785	2.557247
C	-1.179796	1.357929	1.302721
C	-0.737135	2.033672	2.453425
H	0.323304	2.235519	2.574855
C	-1.657002	2.446215	3.418534
H	-1.329544	2.968351	4.314629
C	-3.012906	2.180402	3.202997
H	-3.767669	2.491637	3.920485
C	-3.389254	1.518939	2.030137
C	-4.866862	1.335963	1.720945
H	-5.451557	1.379877	2.651666
H	-5.184615	2.185165	1.103468
C	-0.185322	0.920375	0.251482
H	0.694087	1.570557	0.293608
H	-0.628798	1.050230	-0.737798
C	0.283090	-0.561077	0.355914
H	-0.592639	-1.210093	0.466972
H	0.774397	-0.793791	-0.592868

Table S22. Cartesian coordinates of **RI** in the singlet state.

		angstrom	
Atom	x	y	z
Cu	-3.651610	0.028760	0.597939
Cu	3.538624	-0.063806	0.507812
O	-2.306517	0.049038	1.878949
O	2.260889	-0.027993	2.018152
O	1.692669	-1.102866	2.398978
H	-2.660257	0.065416	2.780137
N	-4.013942	2.092855	0.520434
N	-4.894696	-1.431043	1.419281
N	-2.572308	-0.701412	-1.251282
N	-5.236389	0.057575	-0.829263
N	4.969329	1.018917	1.630631
N	3.839473	-2.111198	0.066858
N	2.496674	1.100884	-1.103922
N	5.140033	0.104052	-0.958952
C	-3.530757	2.983595	1.402710
H	-2.789208	2.594337	2.097078
C	-3.952717	4.316523	1.418463
H	-3.541290	5.008277	2.148063
C	-4.917987	4.724727	0.488246
H	-5.279722	5.750350	0.480293
C	-5.416565	3.791627	-0.431630
H	-6.165128	4.075919	-1.167286
C	-4.929930	2.481756	-0.387652
C	-5.332387	1.423715	-1.400650
H	-6.336030	1.624077	-1.800014
H	-4.633550	1.480588	-2.244014
C	-4.549128	-2.343948	2.342883
H	-3.515882	-2.307591	2.681058
C	-5.458764	-3.284787	2.834451
H	-5.142989	-4.006183	3.582635

C	-6.768887	-3.272556	2.337938
H	-7.502342	-3.991767	2.694953
C	-7.122014	-2.324162	1.367919
H	-8.128774	-2.290617	0.958716
C	-6.153700	-1.413552	0.936534
C	-6.453571	-0.306044	-0.058990
H	-7.280950	-0.593358	-0.723052
H	-6.775503	0.583581	0.496531
C	-1.246758	-0.835669	-1.489900
C	-0.781334	-1.240881	-2.754108
H	0.286748	-1.357069	-2.915053
C	-1.689681	-1.497908	-3.782733
H	-1.343541	-1.807732	-4.766164
C	-3.058047	-1.359675	-3.521704
H	-3.800790	-1.563744	-4.288683
C	-3.452314	-0.973254	-2.237794
C	-4.926230	-0.953553	-1.866323
H	-5.546331	-0.810491	-2.762180
H	-5.178252	-1.938097	-1.454657
C	4.758437	1.680976	2.781933
H	3.750902	1.626380	3.188390
C	5.766433	2.396292	3.434813
H	5.549393	2.913156	4.365208
C	7.042991	2.427903	2.859715
H	7.851980	2.978033	3.334676
C	7.261761	1.740032	1.658988
H	8.240147	1.741614	1.184618
C	6.200198	1.039491	1.078019
C	6.388414	0.197486	-0.174547
H	7.222457	0.588312	-0.775844
H	6.664308	-0.817548	0.137257
C	3.416293	-3.162188	0.792939
H	2.739337	-2.929266	1.611595

C	3.813646	-4.475649	0.523811
H	3.446518	-5.288804	1.143474
C	4.693348	-4.704931	-0.540413
H	5.033467	-5.711054	-0.774520
C	5.137786	-3.611025	-1.294588
H	5.826407	-3.748080	-2.124818
C	4.685560	-2.329884	-0.964580
C	5.079700	-1.113867	-1.788161
H	6.026153	-1.302576	-2.315367
H	4.311710	-0.957515	-2.555854
C	1.180139	1.356367	-1.304041
C	0.737548	2.031359	-2.455239
H	-0.322851	2.233376	-2.576734
C	1.657445	2.442881	-3.420729
H	1.330085	2.964399	-4.317220
C	3.013306	2.176821	-3.205111
H	3.768072	2.487235	-3.922953
C	3.389585	1.516266	-2.031740
C	4.867166	1.333163	-1.722509
H	5.451759	1.375806	-2.653358
H	5.185262	2.183000	-1.106088
C	0.185600	0.919480	-0.252592
H	-0.693605	1.569935	-0.294768
H	0.629206	1.049408	0.736618
C	-0.283230	-0.561875	-0.356763
H	0.592334	-1.211090	-0.467940
H	-0.774345	-0.794437	0.592157

Table S23. Cartesian coordinates of **TS2'** in the triplet state.

		angstrom	
Atom	x	y	z
Cu	3.538438	0.171073	0.707647
Cu	-3.630497	-0.406230	0.391751
O	2.261100	-0.822446	1.604305
O	-2.251607	-1.290873	1.499582
O	-1.726388	-0.662312	2.476851
C	3.501463	1.764080	2.923815
H	3.742324	0.985543	3.640864
H	4.274261	2.492455	2.693441
H	2.229357	-0.639444	2.553757
H	2.464535	2.055056	2.793068
N	3.702106	-1.248028	-0.974545
N	5.291069	-0.742883	1.548733
N	2.348586	1.854096	-0.262538
N	5.042445	1.171434	-0.440178
N	-4.835069	-2.143925	0.415614
N	-4.201037	1.310731	1.491431
N	-2.588717	0.008356	-1.556022
N	-5.309455	0.270259	-0.819475
C	3.241609	-2.507078	-0.978741
H	2.501042	-2.736826	-0.214349
C	3.700495	-3.466496	-1.889718
H	3.301776	-4.476874	-1.865987
C	4.690501	-3.094694	-2.808765
H	5.081417	-3.815892	-3.522951
C	5.181881	-1.781296	-2.788548
H	5.955961	-1.463935	-3.483237
C	4.651531	-0.886249	-1.853382
C	5.040716	0.579565	-1.816150
H	6.011959	0.737931	-2.302158
H	4.294357	1.127655	-2.402493

C	5.294827	-1.833650	2.331370
H	4.319909	-2.168193	2.679412
C	6.472634	-2.510569	2.662240
H	6.435310	-3.384656	3.306204
C	7.683774	-2.040685	2.136476
H	8.619501	-2.545832	2.364407
C	7.671961	-0.913610	1.304260
H	8.592659	-0.526096	0.874438
C	6.448852	-0.287864	1.041153
C	6.358951	0.998184	0.239343
H	6.486763	1.831185	0.940369
H	7.186063	1.060260	-0.479431
C	1.010187	2.017586	-0.387493
C	0.480899	3.148982	-1.034768
H	-0.597078	3.266336	-1.102353
C	1.337969	4.109299	-1.575753
H	0.942222	4.987522	-2.080677
C	2.719343	3.921256	-1.452498
H	3.424715	4.643321	-1.855690
C	3.177139	2.786035	-0.777840
C	4.661951	2.604654	-0.515430
H	5.248188	3.139172	-1.276107
H	4.892905	3.064948	0.451460
C	-4.462040	-3.378656	0.795874
H	-3.440221	-3.481168	1.154680
C	-5.327602	-4.475094	0.747475
H	-4.982586	-5.453418	1.069548
C	-6.631493	-4.276693	0.276303
H	-7.332780	-5.105889	0.218807
C	-7.018893	-2.990804	-0.122362
H	-8.023386	-2.799493	-0.492028
C	-6.093354	-1.946656	-0.030094
C	-6.474585	-0.510677	-0.354563

H	-7.299222	-0.489144	-1.082121
H	-6.845875	-0.043050	0.565889
C	-3.850036	1.611005	2.755381
H	-3.083405	0.978576	3.196638
C	-4.424484	2.667709	3.468862
H	-4.108716	2.865456	4.489241
C	-5.409854	3.440647	2.844027
H	-5.887096	4.264696	3.369353
C	-5.778746	3.127130	1.529310
H	-6.544094	3.701114	1.012545
C	-5.149069	2.058960	0.883603
C	-5.456773	1.715552	-0.564841
H	-6.455875	2.083619	-0.839435
H	-4.734920	2.242075	-1.201535
C	-1.270652	0.135481	-1.846570
C	-0.842779	0.538203	-3.124038
H	0.221618	0.615152	-3.326987
C	-1.781181	0.820679	-4.117458
H	-1.466035	1.135442	-5.109642
C	-3.138585	0.677735	-3.811927
H	-3.905653	0.870793	-4.557314
C	-3.497048	0.258705	-2.527336
C	-4.956536	-0.031734	-2.216743
H	-5.604359	0.501886	-2.927643
H	-5.121930	-1.104527	-2.375332
C	-0.255533	-0.197301	-0.777181
H	0.665738	-0.547520	-1.253415
H	-0.637276	-1.022195	-0.171935
C	0.100101	0.963267	0.199446
H	-0.821428	1.437440	0.554178
H	0.609509	0.491417	1.044491

Table S24. Cartesian coordinates of **TS2'** in the singlet state.

		angstrom	
Atom	x	y	z
Cu	3.557865	0.214415	0.720966
Cu	-3.630604	-0.382744	0.420578
O	2.290572	-0.684292	1.723061
O	-2.270281	-0.912046	1.696145
O	-1.736357	-2.071321	1.498774
C	3.593699	1.946386	2.831338
H	2.516805	2.073749	2.808070
H	4.025447	1.244950	3.538432
H	2.349937	-0.498919	2.670754
H	4.215170	2.769844	2.490054
N	3.632471	-1.285635	-0.894921
N	5.320495	-0.696093	1.543008
N	2.357984	1.845159	-0.318318
N	5.033890	1.133293	-0.519286
N	-4.819456	-2.124363	0.365533
N	-4.139469	1.298415	1.583241
N	-2.618817	0.081815	-1.541392
N	-5.305021	0.351733	-0.713405
C	3.144457	-2.532614	-0.829711
H	2.423322	-2.712795	-0.033972
C	3.551515	-3.540166	-1.712905
H	3.131417	-4.538892	-1.632484
C	4.517718	-3.230876	-2.679332
H	4.868432	-3.990662	-3.374108
C	5.037562	-1.929297	-2.732454
H	5.793959	-1.659462	-3.465676
C	4.558431	-0.983247	-1.819975
C	4.978416	0.474461	-1.863885
H	5.937779	0.588326	-2.384581
H	4.226400	1.010098	-2.454347

C	5.334843	-1.754941	2.368341
H	4.368590	-2.058901	2.765059
C	6.512335	-2.439954	2.683462
H	6.483480	-3.287518	3.362353
C	7.711210	-2.013343	2.096518
H	8.645975	-2.526164	2.310834
C	7.687884	-0.919931	1.220676
H	8.598639	-0.566502	0.743028
C	6.466827	-0.282942	0.976286
C	6.368350	0.971384	0.126908
H	6.525405	1.829240	0.791102
H	7.174478	0.995313	-0.617623
C	1.017649	2.015923	-0.413383
C	0.481961	3.152993	-1.045020
H	-0.596303	3.279629	-1.085760
C	1.333333	4.105469	-1.609155
H	0.932230	4.987791	-2.102631
C	2.715447	3.901866	-1.529181
H	3.415987	4.613861	-1.958086
C	3.180903	2.764348	-0.863269
C	4.672458	2.567345	-0.651251
H	5.235307	3.052463	-1.461232
H	4.951851	3.071189	0.280295
C	-4.442317	-3.383461	0.650014
H	-3.403811	-3.510439	0.947317
C	-5.324266	-4.465835	0.573841
H	-4.975874	-5.465157	0.818346
C	-6.645365	-4.227923	0.176296
H	-7.358259	-5.045674	0.100294
C	-7.035059	-2.916595	-0.127360
H	-8.051856	-2.694060	-0.441686
C	-6.094300	-1.889537	-0.012780
C	-6.467569	-0.434482	-0.242144

H	-7.316921	-0.360290	-0.936486
H	-6.793832	-0.008514	0.714778
C	-3.730483	1.536061	2.842271
H	-2.977946	0.856231	3.235945
C	-4.241807	2.586488	3.610160
H	-3.885188	2.739930	4.624669
C	-5.223002	3.411938	3.046357
H	-5.652291	4.232060	3.617198
C	-5.652885	3.157852	1.736913
H	-6.418614	3.773123	1.270694
C	-5.081904	2.092833	1.033860
C	-5.442943	1.793000	-0.411804
H	-6.452240	2.163251	-0.640853
H	-4.745765	2.338288	-1.059857
C	-1.306903	0.196080	-1.864410
C	-0.909344	0.624819	-3.143537
H	0.150002	0.690376	-3.374676
C	-1.869871	0.948219	-4.102679
H	-1.576894	1.283257	-5.095018
C	-3.220676	0.820690	-3.762703
H	-4.005036	1.046293	-4.480460
C	-3.548730	0.373274	-2.479841
C	-5.002558	0.096583	-2.134491
H	-5.664600	0.669006	-2.799897
H	-5.193748	-0.965965	-2.327445
C	-0.266973	-0.175354	-0.832144
H	0.640593	-0.508024	-1.346671
H	-0.631800	-1.022526	-0.248263
C	0.116453	0.953266	0.172989
H	-0.796387	1.420100	0.558929
H	0.642616	0.459955	0.996932