Supplementary Information

Interactions of copper (II) and zinc (II) with Chlorophyll: insights from Density Functional Theory Studies.

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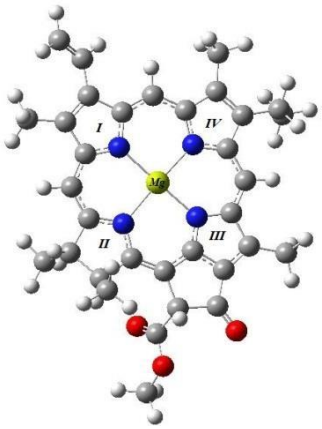
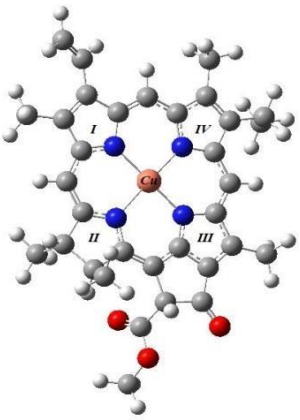
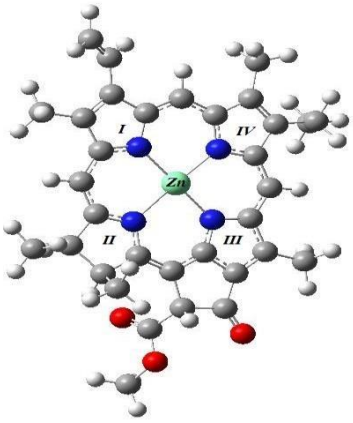


Chla



S(Cu)



S(Zn)

** Cartesian coordinates (xyz)

Chla (Pheo(Mg))

E: -1921.725176 u.a

G: -1921.208806 u.a

C -2.696487 -0.110289 -0.403813

C	-1.953508	1.089872	-0.339160
C	-2.739443	2.272264	-0.383874
C	-4.146026	1.901077	-0.474660
C	-4.162522	0.299305	-0.523184
C	-1.862569	3.351156	-0.332007
C	-0.544178	2.752500	-0.256172
N	-0.648230	1.362303	-0.260864
Mg	0.755861	-0.082463	-0.156532
N	-0.786512	-1.576804	-0.227375
C	-0.519282	-2.902793	-0.105105
C	-1.805917	-3.719708	-0.030434
C	-2.883900	-2.697255	-0.473654
C	-2.141786	-1.373794	-0.360665
C	0.740099	-3.484957	-0.014671
C	2.003389	-2.858256	0.002958
N	2.196535	-1.509167	-0.042008
C	3.555261	-1.280113	0.017628
C	4.254625	-2.560532	0.086674
C	3.281507	-3.542629	0.087360
C	4.151618	-0.023231	0.008116
C	3.524564	1.240635	-0.036870
N	2.174348	1.429551	-0.101965
C	1.957460	2.790842	-0.119426
C	3.230096	3.488583	-0.062934
C	4.208388	2.519123	-0.013622
C	5.695533	2.702056	0.062335
C	3.404938	4.981699	-0.021571
C	3.252113	5.576151	1.392339
C	0.694361	3.399588	-0.190720
C	3.462272	-5.025276	0.203803
C	5.704639	-2.696199	0.179693
C	6.448808	-3.723034	-0.259386
C	-3.389513	-2.952497	-1.906191
C	-2.045337	-4.264862	1.389468
C	-2.196253	4.810643	-0.348723
O	-5.144726	2.591784	-0.517511

C	-5.068149	-0.231265	0.575330
O	-4.704318	-0.627333	1.663195
O	-6.357854	-0.182283	0.187985
C	-7.317499	-0.555545	1.189524
H	5.236215	-0.007215	0.043063
H	5.977975	3.749865	-0.077342
H	6.216053	2.117275	-0.706340
H	6.096479	2.384332	1.034205
H	2.680945	5.460857	-0.693323
H	4.394112	5.245958	-0.414422
H	3.997569	5.154861	2.075595
H	2.262397	5.356353	1.807251
H	3.381278	6.664589	1.374553
H	0.677809	4.485642	-0.199203
H	-1.732650	5.322019	-1.202122
H	-3.278282	4.949119	-0.415403
H	-1.842960	5.315645	0.559481
H	6.225253	-1.863845	0.652756
H	6.023338	-4.572860	-0.783462
H	7.526703	-3.725650	-0.125605
H	4.389641	-5.262823	0.734963
H	3.515944	-5.515502	-0.778353
H	2.633666	-5.488914	0.749852
H	0.746605	-4.568686	0.051004
H	-2.981857	-4.833394	1.428718
H	-1.231167	-4.926627	1.704067
H	-2.116505	-3.445429	2.113515
H	-1.758802	-4.566166	-0.727254
H	-3.879620	-3.931257	-1.968639
H	-4.113578	-2.194213	-2.221534
H	-2.558994	-2.942637	-2.621788
H	-3.736545	-2.710428	0.213961
H	-8.292685	-0.441463	0.715612
H	-7.234944	0.099485	2.060600
H	-7.160996	-1.590536	1.506174
H	-4.614346	0.033123	-1.486384

S(Cu): Pheo(Cu)

E: -3361.879888 u.a

G: -3361.365070 u.a

N	2.105598	1.385672	-0.088681
C	3.460626	1.208183	-0.073130
C	4.151211	2.478588	-0.055617
C	3.178388	3.448684	-0.052227
C	1.908116	2.753313	-0.077318
C	4.095221	-0.037762	-0.053472
C	3.470505	-1.267140	-0.007180
N	2.102463	-1.465250	-0.014386
C	1.918026	-2.817208	0.073610
C	3.187741	-3.513507	0.135908
C	4.164537	-2.545661	0.069844
C	0.676164	-3.458050	0.099099
C	-0.560941	-2.859436	-0.014934
N	-0.793609	-1.531996	-0.182882
C	-2.149837	-1.347409	-0.359472
C	-2.887676	-2.666690	-0.492326
C	-1.850712	-3.663091	0.066133
Cu	0.716372	-0.067187	-0.120343
N	-0.651750	1.319414	-0.201985
C	-1.961878	1.073690	-0.310979
C	-2.739297	2.260172	-0.353003
C	-1.859383	3.327476	-0.265234
C	-0.553831	2.715881	-0.178512
C	-4.146286	1.907412	-0.486931
C	-4.177745	0.310359	-0.562993
C	-2.719243	-0.102413	-0.410644
O	-5.133753	2.613237	-0.543904
C	-5.115343	-0.230002	0.503744
O	-6.394117	-0.156986	0.086269
C	-7.382931	-0.536409	1.056913
C	-2.174842	4.790987	-0.266068
C	0.664736	3.376365	-0.112179

C	-2.152730	-4.093866	1.513236
C	-3.270217	-2.958792	-1.955474
C	5.616782	-2.689412	0.113497
C	6.333828	-3.722112	-0.354739
C	3.352379	-4.994153	0.292584
C	5.641580	2.647300	-0.031312
C	3.352939	4.941172	0.007069
C	3.229120	5.516275	1.431705
O	-4.782478	-0.650393	1.592272
H	5.179249	-0.031646	-0.059496
H	5.925087	3.698732	-0.136102
H	6.126721	2.094445	-0.845454
H	6.078065	2.284976	0.908929
H	2.617182	5.430370	-0.644251
H	4.334490	5.209135	-0.401750
H	3.987742	5.085253	2.094010
H	2.247942	5.291938	1.863973
H	3.359240	6.604682	1.425710
H	0.645745	4.461308	-0.104608
H	-1.691370	5.309609	-1.103802
H	-3.254061	4.941157	-0.350263
H	-1.833427	5.278588	0.655957
H	6.160919	-1.864560	0.572744
H	5.879847	-4.564337	-0.867412
H	7.415512	-3.738363	-0.257513
H	4.318145	-5.228381	0.750934
H	3.312212	-5.520844	-0.671036
H	2.567498	-5.421257	0.926260
H	0.682038	-4.537871	0.201917
H	-3.088210	-4.663936	1.554008
H	-1.351172	-4.722290	1.916181
H	-2.261487	-3.219470	2.164415
H	-1.779119	-4.559284	-0.562539
H	-3.765609	-3.933891	-2.031962
H	-3.954253	-2.201222	-2.352004
H	-2.381293	-2.977568	-2.596699

H	-3.793716	-2.656392	0.122102
H	-8.344489	-0.400222	0.561559
H	-7.313218	0.100836	1.942153
H	-7.247513	-1.579241	1.357009
H	-4.603637	0.059931	-1.542176

S(Zn): Pheo(Zn)

E: -3500.715754 u.a

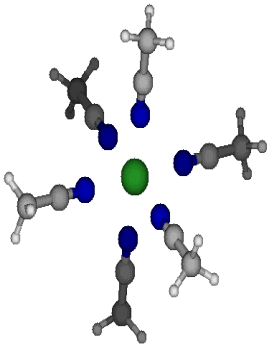
G: -3500.201795 u.a

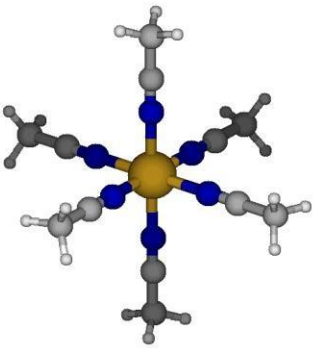
N	2.156960	1.404242	-0.094114
C	3.503585	1.204177	-0.038476
C	4.205436	2.472623	-0.019705
C	3.239396	3.452469	-0.060331
C	1.960259	2.766799	-0.107325
C	4.103051	-0.066101	0.006841
C	3.467837	-1.299223	0.028179
N	2.100475	-1.500977	-0.023991
C	1.893550	-2.852185	0.029465
C	3.160303	-3.553194	0.115357
C	4.145996	-2.587865	0.103788
C	0.637915	-3.480572	0.014006
C	-0.613480	-2.891905	-0.085639
N	-0.854442	-1.565577	-0.214528
C	-2.204638	-1.352695	-0.354762
C	-2.966632	-2.663374	-0.474364
C	-1.907063	-3.696721	-0.017860
C	-2.738255	-0.083762	-0.391577
C	-4.193568	0.354436	-0.520924
C	-4.140997	1.951828	-0.462215
C	-2.727223	2.288709	-0.358966
C	-1.965533	1.091449	-0.313582
C	-1.833155	3.349356	-0.301774
C	-0.528506	2.728833	-0.223634
N	-0.651770	1.335006	-0.226715
C	-5.120531	-0.166197	0.564665
O	-6.405240	-0.080127	0.167636

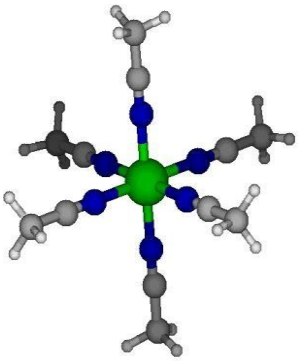
C	-7.382181	-0.441975	1.156741
O	-5.121183	2.668570	-0.508526
C	-2.139825	4.814813	-0.317912
C	0.704872	3.378536	-0.166368
Zn	0.728198	-0.076502	-0.146391
C	-2.163643	-4.232768	1.402297
C	-3.459611	-2.912558	-1.912193
C	5.594722	-2.746381	0.193651
C	6.320211	-3.774943	-0.270784
C	3.317486	-5.037495	0.244809
C	5.695442	2.633358	0.044881
C	3.427400	4.943793	-0.019010
C	3.286168	5.539399	1.395627
O	-4.775246	-0.584150	1.650187
H	4.031182	5.111835	2.075421
H	4.417121	5.199193	-0.416339
H	2.704497	5.429314	-0.687444
H	2.296636	5.328156	1.815351
H	3.424525	6.626676	1.377028
H	6.200924	2.045735	-0.731673
H	6.099624	2.303863	1.011455
H	5.991532	3.677911	-0.090846
H	5.187455	-0.081817	0.033888
H	6.128958	-1.934971	0.687352
H	7.397858	-3.800987	-0.137414
H	5.878568	-4.603385	-0.815626
H	4.262882	-5.284866	0.737584
H	3.317230	-5.541858	-0.731542
H	2.505864	-5.477270	0.834558
H	0.645393	-4.563528	0.085642
H	-1.861857	-4.546165	-0.711161
H	-1.357914	-4.899950	1.727274
H	-3.105190	-4.793249	1.435999
H	-2.234017	-3.409177	2.121575
H	-2.620980	-2.916296	-2.618237
H	-3.964369	-3.883529	-1.979203

H	-3.826520	-2.661904	0.204150
H	-4.168095	-2.143302	-2.236533
H	0.684810	4.464251	-0.175218
H	-1.787606	5.310988	0.595514
H	-1.659126	5.320252	-1.165233
H	-3.218636	4.971645	-0.394943
H	-4.639991	0.102647	-1.490507
H	-7.288353	0.197532	2.038104
H	-8.350275	-0.294452	0.677594
H	-7.256004	-1.485438	1.458761

2. a.2. $[M(CH_3CN)_6]^{2+}$ complexes (M : Mg, Cu, Zn)







(*Mg)* **(*Cu)*** **(*Zn)***

** Cartesian coordinates (xyz)

$[Mg(CH_3CN)_6]^{2+}$

E: -996.375773 u.a

G: -996.157933 u.a

Mg	0.000326	-0.005478	0.005675
N	0.000801	-0.004301	2.194448
N	2.189364	-0.007855	0.006579

N	-0.000518	-0.004509	-2.183042
N	-2.188792	-0.005243	0.007076
N	-0.000352	2.183403	0.003875
N	0.001100	-2.194544	0.004357
C	0.005442	-3.351061	0.003970
C	0.000507	-0.004914	-3.339567
C	-0.001703	3.339926	0.004081
C	-3.345284	-0.013413	0.010690
C	0.002232	-0.004433	3.350974
C	3.345871	-0.001438	0.008384
C	0.008429	-4.807659	0.000777
H	-0.028152	-5.183644	1.028036
H	-0.862720	-5.181337	-0.546456
H	0.918140	-5.178306	-0.481918
C	-0.001473	-0.003094	-4.796152
H	-0.003335	-1.031431	-5.170988
H	-0.892609	0.512796	-5.167282
H	0.889375	0.510934	-5.170459
C	4.802447	0.003709	0.007103
H	5.172354	1.033837	0.006646
H	5.178904	-0.509484	0.897517
H	5.176397	-0.509273	-0.884539
C	0.000599	-0.002411	4.807573
H	0.003519	-1.030705	5.182516
H	0.889160	0.515686	5.181677
H	-0.892890	0.509314	5.178821
C	-4.801852	-0.020907	0.012448
H	-5.170060	-1.051625	0.018705
H	-5.177157	0.496743	0.900764
H	-5.178674	0.486324	-0.881263
C	-0.007118	4.796508	0.002151
H	-0.031580	5.171246	1.030244
H	0.893428	5.173080	-0.492952
H	-0.888124	5.165461	-0.532368

[Cu(CH$_3$CN)$_6$)]$^{2+}$

E: -2436.452967 u.a

G: -2436.243846 u.a

Cu	-0.000227	-0.004197	0.004245
N	-0.000378	-0.004692	1.967546
N	2.194981	-0.010863	0.004569
N	-0.000620	-0.001533	-1.960634
N	-2.195666	0.000155	0.004801
N	-0.001218	2.191237	0.004078
N	0.000612	-2.199816	0.000578
C	0.003989	-3.357036	0.003041
C	0.001019	-0.006765	-3.114716
C	-0.004493	3.348447	0.007863
C	-3.352845	-0.009704	0.007338
C	0.001091	-0.005413	3.121651
C	3.352172	-0.002531	0.007115
C	0.007431	-4.814705	0.002445
H	-0.001292	-5.189843	1.030654
H	-0.877755	-5.190734	-0.520191
H	0.904048	-5.186579	-0.503365
C	0.001024	-0.009039	-4.569942
H	-0.000511	-1.039033	-4.940876
H	-0.889913	0.506662	-4.942545
H	0.893326	0.504053	-4.942831
C	4.809823	0.004119	0.008653
H	5.179791	1.034216	0.011353
H	5.185481	-0.510855	0.898457
H	5.187137	-0.506921	-0.882749
C	0.000691	-0.002685	4.576887
H	-0.001321	-1.031376	4.951432
H	0.893089	0.511312	4.948294
H	-0.890203	0.514555	4.947447
C	-4.810488	-0.018506	0.008690
H	-5.178870	-1.049157	0.014074
H	-5.187101	0.498209	0.897075
H	-5.188465	0.489563	-0.884125
C	-0.007908	4.806103	0.008767

H	0.003273	5.180197	1.037333
H	0.875991	5.182612	-0.515696
H	-0.905693	5.178448	-0.494616

$[Zn(CH_3CN)_6]^{2+}$

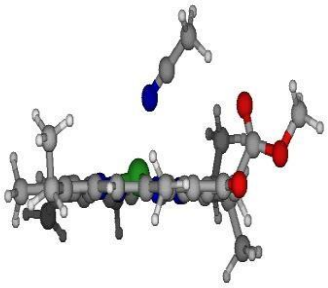
E: -2575.326492 u.a

G: -2575.120253 u.a

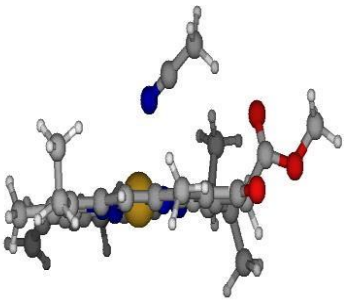
Zn	-0.001031	-0.005010	0.004819
N	-0.000479	-0.005694	2.153301
N	2.150857	-0.010254	0.004992
N	-0.002435	0.001695	-2.143316
N	-2.152921	-0.001695	0.005164
N	0.000731	2.144749	0.006092
N	-0.002763	-2.154824	0.000383
C	0.001364	-3.311400	-0.003180
C	0.000182	-0.001071	-3.299920
C	-0.002664	3.301339	0.006469
C	-3.309522	-0.006547	0.006572
C	0.000771	-0.005056	3.309899
C	3.307456	-0.006243	0.009163
C	0.007140	-4.768199	-0.006196
H	0.088898	-5.143825	1.018854
H	-0.920362	-5.144205	-0.449859
H	0.856107	-5.137332	-0.590512
C	0.002932	-0.005174	-4.756728
H	0.072948	-1.032655	-5.127980
H	-0.920262	0.447481	-5.132673
H	0.856880	0.568957	-5.130370
C	4.764281	-0.001273	0.015588
H	5.135909	1.024899	-0.069993
H	5.134847	-0.439708	0.947745
H	5.142710	-0.588772	-0.827107
C	0.001966	-0.005568	4.766705
H	0.025358	-1.034280	5.140458
H	0.881187	0.529563	5.139641

H	-0.900015	0.489376	5.140861
C	-4.766355	-0.013325	0.007026
H	-5.136288	-1.042896	0.046877
H	-5.141843	0.535234	0.876815
H	-5.141571	0.466264	-0.902757
C	-0.007685	4.758143	0.008668
H	-0.017148	5.130299	1.038166
H	0.886273	5.135509	-0.498211
H	-0.895454	5.129397	-0.513358

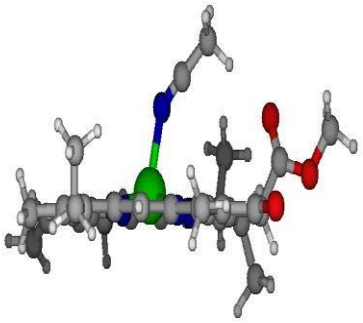
2. a.3. Pheo(M(CH_3CN)) complexes



Pheo(Mg(CH_3CN))



Pheo(Cu(CH_3CN))



Pheo(Zn(CH_3CN))

Pheo(Mg(CH_3CN))

E: -2054.503505 u.a

G: -2053.946737 u.a

C	4.284173	2.511716	-0.091587
C	3.587668	1.236207	-0.065367
N	2.243766	1.430084	-0.158111
C	2.038130	2.787263	-0.264838
C	3.316138	3.482384	-0.213632

C	4.209631	-0.029619	0.009982
C	3.612135	-1.286393	-0.026323
N	2.259094	-1.514576	-0.124274
C	2.070744	-2.862056	-0.162278
C	3.350389	-3.549871	-0.081693
C	4.318518	-2.567763	-0.004033
C	0.814157	-3.496365	-0.263345
C	-0.444634	-2.918757	-0.399302
N	-0.712550	-1.593776	-0.472584
C	-2.054606	-1.383732	-0.662324
C	-2.797339	-2.701344	-0.850817
C	-1.727593	-3.748074	-0.440514
Mg	0.793005	-0.079638	0.004750
N	-0.555569	1.360048	-0.543804
C	-1.854786	1.087459	-0.655502
C	-2.640870	2.269509	-0.753622
C	-1.760882	3.348970	-0.703179
C	-0.450460	2.747470	-0.561188
C	-4.042722	1.900622	-0.847238
C	-4.065172	0.294741	-0.826336
C	-2.600734	-0.115075	-0.704461
O	-5.048322	2.582483	-0.914367
C	-4.941888	-0.146751	0.329298
O	-6.218800	-0.296472	-0.063547
C	-7.164158	-0.588624	0.978341
C	-2.089206	4.808277	-0.779073
C	0.785928	3.396231	-0.434434
C	-2.019779	-4.411753	0.916590
C	-3.281519	-2.890765	-2.300532
C	5.766495	-2.701987	0.113435
C	6.528015	-3.705761	-0.349628
C	3.534457	-5.036340	-0.049222
C	3.500257	4.974306	-0.258317
C	3.299123	5.655490	1.109591
C	5.771920	2.685032	-0.005848
O	-4.577297	-0.313893	1.479969

H	5.293378	-0.015909	0.068405
H	6.063505	3.729509	-0.152387
H	6.294178	2.089357	-0.765317
H	6.163521	2.372195	0.971453
H	2.804683	5.414519	-0.984619
H	4.505048	5.210170	-0.629087
H	4.016582	5.273870	1.844365
H	2.293585	5.464546	1.500255
H	3.434926	6.740626	1.030733
H	0.774587	4.481301	-0.486775
H	-1.651169	5.274896	-1.671260
H	-3.172236	4.950192	-0.821805
H	-1.705308	5.357265	0.090231
H	6.272082	-1.887364	0.631833
H	6.121400	-4.535974	-0.918217
H	7.602558	-3.707226	-0.190416
H	4.444793	-5.302913	0.497764
H	3.623988	-5.466654	-1.056666
H	2.690492	-5.535398	0.439325
H	0.829102	-4.582222	-0.252257
H	-2.956054	-4.981228	0.874700
H	-1.216577	-5.097967	1.205556
H	-2.116876	-3.657078	1.705876
H	-1.646400	-4.535882	-1.200459
H	-3.764985	-3.867999	-2.417831
H	-4.004238	-2.121918	-2.591455
H	-2.439179	-2.841771	-3.000057
H	-3.665024	-2.751325	-0.180601
H	-8.131859	-0.659282	0.481511
H	-7.171875	0.213205	1.721000
H	-6.914129	-1.531961	1.471540
H	-4.547213	-0.022298	-1.757540
N	0.043872	-0.085605	2.133839
C	-0.882804	-0.028857	2.825582
C	-2.081460	0.042824	3.649425
H	-2.959920	-0.047326	2.997507

H	-2.115800	1.001009	4.177005
H	-2.084175	-0.769143	4.383127

Pheo(Cu(CH$_3$CN))

E: -3494.644025 u.a

G: -3494.090112 u.a

N	-0.556710	1.324140	-0.476949
C	-1.863148	1.077325	-0.597309
C	-2.638953	2.264437	-0.677336
C	-1.754982	3.332516	-0.598431
C	-0.455507	2.718702	-0.471321
C	-2.621928	-0.101953	-0.685204
C	-4.077218	0.312310	-0.859416
C	-4.042048	1.913071	-0.815824
C	-2.060446	-1.351624	-0.632155
N	-0.711040	-1.544211	-0.438795
C	-0.478075	-2.871469	-0.299649
C	-1.766703	-3.683379	-0.271549
C	-2.804147	-2.666454	-0.794288
C	0.759170	-3.468424	-0.162426
C	1.999779	-2.824709	-0.123676
N	2.188500	-1.474073	-0.180761
C	3.551031	-1.274473	-0.103049
C	4.244827	-2.555289	-0.020072
C	3.267969	-3.524014	-0.020821
C	4.177441	-0.044299	-0.109485
C	3.546721	1.204135	-0.162601
N	2.197418	1.386045	-0.238375
C	2.002840	2.752847	-0.264605
C	3.275249	3.446426	-0.202037
C	4.242706	2.474132	-0.142768
Cu	0.797503	-0.067142	-0.207330
C	5.731679	2.637826	-0.063989
C	3.453091	4.939312	-0.171725
C	3.274307	5.548387	1.232787

C	0.764976	3.377344	-0.369090
C	3.427298	-5.007743	0.109301
C	5.693600	-2.698240	0.086668
C	6.435019	-3.719655	-0.368618
C	-3.202482	-2.921919	-2.259911
C	-2.078375	-4.188955	1.148405
C	-5.024932	-0.178253	0.217219
O	-4.731166	-0.407697	1.376254
O	-5.035658	2.611406	-0.886309
C	-2.066011	4.796678	-0.643272
O	-6.275517	-0.294958	-0.262107
C	-7.285594	-0.632630	0.703034
H	4.004282	5.130677	1.934653
H	4.451274	5.195185	-0.546743
H	2.745704	5.414905	-0.863389
H	2.275920	5.335955	1.630283
H	3.408125	6.636197	1.206918
H	6.244833	2.076117	-0.854735
H	6.131098	2.281264	0.894783
H	6.023610	3.687301	-0.166629
H	5.260644	-0.039302	-0.064846
H	6.213653	-1.882011	0.587536
H	7.511041	-3.735860	-0.220936
H	6.008107	-4.551906	-0.919490
H	4.373241	-5.252206	0.602486
H	3.428110	-5.513207	-0.866581
H	2.616783	-5.448817	0.699804
H	0.766008	-4.550579	-0.085671
H	-1.686774	-4.547624	-0.942718
H	-1.287025	-4.850239	1.517084
H	-3.022930	-4.745846	1.159422
H	-2.168560	-3.349980	1.847514
H	-2.319497	-2.919491	-2.909282
H	-3.694050	-3.897239	-2.357047
H	-3.707821	-2.672908	-0.173391
H	-3.893792	-2.157931	-2.630289

H	0.749366	4.462429	-0.382616
H	-1.707678	5.316000	0.254709
H	-1.595035	5.284612	-1.506434
H	-3.145914	4.948734	-0.716576
H	-4.500232	0.038001	-1.832499
H	-7.335814	0.130231	1.484043
H	-8.220568	-0.670359	0.143902
H	-7.070616	-1.601633	1.161590
N	0.022388	-0.208298	2.386179
C	-0.987914	-0.010184	2.921310
C	-2.275032	0.235426	3.564907
H	-2.396412	-0.423725	4.430530
H	-2.330869	1.274282	3.905457
H	-3.086212	0.047593	2.851904

Pheo(Zn(CH$_3$CN))

E: -3633.489019 u.a

G: -3632.933766 u.a

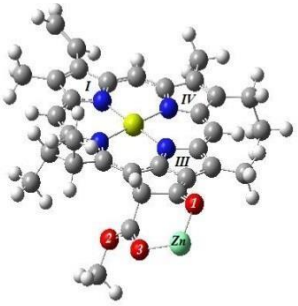
N	-0.561742	1.335592	-0.514122
C	-1.868928	1.091199	-0.631294
C	-2.630073	2.288223	-0.737633
C	-1.732862	3.349597	-0.684421
C	-0.436764	2.726346	-0.534227
C	-2.645699	-0.086852	-0.691168
C	-4.098474	0.351960	-0.832003
C	-4.039031	1.953832	-0.845855
C	-2.122016	-1.361532	-0.648067
N	-0.783875	-1.581635	-0.461973
C	-0.541356	-2.907124	-0.382705
C	-1.831348	-3.724295	-0.415782
C	-2.886663	-2.666957	-0.830727
C	0.711068	-3.491995	-0.253207
C	1.962086	-2.857101	-0.165350
N	2.167249	-1.507901	-0.144013

C	3.528331	-1.307729	-0.047668
C	4.212467	-2.598478	-0.023041
C	3.230027	-3.563425	-0.088157
C	4.165153	-0.073925	-0.014542
C	3.570938	1.199609	-0.077550
N	2.230368	1.406516	-0.160873
C	2.041773	2.765226	-0.254720
C	3.326043	3.447048	-0.210959
C	4.283322	2.465210	-0.102756
Zn	0.782751	-0.059341	0.037314
C	5.773782	2.617590	-0.029180
C	3.523370	4.937196	-0.250634
C	3.335698	5.615018	1.120832
C	0.795682	3.377065	-0.415326
C	3.389396	-5.052500	-0.044338
C	5.659212	-2.757538	0.087624
C	6.400254	-3.763071	-0.402967
C	-3.374016	-2.856294	-2.279218
C	-2.127434	-4.375693	0.946261
C	-5.004778	-0.081065	0.303358
O	-4.662352	-0.277635	1.456115
O	-5.025571	2.662226	-0.921482
C	-2.033768	4.814458	-0.766515
O	-6.279061	-0.187063	-0.110866
C	-7.248309	-0.469524	0.911744
H	4.052957	5.223638	1.850611
H	4.528291	5.165154	-0.625968
H	2.827739	5.386332	-0.971470
H	2.330262	5.432768	1.515870
H	3.481886	6.698998	1.045110
H	6.281148	2.014641	-0.792934
H	6.168903	2.299283	0.944931
H	6.078389	3.657983	-0.178229
H	5.248670	-0.091923	0.038203
H	6.180378	-1.965391	0.624952
H	7.475019	-3.789450	-0.247423

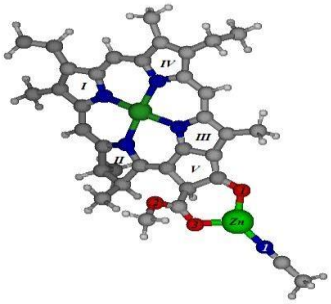
H	5.975422	-4.570374	-0.991157
H	4.318542	-5.327102	0.465108
H	3.425849	-5.496866	-1.048902
H	2.560151	-5.530559	0.488541
H	0.725719	-4.577320	-0.233173
H	-1.759381	-4.517597	-1.170909
H	-1.330705	-5.068347	1.238034
H	-3.069598	-4.935717	0.910425
H	-2.214634	-3.614890	1.730714
H	-2.531274	-2.823778	-2.979155
H	-3.872495	-3.826571	-2.391226
H	-3.754185	-2.699215	-0.159317
H	-4.085182	-2.078230	-2.574234
H	0.781153	4.461842	-0.466718
H	-1.658326	5.356789	0.110650
H	-1.570637	5.273451	-1.649755
H	-3.113281	4.974018	-0.829937
H	-4.568873	0.049897	-1.774203
H	-7.244761	0.319668	1.667818
H	-8.209767	-0.504276	0.399269
H	-7.032477	-1.427677	1.392310
N	0.046092	-0.118454	2.154806
C	-0.906763	-0.054121	2.810676
C	-2.133596	0.025236	3.592056
H	-2.168230	-0.789177	4.322416
H	-2.176648	0.981019	4.123509
H	-2.993671	-0.053447	2.914675

2.b. Chelation

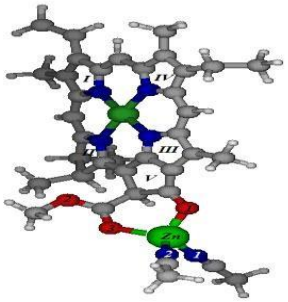
2.b.1. Case of zinc (Zn)



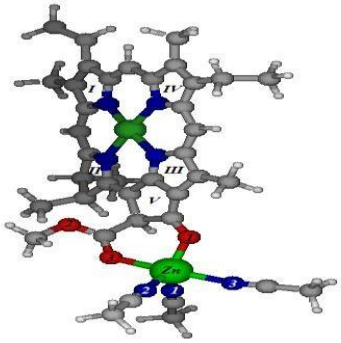
C(Zn)



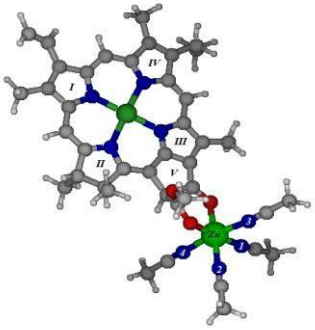
C(Zn(CH₃CN))



C(Zn(CH₃CN)₂)



C(Zn(CH₃CN)₃)



C(Zn(CH₃CN)₄)

C(Zn)

E: -3700.324977 u.a

G: -3699.809073 u.a

C	-2.059502	-0.635265	-0.335952
C	-1.513893	0.660494	-0.258463
C	-2.485927	1.724925	-0.388000
C	-3.726550	1.138711	-0.596027
C	-3.563397	-0.428052	-0.501435
C	-1.761240	2.944963	-0.370260
C	-0.401093	2.543706	-0.226353
N	-0.284251	1.142560	-0.167514
Mg	1.345642	-0.064480	-0.095010

N	0.057370	-1.774802	-0.225712
C	0.550690	-3.054746	-0.216670
C	-0.573193	-4.076840	-0.258300
C	-1.803072	-3.213210	-0.638026
C	-1.301217	-1.804675	-0.373212
C	1.886379	-3.423513	-0.143721
C	3.027123	-2.596874	-0.059726
N	2.986948	-1.236272	-0.028031
C	4.289350	-0.793219	0.055470
C	5.202465	-1.957512	0.077498
C	4.406528	-3.077061	0.011158
C	4.676478	0.535399	0.083352
C	3.841235	1.683731	0.042899
C	4.331536	3.067226	0.058259
C	3.226048	3.870697	-0.010104
C	2.063959	2.973247	-0.062567
N	2.490939	1.650033	-0.023912
C	5.774645	3.457690	0.133768
C	0.742468	3.380279	-0.159772
C	3.161142	5.370806	0.001802
C	2.903385	5.959907	1.404641
C	4.815796	-4.515734	0.049122
C	6.649954	-1.845349	0.183616
C	7.546345	-2.712127	-0.316783
C	-2.222435	-3.404941	-2.112288
C	-0.731642	-4.806478	1.091016
C	-2.304591	4.333858	-0.462779
C	-4.470327	-0.964616	0.601567
O	-5.703266	-0.707356	0.647174
O	-3.911498	-1.719624	1.491975
C	-4.732607	-2.269435	2.580886
H	5.741759	0.730528	0.127881
H	5.897673	4.541810	0.084724
H	6.352881	3.021683	-0.690076
H	6.233441	3.117483	1.070707
H	2.380642	5.713544	-0.689016

H	4.100505	5.774066	-0.390379
H	3.701773	5.682823	2.100258
H	1.956133	5.603276	1.824274
H	2.862239	7.052176	1.353090
H	0.563510	4.449195	-0.199275
H	-1.585001	5.024348	-0.911357
H	-3.217160	4.354714	-1.066207
H	-2.561697	4.727554	0.529980
H	7.025227	-0.968467	0.708384
H	7.260548	-3.583207	-0.897091
H	8.610668	-2.548076	-0.181160
H	5.769828	-4.630735	0.572108
H	4.943359	-4.931616	-0.958960
H	4.075067	-5.133904	0.566080
H	2.075103	-4.491498	-0.158840
H	-1.559770	-5.520917	1.038143
H	0.174084	-5.362743	1.349382
H	-0.934536	-4.098103	1.902626
H	-0.367933	-4.823665	-1.033873
H	-2.524274	-4.443462	-2.280421
H	-3.066712	-2.765079	-2.390359
H	-1.393109	-3.178405	-2.790735
H	-2.657393	-3.444836	0.006950
H	-4.043080	-2.882809	3.155577
H	-5.542007	-2.864322	2.157174
H	-5.126756	-1.448976	3.180988
H	-3.955339	-0.856687	-1.437570
O	-4.845075	1.698896	-0.919340
Zn	-6.369492	0.930539	-0.148763

C(Zn(CH$_3$CN))

E: -3833.183501 u.a

G: -3832.628349 u.a

C	1.422283	-0.816947	-0.015987
C	0.935986	0.517131	0.020693
C	1.958465	1.527908	-0.117079

C	3.167963	0.889618	-0.261231
C	2.936755	-0.667829	-0.111713
C	1.280599	2.793796	-0.117604
C	-0.078604	2.462520	0.024219
N	-0.263976	1.058121	0.091259
Mg	-1.958250	-0.065878	0.051878
N	-0.753926	-1.824618	-0.165690
C	-1.311843	-3.030492	-0.479136
C	-0.243501	-4.038419	-0.872000
C	1.045116	-3.391522	-0.303087
C	0.617876	-1.936045	-0.143455
C	-2.665835	-3.340276	-0.499055
C	-3.764603	-2.485352	-0.276003
N	-3.659708	-1.147919	-0.063515
C	-4.943416	-0.648906	0.049109
C	-5.907777	-1.758710	-0.063883
C	-5.168385	-2.897314	-0.283377
C	-5.260023	0.684881	0.214522
C	-4.366658	1.794225	0.246992
C	-4.787835	3.192078	0.332717
C	-3.644572	3.945851	0.288743
C	-2.527939	3.002223	0.186584
N	-3.022762	1.697925	0.171319
C	-6.210571	3.651068	0.431871
C	-1.193940	3.346272	0.105931
C	-3.518115	5.442768	0.295010
C	-3.448964	6.053433	-1.119902
C	-5.654012	-4.290393	-0.533531
C	-7.354592	-1.588607	0.006840
C	-8.231287	-2.490359	0.474431
C	1.453678	-4.055241	1.027513
C	-0.204321	-4.236357	-2.400473
C	1.903821	4.146114	-0.246691
O	4.351231	1.387092	-0.484863
Zn	5.832512	0.348947	-0.134941
O	5.059872	-1.004357	1.004115

C	3.798509	-1.079365	1.067416
O	3.199992	-1.458311	2.148978
C	3.996589	-1.784205	3.334619
H	-6.313033	0.928301	0.299992
H	-6.272798	4.734002	0.563578
H	-6.726454	3.185617	1.280487
H	-6.778633	3.399088	-0.472631
H	-2.628759	5.738535	0.865353
H	-4.370196	5.875043	0.830492
H	-4.354292	5.824114	-1.691021
H	-2.593144	5.664992	-1.682970
H	-3.351972	7.142106	-1.060101
H	-0.966847	4.406910	0.104841
H	1.162493	4.946719	-0.194729
H	2.640230	4.320451	0.547481
H	2.434464	4.245455	-1.201791
H	-7.741353	-0.633292	-0.344408
H	-7.924984	-3.445824	0.888107
H	-9.295683	-2.277579	0.482054
H	-6.674185	-4.278471	-0.927985
H	-5.665192	-4.891422	0.385330
H	-5.020781	-4.814793	-1.256758
H	-2.903638	-4.373864	-0.727194
H	0.588240	-4.941899	-2.671933
H	-1.153203	-4.636763	-2.769584
H	-0.014793	-3.288905	-2.918260
H	-0.436622	-5.007703	-0.399283
H	1.652477	-5.119053	0.861979
H	2.352565	-3.607689	1.455687
H	0.650885	-3.972177	1.768302
H	1.875379	-3.476994	-1.015313
H	3.265592	-2.107161	4.071948
H	4.524883	-0.890425	3.668852
H	4.698701	-2.582497	3.092729
H	3.365077	-1.169568	-0.994510
N	7.676001	0.431975	-0.589583

C	8.795143	0.526675	-0.866889
C	10.195602	0.643442	-1.219457
H	10.633699	-0.355745	-1.322692
H	10.726864	1.193521	-0.434272
H	10.290956	1.183357	-2.168423

C(Zn(CH$_3$CN)$_2$)

E: -3966.006222 u.a

G: -3965.411644 u.a

C	-0.996129	-0.871429	-0.067936
C	-0.540168	0.473921	0.004424
C	-1.579264	1.444629	0.209317
C	-2.789649	0.776252	0.288079
C	-2.514955	-0.764605	0.027410
C	-0.932630	2.718764	0.303458
C	0.438622	2.430424	0.144050
N	0.651907	1.042976	-0.022958
Mg	2.368320	-0.042619	-0.074008
N	1.203751	-1.839507	0.006526
C	1.785163	-3.051315	0.229072
C	0.736603	-4.108125	0.541540
C	-0.559550	-3.451549	0.002348
C	-0.168589	-1.976977	-0.030406
C	3.146419	-3.334554	0.230333
C	4.225958	-2.443067	0.073077
N	4.093340	-1.095333	-0.039104
C	5.365688	-0.562601	-0.116524
C	6.352189	-1.655996	-0.088302
C	5.637753	-2.823554	0.047724
C	5.654307	0.786957	-0.182767
C	4.739661	1.876434	-0.131467
C	5.129109	3.283981	-0.114436
C	3.968890	4.007463	-0.012436
C	2.874611	3.035999	0.022052
N	3.396854	1.746886	-0.060319
C	6.540773	3.782277	-0.181660

C	1.531417	3.342358	0.129689
C	3.811884	5.498171	0.091175
C	3.749019	6.004324	1.546786
C	6.154335	-4.220691	0.192217
C	7.795686	-1.452242	-0.150560
C	8.686855	-2.294934	-0.694009
C	-0.921087	-4.013606	-1.387194
C	0.687916	-4.406530	2.052762
C	-1.584036	4.044657	0.530956
O	-3.970779	1.225101	0.514003
Zn	-5.516796	0.176659	0.143571
O	-4.620093	-1.059813	-1.125233
C	-3.367491	-1.108125	-1.178353
O	-2.741552	-1.398103	-2.280949
C	-3.523632	-1.654510	-3.486390
H	6.702119	1.057252	-0.251643
H	6.576791	4.872481	-0.247809
H	7.069301	3.381565	-1.055119
H	7.113838	3.490160	0.707549
H	2.909072	5.815584	-0.445429
H	4.647803	5.986274	-0.421783
H	4.665837	5.752430	2.089508
H	2.908232	5.558490	2.089760
H	3.630114	7.092448	1.567979
H	1.280940	4.394800	0.210794
H	-0.864811	4.866602	0.504915
H	-2.349450	4.244713	-0.228826
H	-2.087550	4.074132	1.505519
H	8.165781	-0.521339	0.276367
H	8.395621	-3.218973	-1.183196
H	9.747108	-2.062118	-0.688468
H	7.178481	-4.215875	0.576259
H	6.166788	-4.754497	-0.767309
H	5.539462	-4.808378	0.882087
H	3.405558	-4.377509	0.379943
H	-0.090340	-5.146352	2.269895

H	1.642822	-4.807713	2.405373
H	0.471649	-3.498990	2.628556
H	0.955761	-5.039823	0.008305
H	-1.094716	-5.092435	-1.315458
H	-1.820046	-3.551814	-1.798833
H	-0.103496	-3.849278	-2.097688
H	-1.400981	-3.617915	0.686829
H	-2.784838	-1.902155	-4.245239
H	-4.077743	-0.754587	-3.757181
H	-4.206540	-2.486771	-3.311784
H	-2.936237	-1.333090	0.870894
N	-6.957838	1.180884	-0.787458
C	-7.748780	1.829291	-1.326571
C	-8.745673	2.641816	-2.002064
H	-9.514827	1.996596	-2.439549
H	-8.269282	3.225748	-2.796628
H	-9.212482	3.324922	-1.284502
N	-6.429881	-0.720091	1.667351
C	-6.946178	-1.202581	2.582686
C	-7.599328	-1.806215	3.731269
H	-7.174810	-1.397065	4.654230
H	-7.450220	-2.891011	3.714153
H	-8.672537	-1.590104	3.701572

C(Zn(CH$_3$CN)$_3$)

E: -4098.793135 u.a

G: -4098.160188 u.a

N	-3.750654	1.758097	0.151616
C	-5.093155	1.903792	0.216494
C	-5.459880	3.315193	0.282884
C	-4.286834	4.024554	0.239664
C	-3.208121	3.040226	0.156242
C	-6.023195	0.827986	0.192345
C	-5.753077	-0.520764	0.053604
N	-4.488265	-1.067897	-0.036729

C	-4.638536	-2.406720	-0.220424
C	-6.055916	-2.765148	-0.233411
C	-6.754607	-1.595001	-0.045963
C	-3.571322	-3.305799	-0.406551
C	-2.204823	-3.044096	-0.375425
N	-1.609330	-1.854279	-0.093913
C	-0.237387	-2.012085	-0.049330
C	0.133542	-3.488808	-0.148315
C	-1.169247	-4.105099	-0.718592
Mg	-2.747036	-0.045471	0.071644
N	-1.016935	1.015309	0.098199
C	0.169017	0.430384	0.048889
C	1.223302	1.392501	-0.078285
C	0.600299	2.677841	-0.096827
C	-0.781041	2.403949	0.024765
C	2.430972	0.706060	-0.175254
C	2.127136	-0.835613	0.000393
C	0.604818	-0.924073	0.050769
O	3.615191	1.143755	-0.346041
Zn	5.262585	0.142492	-0.103907
N	6.271256	1.507847	-1.390200
C	6.646781	2.340020	-2.100111
C	7.124722	3.385573	-2.993512
C	2.944656	-1.222151	1.219776
O	2.261865	-1.533243	2.296017
C	3.001299	-1.816563	3.514130
C	1.272882	4.006399	-0.229172
C	-1.857647	3.330753	0.084185
C	-1.114510	-4.351114	-2.238778
C	0.490700	-4.116426	1.213513
C	-8.195955	-1.372311	0.005898
C	-9.109353	-2.227835	0.488736
C	-6.591795	-4.144463	-0.457643
C	-6.864034	3.832508	0.366495
C	-4.105047	5.516191	0.232666
C	-4.010393	6.112227	-1.186539

O	4.184460	-1.173614	1.203652
N	5.877207	-1.466784	-1.215437
C	6.279875	-2.366699	-1.819137
C	6.784607	-3.499075	-2.580621
H	-7.067947	1.109269	0.264247
H	-6.882892	4.916749	0.502749
H	-7.409856	3.385592	1.206287
H	-7.431566	3.608529	-0.545799
H	-3.205921	5.783872	0.801726
H	-4.941157	5.985624	0.762570
H	-4.922710	5.911832	-1.757639
H	-3.169167	5.685402	-1.743902
H	-3.872105	7.197287	-1.137494
H	-1.589655	4.382138	0.074005
H	0.575951	4.836413	-0.090074
H	2.077709	4.116201	0.507507
H	1.730074	4.120320	-1.220735
H	-8.544567	-0.413971	-0.376242
H	-8.841229	-3.181820	0.931506
H	-10.165593	-1.977422	0.478648
H	-7.610032	-4.103616	-0.855233
H	-6.626877	-4.727194	0.472478
H	-5.975535	-4.705345	-1.168324
H	-3.843939	-4.336913	-0.606155
H	-0.347661	-5.096524	-2.477168
H	-2.073567	-4.722060	-2.612832
H	-0.877538	-3.427522	-2.779880
H	-1.406150	-5.051402	-0.219491
H	0.654265	-5.192840	1.093877
H	1.393109	-3.679664	1.644699
H	-0.325021	-3.976437	1.931423
H	0.973217	-3.633451	-0.839969
H	2.240270	-2.062202	4.252025
H	3.564943	-0.931848	3.815431
H	3.677208	-2.657947	3.352672
H	2.570661	-1.373001	-0.850217

H	7.839933	-3.340417	-2.825006
H	6.214795	-3.605435	-3.509392
H	6.687467	-4.416552	-1.991421
H	6.920040	4.368377	-2.557141
H	6.614152	3.311242	-3.958917
H	8.203008	3.280741	-3.149690
N	6.512064	0.555550	1.458617
C	7.210675	0.818083	2.340997
C	8.088186	1.148260	3.453503
H	8.163488	0.293852	4.133704
H	7.685972	2.007871	3.999387
H	9.086221	1.397148	3.078822

C(Zn(CH$_3$CN)$_4$)

E: -4231.565849 u.a

G: -4230.898298 u.a

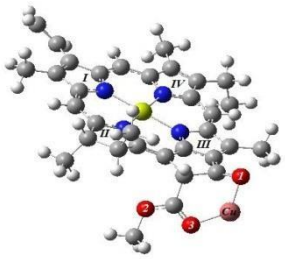
N	4.064106	1.740683	-0.098930
C	5.407987	1.884491	-0.167297
C	5.777470	3.295474	-0.178546
C	4.605929	4.005558	-0.098382
C	3.526090	3.022063	-0.047968
C	6.333212	0.806107	-0.193258
C	6.059533	-0.547086	-0.106269
N	4.793874	-1.093379	-0.027631
C	4.940779	-2.439272	0.103040
C	6.356383	-2.801542	0.090636
C	7.057469	-1.626582	-0.056873
C	3.871866	-3.340969	0.262985
C	2.505777	-3.073583	0.250880
N	1.912700	-1.873133	0.018148
C	0.538782	-2.024541	-0.022814
C	0.167212	-3.504294	0.013473
C	1.467880	-4.142564	0.563172
Mg	3.054597	-0.061986	-0.084875
N	1.328269	1.002178	-0.054441
C	0.137602	0.420403	-0.016704

C	-0.908733	1.378686	0.153924
C	-0.284360	2.656651	0.215380
C	1.099612	2.384694	0.073729
C	-2.130680	0.695840	0.224957
C	-1.823797	-0.846584	0.004828
C	-0.301740	-0.932127	-0.070118
O	-3.303155	1.128765	0.398323
Zn	-5.015900	0.114353	0.116946
N	-6.128181	1.517904	1.279043
C	-6.604890	2.350148	1.924354
C	-7.209336	3.397218	2.737074
C	-2.666180	-1.219566	-1.197670
O	-2.005650	-1.475216	-2.306524
C	-2.779258	-1.754960	-3.501717
C	-0.944699	3.983470	0.418579
C	2.174589	3.311312	0.044639
C	1.415074	-4.433187	2.075234
C	-0.178512	-4.074271	-1.376379
C	8.499454	-1.407315	-0.112381
C	9.405478	-2.245579	-0.637352
C	6.890489	-4.189955	0.256264
C	7.182195	3.813564	-0.249740
C	4.429610	5.496428	-0.029038
C	4.356001	6.035712	1.413766
O	-3.903612	-1.213477	-1.145725
N	-4.810210	-1.133779	1.913729
C	-4.747467	-1.704897	2.918061
C	-4.672139	-2.427033	4.181793
H	7.378612	1.086236	-0.261564
H	7.202257	4.902016	-0.347489
H	7.723975	3.396064	-1.107092
H	7.753456	3.556585	0.651501
H	3.523761	5.789687	-0.574420
H	5.260213	5.984401	-0.551078
H	5.274756	5.808818	1.964378
H	3.520266	5.589803	1.964492

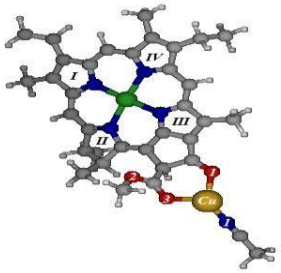
H	4.221783	7.122500	1.410713
H	1.907638	4.361746	0.101580
H	-0.323024	4.810257	0.063562
H	-1.903514	4.028424	-0.108694
H	-1.154858	4.164841	1.481430
H	8.855195	-0.466483	0.305199
H	9.129676	-3.179817	-1.116077
H	10.462796	-1.999676	-0.626216
H	7.911756	-4.167124	0.647517
H	6.917160	-4.735882	-0.696227
H	6.277928	-4.777091	0.948780
H	4.142145	-4.379900	0.421607
H	0.645907	-5.182629	2.293414
H	2.373631	-4.818131	2.436351
H	1.183190	-3.524538	2.643469
H	1.700882	-5.074644	0.036195
H	-0.346759	-5.154221	-1.303266
H	-1.074206	-3.615380	-1.797708
H	0.645363	-3.907558	-2.079178
H	-0.677282	-3.679301	0.692230
H	-2.039847	-1.902224	-4.286576
H	-3.429657	-0.908522	-3.728554
H	-3.377522	-2.656152	-3.355258
H	-2.251562	-1.396031	0.853523
H	-5.632967	-2.368058	4.702676
H	-3.896040	-1.988780	4.817047
H	-4.432262	-3.479013	3.998272
H	-6.449872	3.853568	3.379664
H	-8.001143	2.974915	3.363602
H	-7.640184	4.169109	2.091803
N	-6.734673	-1.036241	-0.385868
C	-7.644378	-1.677054	-0.698434
C	-8.790645	-2.484431	-1.094308
H	-8.994685	-3.243334	-0.332579
H	-8.583925	-2.982719	-2.046602
H	-9.673958	-1.848390	-1.208805

N	-5.413866	1.335806	-1.666141
C	-5.544196	2.073885	-2.547188
C	-5.712749	3.000806	-3.659610
H	-6.222628	2.502216	-4.489801
H	-4.735552	3.355113	-4.002215
H	-6.310124	3.860988	-3.341771

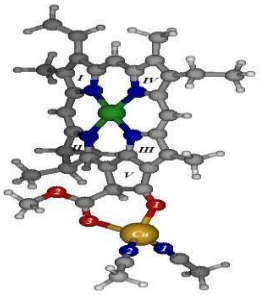
2.b.2. Case of cooper (Cu)



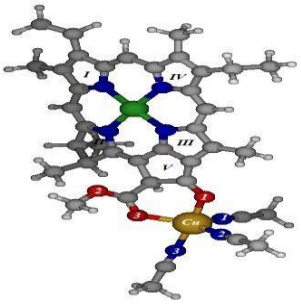
C(Cu)



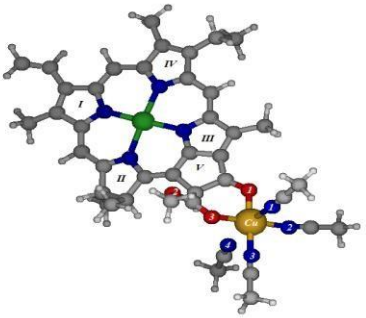
C(Cu(CH₃CN))



C(Cu(CH₃CN)₂)



C(Cu(CH₃CN)₃)



C(Cu(CH₃CN)₄)

Cartesian coordinates

C(Cu)

E: -3561.506307 u.a

G: -3560.991516 u.a

C	-2.154132	-0.703163	-0.364970
C	-1.630367	0.611096	-0.263076
C	-2.597123	1.647723	-0.486537
C	-3.862319	1.040184	-0.767389
C	-3.677101	-0.527821	-0.515477

C	-1.911337	2.859621	-0.499855
C	-0.515250	2.488821	-0.266243
N	-0.401447	1.101697	-0.138660
Mg	1.247450	-0.071627	-0.066492
N	-0.004887	-1.799637	-0.261871
C	0.498862	-3.053828	-0.278014
C	-0.590723	-4.102237	-0.397568
C	-1.829677	-3.255582	-0.782646
C	-1.379970	-1.847784	-0.437412
C	1.858790	-3.412968	-0.166775
C	2.971904	-2.588832	-0.034389
N	2.913893	-1.211755	0.014982
C	4.192270	-0.763784	0.129433
C	5.130139	-1.904574	0.165093
C	4.360996	-3.040220	0.066793
C	4.568761	0.594774	0.166898
C	3.737809	1.712401	0.099156
C	4.194455	3.108700	0.104012
C	3.071080	3.884407	-0.007528
C	1.937143	2.955727	-0.070026
N	2.366768	1.661587	-0.000558
C	5.624279	3.535647	0.209369
C	0.581763	3.341400	-0.214199
C	2.966691	5.382703	-0.028533
C	2.627880	5.992408	1.347624
C	4.800140	-4.469102	0.096155
C	6.573505	-1.762840	0.310712
C	7.498949	-2.591314	-0.199338
C	-2.183381	-3.381797	-2.282127
C	-0.767570	-4.893186	0.916087
C	-2.444851	4.234841	-0.715997
C	-4.478718	-0.983705	0.724184
O	-5.399780	-0.316069	1.244712
O	-4.139127	-2.147365	1.195117
C	-4.886526	-2.672771	2.344606
H	5.632502	0.793087	0.233264

H	5.724443	4.620201	0.130405
H	6.236455	3.087922	-0.582838
H	6.060764	3.234105	1.169862
H	2.212177	5.691429	-0.763367
H	3.912594	5.802873	-0.385110
H	3.398579	5.749390	2.085806
H	1.670456	5.621556	1.731128
H	2.562623	7.081948	1.271402
H	0.387934	4.404648	-0.307244
H	-1.859886	4.774826	-1.469274
H	-3.483747	4.204349	-1.051252
H	-2.398085	4.825201	0.209036
H	6.915887	-0.900591	0.880682
H	7.244965	-3.444550	-0.819935
H	8.556071	-2.413400	-0.029391
H	5.747281	-4.568779	0.634537
H	4.955747	-4.868106	-0.914832
H	4.062970	-5.109509	0.590715
H	2.054361	-4.479405	-0.202078
H	-1.569443	-5.629511	0.802009
H	0.145046	-5.433583	1.184299
H	-1.023171	-4.226887	1.747844
H	-0.335150	-4.809909	-1.195154
H	-2.455407	-4.416647	-2.512023
H	-3.030409	-2.746606	-2.560390
H	-1.333610	-3.104283	-2.915052
H	-2.701917	-3.539590	-0.188648
H	-4.433781	-3.640631	2.546214
H	-5.938050	-2.774453	2.074545
H	-4.770393	-1.994261	3.190048
H	-4.098004	-1.068710	-1.374922
O	-4.839892	1.572457	-1.402956
Cu	-5.718184	1.185942	0.158043

C(Cu(CH3CN))

E: -3694.351283 u.a

G: -3693.796654 u.a

C	1.489154	-0.697631	0.104747
C	0.944188	0.612809	0.105513
C	1.922735	1.657355	0.013883
C	3.217615	1.054934	-0.050757
C	3.006878	-0.512177	0.082216
C	1.240282	2.869848	0.003978
C	-0.172622	2.488949	0.091176
N	-0.292766	1.099171	0.140051
Mg	-1.931848	-0.080177	0.075233
N	-0.657071	-1.792781	-0.081948
C	-1.145879	-3.013312	-0.389706
C	-0.038210	-3.997404	-0.709078
C	1.211315	-3.285351	-0.130634
C	0.729760	-1.847919	-0.016747
C	-2.507001	-3.380981	-0.459162
C	-3.634441	-2.580559	-0.305730
N	-3.591893	-1.217921	-0.102029
C	-4.878589	-0.779399	-0.060545
C	-5.807084	-1.918104	-0.208874
C	-5.024308	-3.036322	-0.375696
C	-5.263835	0.568745	0.085518
C	-4.435572	1.689533	0.150682
C	-4.897865	3.081936	0.219971
C	-3.773803	3.864526	0.216006
C	-2.633392	2.943666	0.155547
N	-3.061666	1.647116	0.125406
C	-6.333589	3.500168	0.267395
C	-1.273400	3.338255	0.121693
C	-3.677490	5.363695	0.230648
C	-3.507968	5.978410	-1.174393
C	-5.454793	-4.445825	-0.626764
C	-7.259288	-1.787668	-0.210635
C	-8.130009	-2.709335	0.230335
C	1.620418	-3.898054	1.226474
C	0.048451	-4.261250	-2.228365

C	1.788125	4.252865	-0.087421
O	4.339472	1.571088	-0.144803
Cu	5.928651	0.450629	-0.086407
O	5.080330	-0.785286	1.240899
C	3.850953	-0.882390	1.294783
O	3.189581	-1.199701	2.384428
C	3.974429	-1.448408	3.590842
H	-6.330278	0.759467	0.125386
H	-6.431386	4.582528	0.376090
H	-6.860177	3.033178	1.108500
H	-6.863651	3.213301	-0.649582
H	-2.843042	5.675035	0.871813
H	-4.577483	5.777038	0.697325
H	-4.360749	5.733808	-1.815485
H	-2.602602	5.610976	-1.670763
H	-3.437343	7.068085	-1.104251
H	-1.077912	4.405212	0.113983
H	1.489547	4.854552	0.780307
H	2.878752	4.239827	-0.136547
H	1.410262	4.768306	-0.979387
H	-7.657147	-0.851560	-0.599063
H	-7.815908	-3.646900	0.677747
H	-9.199376	-2.530303	0.180914
H	-6.447076	-4.468678	-1.086653
H	-5.511956	-5.025889	0.303670
H	-4.762186	-4.968336	-1.294353
H	-2.686984	-4.430757	-0.665158
H	0.869415	-4.953671	-2.439424
H	-0.874904	-4.709480	-2.607258
H	0.228565	-3.333568	-2.783220
H	-0.219763	-4.951580	-0.201530
H	1.884836	-4.950672	1.085031
H	2.477224	-3.386228	1.665361
H	0.793847	-3.847838	1.943769
H	2.060837	-3.351092	-0.820865
H	3.241175	-1.712706	4.349771

H	4.516441	-0.542216	3.865661
H	4.673992	-2.266455	3.413703
H	3.488603	-0.988279	-0.782877
N	7.486483	0.309969	-0.982322
C	8.526072	0.264077	-1.493705
C	9.823419	0.203854	-2.148388
H	10.220062	-0.815782	-2.106701
H	10.523929	0.878059	-1.644535
H	9.729135	0.509624	-3.195528

C(Cu(CH$_3$CN)$_2$)

E: -3827.153670 u.a

G: -3826.564088 u.a

C	-0.999973	-0.838511	-0.044164
C	-0.523106	0.493419	0.013542
C	-1.549872	1.479410	0.196312
C	-2.815720	0.799477	0.272519
C	-2.525220	-0.738297	0.034971
C	-0.931528	2.718650	0.255060
C	0.498665	2.419219	0.101291
N	0.688061	1.045076	-0.031211
Mg	2.384101	-0.049145	-0.083547
N	1.204627	-1.830309	0.014552
C	1.765297	-3.042376	0.232833
C	0.715781	-4.097442	0.524745
C	-0.581951	-3.417451	0.019110
C	-0.176132	-1.952995	-0.015120
C	3.141214	-3.340698	0.240051
C	4.221899	-2.471950	0.096543
N	4.104158	-1.106922	-0.027655
C	5.367016	-0.598242	-0.089067
C	6.354314	-1.694597	-0.037219
C	5.634314	-2.858671	0.093831
C	5.677673	0.770991	-0.172881
C	4.790011	1.849980	-0.147112
C	5.178420	3.266311	-0.157216

C	4.017773	3.987604	-0.069209
C	2.927396	3.007196	-0.018448
N	3.423837	1.734385	-0.075224
C	6.588413	3.761380	-0.233582
C	1.553072	3.326756	0.084097
C	3.845795	5.478340	0.001764
C	3.716080	6.010296	1.444119
C	6.142419	-4.256313	0.250045
C	7.797782	-1.491358	-0.079645
C	8.693974	-2.340970	-0.605533
C	-0.988918	-3.961281	-1.367729
C	0.684437	-4.446719	2.028238
C	-1.541921	4.065926	0.445548
O	-3.949694	1.246455	0.454782
Cu	-5.666130	0.202979	0.235595
O	-4.608169	-1.080375	-1.093104
C	-3.383576	-1.084529	-1.174202
O	-2.717841	-1.279104	-2.301025
C	-3.511828	-1.505767	-3.498935
H	6.730593	1.020636	-0.238906
H	6.626153	4.850084	-0.314051
H	7.113693	3.346040	-1.102055
H	7.160162	3.478612	0.659453
H	2.965310	5.777664	-0.580814
H	4.699310	5.962768	-0.483871
H	4.611042	5.777961	2.030014
H	2.856131	5.570478	1.961894
H	3.587757	7.097052	1.436783
H	1.302691	4.379509	0.159721
H	-1.297701	4.733423	-0.390354
H	-2.628816	3.993878	0.521753
H	-1.165288	4.544664	1.358249
H	8.164370	-0.559837	0.348666
H	8.406927	-3.265929	-1.095345
H	9.754762	-2.112125	-0.584488
H	7.156267	-4.253991	0.660629

H	6.179520	-4.785968	-0.710997
H	5.508284	-4.844353	0.921405
H	3.382763	-4.388942	0.381007
H	-0.095532	-5.189781	2.222551
H	1.639373	-4.866858	2.357955
H	0.475269	-3.560027	2.637402
H	0.928274	-5.012424	-0.039744
H	-1.204192	-5.031725	-1.290561
H	-1.873532	-3.459032	-1.759643
H	-0.177379	-3.828197	-2.091654
H	-1.412090	-3.569770	0.719203
H	-2.784371	-1.658899	-4.293787
H	-4.132620	-0.630829	-3.699536
H	-4.142014	-2.386949	-3.367414
H	-2.957078	-1.288156	0.882178
N	-6.987008	0.943267	-0.903746
C	-7.862381	1.383620	-1.521650
C	-8.970131	1.932573	-2.291535
H	-9.571653	1.120772	-2.712919
H	-8.590879	2.554607	-3.108464
H	-9.606346	2.545977	-1.645471
N	-6.400415	-0.473239	1.833256
C	-6.968353	-0.813196	2.784658
C	-7.694513	-1.234665	3.974581
H	-7.289755	-0.733135	4.859458
H	-7.603371	-2.317518	4.106900
H	-8.754405	-0.978647	3.876481

C(Cu(CH$_3$CN)$_3$)

E: -3959.930353 u.a

G: -3959.298827 u.a

N	3.736740	1.702636	-0.158486
C	5.082500	1.816524	-0.206156
C	5.485124	3.219203	-0.245198
C	4.329576	3.956847	-0.204040
C	3.225805	2.998090	-0.149049

C	5.986114	0.717026	-0.189786
C	5.682101	-0.626116	-0.075929
N	4.402820	-1.143655	-0.006972
C	4.519004	-2.487636	0.156889
C	5.926473	-2.881875	0.178038
C	6.656013	-1.726620	0.016179
C	3.427010	-3.363752	0.319354
C	2.069058	-3.069377	0.277703
N	1.504839	-1.859079	0.007732
C	0.132921	-1.983984	-0.055928
C	-0.275156	-3.452142	0.011885
C	1.002811	-4.107817	0.593929
Mg	2.689365	-0.076803	-0.122172
N	0.986058	1.026874	-0.148583
C	-0.214184	0.469546	-0.121705
C	-1.246290	1.455863	0.005639
C	-0.594058	2.725286	0.045964
C	0.782621	2.418672	-0.058391
C	-2.472552	0.796463	0.049671
C	-2.201073	-0.750124	-0.117095
C	-0.682809	-0.872376	-0.153448
O	-3.652067	1.271201	0.127454
Cu	-5.215437	0.166718	0.121187
N	-5.094421	-0.140091	2.160510
C	-5.072107	-0.161208	3.316874
C	-5.042823	-0.190005	4.772437
C	-3.035261	-1.113044	-1.331450
O	-2.381109	-1.436990	-2.417279
C	-3.149117	-1.684452	-3.629848
C	-1.236006	4.068449	0.182192
C	1.882297	3.320298	-0.089020
C	0.919479	-4.369514	2.110300
C	-0.619918	-4.047464	-1.367924
C	8.102553	-1.538902	-0.018869
C	8.998978	-2.410568	-0.505048
C	6.425508	-4.277574	0.385290

C	6.902783	3.701741	-0.303945
C	4.184624	5.452197	-0.175500
C	4.084812	6.028038	1.251785
O	-4.273733	-1.031379	-1.292104
N	-6.808862	-1.000237	-0.064506
C	-7.727417	-1.683289	-0.217014
C	-8.885180	-2.543520	-0.411274
H	7.038060	0.973899	-0.246502
H	6.951062	4.788154	-0.412221
H	7.444296	3.262102	-1.150362
H	7.455857	3.439855	0.607077
H	3.300603	5.751228	-0.752556
H	5.039498	5.908581	-0.686329
H	4.983454	5.795505	1.832287
H	3.224936	5.614676	1.790571
H	3.974960	7.116846	1.217848
H	1.639863	4.377599	-0.066583
H	-0.514220	4.882066	0.077858
H	-2.014730	4.210407	-0.576772
H	-1.720673	4.178643	1.160905
H	8.471232	-0.594650	0.379038
H	8.711570	-3.351478	-0.963336
H	10.060883	-2.186427	-0.482341
H	7.439432	-4.268488	0.795668
H	6.457669	-4.845334	-0.554091
H	5.787227	-4.834911	1.079061
H	3.672821	-4.403731	0.507186
H	0.129211	-5.096198	2.328709
H	1.862625	-4.770967	2.493177
H	0.700240	-3.445968	2.659083
H	1.223189	-5.054198	0.087704
H	-0.816032	-5.120370	-1.268784
H	-1.499976	-3.578547	-1.810815
H	0.215005	-3.919368	-2.065677
H	-1.131537	-3.588488	0.684444
H	-2.403957	-1.920124	-4.386669

H	-3.710409	-0.787618	-3.896838
H	-3.828112	-2.523783	-3.472224
H	-2.657224	-1.280560	0.731877
H	-9.737423	-2.154872	0.155212
H	-8.657976	-3.557155	-0.066099
H	-9.147355	-2.577923	-1.473567
H	-4.167408	0.355873	5.138114
H	-4.994113	-1.225047	5.125227
H	-5.947683	0.280195	5.170657
N	-6.302428	1.824011	-0.485235
C	-6.814540	2.804219	-0.822342
C	-7.458117	4.038992	-1.248690
H	-7.892076	3.908729	-2.245096
H	-6.722153	4.848391	-1.282446
H	-8.252635	4.307809	-0.545437

C(Cu(CH$_3$CN)$_4$)

E: -4092.699354 u.a

G: -4092.030260 u.a

N	4.035470	1.735687	-0.065869
C	5.381326	1.860312	-0.113328
C	5.773894	3.265021	-0.072655
C	4.613364	3.991096	0.018320
C	3.516916	3.023862	0.022807
C	6.290658	0.768227	-0.162324
C	5.994861	-0.581772	-0.118351
N	4.719565	-1.109555	-0.070876
C	4.843645	-2.460084	0.026245
C	6.253603	-2.845328	0.022208
C	6.975175	-1.678732	-0.085858
C	3.757963	-3.347837	0.150497
C	2.397055	-3.057823	0.125141
N	1.825809	-1.842831	-0.091204
C	0.451124	-1.973014	-0.158396
C	0.057766	-3.447686	-0.162115
C	1.337829	-4.115071	0.401172

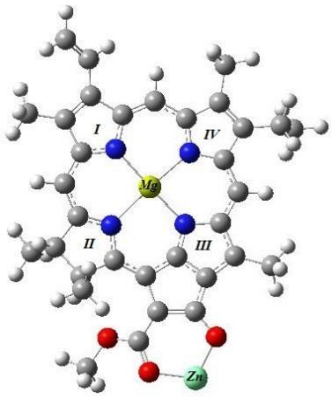
Mg	2.998199	-0.049493	-0.124290
N	1.287973	1.041553	-0.081569
C	0.089975	0.477077	-0.081438
C	-0.944963	1.446608	0.113371
C	-0.300357	2.713319	0.230915
C	1.078381	2.423569	0.096083
C	-2.169554	0.776668	0.139650
C	-1.892074	-0.751589	-0.131115
C	-0.371357	-0.865575	-0.190447
O	-3.344954	1.228042	0.304743
Cu	-4.939474	0.191101	0.019946
N	-5.840028	1.253687	1.459675
C	-6.268475	1.963992	2.262695
C	-6.808937	2.854505	3.280121
C	-2.728083	-1.048530	-1.358008
O	-2.085289	-1.396497	-2.443154
C	-2.857072	-1.601661	-3.659763
C	-0.947434	4.040636	0.465630
C	2.170541	3.332378	0.111261
C	1.252951	-4.428389	1.907361
C	-0.263707	-3.986846	-1.570235
C	8.420884	-1.481281	-0.118646
C	9.319234	-2.320556	-0.655189
C	6.762776	-4.246193	0.158292
C	7.187818	3.760842	-0.109706
C	4.459900	5.481324	0.136973
C	4.371844	5.970767	1.596734
O	-3.964368	-0.911121	-1.342389
N	-4.470660	-1.563631	1.972852
C	-4.433139	-2.201269	2.941164
C	-4.389511	-3.004942	4.159437
H	7.340947	1.033914	-0.209567
H	7.227571	4.851485	-0.168288
H	7.732346	3.364608	-0.975353
H	7.743631	3.461838	0.788189
H	3.568042	5.808609	-0.412064

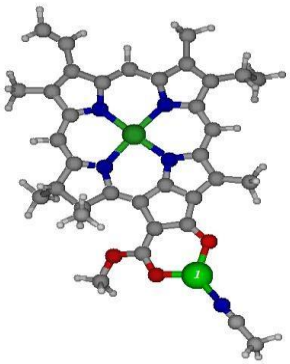
H	5.306741	5.972847	-0.354577
H	5.277204	5.707930	2.153442
H	3.519280	5.521442	2.118173
H	4.257005	7.059214	1.629749
H	1.921575	4.384704	0.201050
H	-0.249087	4.869601	0.325763
H	-1.792513	4.192228	-0.215811
H	-1.344538	4.112107	1.486865
H	8.786694	-0.557411	0.327050
H	9.033857	-3.237327	-1.161248
H	10.380147	-2.092333	-0.626132
H	7.779314	-4.250382	0.562218
H	6.792152	-4.767792	-0.807620
H	6.132233	-4.840583	0.828100
H	4.009103	-4.394279	0.289719
H	0.468175	-5.168836	2.099015
H	2.198438	-4.834814	2.279194
H	1.025343	-3.525350	2.486180
H	1.566293	-5.042317	-0.136038
H	-0.442967	-5.066299	-1.520692
H	-1.146571	-3.512358	-2.000389
H	0.576296	-3.815303	-2.252497
H	-0.803770	-3.623892	0.494312
H	-2.116431	-1.834619	-4.422002
H	-3.403566	-0.689984	-3.905335
H	-3.551114	-2.432153	-3.520793
H	-2.347077	-1.326762	0.686939
H	-5.168918	-3.772666	4.133020
H	-4.548182	-2.369354	5.036021
H	-3.415505	-3.495047	4.252733
H	-5.993241	3.395892	3.769524
H	-7.356279	2.276474	4.031191
H	-7.490595	3.576507	2.819721
N	-6.549106	-0.937270	-0.273607
C	-7.473490	-1.588199	-0.505841
C	-8.639821	-2.409789	-0.796795

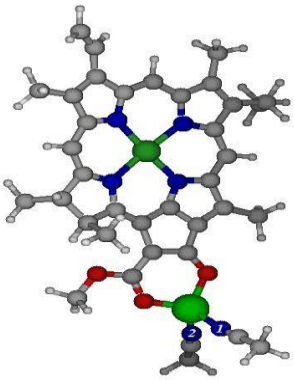
H	-8.680743	-3.258374	-0.106819
H	-8.582354	-2.786442	-1.822851
H	-9.551786	-1.814780	-0.686012
N	-5.637464	1.627568	-1.702433
C	-5.888865	2.453754	-2.474206
C	-6.209309	3.489113	-3.451006
H	-5.666690	3.306662	-4.383656
H	-5.924743	4.471946	-3.062881
H	-7.283384	3.488145	-3.660795

2.c. Deprotonation

2.c.1. Case of zinc







D(Zn) *D(Zn(CH3CN))* *D(Zn(CH3CN)2)*

Cartesian coordinates

D(Zn)

E: -3700.031889 u.a

G: -3699.527989 u.a

C	-3.558562	-0.097730	-0.092074
C	-2.112942	-0.464705	-0.012521
C	-1.443477	0.805416	-0.032809
C	-2.338664	1.896965	-0.181674

C	-3.648449	1.361989	-0.256940
C	-1.564360	3.070853	-0.241007
C	-0.213819	2.608638	-0.127731
N	-0.178403	1.209287	-0.015622
Mg	1.373356	-0.074125	0.014177
N	-0.041595	-1.708835	-0.024161
C	0.396265	-2.996957	-0.070789
C	-0.762134	-3.980397	-0.098898
C	-1.979127	-3.062757	-0.354653
C	-1.420790	-1.671713	-0.087072
C	1.716860	-3.437285	-0.064559
C	2.909063	-2.688486	-0.022115
N	2.957949	-1.330800	0.008804
C	4.289287	-0.967240	0.032282
C	5.121054	-2.175150	0.019747
C	4.255428	-3.247620	-0.010236
C	4.753489	0.338220	0.029246
C	3.990729	1.533511	0.000731
N	2.633860	1.573805	-0.021255
C	2.277504	2.909780	-0.071992
C	3.473458	3.739080	-0.073891
C	4.545144	2.876880	-0.025622
C	3.492920	5.242099	-0.081686
C	3.330776	5.861034	1.321144
C	0.964195	3.376947	-0.135156
C	6.007884	3.205836	-0.002619
C	6.579902	-2.160903	0.066203
C	7.401127	-3.069888	-0.480253
C	4.582337	-4.708420	0.014046
C	-2.036020	4.477691	-0.426653
C	-2.528161	-3.175888	-1.790429
C	-0.870296	-4.778053	1.214068
O	-4.708999	2.118963	-0.414505
Zn	-6.281433	1.235022	-0.071446
O	-5.927797	-0.577856	0.031230
C	-4.678798	-0.881979	0.256769

O	-4.464294	-2.036774	0.881360
C	-5.590704	-2.912807	1.113991
H	2.384962	5.556856	1.782867
H	2.700910	5.621609	-0.739786
H	4.434228	5.591383	-0.520700
H	3.346584	6.954685	1.264032
H	4.141059	5.542931	1.985506
H	6.177162	4.280387	-0.110876
H	6.548601	2.704918	-0.815116
H	6.477698	2.894818	0.939313
H	5.830552	0.467597	0.028979
H	7.038789	-3.912598	-1.060282
H	8.478291	-2.975923	-0.381964
H	7.029194	-1.319356	0.592035
H	4.630413	-5.136524	-0.996356
H	3.833142	-5.279084	0.572716
H	5.554865	-4.879216	0.485607
H	1.839106	-4.514803	-0.107137
H	0.838855	4.452950	-0.205712
H	-2.213682	4.696741	-1.488193
H	-1.309196	5.207452	-0.058269
H	-2.982847	4.644413	0.096082
H	-1.722859	-5.465335	1.173050
H	0.030985	-5.371832	1.396838
H	-1.011133	-4.108148	2.070116
H	-0.626651	-4.688576	-0.925713
H	-2.780795	-3.292746	0.345432
H	-2.896528	-4.190808	-1.977337
H	-1.747918	-2.958020	-2.528685
H	-3.352909	-2.476470	-1.961081
H	-5.156747	-3.815752	1.541968
H	-6.104566	-3.136971	0.176736
H	-6.287521	-2.456394	1.819086

D(Zn(CH$_3$CN))

E: -3832.871468 u.a

G: -3832.327286 u.a

C	-2.918584	-0.621616	0.080010
C	-1.417555	-0.822615	0.093584
C	-0.907511	0.513556	0.077441
C	-1.927423	1.494370	-0.015396
C	-3.172138	0.811220	-0.032928
C	-1.300328	2.751238	-0.078498
C	0.099481	2.451929	-0.023765
N	0.305161	1.071433	0.065239
Mg	2.000462	-0.009343	0.029406
N	0.797727	-1.797804	0.011578
C	1.387177	-3.020669	-0.040549
C	0.358421	-4.139106	-0.023392
C	-0.966159	-3.382468	-0.262448
C	-0.584471	-1.929027	-0.010842
C	2.751404	-3.302355	-0.073697
C	3.842010	-2.414826	-0.066347
N	3.728825	-1.060599	-0.033212
C	5.007114	-0.537133	-0.049082
C	5.977142	-1.637311	-0.091447
C	5.247789	-2.805446	-0.096862
C	5.310372	0.812433	-0.059483
C	4.404708	1.905812	-0.053227
N	3.054462	1.780179	-0.026833
C	2.533010	3.064017	-0.051011
C	3.619220	4.031563	-0.089891
C	4.788658	3.306757	-0.088566
C	3.456377	5.526112	-0.088138
C	3.284375	6.121037	1.323610
C	1.173760	3.363686	-0.059785
C	6.200505	3.811920	-0.115872
C	7.424645	-1.447373	-0.090168
C	8.334145	-2.249288	-0.663815
C	5.749368	-4.216232	-0.084942
C	-1.941221	4.096759	-0.213904
C	-1.514095	-3.572096	-1.689782

C	0.377783	-4.914275	1.307376
O	-4.321431	1.441112	-0.109804
Zn	-5.838704	0.418141	-0.036565
O	-5.232517	-1.294344	0.290607
C	-3.947050	-1.527134	0.366016
O	-3.620678	-2.758136	0.771770
C	-4.675646	-3.705141	1.015446
H	2.405362	5.702151	1.825770
H	2.594226	5.807270	-0.706503
H	4.327285	5.988342	-0.567036
H	3.163225	7.208804	1.273160
H	4.157152	5.904467	1.948709
H	6.234329	4.898706	-0.232359
H	6.771556	3.374951	-0.944566
H	6.737065	3.566906	0.810012
H	6.362854	1.073053	-0.094952
H	8.059573	-3.129530	-1.236312
H	9.394545	-2.025488	-0.596347
H	7.784393	-0.557405	0.425072
H	5.812991	-4.640168	-1.096440
H	5.093198	-4.870338	0.499102
H	6.751280	-4.267180	0.352208
H	3.000809	-4.357609	-0.118365
H	0.912027	4.416436	-0.108848
H	-2.140782	4.338723	-1.266938
H	-1.309978	4.894352	0.189577
H	-2.902090	4.124697	0.309190
H	-0.388000	-5.698497	1.303232
H	1.348252	-5.390940	1.479121
H	0.177237	-4.245491	2.152444
H	0.561186	-4.844410	-0.839070
H	-1.723336	-3.707181	0.448555
H	-1.756951	-4.626107	-1.868411
H	-0.774809	-3.264257	-2.438383
H	-2.419975	-2.979246	-1.850464
H	-4.164739	-4.627362	1.292256

H	-5.277461	-3.859303	0.116608
H	-5.316259	-3.368941	1.833826
N	-7.671184	0.954148	-0.258437
C	-8.760377	1.312451	-0.401428
C	-10.128617	1.762529	-0.581213
H	-10.661681	1.709040	0.374197
H	-10.130420	2.796956	-0.941322
H	-10.632140	1.122250	-1.313603

D(Zn(CH$_3$CN)$_2$)

E: -3965.675618 u.a

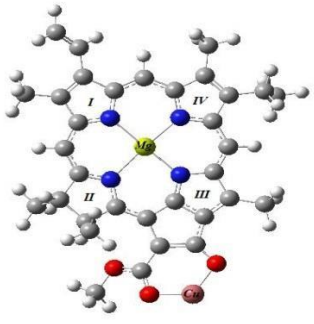
G: -3965.094543 u.a

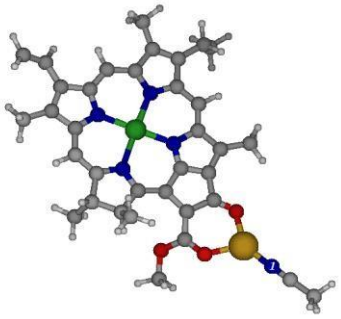
C	2.519076	-0.692098	-0.137876
C	1.014074	-0.871481	-0.153721
C	0.522238	0.469408	-0.099549
C	1.555592	1.431932	0.021475
C	2.803031	0.726993	0.021450
C	0.949770	2.688500	0.128111
C	-0.461197	2.413428	0.067925
N	-0.684634	1.041696	-0.063696
Mg	-2.394496	-0.014562	-0.051655
N	-1.215993	-1.819486	-0.089268
C	-1.821169	-3.034508	-0.066797
C	-0.806571	-4.165863	-0.116979
C	0.529410	-3.432726	0.133276
C	0.165534	-1.967866	-0.076815
C	-3.189300	-3.298721	-0.036106
C	-4.268354	-2.397201	-0.015991
N	-4.137065	-1.043254	-0.011999
C	-5.407412	-0.502573	0.021999
C	-6.391436	-1.588753	0.036915
C	-5.678072	-2.767704	0.008062
C	-5.691438	0.851941	0.070973
C	-4.772734	1.931720	0.093126
N	-3.421817	1.788872	0.059058
C	-2.883110	3.061842	0.121628

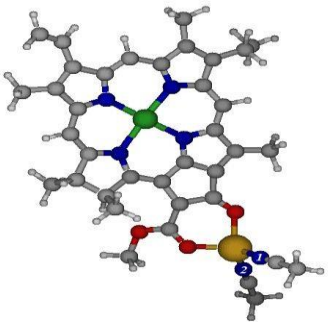
C	-3.953375	4.042536	0.192476
C	-5.134690	3.335252	0.171563
C	-3.768501	5.534124	0.233585
C	-3.594917	6.166991	-1.161227
C	-1.515519	3.339792	0.137469
C	-6.538159	3.862627	0.217514
C	-7.836212	-1.379358	0.044905
C	-8.757924	-2.186644	0.591118
C	-6.201041	-4.170121	-0.041380
C	1.602901	4.028183	0.279046
C	1.085372	-3.667738	1.550310
C	-0.842348	-4.907352	-1.466221
O	3.948911	1.331578	0.120293
Zn	5.517126	0.297555	0.078960
O	4.813676	-1.396041	-0.386977
C	3.537712	-1.600457	-0.465368
O	3.175018	-2.806098	-0.932408
C	4.210061	-3.752713	-1.237462
H	-2.724901	5.748628	-1.679248
H	-2.898491	5.784550	0.854240
H	-4.629708	5.995854	0.730583
H	-3.457136	7.251242	-1.081696
H	-4.473920	5.980480	-1.787395
H	-6.553853	4.944729	0.375661
H	-7.117610	3.404060	1.028584
H	-7.078619	3.662591	-0.717019
H	-6.740354	1.125567	0.116852
H	-8.496958	-3.090295	1.132659
H	-9.814871	-1.944652	0.531629
H	-8.183699	-0.467178	-0.439129
H	-6.274274	-4.619563	0.958503
H	-5.552975	-4.818744	-0.640442
H	-7.202410	-4.194884	-0.482304
H	-3.452582	-4.351564	-0.018403
H	-1.233558	4.385800	0.219432
H	1.250921	4.551821	1.176647

H	1.387452	4.681319	-0.576759
H	2.687809	3.919228	0.353184
H	-0.087129	-5.701779	-1.486205
H	-1.820167	-5.366113	-1.645700
H	-0.636368	-4.219938	-2.294930
H	-1.014064	-4.889053	0.681924
H	1.278455	-3.747741	-0.590737
H	1.316354	-4.729229	1.699721
H	0.355833	-3.370157	2.312730
H	2.000047	-3.090170	1.717777
H	3.683894	-4.652853	-1.556781
H	4.822224	-3.963560	-0.356877
H	4.848896	-3.384450	-2.043893
N	6.878143	0.977703	-1.249949
C	7.497583	1.391049	-2.133315
C	8.279776	1.910956	-3.243670
H	7.625868	2.461692	-3.927374
H	9.056226	2.584724	-2.868063
H	8.750531	1.083838	-3.784332
N	6.558496	0.294712	1.811946
C	6.972146	0.269350	2.890528
C	7.497416	0.239208	4.246339
H	8.089480	-0.669389	4.394491
H	8.131019	1.114982	4.418301
H	6.668803	0.249367	4.961628

2.c.2 Case of cooper (Cu)







D(Cu) *D(Cu(CH_3CN))* *D(Cu($CH_3CN)_2$)*

D(Cu)

E: -3561.202578 u.a

G: -3560.700105 u.a

C	4.591080	2.776445	-0.019358
C	4.000559	1.449337	0.001336
N	2.634766	1.535802	-0.019195
C	2.327955	2.871114	-0.061374
C	3.541107	3.669195	-0.062273
C	4.715818	0.239023	0.021071
C	4.209949	-1.064034	0.014182
N	2.873910	-1.380306	-0.013122
C	2.781593	-2.740135	-0.061250
C	4.104083	-3.339099	-0.056577
C	5.004786	-2.289570	-0.011591
C	1.562603	-3.442243	-0.114051
C	0.249466	-2.966254	-0.112680
N	-0.146178	-1.668783	-0.039706
C	-1.520274	-1.586704	-0.085702
C	-2.130508	-2.950309	-0.373590
C	-0.938877	-3.913412	-0.157376
Mg	1.332037	-0.075151	0.012193
N	-0.182875	1.255497	0.002957
C	-1.454313	0.904244	-0.008496
C	-2.323001	2.022903	-0.127758
C	-1.531781	3.161716	-0.189612
C	-0.172440	2.663153	-0.100656
C	-3.673073	1.525689	-0.160692
C	-3.585254	0.043510	0.000548
C	-2.173475	-0.354519	0.021052
C	-4.711226	-0.789776	0.390318
O	-4.405165	-1.822470	1.175492
C	-5.497070	-2.677931	1.590302
O	-4.695385	2.279794	-0.297351
Cu	-6.113222	1.136356	-0.378921

O	-5.927579	-0.625828	0.068566
C	-1.959150	4.588648	-0.321058
C	1.011371	3.385896	-0.118147
C	-1.059006	-4.748637	1.130834
C	-2.708616	-3.013895	-1.801730
C	6.463108	-2.321048	0.038970
C	7.258186	-3.260281	-0.495184
C	4.393113	-4.808123	-0.052532
C	3.601105	5.171520	-0.064696
C	3.457805	5.790516	1.340043
C	6.061011	3.068431	0.006992
H	2.502970	5.515270	1.801660
H	2.820125	5.575242	-0.721531
H	4.551195	5.495650	-0.503876
H	3.507016	6.883105	1.285679
H	4.257949	5.446148	2.003531
H	6.259681	4.131717	-0.150101
H	6.597971	2.515476	-0.773089
H	6.510069	2.791254	0.969437
H	5.796904	0.331044	0.020904
H	6.874363	-4.097941	-1.068385
H	8.337113	-3.197606	-0.392419
H	6.937596	-1.490509	0.559988
H	4.484541	-5.212069	-1.069703
H	3.604617	-5.374870	0.452829
H	5.336169	-5.013862	0.463316
H	1.649698	-4.522788	-0.172734
H	0.920152	4.465735	-0.188083
H	-1.512405	5.061458	-1.204133
H	-1.653116	5.179005	0.551810
H	-3.045561	4.655245	-0.410581
H	-1.932781	-5.407312	1.075894
H	-0.175984	-5.377093	1.286176
H	-1.171468	-4.102729	2.009163
H	-0.835073	-4.597996	-1.008231
H	-2.927549	-3.169548	0.335988

H	-3.110600	-4.013057	-2.002503
H	-1.936243	-2.802911	-2.550274
H	-3.517027	-2.289164	-1.942428
H	-5.028459	-3.461973	2.183674
H	-6.007067	-3.095806	0.719986
H	-6.207943	-2.111317	2.194672

D(Cu(CH_3CN))

E: -3694.035832 u.a

G: -3693.494684 u.a

C	-2.868591	-0.568702	0.172560
C	-1.429424	-0.771052	0.136450
C	-0.894057	0.577434	0.108023
C	-1.906414	1.571386	0.073453
C	-3.176981	0.883905	0.088274
C	-1.273830	2.808350	0.019534
C	0.139176	2.493935	0.025250
N	0.320506	1.098431	0.077494
Mg	2.005065	-0.011736	0.022139
N	0.757268	-1.795856	0.029311
C	1.332196	-3.037209	-0.036356
C	0.280250	-4.134209	0.004284
C	-1.035575	-3.348068	-0.201727
C	-0.605151	-1.907656	0.027071
C	2.687138	-3.324031	-0.098078
C	3.802624	-2.453250	-0.113283
N	3.708059	-1.098486	-0.071269
C	4.992786	-0.597664	-0.107538
C	5.942670	-1.704774	-0.175711
C	5.191385	-2.867055	-0.175000
C	5.313399	0.755967	-0.114338
C	4.437059	1.862761	-0.083012
N	3.076338	1.761666	-0.036492
C	2.586643	3.046290	-0.039333
C	3.679811	3.998163	-0.085436
C	4.841824	3.253915	-0.110383

C	3.541784	5.495385	-0.065770
C	3.432773	6.080979	1.356077
C	1.216133	3.373701	-0.021222
C	6.258512	3.743662	-0.152584
C	7.392363	-1.539429	-0.202029
C	8.278558	-2.367962	-0.774891
C	5.677410	-4.283787	-0.185698
C	-1.893160	4.169196	-0.036848
C	-1.635057	-3.536160	-1.609678
C	0.314867	-4.914424	1.331630
O	-4.311411	1.430585	0.065877
Cu	-5.979866	0.528241	-0.115777
O	-5.155380	-1.232530	0.168442
C	-3.959044	-1.480849	0.430851
O	-3.639053	-2.630822	1.037860
C	-4.727758	-3.535760	1.323807
H	2.564481	5.675978	1.887621
H	2.663667	5.797102	-0.650687
H	4.402286	5.946035	-0.573303
H	3.330757	7.170811	1.317394
H	4.323386	5.843441	1.947393
H	6.301891	4.827596	-0.288274
H	6.821402	3.287516	-0.976013
H	6.795523	3.510565	0.775933
H	6.370245	0.996890	-0.165417
H	7.981616	-3.255554	-1.323901
H	9.342998	-2.158931	-0.730498
H	7.776923	-0.646788	0.289649
H	5.769729	-4.680253	-1.205830
H	5.000620	-4.948491	0.360844
H	6.665075	-4.356190	0.280259
H	2.924355	-4.382223	-0.148618
H	0.973976	4.432048	-0.052958
H	-1.577688	4.716989	-0.933344
H	-1.605497	4.776325	0.830665
H	-2.982770	4.093203	-0.050096

H	-0.468538	-5.680411	1.342875
H	1.277705	-5.415424	1.475904
H	0.151498	-4.246209	2.184961
H	0.444377	-4.840048	-0.819113
H	-1.780287	-3.642493	0.537020
H	-1.910340	-4.585257	-1.764535
H	-0.913509	-3.257558	-2.386363
H	-2.531902	-2.925220	-1.751215
H	-4.259089	-4.408250	1.777903
H	-5.250752	-3.809064	0.404803
H	-5.430596	-3.072648	2.019547
N	-7.693261	0.921048	-0.430129
C	-8.807946	1.175577	-0.630958
C	-10.202777	1.505273	-0.883880
H	-10.773259	1.451497	0.049161
H	-10.285777	2.518916	-1.289754
H	-10.634377	0.799431	-1.601066

D(Cu(CH$_3$CN)$_2$)

E: -3826.825099 u.a

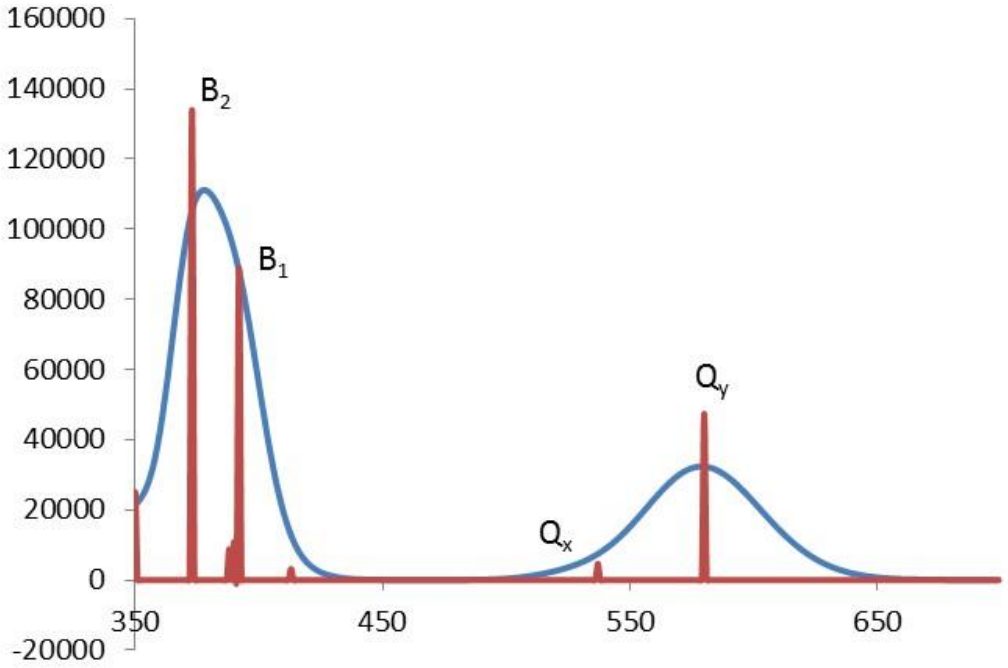
G: -3826.245613 u.a

C	2.455281	-0.673761	-0.176041
C	1.009869	-0.843735	-0.135633
C	0.501164	0.510150	-0.137740
C	1.529299	1.485236	-0.120140
C	2.793606	0.776149	-0.118848
C	0.917844	2.733340	-0.101073
C	-0.501210	2.444496	-0.107771
N	-0.707250	1.055962	-0.126597
Mg	-2.410810	-0.020161	-0.056702
N	-1.199043	-1.824865	-0.013832
C	-1.798393	-3.055022	0.082775
C	-0.765376	-4.170963	0.076556
C	0.563209	-3.403287	0.265039
C	0.160436	-1.961264	-0.003148
C	-3.155768	-3.316907	0.145746

C	-4.254853	-2.423688	0.131300
N	-4.135290	-1.073481	0.056799
C	-5.412218	-0.546459	0.072517
C	-6.381701	-1.635307	0.161440
C	-5.651892	-2.810005	0.193791
C	-5.707684	0.809947	0.044153
C	-4.809361	1.900858	-0.009509
N	-3.451804	1.773527	-0.045084
C	-2.936195	3.049493	-0.072882
C	-4.012489	4.020592	-0.057537
C	-5.188196	3.298412	-0.019937
C	-3.848117	5.514262	-0.114478
C	-3.731459	6.063220	-1.550159
C	-1.561718	3.348367	-0.091835
C	-6.595953	3.815534	0.001812
C	-7.828278	-1.443442	0.173978
C	-8.735155	-2.242334	0.756645
C	-6.163144	-4.217464	0.233905
C	1.561993	4.083785	-0.065005
C	1.156531	-3.563858	1.678790
C	-0.808340	-4.987071	-1.228660
O	3.932162	1.299328	-0.103646
Cu	5.670284	0.384853	0.152145
O	4.726700	-1.385874	-0.169712
C	3.527093	-1.611865	-0.414998
O	3.173740	-2.773044	-0.995476
C	4.238379	-3.707362	-1.258147
H	-2.871600	5.629326	-2.072526
H	-2.963253	5.814732	0.460907
H	-4.699487	5.993157	0.382970
H	-3.610004	7.151903	-1.539172
H	-4.627247	5.826833	-2.134182
H	-6.620039	4.901552	0.126860
H	-7.176723	3.378533	0.823221
H	-7.128189	3.583992	-0.930000
H	-6.759979	1.072256	0.082859

H	-8.460221	-3.123807	1.326618
H	-9.794982	-2.013679	0.698813
H	-8.192272	-0.554100	-0.339021
H	-6.267321	-4.590184	1.261952
H	-5.494972	-4.905602	-0.294095
H	-7.149604	-4.283347	-0.235708
H	-3.412884	-4.368791	0.223094
H	-1.297991	4.402140	-0.088070
H	1.388336	4.584413	0.896576
H	1.165416	4.742124	-0.847110
H	2.641873	3.995640	-0.206482
H	-0.037187	-5.765644	-1.216827
H	-1.779104	-5.475504	-1.362605
H	-0.631608	-4.344669	-2.099043
H	-0.945046	-4.850992	0.918337
H	1.304862	-3.730220	-0.462769
H	1.412503	-4.613204	1.863504
H	0.438342	-3.250750	2.445544
H	2.063899	-2.964995	1.804581
H	3.751338	-4.580337	-1.692526
H	4.756125	-3.973324	-0.333447
H	4.954643	-3.279373	-1.963206
N	7.055688	0.428847	-1.144811
C	7.909839	0.440925	-1.927616
C	8.983513	0.456220	-2.912018
H	9.806959	-0.186030	-2.582521
H	8.615685	0.092680	-3.877232
H	9.361286	1.476023	-3.040548
N	6.340407	0.869630	1.859379
C	6.737180	1.223169	2.889083
C	7.243487	1.672176	4.179249
H	7.828601	0.876539	4.651441
H	7.883172	2.550732	4.047318
H	6.411060	1.937328	4.838739

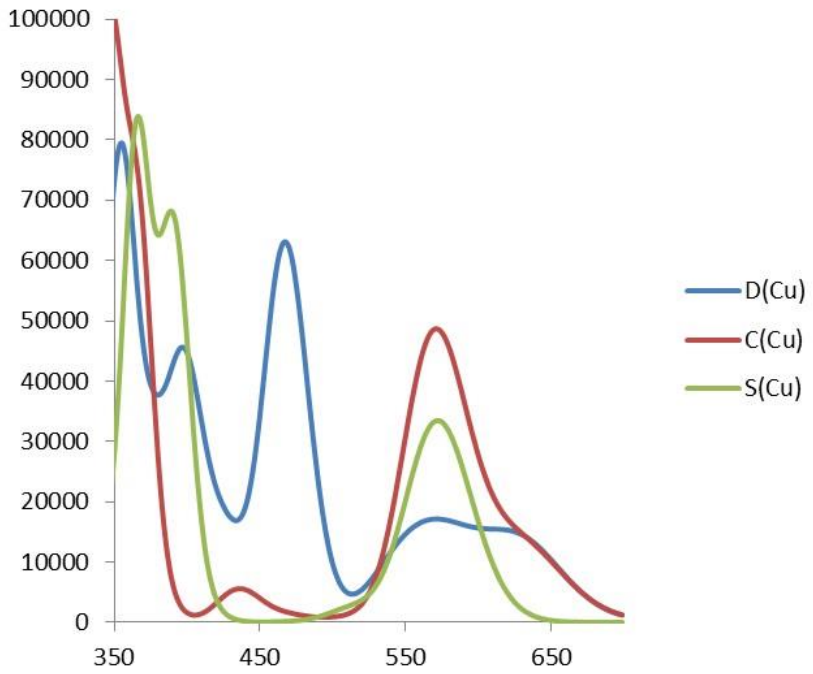
2. Simulation of the UV-visible spectra using the Chla model used. The computed transitions are superimposed.



3. Q_y-state of Chla, S(Cu) and S(Zn) using different levels (single point TD-DFT calculations carried out on geometry optimized at the corresponding DFT level).

	B3LYP/6-31G*	***CAM-B3LYP/6-31G****	***BP86/6-31+G*** **
	Chla (Pheo(Mg))		
γ (nm) Q_y-state	579.64	590.67	616.52
f (Intensity)	0.2369	0.2441	0.2046
	S(Cu) (Pheo(Cu))		
γ (nm) Q_y-state	572.35	579.64	608.55
f (Intensity)	0.2471	0.2511	0.1959
	S(Zn)(Pheo(Zn))		
γ (nm) Q_y-state	571.92	580.91	609.97
f (Intensity)	0.2386	0.2460	0.2058

4. Superposition of the simulated UV-visible spectra of the Cu substituted (green), Cu-chelated (red) and Cu-deprotonated (blue) .



5. Gibbs free energies for processes 2a, 2b and 2c, computed without PCM or when using single point calculation within the standard PCM model implemented in Gaussian09.[28b] Values in parenthesis refer to the standard implementation in Gaussian 03.[29]

	Cu		Zn	
	Without PCM	With PCM	Without PCM	With PCM
2a	-44.1	-55.1 (-35.2)	-19.2	-25.6 (-17.3)
2b	-27.7	-11.0	-22.5	1.8
2c	-15.6	7.9	+1.5	24.7