

SUPPORTING INFORMATION

Dicopper(I) Complexes Incorporating Acetylide-functionalized Pyridinyl-based Ligands: Synthesis, Structural and Photovoltaic Studies

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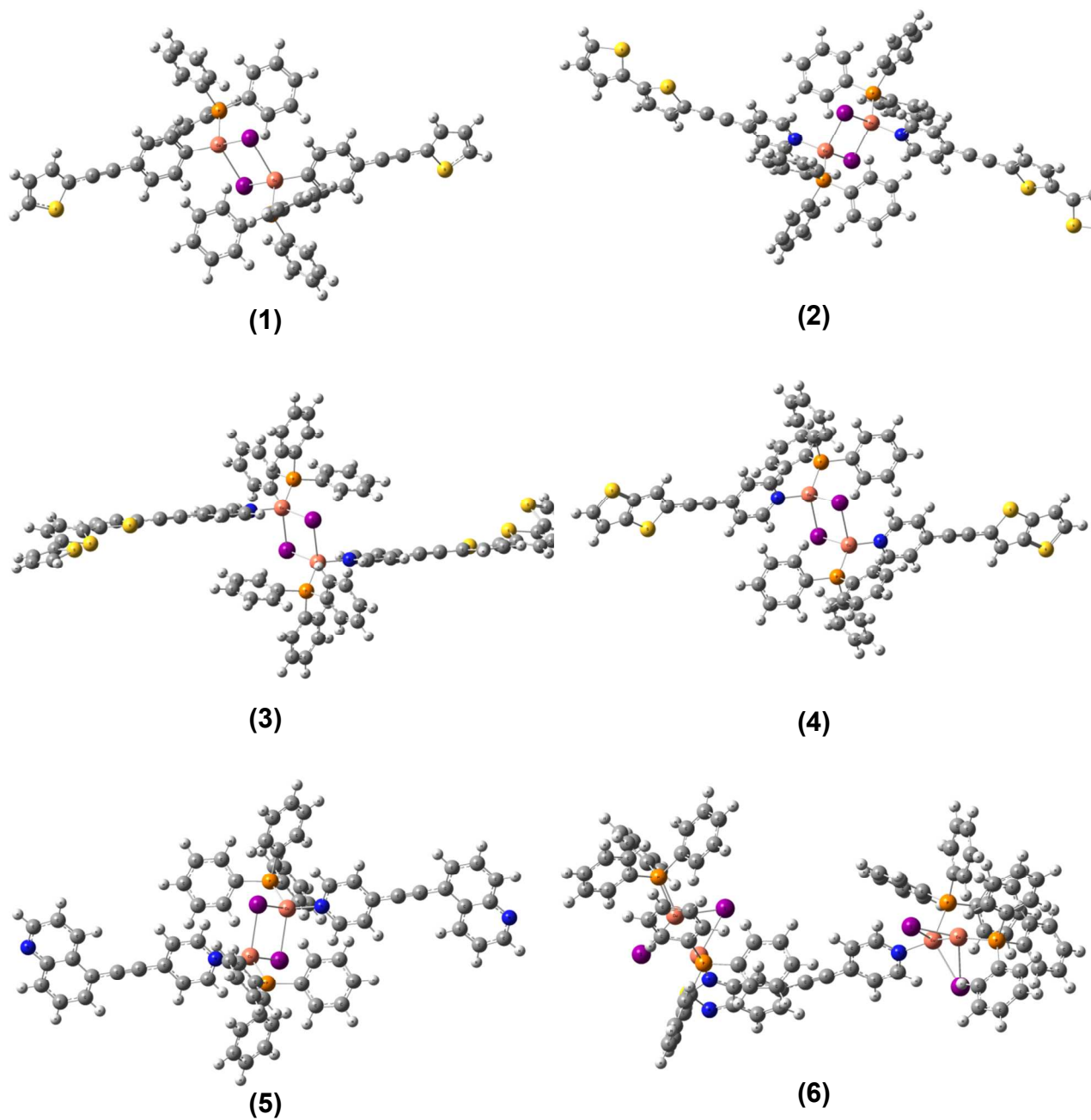
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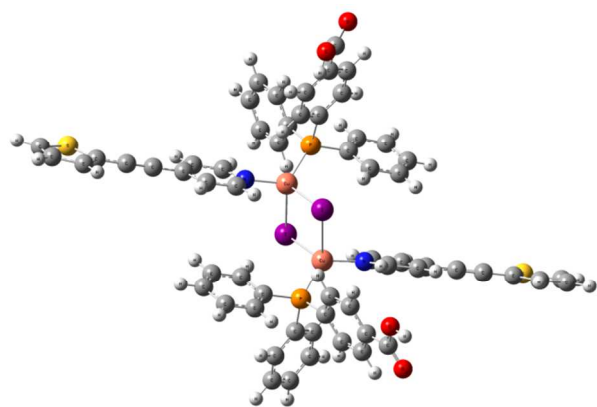
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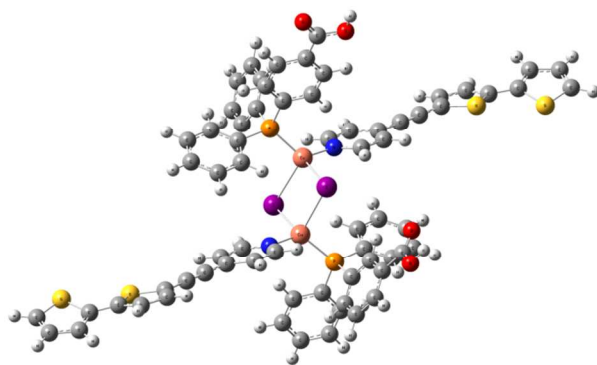
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Figure S1: Fully optimized geometries of the Cu-complexes **1-10**, obtained by the B3LYP level of theory with the Lanl2dz for I and 6-31G(d) for all other atoms. C, H, S, N, O, I, Cu/P atoms are shown in grey, white, yellow, blue, red, purple, and orange, respectively.

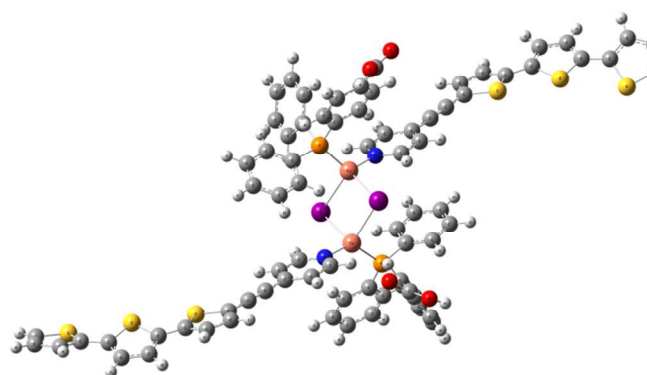




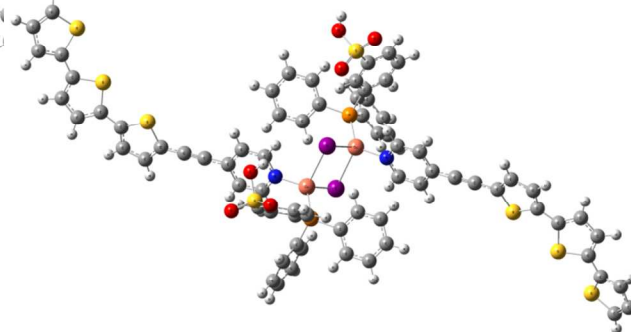
(7)



(8)

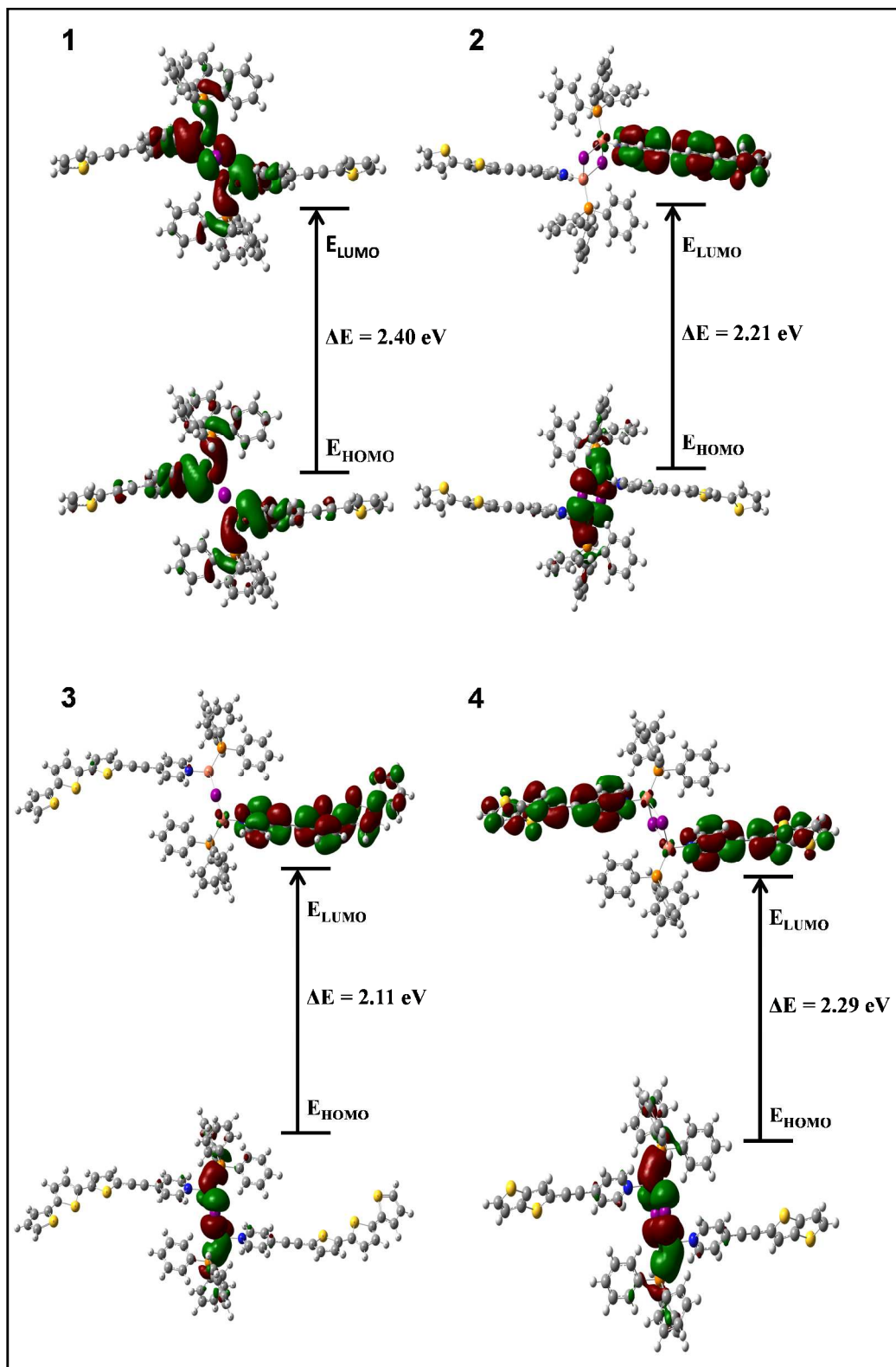


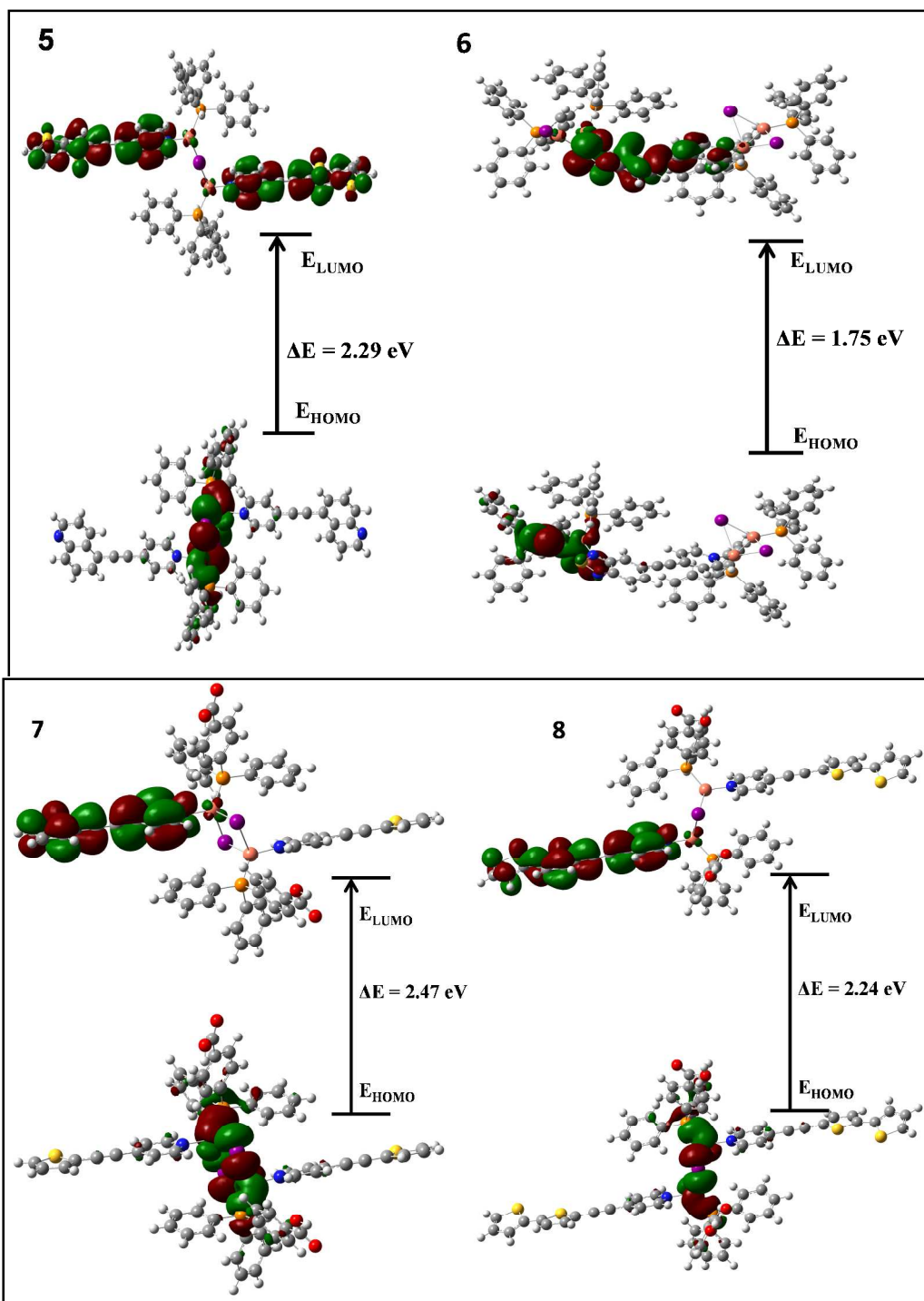
(9)



(10)

Figure S2: Frontier molecular orbital and their energies of complexes **1-10** at the B3LYP/6-31G(d)+LanI2dz.





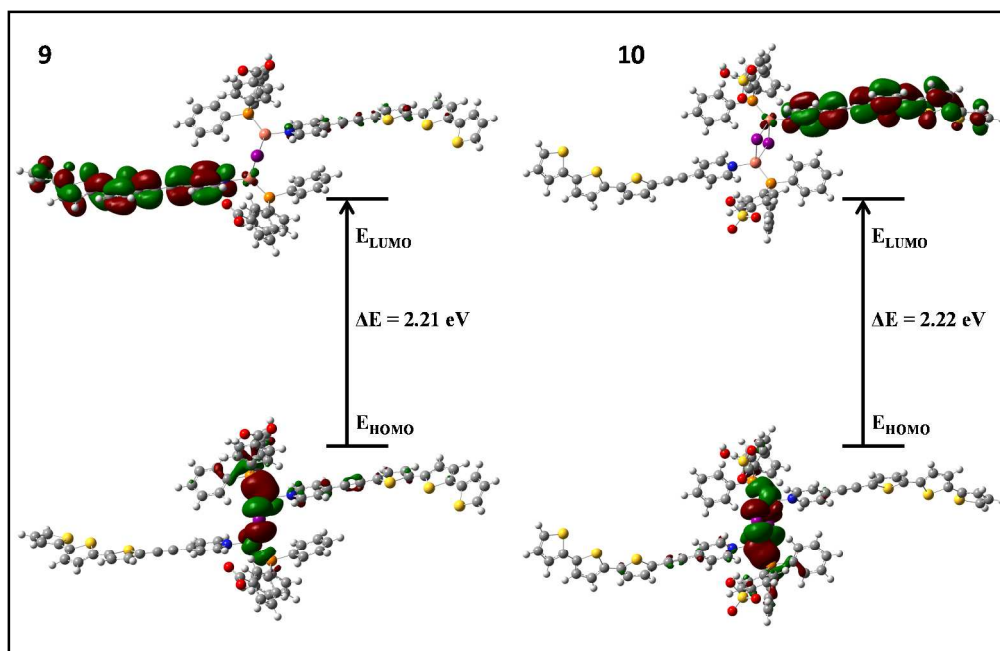
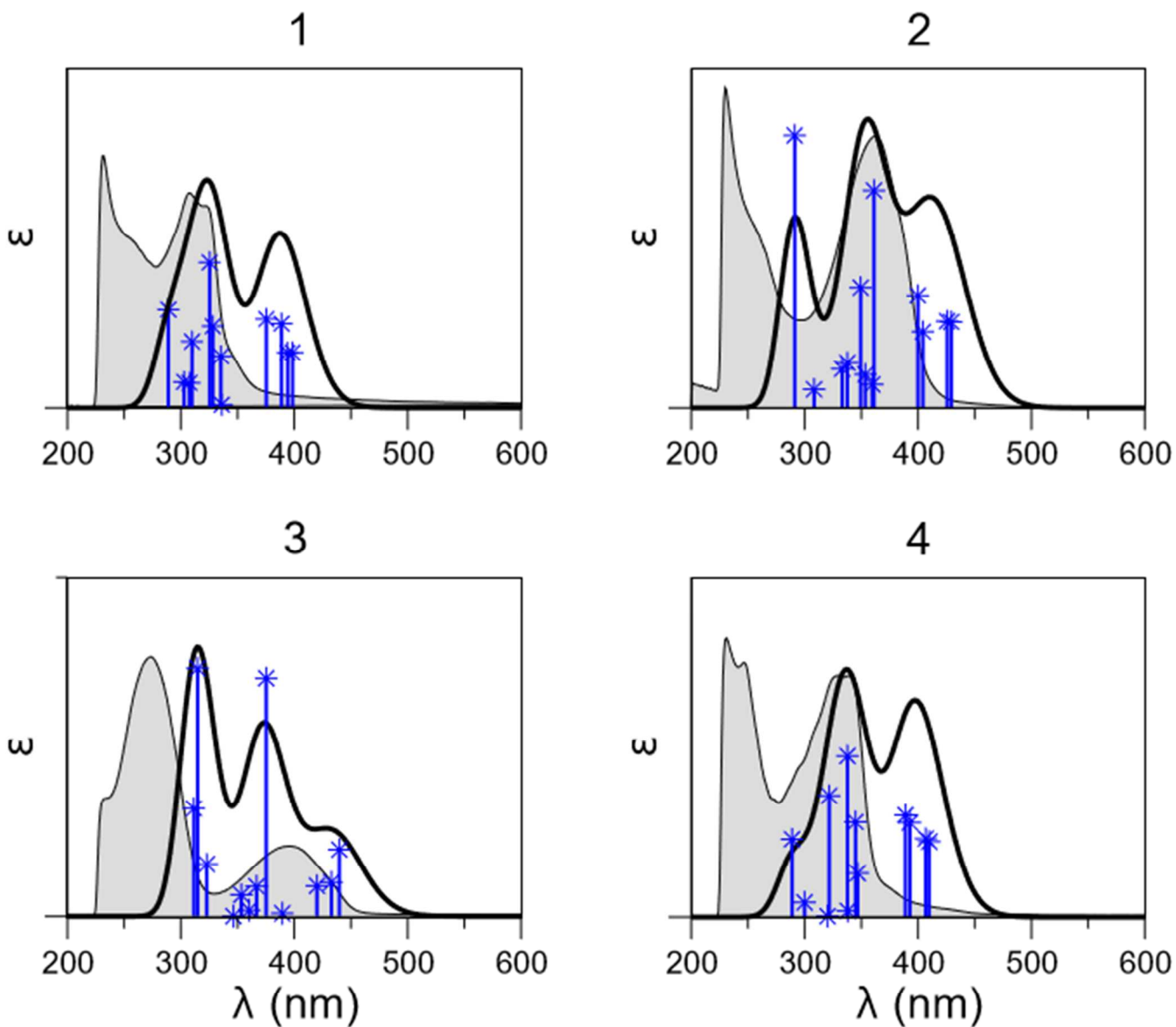


Figure S3: Simulated UV-Vis absorption spectra of **Cu(I) complexes** in dichloromethane from time-dependent density-functional theory (TD-DFT) using the B3LYP level of theory. Each plot shows the simulated absorption profile obtained from the spin-allowed singlet states (blue). These plots were prepared using the GaussView 6 visualization software.²⁵



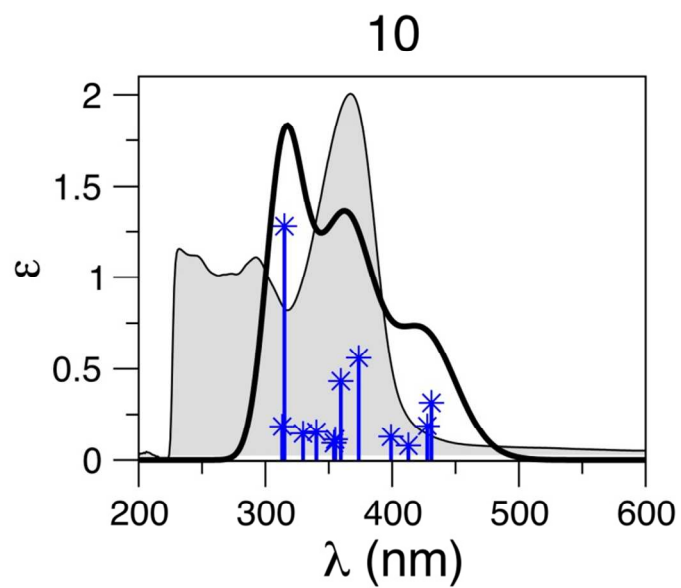
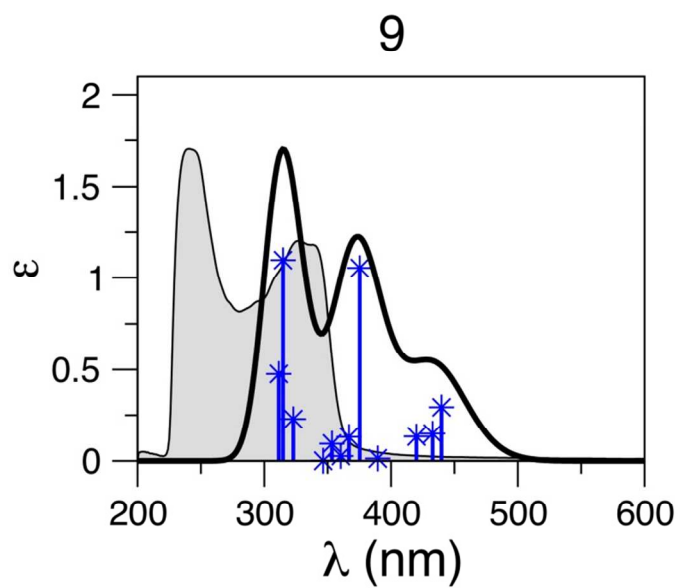
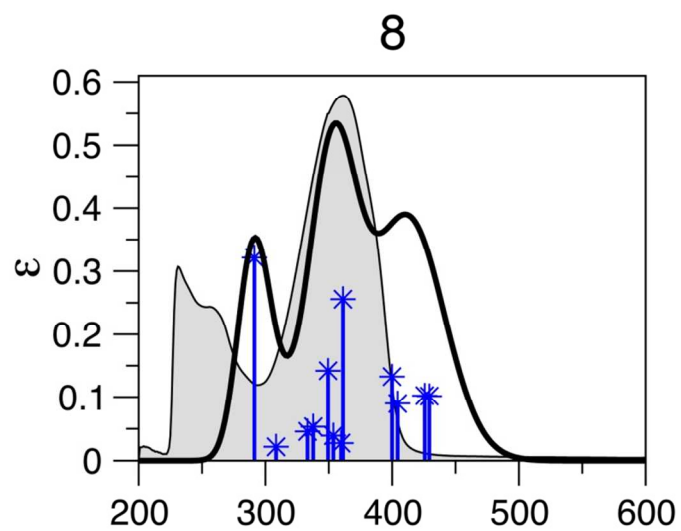
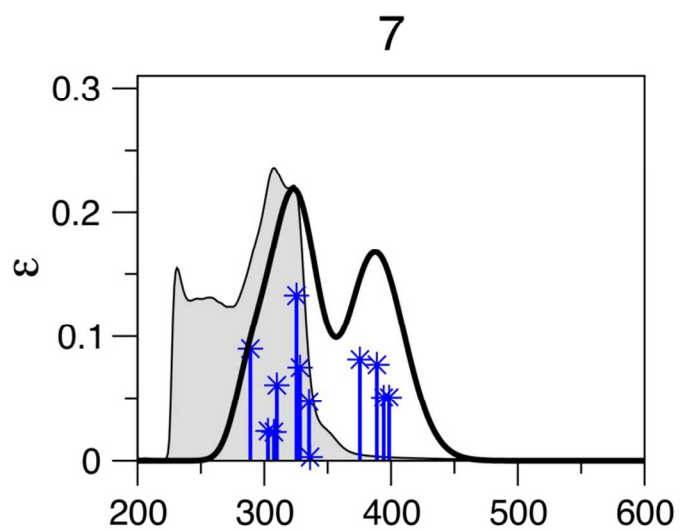


Figure S4: Cyclic voltammetry (CV) obtained at a 3 mm diameter glassy carbon disc electrode for complexes **1-6** at the scan rate of 100 mV/s, approximately 1 mM in anhydrous acetonitrile with 0.1 M NBu₄PF₆ electrolyte using silver (Ag) wire as a quasi-reference electrode. All the potentials are referred to Fc/Fc⁺ couple.

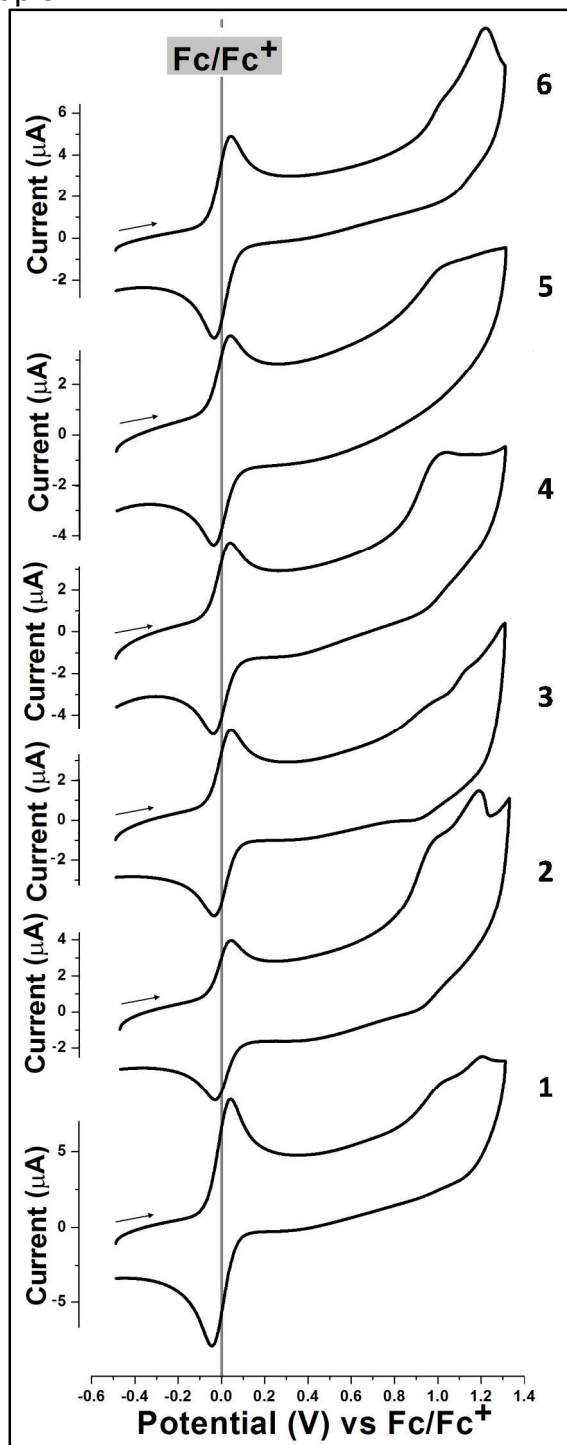


Table ST1: Cartesian coordinates of the optimized geometries.

Complex 1

I	0.17933596	0.39535261	2.047904
Cu	1.65020052	-0.95488454	-0.03044
P	1.54825378	-3.20532235	0.13605
C	3.51472637	-0.57476319	0.080266
C	4.08402291	0.09528917	1.177541
H	3.47749276	0.33500612	2.04637
C	5.42288293	0.48120343	1.177002
H	5.83829781	1.01325237	2.028613
C	5.69404287	-0.49849207	-1.02069
H	6.31988583	-0.73221847	-1.87759
C	4.354271	-0.8824324	-1.00302
H	3.9666385	-1.42877917	-1.8596
C	6.25156143	0.19437571	0.07263
C	7.61843896	0.5861541	0.066287
C	8.78828089	0.92741682	0.07285
C	10.13928512	1.31447766	0.05914
C	12.52569793	1.74018095	-0.57508
H	13.47365796	1.79467401	-1.09365
C	12.22174296	2.19077288	0.682765
H	12.94126506	2.6791039	1.331084
C	2.52706112	-4.00210641	-1.18931
C	3.61042539	-4.85478833	-0.93837
H	3.88965591	-5.09491184	0.082089
C	4.33790447	-5.39876536	-1.99952
H	5.17682959	-6.05741063	-1.79186
C	3.99060652	-5.10032255	-3.31736
H	4.55970725	-5.52367299	-4.14052
C	2.90890003	-4.25348844	-3.57545
H	2.6322293	-4.01613724	-4.59896
C	2.18208861	-3.7038175	-2.52066
H	1.34519129	-3.04289501	-2.73114
C	-0.13743728	-3.90819412	-0.0309
C	-0.39967324	-5.06664737	-0.77981
H	0.40733268	-5.58030326	-1.29172
C	-1.70084558	-5.56214497	-0.87549
H	-1.89139232	-6.45829087	-1.46003
C	-2.75158144	-4.91023819	-0.22725

H	-3.76513967	-5.29270792	-0.31168
C	-2.4980727	-3.76059633	0.524156
H	-3.31087295	-3.23902035	1.020893
C	-1.19968744	-3.2609793	0.62301
H	-1.01901599	-2.35789873	1.198389
C	2.1903853	-3.83591021	1.730516
C	3.45587354	-3.40855065	2.170671
H	4.03398136	-2.71584796	1.567736
C	3.96767474	-3.86180148	3.385947
H	4.94693436	-3.52412431	3.713763
C	3.22146582	-4.73408364	4.182018
H	3.61867047	-5.07887884	5.132899
C	1.9619796	-5.15622982	3.754529
H	1.3746266	-5.83246749	4.369731
C	1.44771489	-4.71363997	2.534834
H	0.46779603	-5.04931893	2.213369
I	-0.08887647	-0.161409	-2.0177
Cu	-1.60996645	1.11181456	0.059291
P	-1.66250081	3.3676198	-0.08177
C	-3.44431278	0.59486325	-0.01347
C	-3.99174982	-0.11468971	-1.09686
H	-3.39148553	-0.31058881	-1.98067
C	-5.29985869	-0.59429011	-1.06502
H	-5.6968836	-1.15380065	-1.90779
C	-5.58649077	0.36485172	1.139446
H	-6.20674768	0.55492745	2.011106
C	-4.27791518	0.84234586	1.089885
H	-3.90951986	1.41551944	1.937437
C	-6.11994981	-0.36686411	0.059324
C	-7.45488641	-0.85538633	0.097994
S	-10.58692351	-2.65265959	-1.18801
C	-8.60012002	-1.26958134	0.141868
C	-9.91840828	-1.75593916	0.172411
C	-10.86224396	-1.63984167	1.176216
H	-10.6565498	-1.12237853	2.106111
C	-12.10184076	-2.25994188	0.859623
H	-12.95711952	-2.26933703	1.526652
C	-12.10610032	-2.84670769	-0.37861
H	-12.91285744	-3.38132381	-0.86218

C	-2.66408487	4.08894178	1.270734
C	-3.80177109	4.87606379	1.047968
H	-4.11400894	5.10657814	0.034877
C	-4.54027984	5.36644485	2.127484
H	-5.42134403	5.97476225	1.941786
C	-4.14980966	5.07945398	3.435761
H	-4.72715293	5.46145799	4.273323
C	-3.01399939	4.29789189	3.665744
H	-2.70352285	4.06992555	4.681677
C	-2.27563005	3.80188051	2.592461
H	-1.39630031	3.19131728	2.781213
C	-0.02594329	4.1846301	0.056962
C	0.1664975	5.37124867	0.782404
H	-0.66652829	5.83635927	1.299384
C	1.43130752	5.95765189	0.848505
H	1.56831049	6.87445385	1.415773
C	2.51414087	5.37012332	0.191575
H	3.49928191	5.82485237	0.25077
C	2.3294599	4.19261896	-0.5363
H	3.16807022	3.72368766	-1.04282
C	1.06841687	3.60055544	-0.60274
H	0.94139729	2.67500101	-1.15686
C	-2.37778018	3.97705063	-1.65418
C	-3.60614518	3.44969982	-2.09134
H	-4.1135313	2.6944637	-1.49982
C	-4.17274102	3.88482081	-3.28887
H	-5.12235536	3.46885828	-3.61394
C	-3.51817446	4.83940483	-4.07086
H	-3.95723551	5.17051697	-5.00809
C	-2.2955455	5.36161685	-3.64674
H	-1.77898397	6.10242864	-4.25103
C	-1.72746793	4.93700317	-2.44462
H	-0.77707709	5.35163297	-2.12639
H	10.43149643	2.23148513	1.998025
C	10.86843496	1.9511437	1.046566
S	11.15698447	1.00978154	-1.34548

Complex 2

I	0.249508	-0.03165	-2.42799
Cu	-0.97563	-1.2794	-0.10169
S	-10.7261	0.061087	0.428085
S	-13.7508	1.05899	1.566825
P	-0.45311	-3.3701	0.082281
N	-2.89468	-0.8693	-0.28487
C	-3.48195	-0.86356	-1.50274
H	-2.81051	-0.96341	-2.35078
C	-4.84659	-0.72103	-1.68952
H	-5.26025	-0.72937	-2.69302
C	-5.69118	-0.56229	-0.57052
C	-5.07281	-0.56042	0.696657
H	-5.66596	-0.43572	1.59692
C	-3.6992	-0.71123	0.790087
H	-3.19684	-0.69215	1.753052
C	-7.08871	-0.39666	-0.71794
C	-8.29493	-0.26926	-0.83712
C	-9.6801	-0.12246	-0.97695
C	-10.4331	-0.10191	-2.14042
H	-9.97946	-0.19487	-3.12105
C	-11.8146	0.073223	-1.91532
H	-12.5481	0.15625	-2.71025
C	-12.1539	0.182893	-0.57743
C	-13.4801	0.343125	-0.01816
C	-14.6866	0.000239	-0.59214
H	-14.7557	-0.48049	-1.56294
C	-15.814	0.299064	0.22173
H	-16.8387	0.088778	-0.06594
C	-15.469	0.865905	1.41907
H	-16.1073	1.190325	2.230037
C	1.31807	-3.84082	0.269428
C	2.178616	-2.9478	0.925611
H	1.789578	-2.00582	1.3026
C	3.527118	-3.26336	1.103514
H	4.179595	-2.55511	1.609393
C	4.035986	-4.46997	0.622002
H	5.089618	-4.70966	0.7496
C	3.187219	-5.36581	-0.0327

H	3.574801	-6.30965	-0.4107
C	1.838245	-5.05519	-0.20507
H	1.191003	-5.7581	-0.72232
C	-1.02067	-4.44274	-1.30883
C	-1.5512	-5.72997	-1.12293
H	-1.67801	-6.12461	-0.11883
C	-1.92918	-6.50973	-2.21768
H	-2.33848	-7.5045	-2.05337
C	-1.77701	-6.01875	-3.5157
H	-2.07575	-6.62537	-4.36806
C	-1.23958	-4.74553	-3.71252
H	-1.11281	-4.35415	-4.71962
C	-0.86187	-3.96369	-2.61993
H	-0.4475	-2.97219	-2.78701
C	-1.26654	-4.10773	1.562059
C	-2.67003	-4.19136	1.586015
H	-3.24364	-3.89853	0.709008
C	-3.33812	-4.65934	2.716496
H	-4.42422	-4.72389	2.71244
C	-2.61555	-5.04131	3.849734
H	-3.13599	-5.39804	4.735822
C	-1.22351	-4.9541	3.839224
H	-0.65138	-5.2479	4.716672
C	-0.5525	-4.49122	2.705303
H	0.531218	-4.42394	2.715803
I	-0.26335	0.062096	2.427509
Cu	0.972893	1.302402	0.102556
S	10.71214	-0.11192	-0.43112
S	13.72659	-1.1364	-1.57349
P	0.463479	3.396721	-0.07984
N	2.889661	0.878305	0.285247
C	3.476964	0.867219	1.503023
H	2.806275	0.970669	2.351247
C	4.840626	0.715165	1.689409
H	5.254524	0.719508	2.692834
C	5.683924	0.551887	0.570063
C	5.065395	0.555953	-0.69704
H	5.657543	0.428394	-1.59756
C	3.69281	0.716177	-0.79006

H	3.190131	0.701705	-1.75296
C	7.080261	0.376225	0.717043
C	8.285329	0.238408	0.836787
C	9.669356	0.079965	0.975246
C	10.42346	0.05239	2.137805
H	9.971863	0.148793	3.119026
C	11.80316	-0.13453	1.91102
H	12.53689	-0.22422	2.705055
C	12.13995	-0.24654	0.572693
C	13.46411	-0.41801	0.011737
C	14.67423	-0.08533	0.584072
H	14.7487	0.394947	1.554697
C	15.79798	-0.3939	-0.23124
H	16.82476	-0.19231	0.055044
C	15.4465	-0.95795	-1.42803
H	16.08101	-1.28792	-2.23978
C	-1.30448	3.879473	-0.26628
C	-2.17129	2.992808	-0.92284
H	-1.78884	2.048519	-1.30076
C	-3.51768	3.317672	-1.10005
H	-4.17512	2.614229	-1.60621
C	-4.01815	4.527381	-0.61752
H	-5.07017	4.77433	-0.74459
C	-3.16308	5.416962	0.037508
H	-3.5441	6.36316	0.41629
C	-1.81621	5.09703	0.209216
H	-1.16404	5.795133	0.726788
C	1.038493	4.464417	1.312007
C	1.577824	5.748116	1.126992
H	1.707326	6.142582	0.123173
C	1.961275	6.524452	2.222272
H	2.377393	7.516494	2.058653
C	1.80586	6.033575	3.519951
H	2.108846	6.637494	4.372724
C	1.259735	4.763918	3.71589
H	1.130384	4.372679	4.722711
C	0.876544	3.985499	2.622772
H	0.455383	2.996739	2.789154
C	1.281774	4.129862	-1.55913

C	2.685793	4.203822	-1.5832
H	3.257467	3.90629	-0.7065
C	3.356951	4.668046	-2.71341
H	4.443469	4.725084	-2.70946
C	2.636881	5.055846	-3.84626
H	3.159657	5.409662	-4.73215
C	1.244274	4.978218	-3.83564
H	0.674071	5.276611	-4.71279
C	0.570233	4.51912	-2.70198
H	-0.51392	4.459319	-2.71237

Complex 3

I	-0.26439	-0.35326	2.273921
Cu	0.78426	-1.66573	-0.23383
S	10.57938	-1.05625	0.190319
S	13.66737	0.185305	-0.22854
P	-0.3661	-3.47503	-0.48937
N	2.700959	-1.6803	0.04628
C	3.208124	-2.3608	1.10018
H	2.486632	-2.85578	1.741202
C	4.562511	-2.44201	1.374619
H	4.908592	-3.0031	2.235529
C	5.483642	-1.78631	0.531138
C	4.952275	-1.07346	-0.5619
H	5.607224	-0.5386	-1.24064
C	3.580561	-1.04316	-0.75746
H	3.145932	-0.48339	-1.57986
C	6.877387	-1.83386	0.777807
C	8.075068	-1.87236	1.004773
C	9.453821	-1.90012	1.247426
C	10.14023	-2.53186	2.272614
H	9.633651	-3.10726	3.038844
C	11.53567	-2.33202	2.223931
H	12.22341	-2.72663	2.963227
C	11.95165	-1.54962	1.15784
C	13.3068	-1.17127	0.82315
C	14.47954	-1.76279	1.254834
H	14.49427	-2.63396	1.90031
C	15.64815	-1.13302	0.76632

H	16.65314	-1.44705	1.025281
C	15.39511	-0.05636	-0.06162
C	-2.20301	-3.3851	-0.48063
C	-2.79194	-2.31404	-1.173
H	-2.16196	-1.55791	-1.63507
C	-4.18019	-2.20642	-1.25794
H	-4.62122	-1.37329	-1.79832
C	-4.99923	-3.15859	-0.64613
H	-6.08087	-3.07019	-0.70885
C	-4.42232	-4.22251	0.049016
H	-5.05227	-4.96679	0.529737
C	-3.03246	-4.33939	0.126626
H	-2.59619	-5.17241	0.669076
C	0.032179	-4.72728	0.80107
C	0.737995	-5.90706	0.523103
H	1.011365	-6.14662	-0.49942
C	1.091234	-6.78179	1.554025
H	1.637314	-7.69251	1.321197
C	0.742554	-6.49226	2.873564
H	1.016723	-7.1747	3.673884
C	0.040514	-5.31808	3.160786
H	-0.23275	-5.08143	4.185755
C	-0.30871	-4.43911	2.135988
H	-0.83859	-3.52034	2.372055
C	0.008439	-4.33321	-2.07442
C	1.218027	-4.02558	-2.71439
H	1.870811	-3.27817	-2.27308
C	1.572834	-4.65476	-3.90842
H	2.511738	-4.40194	-4.39358
C	0.714724	-5.59375	-4.48302
C	-0.49716	-5.90097	-3.85906
H	-1.172	-6.62586	-4.30703
C	-0.8487	-5.27595	-2.66224
H	-1.79645	-5.51555	-2.18907
I	0.257073	0.363079	-2.243
Cu	-0.78853	1.677135	0.266628
S	-10.5823	1.021421	-0.24724
S	-13.6655	-0.29511	0.039174
P	0.364225	3.484785	0.522642

N	-2.70475	1.693424	-0.01702
C	-3.20819	2.377337	-1.0705
H	-2.48467	2.876958	-1.70559
C	-4.56125	2.455821	-1.35187
H	-4.90435	3.019459	-2.21231
C	-5.48496	1.79308	-0.51675
C	-4.95756	1.077533	0.576403
H	-5.61454	0.537649	1.249174
C	-3.5868	1.0507	0.779477
H	-3.15497	0.489039	1.602059
C	-6.87712	1.836161	-0.77321
C	-8.0726	1.870955	-1.01196
C	-9.44845	1.894286	-1.2715
C	-10.1249	2.541988	-2.29336
H	-9.61168	3.136473	-3.04037
C	-11.5194	2.330588	-2.2691
H	-12.2002	2.732726	-3.01081
C	-11.9441	1.524083	-1.22492
C	-13.3008	1.12736	-0.91947
C	-14.4713	1.745755	-1.3179
H	-14.4817	2.660206	-1.90064
C	-15.6416	1.105655	-0.84672
H	-16.6443	1.476028	-1.02911
C	-15.3914	-0.01645	-0.08057
C	2.201002	3.392352	0.513302
C	2.788743	2.319012	1.203113
H	2.157864	1.562937	1.664014
C	4.17688	2.209055	1.286915
H	4.61697	1.374059	1.825188
C	4.996986	3.161226	0.676556
H	6.078521	3.07097	0.7383
C	4.421266	4.227504	-0.01598
H	5.052051	4.971799	-0.49557
C	3.031545	4.346643	-0.09249
H	2.596211	5.181408	-0.63303
C	-0.03237	4.738247	-0.7672
C	-0.73595	5.919223	-0.48863
H	-1.00865	6.158919	0.534032
C	-1.08785	6.794963	-1.51916

H	-1.6322	7.706603	-1.28586
C	-0.74003	6.505276	-2.83888
H	-1.01316	7.188494	-3.63889
C	-0.04017	5.329934	-3.1267
C	0.307724	4.449964	-2.1023
H	0.8359	3.530324	-2.33882
C	-0.0094	4.342748	2.108012
C	-1.22116	4.038896	2.745744
H	-1.87598	3.294265	2.302736
C	-1.57563	4.668328	3.939733
H	-2.51624	4.418504	4.423143
C	-0.71505	5.6037	4.516575
H	-0.98459	6.089175	5.450939
C	0.498939	5.907079	3.894857
H	1.175662	6.629134	4.344567
C	0.850151	5.28188	2.698022
H	1.799473	5.518529	2.226543
C	-16.3583	-0.90068	0.539621
C	-17.6607	-1.13176	0.145662
C	-17.5784	-2.5174	2.01316
H	-18.0937	-0.67742	-0.73861
C	-18.353	-2.04694	0.986907
H	-17.8448	-3.22486	2.786812
H	-19.3813	-2.35233	0.826846
C	16.36025	0.78243	-0.74491
C	17.64947	0.453603	-1.11154
C	17.5864	2.649329	-1.87889
H	18.07041	-0.53248	-0.94961
C	18.34526	1.517006	-1.75161
H	17.85816	3.593685	-2.33089
H	19.36444	1.437682	-2.11391
S	-15.987	-1.83213	1.979491
S	16.00635	2.440025	-1.19852
H	0.98449	-6.07908	-5.4174
H	0.232422	5.093166	-4.15182

Complex 4

I	-0.11058	0.17651	-2.28241
Cu	1.00639	1.56116	0.11549
S	10.61288	-0.51444	0.26134
P	0.14458	3.53878	0.1683
N	2.91695	1.2722	-0.04495
C	3.56683	1.79503	-1.11043
H	2.95911	2.35151	-1.8158
C	4.92736	1.64976	-1.31956
H	5.3922	2.09293	-2.1932
C	5.69898	0.91878	-0.39248
C	5.01899	0.36985	0.7123
H	5.55398	-0.21195	1.4546
C	3.65207	0.56328	0.8393
H	3.10121	0.13489	1.67114
C	7.09311	0.74091	-0.57172
C	8.29078	0.59388	-0.74597
C	9.66857	0.41033	-0.92647
C	10.4578	0.87236	-1.96521
H	10.05906	1.45596	-2.78591
C	11.81007	0.48682	-1.80851
C	12.06693	-0.26598	-0.66106
C	-1.68234	3.73899	0.08335
C	-2.46046	2.84274	0.83493
H	-1.97822	2.04311	1.39183
C	-3.85013	2.96298	0.85889
H	-4.43873	2.26312	1.44576
C	-4.48272	3.97188	0.12834
H	-5.56599	4.0611	0.14486
C	-3.71761	4.86316	-0.62538
H	-4.20177	5.64998	-1.19841
C	-2.32534	4.75137	-0.64421
H	-1.74142	5.45029	-1.23508
C	0.77623	4.58665	-1.20905
C	1.642	5.67158	-1.00574
H	1.91221	5.96894	0.00239
C	2.16003	6.37966	-2.09348
H	2.82857	7.21868	-1.91768
C	1.81883	6.01714	-3.39674

H	2.22094	6.57038	-4.24149
C	0.95858	4.93613	-3.60984
H	0.68994	4.64252	-4.62121
C	0.4445	4.22238	-2.52775
H	-0.20801	3.37205	-2.70611
C	0.60419	4.47201	1.6868
C	1.71796	4.02725	2.41408
H	2.24535	3.14006	2.07595
C	2.13342	4.70088	3.56352
H	2.99576	4.34102	4.11826
C	1.43183	5.82377	4.00509
C	0.3153	6.27022	3.29335
H	-0.23838	7.13978	3.63806
C	-0.09633	5.59966	2.14113
H	-0.96971	5.94946	1.59846
I	0.11315	-0.17783	2.28272
Cu	-1.00375	-1.56251	-0.11531
S	-10.6103	0.51295	-0.26039
P	-0.14188	-3.5401	-0.16801
N	-2.91429	-1.27354	0.04527
C	-3.56407	-1.7963	1.11084
H	-2.95627	-2.35269	1.81622
C	-4.92459	-1.65106	1.32006
H	-5.38934	-2.09418	2.19377
C	-5.69631	-0.92019	0.39297
C	-5.01641	-0.37131	-0.71189
H	-5.55149	0.21041	-1.4542
C	-3.6495	-0.56471	-0.83898
H	-3.09871	-0.13634	-1.67089
C	-7.09043	-0.74236	0.5723
C	-8.2881	-0.5954	0.74663
C	-9.66588	-0.41193	0.92724
C	-10.455	-0.87411	1.96598
H	-10.0562	-1.45779	2.78658
C	-11.8073	-0.48862	1.80942
C	-12.0643	0.26431	0.66208
C	1.68504	-3.74028	-0.08306
C	2.46315	-2.84407	-0.83469
H	1.9809	-2.04447	-1.39163

C	3.85282	-2.9643	-0.85866
H	4.44141	-2.26446	-1.44558
C	4.48542	-3.97315	-0.12808
H	5.56869	-4.06237	-0.1446
C	3.72033	-4.8644	0.6257
H	4.2045	-5.65119	1.19877
C	2.32806	-4.75262	0.64454
H	1.74415	-5.45151	1.23546
C	-0.77353	-4.58794	1.20936
C	-1.63935	-5.67283	1.00607
H	-1.90959	-5.97019	-0.00205
C	-2.1574	-6.38087	2.09384
H	-2.82599	-7.21986	1.91805
C	-1.81616	-6.01835	3.39709
H	-2.21828	-6.57157	4.24185
C	-0.95586	-4.93739	3.61016
C	-0.44176	-4.22367	2.52805
H	0.21078	-3.37337	2.70639
C	-0.60146	-4.47337	-1.68651
C	-1.715	-4.02841	-2.41401
H	-2.24224	-3.14108	-2.07603
C	-2.13041	-4.70204	-3.56347
H	-2.99257	-4.34202	-4.11839
C	-1.42901	-5.82513	-4.00482
H	-1.74528	-6.34666	-4.90445
C	-0.31271	-6.27178	-3.29284
H	0.24082	-7.14151	-3.63738
C	0.09888	-5.60122	-2.14062
H	0.97209	-5.95117	-1.59776
H	1.74813	6.3453	4.90471
H	-0.68719	-4.64378	4.62151
S	-13.2715	-0.73254	2.72794
C	-13.4279	0.64786	0.51309
C	-14.1875	0.18023	1.55044
H	-13.8252	1.23265	-0.30799
H	-15.2502	0.31757	1.70048
S	13.27431	0.73055	-2.72698
C	13.43048	-0.64955	-0.51191
C	14.19021	-0.18213	-1.54928

H	13.82773	-1.23424	0.30929
H	15.2529	-0.31955	-1.69923

Complex 5

I	1.721726	-1.24383	-0.93081
Cu	0.987176	1.513664	-0.38219
P	0.620796	2.723657	-2.13275
N	2.128725	2.093435	1.066932
N	9.471532	4.055794	7.738652
C	1.831752	3.240395	1.719876
H	0.911329	3.733125	1.425795
C	2.634369	3.780192	2.710977
H	2.345783	4.704716	3.198508
C	3.825404	3.121092	3.077557
C	4.123999	1.921095	2.40425
H	5.018589	1.359582	2.649944
C	3.259663	1.449733	1.428361
H	3.455016	0.515818	0.91028
C	4.679827	3.646033	4.082414
C	5.402172	4.111946	4.944926
C	6.239592	4.665402	5.952086
C	5.87122	5.844899	6.593417
H	4.940629	6.327948	6.312933
C	6.685958	6.413797	7.593965
H	6.36922	7.334828	8.074784
C	7.870271	5.812223	7.960536
H	8.514549	6.230288	8.727253
C	8.288997	4.607635	7.335556
C	7.471755	4.019907	6.319387
C	7.931339	2.819094	5.725232
H	7.335157	2.346756	4.950373
C	9.124361	2.276063	6.142069
H	9.507243	1.357124	5.708519
C	9.858281	2.938621	7.157336
H	10.80515	2.520262	7.497762
C	2.084472	2.874517	-3.23917
C	3.220752	2.119236	-2.92065
H	3.194307	1.483253	-2.04092

C	4.356184	2.164055	-3.73266
H	5.227365	1.568328	-3.47421
C	4.362918	2.963008	-4.87593
H	5.243888	2.998463	-5.51162
C	3.23027	3.712844	-5.20922
H	3.229805	4.329874	-6.10409
C	2.096272	3.665311	-4.39963
H	1.218056	4.243927	-4.67273
C	0.234716	4.449834	-1.6297
C	1.195109	5.472647	-1.66487
H	2.173663	5.283049	-2.09438
C	0.901463	6.739996	-1.15555
H	1.655409	7.522107	-1.19616
C	-0.35149	7.002885	-0.60038
H	-0.57911	7.989989	-0.20659
C	-1.31041	5.987336	-0.54944
H	-2.28625	6.178825	-0.11104
C	-1.02045	4.719605	-1.05319
H	-1.76545	3.931931	-0.98862
C	-0.72986	2.272309	-3.29903
C	-1.52958	3.209389	-3.96988
H	-1.41333	4.269092	-3.76421
C	-2.49016	2.79107	-4.89286
H	-3.10604	3.52913	-5.40062
C	-2.65526	1.432104	-5.16578
H	-3.40045	1.107313	-5.88754
C	-1.8603	0.492184	-4.5062
H	-1.98392	-0.56764	-4.71148
C	-0.9064	0.906846	-3.5759
H	-0.30328	0.166277	-3.05641
I	-1.72173	1.243825	0.93081
Cu	-0.98718	-1.51366	0.382186
P	-0.6208	-2.72366	2.132754
N	-2.12873	-2.09344	-1.06693
N	-9.47153	-4.05579	-7.73865
C	-1.83175	-3.2404	-1.71988
H	-0.91133	-3.73313	-1.4258
C	-2.63437	-3.78019	-2.71098
H	-2.34578	-4.70472	-3.19851

C	-3.8254	-3.12109	-3.07756
C	-4.124	-1.9211	-2.40425
H	-5.01859	-1.35958	-2.64994
C	-3.25966	-1.44973	-1.42836
H	-3.45502	-0.51582	-0.91028
C	-4.67983	-3.64603	-4.08241
C	-5.40217	-4.11195	-4.94493
C	-6.23959	-4.6654	-5.95209
C	-5.87122	-5.8449	-6.59342
H	-4.94063	-6.32795	-6.31293
C	-6.68596	-6.4138	-7.59397
H	-6.36922	-7.33483	-8.07478
C	-7.87027	-5.81222	-7.96054
H	-8.51455	-6.23029	-8.72725
C	-8.289	-4.60764	-7.33556
C	-7.47176	-4.01991	-6.31939
C	-7.93134	-2.81909	-5.72523
H	-7.33516	-2.34676	-4.95037
C	-9.12436	-2.27606	-6.14207
H	-9.50724	-1.35712	-5.70852
C	-9.85828	-2.93862	-7.15734
H	-10.8051	-2.52026	-7.49776
C	-2.08447	-2.87452	3.239166
C	-3.22075	-2.11924	2.920652
H	-3.19431	-1.48325	2.040916
C	-4.35618	-2.16406	3.732658
H	-5.22737	-1.56833	3.474211
C	-4.36292	-2.96301	4.875927
H	-5.24389	-2.99846	5.511621
C	-3.23027	-3.71284	5.209217
H	-3.22981	-4.32987	6.104091
C	-2.09627	-3.66531	4.399627
H	-1.21806	-4.24393	4.672729
C	-0.23472	-4.44983	1.629697
C	-1.19511	-5.47265	1.664868
H	-2.17366	-5.28305	2.094383
C	-0.90146	-6.74	1.155546
H	-1.65541	-7.52211	1.196158
C	0.351487	-7.00289	0.600378

H	0.57911	-7.98999	0.206593
C	1.310408	-5.98734	0.549444
H	2.286247	-6.17883	0.111043
C	1.020453	-4.71961	1.053189
H	1.76545	-3.93193	0.988621
C	0.729861	-2.27231	3.299031
C	1.529578	-3.20939	3.969877
H	1.413333	-4.26909	3.764213
C	2.490159	-2.79107	4.892856
H	3.106037	-3.52913	5.400623
C	2.655263	-1.4321	5.165782
H	3.400445	-1.10731	5.887543
C	1.860295	-0.49218	4.506204
H	1.983915	0.567638	4.711481
C	0.906395	-0.90685	3.575901
H	0.303278	-0.16628	3.056409

Complex 6

Cu	5.739653	-0.21538	-0.7947
Cu	-6.29398	-1.38826	-0.60236
I	-9.31488	-1.38827	-0.76208
I	7.218514	-2.55084	-1.09384
S	-7.19046	-3.0962	-3.16702
P	-5.68264	-1.99392	1.419058
P	6.297628	1.78414	-1.49606
N	3.913779	-0.84961	-1.31392
N	-5.97175	-2.42149	-2.23371
N	-6.26569	-3.75079	-4.34734
C	3.736207	-1.73822	-2.31387
H	4.640551	-2.14244	-2.75674
C	2.488211	-2.15581	-2.75153
H	2.408827	-2.87558	-3.55854
C	1.33296	-1.64639	-2.13058
C	1.520051	-0.72502	-1.08341
H	0.665169	-0.30538	-0.56574
C	2.80637	-0.35972	-0.71844
H	2.974908	0.332684	0.098321
C	0.028741	-2.04032	-2.52966
C	-1.10624	-2.3498	-2.83865

C	-2.42711	-2.71212	-3.21738
C	-2.61805	-3.47628	-4.42923
H	-1.7367	-3.74999	-5.00001
C	-3.8611	-3.84666	-4.85719
H	-4.01272	-4.4185	-5.76615
C	-4.98984	-3.46368	-4.07447
C	-4.80688	-2.70172	-2.85999
C	-3.5081	-2.32742	-2.43779
H	-3.36341	-1.74758	-1.53444
C	-3.85205	-2.03278	1.592517
C	-3.13435	-3.19192	1.922843
H	-3.65999	-4.1228	2.107897
C	-1.74108	-3.15732	2.018822
H	-1.19826	-4.06361	2.273251
C	-1.04807	-1.96643	1.79758
H	0.034859	-1.94129	1.882008
C	-1.75526	-0.8085	1.462125
H	-1.22707	0.125563	1.288499
C	-3.14526	-0.84071	1.34808
H	-3.68106	0.060263	1.061532
C	-6.2628	-1.02766	2.877185
C	-5.40294	-0.46481	3.830633
H	-4.32851	-0.57514	3.729796
C	-5.92253	0.240488	4.920474
H	-5.2441	0.669835	5.653241
C	-7.30176	0.387619	5.070358
H	-7.70365	0.939747	5.915498
C	-8.1658	-0.17496	4.126899
H	-9.24022	-0.05744	4.230502
C	-7.65192	-0.87824	3.038207
H	-8.33431	-1.30986	2.310993
C	-6.25062	-3.69248	1.832829
C	-6.23891	-4.1926	3.145399
H	-5.90397	-3.56205	3.963957
C	-6.6666	-5.49368	3.407966
H	-6.65535	-5.86929	4.427662
C	-7.11413	-6.3101	2.365281
H	-7.45196	-7.32172	2.573583
C	-7.13494	-5.82057	1.059038

H	-7.49272	-6.44496	0.245163
C	-6.70772	-4.51788	0.796346
H	-6.74079	-4.12503	-0.21428
C	7.578421	1.820206	-2.82349
C	7.900888	0.626098	-3.48732
H	7.468001	-0.31538	-3.16265
C	8.808503	0.625581	-4.54918
H	9.047638	-0.31067	-5.04545
C	9.413493	1.814214	-4.95668
H	10.12144	1.813034	-5.78145
C	9.110893	3.006726	-4.29373
H	9.581739	3.93724	-4.60041
C	8.199049	3.010626	-3.23825
H	7.97728	3.945237	-2.73388
C	6.740388	3.190896	-0.39635
C	7.460966	2.930388	0.774158
H	7.647336	1.895501	1.050325
C	7.896173	3.969757	1.596044
H	8.45051	3.740051	2.500337
C	7.602306	5.291025	1.258627
H	7.933601	6.103544	1.899874
C	6.869654	5.566492	0.101378
H	6.628694	6.593337	-0.16091
C	6.44224	4.525353	-0.72281
H	5.865414	4.753334	-1.61358
C	4.792331	2.418369	-2.35364
C	4.635943	2.349978	-3.74487
H	5.449382	1.989226	-4.3663
C	3.438278	2.752601	-4.3418
H	3.333228	2.69868	-5.42222
C	2.384722	3.226558	-3.55962
H	1.455266	3.541011	-4.02624
C	2.530784	3.293239	-2.17128
H	1.715278	3.661845	-1.55463
C	3.721563	2.8859	-1.57129
H	3.826776	2.941033	-0.49057
Cu	7.340062	-0.20615	0.888362
Cu	-7.58154	0.590599	-0.33569
I	-5.22632	1.159912	-1.52388

I	5.108318	0.080585	2.305097
P	-8.38918	2.441659	0.53111
C	-7.13344	3.618194	1.167757
C	-6.21215	3.135731	2.112694
C	-7.03804	4.951248	0.746959
C	-5.22848	3.974085	2.634877
H	-6.26032	2.099991	2.438547
C	-6.04319	5.785686	1.261867
H	-7.73603	5.339575	0.012364
C	-5.13963	5.30161	2.20836
H	-4.52526	3.586782	3.367414
H	-5.97675	6.815587	0.920995
H	-4.36632	5.952491	2.607818
C	-9.24801	3.334121	-0.825
C	-10.2911	4.249469	-0.61955
C	-8.81248	3.075066	-2.13337
C	-10.8836	4.894239	-1.70659
H	-10.6478	4.449905	0.386488
C	-9.40222	3.723892	-3.21774
H	-8.01334	2.355456	-2.28588
C	-10.4392	4.634527	-3.00558
H	-11.6944	5.598403	-1.53878
H	-9.05672	3.510955	-4.22555
H	-10.9051	5.13612	-3.84972
C	-9.6616	2.367549	1.857625
C	-10.781	1.546027	1.637329
C	-9.56817	3.07526	3.064145
C	-11.7781	1.433028	2.605356
H	-10.8688	0.988315	0.709502
C	-10.5682	2.958792	4.033321
H	-8.71312	3.715934	3.252895
C	-11.6741	2.137801	3.808337
H	-12.6363	0.792744	2.419537
H	-10.4819	3.515721	4.962947
H	-12.4518	2.049203	4.562455
P	9.431757	-0.39458	1.444253
C	10.61662	-0.40082	0.046999
C	10.70382	0.753555	-0.74964
C	11.37227	-1.52678	-0.30412

C	11.5512	0.789077	-1.8555
H	10.1062	1.628646	-0.50655
C	12.21402	-1.49141	-1.41793
H	11.29944	-2.43439	0.284997
C	12.31056	-0.33473	-2.1914
H	11.60419	1.687905	-2.46281
H	12.7919	-2.3735	-1.68069
H	12.96704	-0.31026	-3.05724
C	10.05414	0.918658	2.584334
C	11.2564	1.617386	2.409349
C	9.27263	1.188995	3.722064
C	11.66305	2.574158	3.343641
H	11.87759	1.421093	1.541733
C	9.684895	2.137505	4.657566
H	8.332571	0.662657	3.871082
C	10.88163	2.835704	4.469375
H	12.59611	3.110361	3.190541
H	9.069522	2.332223	5.531838
H	11.20135	3.577601	5.196383
C	9.776668	-1.92091	2.407829
C	8.778411	-2.89962	2.508763
C	10.99721	-2.11647	3.075776
C	9.000221	-4.0595	3.254222
H	7.831503	-2.75483	1.999591
C	11.21721	-3.27632	3.817067
H	11.77311	-1.35758	3.024091
C	10.21821	-4.25045	3.906442
H	8.217258	-4.8094	3.322634
H	12.16509	-3.41768	4.329778
H	10.38975	-5.15253	4.48801

Complex 7

I	-0.0217	-0.12092	1.953099
Cu	-1.42959	1.140597	-0.29328
P	-1.03746	3.263993	-0.32842
C	-3.70614	-0.37756	0.721229
H	-2.98344	-0.67214	1.475965
C	-5.01259	-0.83875	0.764867
H	-5.3252	-1.50245	1.563335

C	-5.4331	0.406309	-1.24604
H	-6.083	0.738976	-2.04772
C	-4.11243	0.819855	-1.20889
H	-3.72274	1.478507	-1.97771
C	-5.92319	-0.44696	-0.23608
C	-7.26973	-0.88817	-0.22834
C	-8.42663	-1.27034	-0.20712
C	-9.7637	-1.6974	-0.20019
C	-12.1714	-2.09617	-0.7333
H	-13.1527	-2.09923	-1.18931
C	-11.7705	-2.73559	0.412151
H	-12.4315	-3.34638	1.016853
C	-2.03406	4.131258	-1.60965
C	-3.01863	5.08443	-1.31051
H	-3.18986	5.387772	-0.28273
C	-3.78629	5.654656	-2.32953
H	-4.54526	6.391616	-2.08005
C	-3.57794	5.285661	-3.65862
H	-4.17471	5.731954	-4.44967
C	-2.59882	4.336923	-3.96726
H	-2.43037	4.041159	-4.99935
C	-1.83546	3.759219	-2.9531
H	-1.08776	3.010549	-3.20279
C	0.676053	3.880248	-0.5857
C	1.0135	4.922637	-1.46043
H	0.244446	5.40632	-2.05426
C	2.340571	5.342731	-1.58164
H	2.588047	6.149142	-2.26723
C	3.341756	4.734608	-0.82356
H	4.37329	5.064153	-0.91694
C	3.012421	3.698999	0.05488
H	3.786352	3.218692	0.64735
C	1.690768	3.269899	0.171557
H	1.446495	2.45192	0.844771
C	-1.52921	4.082474	1.24904
C	-2.4693	3.429948	2.058519
H	-2.86605	2.470952	1.740579
C	-2.8783	3.988771	3.267511
H	-3.6318	3.469884	3.856065

C	-2.35075	5.215482	3.693401
C	-1.42524	5.88125	2.878022
H	-1.0372	6.839322	3.208307
C	-1.01101	5.31619	1.675715
H	-0.27623	5.834475	1.067149
I	-0.16211	-0.06691	-2.6597
Cu	1.302313	-1.28897	-0.4698
P	1.003087	-3.42181	-0.32595
C	3.579464	0.166768	-1.54425
H	2.90994	0.28445	-2.39091
C	4.870485	0.669202	-1.58216
H	5.227095	1.178782	-2.47034
C	5.160347	-0.13345	0.663895
H	5.751079	-0.26899	1.563007
C	3.8599	-0.60669	0.611625
H	3.422002	-1.10807	1.468217
C	5.707222	0.522424	-0.45841
C	7.036212	1.014231	-0.45427
S	10.1573	2.742691	-1.85389
C	8.18185	1.429253	-0.44197
C	9.499446	1.913111	-0.44865
C	10.44989	1.83653	0.554204
H	10.24943	1.362103	1.507815
C	11.68753	2.43462	0.199438
H	12.54951	2.470983	0.856191
C	11.68027	2.963968	-1.066
H	12.48526	3.472189	-1.58021
C	1.975328	-4.12763	1.068453
C	3.143552	-4.88081	0.867543
H	3.458183	-5.13656	-0.13874
C	3.903606	-5.31037	1.952297
H	4.805186	-5.89597	1.803931
C	3.51159	-4.99765	3.259878
C	2.348177	-4.24167	3.469661
H	2.042444	-3.99126	4.479527
C	1.591977	-3.80757	2.385133
H	0.70459	-3.206	2.558859
C	-0.69279	-4.08761	-0.07778
C	-0.99812	-5.16808	0.763289

H	-0.21604	-5.64055	1.3493
C	-2.30918	-5.63929	0.864529
H	-2.53077	-6.47389	1.524792
C	-3.32782	-5.04489	0.118272
H	-4.34724	-5.41419	0.195615
C	-3.03135	-3.97353	-0.72773
H	-3.81852	-3.50475	-1.31198
C	-1.72475	-3.49437	-0.82421
H	-1.50653	-2.65074	-1.47408
C	1.612207	-4.33209	-1.804
C	2.523084	-3.67447	-2.64386
H	2.809283	-2.65324	-2.41031
C	3.041411	-4.31309	-3.77124
H	3.743528	-3.78902	-4.41394
C	2.645274	-5.61593	-4.07725
H	3.040939	-6.11308	-4.95895
C	1.730775	-6.27674	-3.25281
H	1.414201	-7.28858	-3.49205
C	1.217222	-5.64039	-2.12256
H	0.500552	-6.1598	-1.49312
H	-9.89164	-2.92574	1.579978
C	-10.4026	-2.51152	0.718588
S	-10.8835	-1.20421	-1.46432
C	4.357982	-5.48389	4.3789
O	5.379882	-6.13064	4.251679
O	3.878963	-5.13365	5.600925
H	4.510992	-5.50356	6.244959
C	-2.7529	5.873806	4.979154
O	-3.2488	5.059925	5.951155
H	-3.10929	4.12976	5.708785
O	-2.65668	7.062081	5.177299
N	-3.24275	0.452412	-0.23925
N	3.065722	-0.48216	-0.4763

Complex 8

I	-0.26898	0.2911	-2.35646
Cu	0.93526	1.58769	0.09062
S	10.55428	-0.41098	0.33218
S	13.44575	-2.02072	1.0365

P	0.11859	3.58286	0.16429
N	2.8326	1.24758	-0.10672
C	3.47237	1.67295	-1.2204
H	2.85655	2.15948	-1.96928
C	4.83242	1.51433	-1.42492
H	5.28997	1.88037	-2.33734
C	5.61406	0.87429	-0.44036
C	4.94242	0.41865	0.71128
H	5.48453	-0.09412	1.49796
C	3.57574	0.61658	0.82939
H	3.03228	0.25544	1.69729
C	7.00899	0.69359	-0.60603
C	8.20919	0.54394	-0.76104
C	9.58948	0.36391	-0.91851
C	10.39156	0.72668	-1.98839
H	9.99426	1.218	-2.86907
C	11.74852	0.37528	-1.81949
H	12.51249	0.55093	-2.56839
C	12.01576	-0.25466	-0.61607
C	13.30084	-0.72381	-0.13582
C	14.55221	-0.27527	-0.50766
H	14.6984	0.54166	-1.20555
C	15.61552	-0.9617	0.14172
H	16.66441	-0.73999	-0.022
C	15.17532	-1.92497	1.00967
H	15.76154	-2.58505	1.63469
C	-1.70082	3.82098	0.05375
C	-2.51029	2.88421	0.71689
H	-2.05151	2.04282	1.22995
C	-3.89855	3.02198	0.71097
H	-4.51245	2.28961	1.22811
C	-4.49677	4.08999	0.03815
H	-5.57885	4.19282	0.0298
C	-3.69976	5.02342	-0.62664
H	-4.15805	5.85643	-1.15364
C	-2.30926	4.89334	-0.61568
H	-1.7	5.62474	-1.13773
C	0.7944	4.67107	-1.15817
C	1.65936	5.74535	-0.90371

H	1.91422	6.00945	0.1176
C	2.19828	6.4865	-1.95875
H	2.86591	7.31705	-1.74413
C	1.87812	6.168	-3.27866
H	2.29653	6.74733	-4.09755
C	1.01743	5.09845	-3.54211
H	0.76387	4.84058	-4.567
C	0.48234	4.35184	-2.49311
H	-0.17408	3.51315	-2.70939
C	0.57185	4.45335	1.72533
C	1.74342	4.04185	2.37993
H	2.31634	3.21774	1.96537
C	2.15877	4.65906	3.55706
H	3.06313	4.33117	4.05734
C	1.39506	5.69827	4.10538
C	0.21892	6.10889	3.46318
H	-0.36269	6.91154	3.90484
C	-0.18816	5.49296	2.28353
H	-1.10367	5.81657	1.79842
I	0.02535	-0.0973	2.24517
Cu	-1.06132	-1.4626	-0.18033
S	-10.7591	0.12582	-0.34668
S	-13.728	1.54492	-1.12921
P	-0.14551	-3.41475	-0.20326
N	-2.97082	-1.18764	0.03423
C	-3.56468	-1.53109	1.20021
H	-2.90804	-1.91074	1.97556
C	-4.925	-1.40882	1.42762
H	-5.34356	-1.7034	2.38357
C	-5.75704	-0.89422	0.41145
C	-5.13292	-0.52059	-0.79556
H	-5.71546	-0.10372	-1.60961
C	-3.76276	-0.67604	-0.93392
H	-3.25664	-0.37337	-1.84557
C	-7.15379	-0.75349	0.59812
C	-8.35537	-0.63601	0.76965
C	-9.73795	-0.49485	0.94469
C	-10.5022	-0.78858	2.06244
H	-10.067	-1.18164	2.97402

C	-11.8753	-0.50593	1.89581
H	-12.6158	-0.64169	2.6759
C	-12.1929	0.00091	0.64726
C	-13.5057	0.3742	0.15821
C	-14.7298	-0.08211	0.60415
H	-14.828	-0.83186	1.38135
C	-15.8336	0.49813	-0.08013
H	-16.869	0.25491	0.13178
C	-15.4514	1.38816	-1.04801
H	-16.077	1.96269	-1.71769
C	1.68367	-3.58118	-0.29423
C	2.369	-2.64814	-1.08951
H	1.82155	-1.8385	-1.56484
C	3.75046	-2.74498	-1.26068
H	4.26586	-2.01445	-1.87823
C	4.46759	-3.76715	-0.63538
H	5.54461	-3.83694	-0.76429
C	3.79583	-4.69618	0.16101
H	4.34662	-5.49239	0.65513
C	2.41212	-4.60778	0.32651
H	1.90449	-5.335	0.95261
C	-0.62093	-4.39881	1.28048
C	-1.66302	-5.33922	1.23859
H	-2.14782	-5.56627	0.29427
C	-2.08233	-5.99299	2.3997
H	-2.88908	-6.71905	2.34676
C	-1.46578	-5.72654	3.61955
H	-1.78099	-6.23558	4.52341
C	-0.42065	-4.79294	3.67392
C	-0.01026	-4.12598	2.51357
H	0.78528	-3.3928	2.59492
C	-0.73724	-4.44417	-1.61271
C	-1.90537	-4.03151	-2.26993
H	-2.39171	-3.11771	-1.94203
C	-2.42433	-4.77099	-3.33393
H	-3.32859	-4.43585	-3.83477
C	-1.77203	-5.92898	-3.75971
H	-2.16845	-6.50274	-4.59334
C	-0.60179	-6.34399	-3.11821

H	-0.08661	-7.24075	-3.45265
C	-0.08722	-5.60784	-2.05085
H	0.82833	-5.93343	-1.56583
C	1.78243	6.39013	5.36273
O	1.15939	7.29653	5.8803
O	2.93263	5.91042	5.9024
H	3.07756	6.43198	6.71358
C	0.29669	-4.48812	4.94144
O	1.28371	-3.78828	5.03601
O	-0.26396	-5.09	6.0251
H	0.28748	-4.82088	6.78314

Complex 9

I	-0.38701	-0.05094	-2.2846
Cu	0.95196	1.22796	-0.01618
S	10.67109	-0.18389	-0.08673
S	13.68263	-1.45933	0.68964
P	0.1432	3.21478	0.21109
N	2.85305	0.96376	-0.28864
C	3.41298	1.33088	-1.46428
H	2.73309	1.70868	-2.22065
C	4.7703	1.24434	-1.72246
H	5.16067	1.55949	-2.68383
C	5.63681	0.74323	-0.72883
C	5.04898	0.34765	0.489
H	5.65984	-0.05672	1.28838
C	3.67892	0.46699	0.65896
H	3.20225	0.15147	1.58196
C	7.03187	0.63652	-0.94692
C	8.23238	0.54892	-1.14369
C	9.6138	0.4424	-1.34615
C	10.35257	0.77945	-2.46956
H	9.89304	1.18436	-3.36383
C	11.73349	0.52686	-2.33278
H	12.45599	0.70115	-3.122
C	12.08573	-0.00174	-1.10068
C	13.41235	-0.35393	-0.64498
C	14.6216	0.07968	-1.15586
H	14.69247	0.78677	-1.97495

C	15.74699	-0.47398	-0.50178
H	16.77169	-0.26541	-0.78839
C	15.42339	-1.33038	0.53294
C	-1.67876	3.44808	0.2723
C	-2.42561	2.50897	1.0033
H	-1.92425	1.67009	1.47875
C	-3.80992	2.64133	1.11557
H	-4.37378	1.90664	1.6838
C	-4.46787	3.70512	0.49372
H	-5.5474	3.80221	0.57541
C	-3.73357	4.64136	-0.23629
H	-4.23825	5.47164	-0.7237
C	-2.34643	4.51799	-0.34207
H	-1.78637	5.25324	-0.91142
C	0.69462	4.35674	-1.1248
C	1.47079	5.50275	-0.89997
H	1.7478	5.78435	0.11063
C	1.89633	6.29259	-1.97136
H	2.49933	7.17628	-1.77907
C	1.54582	5.95382	-3.27843
H	1.87643	6.57039	-4.11016
C	0.76735	4.81676	-3.51217
H	0.48846	4.5443	-4.52668
C	0.34708	4.02101	-2.44702
H	-0.24633	3.13134	-2.64206
C	0.73284	4.02488	1.75957
C	2.07904	3.8476	2.12773
H	2.73011	3.24074	1.50485
C	2.58496	4.42655	3.28572
H	3.62652	4.30384	3.56391
C	1.74697	5.16849	4.12979
C	0.4054	5.34917	3.76814
H	-0.25653	5.96389	4.37481
C	-0.09411	4.79039	2.59207
H	-1.1325	4.95353	2.32402
I	0.2419	-0.40934	2.32167
Cu	-1.09916	-1.7798	0.09296
S	-10.7205	0.13457	-0.18249
S	-13.6162	1.57151	-1.11183

P	-0.01265	-3.61621	-0.26484
N	-2.99382	-1.46532	0.35059
C	-3.60922	-1.71415	1.53099
H	-2.99454	-2.08371	2.34398
C	-4.96715	-1.52899	1.73522
H	-5.39697	-1.75638	2.70423
C	-5.77267	-1.04879	0.68295
C	-5.12631	-0.7744	-0.53927
H	-5.68677	-0.38975	-1.3841
C	-3.76306	-0.98839	-0.65583
H	-3.24267	-0.75996	-1.58062
C	-7.16459	-0.84549	0.84619
C	-8.3624	-0.67255	0.99668
C	-9.73927	-0.46813	1.14817
C	-10.5273	-0.68043	2.26857
H	-10.1179	-1.0502	3.20157
C	-11.8851	-0.35199	2.07299
H	-12.6378	-0.42459	2.84985
C	-12.17	0.11064	0.79777
C	-13.4578	0.51589	0.27965
C	-14.7073	0.17884	0.76604
H	-14.8472	-0.48734	1.61018
C	-15.7755	0.7374	0.02564
H	-16.8209	0.54594	0.24082
C	-15.3662	1.51484	-1.04056
C	1.82016	-3.56506	-0.3523
C	2.41089	-2.94347	-1.46664
H	1.7831	-2.53876	-2.25515
C	3.79739	-2.83168	-1.55765
H	4.24082	-2.35104	-2.42548
C	4.61334	-3.32645	-0.53606
H	5.69398	-3.23715	-0.60965
C	4.03307	-3.92992	0.5799
H	4.65948	-4.31153	1.38212
C	2.64428	-4.04862	0.67307
H	2.20689	-4.51741	1.54864
C	-0.37079	-4.84659	1.06898
C	-0.13433	-6.22732	0.97222
H	0.31188	-6.64161	0.0731

C	-0.4947	-7.07989	2.01633
H	-0.32475	-8.14911	1.92593
C	-1.09526	-6.56803	3.16832
H	-1.41661	-7.25401	3.9492
C	-1.33732	-5.19222	3.27973
C	-0.97156	-4.34668	2.22601
H	-1.15386	-3.28142	2.30599
C	-0.50012	-4.51161	-1.79805
C	-1.7966	-4.29039	-2.28652
H	-2.43395	-3.56889	-1.78298
C	-2.25765	-4.9677	-3.41528
H	-3.26317	-4.78215	-3.78298
C	-1.42256	-5.869	-4.07829
H	-1.77699	-6.39135	-4.96294
C	-0.12547	-6.08734	-3.60913
H	0.53261	-6.77942	-4.12818
C	0.33396	-5.41415	-2.47574
H	1.35105	-5.57701	-2.13151
C	-16.1986	2.23313	-1.98532
C	-17.48	2.70592	-1.78712
C	-17.1648	3.37873	-3.99216
H	-17.9969	2.61418	-0.83832
C	-18.0283	3.35228	-2.93002
H	-17.3169	3.81178	-4.9716
H	-19.0199	3.79085	-2.95595
C	16.33161	-2.03518	1.41634
C	17.6246	-1.68352	1.74657
C	17.44298	-3.65244	2.97313
H	18.09347	-0.77403	1.3876
C	18.25514	-2.60586	2.62769
H	17.66005	-4.48364	3.63034
H	19.26714	-2.48779	2.99939
S	-15.6659	2.59366	-3.6178
S	15.89158	-3.53719	2.20919
C	-2.05403	-4.58656	4.44753
C	2.34635	5.76155	5.36837
O	-1.94955	-5.2431	5.63388
H	-1.26366	-5.92812	5.57234
O	1.48442	6.06118	6.37933

H	0.61103	5.67928	6.19337
O	3.52819	5.97883	5.49898
O	-2.71808	-3.57788	4.37401

Complex 10

I	-0.3495	-0.02778	-2.49609
Cu	0.96168	1.39384	-0.27211
S	10.66867	-0.06916	0.13629
S	13.6242	-1.41026	0.99229
P	0.18749	3.40148	-0.11135
N	2.87757	1.14127	-0.45775
C	3.51534	1.61693	-1.55237
H	2.88964	2.08147	-2.30699
C	4.88591	1.54152	-1.7308
H	5.33917	1.94457	-2.62968
C	5.68444	0.93791	-0.73621
C	5.01656	0.4341	0.3976
H	5.57213	-0.04836	1.19399
C	3.63846	0.55081	0.49032
H	3.10203	0.16021	1.34933
C	7.09027	0.8434	-0.87277
C	8.30108	0.76999	-1.00005
C	9.69257	0.6778	-1.12266
C	10.5007	1.11776	-2.15961
H	10.0981	1.60724	-3.03892
C	11.87047	0.84902	-1.95952
H	12.64126	1.09575	-2.68074
C	12.14445	0.2044	-0.76287
C	13.43965	-0.19443	-0.2582
C	14.67926	0.27332	-0.6534
H	14.80283	1.04699	-1.40302
C	15.76055	-0.34084	0.02045
H	16.80145	-0.11526	-0.18265
C	15.37139	-1.28015	0.95603
C	-1.62383	3.69172	0.0112
C	-2.39209	2.74707	0.71167
H	-1.91149	1.87494	1.14675
C	-3.77056	2.91971	0.84761
H	-4.35157	2.18183	1.39416

C	-4.40023	4.02713	0.27563
H	-5.4749	4.15598	0.37509
C	-3.64445	4.96661	-0.42839
H	-4.12808	5.82973	-0.87846
C	-2.26408	4.80374	-0.55641
H	-1.68811	5.54153	-1.10627
C	0.71834	4.51289	-1.47997
C	1.18636	5.82285	-1.29338
H	1.27047	6.23399	-0.29239
C	1.55414	6.60831	-2.38832
H	1.92016	7.61864	-2.22524
C	1.44725	6.10151	-3.68448
H	1.73361	6.71432	-4.53513
C	0.96981	4.80381	-3.88243
H	0.87884	4.40187	-4.888
C	0.60864	4.01377	-2.79047
H	0.24521	3.00205	-2.95513
C	0.87929	4.1932	1.4018
C	2.27608	4.35135	1.49367
H	2.90825	4.07864	0.65321
C	2.86497	4.85585	2.64735
H	3.9391	4.995	2.70964
C	2.04858	5.18923	3.73282
C	0.66445	5.03949	3.67068
H	0.05053	5.31884	4.5202
C	0.08513	4.54531	2.50091
H	-0.9922	4.43166	2.45182
I	0.18152	-0.19222	2.059
Cu	-1.09746	-1.63616	-0.13465
S	-10.7699	0.08332	-0.11894
S	-13.7464	1.39755	-0.96168
P	-0.21038	-3.59828	-0.23904
N	-2.99087	-1.31194	0.11068
C	-3.55563	-1.58638	1.30915
H	-2.88435	-1.94227	2.08361
C	-4.90558	-1.42542	1.57077
H	-5.30003	-1.66634	2.55166
C	-5.75875	-0.94473	0.55514
C	-5.16376	-0.64062	-0.68604

H	-5.76273	-0.25144	-1.50186
C	-3.80188	-0.82978	-0.85696
H	-3.31725	-0.57879	-1.79576
C	-7.14644	-0.77161	0.77448
C	-8.34119	-0.62891	0.97426
C	-9.71566	-0.46134	1.18036
C	-10.4492	-0.67385	2.33742
H	-9.99	-1.01108	3.25955
C	-11.8232	-0.39095	2.19345
H	-12.54	-0.46999	3.00291
C	-12.1757	0.03545	0.92213
C	-13.4961	0.38822	0.45034
C	-14.7126	0.02788	0.99976
H	-14.7958	-0.61695	1.86765
C	-15.8283	0.53173	0.291
H	-16.8569	0.31511	0.55655
C	-15.4891	1.28959	-0.81339
C	1.61715	-3.79399	-0.1925
C	2.36417	-2.90309	-0.98171
H	1.85936	-2.11792	-1.53871
C	3.75293	-3.0129	-1.04789
H	4.31671	-2.31674	-1.66272
C	4.41644	-4.00585	-0.32319
H	5.49935	-4.08553	-0.37043
C	3.68272	-4.89357	0.46452
H	4.19029	-5.66803	1.03358
C	2.29068	-4.79369	0.52465
H	1.73637	-5.4936	1.14194
C	-0.81685	-4.66294	1.14088
C	-1.78815	-5.65652	0.94156
H	-2.14335	-5.86509	-0.06215
C	-2.3077	-6.38451	2.01482
H	-3.06475	-7.14284	1.83617
C	-1.85519	-6.14882	3.31045
H	-2.24489	-6.70205	4.15783
C	-0.88794	-5.15936	3.50381
C	-0.37683	-4.40167	2.45093
H	0.34486	-3.61562	2.65202
C	-0.69648	-4.52619	-1.751

C	-1.73867	-3.99682	-2.52437
H	-2.18888	-3.05876	-2.21527
C	-2.17105	-4.64958	-3.67974
H	-2.97627	-4.22348	-4.27181
C	-1.55604	-5.83698	-4.07829
H	-1.88477	-6.3445	-4.98138
C	-0.50787	-6.36796	-3.32053
H	-0.02075	-7.28747	-3.63441
C	-0.07842	-5.71704	-2.16411
H	0.74529	-6.13049	-1.58892
S	2.79903	5.80569	5.22943
S	-0.28455	-4.873	5.16044
O	3.96096	6.60752	4.8788
O	1.7472	6.29515	6.12034
O	3.41201	4.43753	5.91106
H	2.74884	4.10475	6.5452
O	1.01622	-5.89419	5.15991
H	0.98492	-6.36928	6.01268
O	0.20665	-3.50809	5.26777
O	-1.23055	-5.42177	6.13533
C	-16.3822	1.95368	-1.7422
C	-17.6689	2.39245	-1.50441
C	-17.4648	3.00955	-3.73858
H	-18.1443	2.31317	-0.53304
C	-18.2833	2.98783	-2.64127
H	-17.6704	3.40843	-4.72276
H	-19.2887	3.39464	-2.63846
C	16.2208	-2.06486	1.83044
C	17.49117	-1.75293	2.27034
C	17.22759	-3.81837	3.30868
H	17.98425	-0.81974	2.02166
C	18.06253	-2.75244	3.10642
H	17.40087	-4.70469	3.90398
H	19.04933	-2.67469	3.5496
S	-15.9278	2.28237	-3.40481
S	15.72807	-3.62606	2.46168