

Supplementary Information

Emission energy of azole-based ionic iridium(III) complexes: A theoretical study

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Table S1. Cartesian coordinates (x, y, z , in Å) calculated for the minimum-energy optimized structures of **1**, **2a-c**, **3a-c**, **4a-c**, **2b'**, **2b''** and **3b'** complexes in the singlet ground state (S_0) and in the lowest-energy T_1 triplet state. All calculations performed at the B3LYP/(6-31G**+LANL2DZ) level in the presence of the solvent (acetonitrile).

Complex 1

	State S_0			State T_1		
C	1.464549	1.864851	-2.045231	-1.814010	-1.550403	1.993568
N	1.609279	0.990452	-1.034668	-0.891167	-1.607001	1.002884
C	2.851931	0.725646	-0.553454	-0.476418	-2.849721	0.527000
C	3.977033	1.354635	-1.096651	-1.023843	-4.026721	1.115323
C	3.822537	2.257279	-2.144347	-1.951758	-3.943766	2.123168
C	2.543393	2.517854	-2.630742	-2.368591	-2.665848	2.582556
C	2.930245	-0.250672	0.559544	0.479614	-2.849082	-0.527399
N	1.745908	-0.715925	1.035695	0.892814	-1.605812	-1.003183
C	1.742779	-1.604614	2.044292	1.815546	-1.547985	-1.993917
C	2.911835	-2.073561	2.632943	2.371486	-2.662693	-2.583011
C	4.132788	-1.605790	2.152187	1.956279	-3.941167	-2.123689
C	4.141158	-0.688004	1.106329	1.028514	-4.025349	-1.115809
C	-1.998745	2.118489	-0.538307	-2.352918	1.756465	0.464620
C	-3.012023	2.855591	-1.174317	-3.205935	2.685033	1.069003
C	-3.632502	2.350680	-2.312235	-2.813920	3.326129	2.244444
C	-3.238655	1.105734	-2.815053	-1.567759	3.044722	2.822948
C	-2.231642	0.370668	-2.184569	-0.711562	2.124380	2.226649
C	-1.582826	0.853330	-1.035964	-1.071213	1.467477	1.031175
C	-1.296344	2.585074	0.659229	-2.683176	1.030909	-0.765969
N	-0.325896	1.734704	1.113754	-1.697438	0.192998	-1.203106
C	0.385083	2.053887	2.213789	-1.876241	-0.544275	-2.313729
C	0.175596	3.227454	2.922017	-3.047040	-0.479037	-3.058264
C	-0.809678	4.109764	2.473042	-4.064712	0.374981	-2.633225
C	-1.543626	3.784775	1.340330	-3.880839	1.131006	-1.480738
C	-0.118866	-4.188295	-2.469811	4.064242	0.378592	2.633238
C	0.706711	-3.155473	-2.919765	3.047405	-0.476480	3.058156
C	0.717755	-1.962194	-2.213607	1.876652	-0.542716	2.313634
N	-0.037287	-1.763601	-1.114431	1.697134	0.194543	1.203120
C	-0.854251	-2.762252	-0.659635	2.682040	1.033503	0.766118
C	-0.898256	-3.987464	-1.338677	3.879611	1.134647	1.480889
C	-1.625862	-2.416221	0.536171	2.351041	1.758969	-0.464321
C	-1.423863	-1.099471	1.032806	1.069635	1.468762	-1.030952
C	-2.145050	-0.727834	2.179370	0.709308	2.125544	-2.226298
C	-3.019314	-1.617089	2.809364	1.564547	3.046908	-2.822386
C	-3.202813	-2.910385	2.307894	2.810410	3.329490	-2.243807
C	-2.505796	-3.308521	1.171837	3.203090	2.688552	-1.068498
Ir	-0.070257	-0.005228	-0.000834	-0.000095	0.130575	-0.000015
H	0.448487	2.032446	-2.382227	-2.094994	-0.555041	2.316987
H	4.965302	1.150997	-0.706111	-0.703313	-4.997831	0.757660

H	4.690082	2.749239	-2.570334	-2.362256	-4.847328	2.562464
H	2.375037	3.213160	-3.444623	-3.097874	-2.553231	3.375693
H	0.766756	-1.937245	2.377146	2.095269	-0.552257	-2.317305
H	2.856583	-2.788686	3.445199	3.100573	-2.549104	-3.376190
H	5.067640	-1.949832	2.580917	2.367899	-4.844183	-2.563054
H	5.084204	-0.324814	0.719713	0.709228	-4.996879	-0.758179
H	-3.319042	3.822795	-0.787865	-4.173477	2.917834	0.637396
H	-4.415441	2.919896	-2.803544	-3.480486	4.043074	2.712639
H	-3.720828	0.705539	-3.703228	-1.271991	3.548636	3.737898
H	-1.950284	-0.591993	-2.600723	0.247148	1.916203	2.689192
H	1.134084	1.336238	2.522149	-1.053430	-1.188597	-2.594779
H	0.772181	3.437474	3.801668	-3.149230	-1.087833	-3.948409
H	-1.002915	5.037776	3.000827	-4.991640	0.450462	-3.191334
H	-2.312853	4.456245	0.979609	-4.662399	1.795430	-1.134396
H	-0.154490	-5.136539	-2.995804	4.991107	0.454878	3.191342
H	1.330905	-3.265119	-3.798511	3.150201	-1.085330	3.948195
H	1.337287	-1.130507	-2.522632	1.054453	-1.187861	2.594578
H	-1.545985	-4.776672	-0.977593	4.660515	1.799901	1.134658
H	-2.025694	0.268536	2.594165	-0.249182	1.916460	-2.688884
H	-3.562427	-1.300168	3.695978	1.268266	3.550711	-3.737231
H	-3.883017	-3.599453	2.798703	3.476224	4.047241	-2.711835
H	-2.649481	-4.313390	0.786233	4.170379	2.922281	-0.636825

Complex 2a

	State S ₀			State T ₁		
C	-1.622505	2.265570	1.438635	-1.559904	2.311273	1.382505
N	-1.699470	1.134041	0.718702	-1.620518	1.152025	0.684811
C	-2.917157	0.624149	0.399290	-2.863810	0.612946	0.360952
C	-4.088918	1.263300	0.816833	-4.038846	1.307707	0.769194
C	-4.005632	2.434931	1.563146	-3.953133	2.483004	1.472945
C	-2.750205	2.948335	1.880731	-2.673873	3.008720	1.796662
C	-2.917012	-0.625501	-0.398785	-2.863823	-0.612882	-0.360965
N	-1.699192	-1.134726	-0.718583	-1.620542	-1.151981	-0.684833
C	-1.621774	-2.266169	-1.438576	-1.559951	-2.311230	-1.382529
C	-2.749240	-2.949554	-1.880341	-2.673934	-3.008659	-1.796678
C	-4.004851	-2.436882	-1.562285	-3.953183	-2.482923	-1.472950
C	-4.088562	-1.265309	-0.815930	-4.038873	-1.307625	-0.769198
N	1.084233	2.239209	-1.523057	1.037769	2.225974	-1.599196
C	1.095101	2.988040	-2.653999	1.003414	2.946947	-2.752674
C	0.148643	2.458642	-3.515094	0.104307	2.329807	-3.599933
C	-0.411861	1.367516	-2.832047	-0.386313	1.217487	-2.890431
N	0.160863	1.242527	-1.629646	0.185251	1.164857	-1.686705
C	1.814166	2.297949	-0.303990	1.737051	2.366972	-0.382417
C	1.489674	1.283136	0.623354	1.442539	1.371226	0.594165
C	2.184940	1.321975	1.841075	2.101943	1.489917	1.835547

C	3.137701	2.310654	2.111183	3.011176	2.514776	2.073409
C	3.426378	3.295085	1.163340	3.280686	3.466062	1.077418
C	2.758368	3.295242	-0.061425	2.643300	3.399575	-0.162131
C	0.151402	-2.457871	3.515589	0.104221	-2.329804	3.599932
C	-0.410441	-1.367608	2.832229	-0.386371	-1.217478	2.890421
N	0.161571	-1.242725	1.629495	0.185201	-1.164866	1.686698
N	1.085793	-2.238628	1.522980	1.037698	-2.226001	1.599200
C	1.097934	-2.986849	2.654314	1.003323	-2.946966	2.752682
C	1.815358	-2.297196	0.303662	1.736993	-2.367013	0.382431
C	2.185183	-1.321107	-1.841516	2.101934	-1.489964	-1.835529
C	3.138366	-2.309363	-2.111777	3.011150	-2.514840	-2.073378
C	3.427674	-3.293636	-1.164009	3.280629	-3.466131	-1.077383
C	2.759917	-3.294078	0.060916	2.643227	-3.399632	0.162158
H	-0.621739	2.617532	1.658703	-0.563740	2.672396	1.608733
H	-5.059086	0.855511	0.565546	-5.010646	0.899619	0.518264
H	-4.909920	2.936484	1.889970	-4.855428	3.003374	1.777881
H	-2.637144	3.857714	2.459019	-2.558605	3.931354	2.352611
H	-0.620866	-2.617525	-1.658969	-0.563795	-2.672368	-1.608765
H	-2.635859	-3.858862	-2.458675	-2.558685	-3.931293	-2.352630
H	-4.908970	-2.938977	-1.888755	-4.855489	-3.003279	-1.777878
H	-5.058880	-0.858106	-0.564268	-5.010664	-0.899522	-0.518260
H	1.762068	3.827907	-2.766021	1.608942	3.829575	-2.883113
H	-0.100945	2.812880	-4.502779	-0.163795	2.638027	-4.597939
H	-1.181812	0.677881	-3.141810	-1.105672	0.468433	-3.183847
H	1.977448	0.571114	2.597790	1.899107	0.764851	2.616074
H	3.656597	2.311584	3.065650	3.516934	2.581502	3.031173
H	4.165095	4.062224	1.371993	3.988032	4.266297	1.267730
H	2.973008	4.059842	-0.801121	2.854706	4.140380	-0.924967
H	-0.097381	-2.811827	4.503579	-0.163895	-2.638014	4.597937
H	-1.181067	-0.678659	3.141863	-1.105721	-0.468410	3.183826
H	1.765826	-3.825967	2.766465	1.608830	-3.829607	2.883128
H	3.657106	-2.310026	-3.066325	3.516921	-2.581575	-3.031135
H	4.166676	-4.060465	-1.372811	3.987963	-4.266379	-1.267683
H	2.974955	-4.058611	0.800568	2.854607	-4.140440	0.924996
C	1.490228	-1.282501	-0.623646	1.442514	-1.371259	-0.594156
H	1.977227	-0.570324	-2.598239	1.899122	-0.764894	-2.616058
Ir	0.040050	-0.000060	-0.000076	0.106086	-0.000002	-0.000004

Complex 2b

	State S ₀			State T ₁		
C	-1.612477	2.277641	1.418449	1.552055	2.349849	-1.315302
N	-1.691654	1.146198	0.699843	1.614051	1.174029	-0.644953
C	-2.908575	0.626367	0.396030	2.857027	0.622230	-0.343893
C	-4.079325	1.258050	0.826099	4.031286	1.323604	-0.741032
C	-3.994918	2.431685	1.569258	3.945369	2.516956	-1.413334

C	-2.739632	2.953500	1.872209	2.665733	3.053774	-1.716436
C	-2.908574	-0.626367	-0.396040	2.857027	-0.622229	0.343894
N	-1.691652	-1.146204	-0.699838	1.614052	-1.174029	0.644954
C	-1.612471	-2.277650	-1.418438	1.552055	-2.349848	1.315303
C	-2.739624	-2.953505	-1.872210	2.665733	-3.053773	1.716438
C	-3.994911	-2.431682	-1.569277	3.945370	-2.516955	1.413335
C	-4.079322	-1.258044	-0.826121	4.031286	-1.323603	0.741033
N	1.073736	2.182546	-1.593272	-1.027434	2.194982	1.635083
C	1.045441	2.869372	-2.758901	-0.968479	2.863432	2.811257
C	0.077405	2.238793	-3.517453	-0.064849	2.150851	3.575051
N	-0.448219	1.206534	-2.811436	0.394265	1.090630	2.861183
N	0.161125	1.184284	-1.655804	-0.191189	1.129649	1.700715
C	1.815391	2.287284	-0.381727	-1.732451	2.365641	0.417188
C	1.492169	1.305379	0.579242	-1.437124	1.387172	-0.573547
C	2.193356	1.388416	1.791188	-2.095044	1.530862	-1.812830
C	3.147678	2.385945	2.016455	-3.006306	2.560562	-2.027317
C	3.434407	3.335775	1.032170	-3.278195	3.489796	-1.013399
C	2.760883	3.293036	-0.187508	-2.638006	3.399253	0.226424
C	0.077385	-2.238824	3.517440	-0.064847	-2.150851	-3.575051
N	-0.448231	-1.206556	2.811430	0.394267	-1.090630	-2.861183
N	0.161127	-1.184289	1.655806	-0.191188	-1.129649	-1.700714
N	1.073741	-2.182549	1.593272	-1.027432	-2.194983	-1.635083
C	1.045433	-2.869390	2.758892	-0.968477	-2.863433	-2.811258
C	1.815401	-2.287278	0.381729	-1.732450	-2.365642	-0.417189
C	2.193370	-1.388399	-1.791181	-2.095045	-1.530862	1.812829
C	3.147702	-2.385919	-2.016447	-3.006307	-2.560563	2.027315
C	3.434434	-3.335749	-1.032164	-3.278194	-3.489797	1.013398
C	2.760904	-3.293020	0.187512	-2.638005	-3.399254	-0.226425
H	-0.612206	2.635703	1.629606	0.556982	2.719183	-1.530817
H	-5.049317	0.841461	0.589200	5.002832	0.904513	-0.508327
H	-4.898619	2.927418	1.906345	4.847299	3.042047	-1.710835
H	-2.625724	3.863643	2.448982	2.549745	3.989932	-2.249044
H	-0.612200	-2.635718	-1.629582	0.556983	-2.719182	1.530819
H	-2.625714	-3.863651	-2.448978	2.549746	-3.989931	2.249046
H	-4.898610	-2.927410	-1.906374	4.847300	-3.042046	1.710836
H	-5.049314	-0.841450	-0.589236	5.002832	-0.904513	0.508326
H	1.683655	3.714391	-2.955783	-1.543950	3.752150	3.010223
H	-0.261128	2.469576	-4.515166	0.272624	2.340127	4.581540
H	1.991348	0.668433	2.578294	-1.887824	0.828011	-2.612104
H	3.671648	2.421689	2.967211	-3.509966	2.647650	-2.984294
H	4.175650	4.107665	1.210230	-3.986881	4.292291	-1.186698
H	2.970275	4.027213	-0.958495	-2.849940	4.120941	1.007060
H	-0.261159	-2.469620	4.515145	0.272627	-2.340127	-4.581539
H	1.683647	-3.714409	2.955773	-1.543947	-3.752150	-3.010224
H	3.671677	-2.421654	-2.967200	-3.509967	-2.647651	2.984292
H	4.175685	-4.107632	-1.210222	-3.986881	-4.292292	1.186696

H	2.970299	-4.027198	0.958497	-2.849938	-4.120942	-1.007061
C	1.492176	-1.305372	-0.579238	-1.437124	-1.387173	0.573547
H	1.991359	-0.668415	-2.578285	-1.887826	-0.828011	2.612103
Ir	0.038918	-0.000001	0.000003	-0.102985	0.000000	0.000000

Complex 2c

	State S ₀			State T ₁		
C	-1.609084	2.285853	1.407138	1.543680	2.341076	-1.330040
N	-1.689327	1.151856	0.692284	1.608467	1.176183	-0.638349
C	-2.906205	0.628290	0.392743	2.852203	0.622154	-0.343199
C	-4.076242	1.260572	0.822369	4.025277	1.317938	-0.752482
C	-3.991347	2.437489	1.560495	3.937519	2.502619	-1.439203
C	-2.736425	2.961917	1.859653	2.656933	3.036089	-1.744777
C	-2.906205	-0.628288	-0.392751	2.852212	-0.622106	0.343207
N	-1.689328	-1.151861	-0.692282	1.608484	-1.176154	0.638352
C	-1.609084	-2.285860	-1.407130	1.543712	-2.341049	1.330043
C	-2.736425	-2.961920	-1.859654	2.656975	-3.036044	1.744785
C	-3.991346	-2.437483	-1.560509	3.937554	-2.502553	1.439215
C	-4.076242	-1.260564	-0.822388	4.025295	-1.317871	0.752494
N	1.063349	2.159463	-1.621958	-1.015958	2.153796	1.688867
C	0.978300	2.794635	-2.803600	-0.904543	2.752334	2.888891
N	0.053954	2.200703	-3.548836	-0.039170	2.071674	3.628643
N	-0.442217	1.185212	-2.823004	0.393982	1.040906	2.882626
N	0.158461	1.154430	-1.669296	-0.185986	1.084883	1.724301
C	1.815762	2.286407	-0.417897	-1.732834	2.360312	0.479621
C	1.496113	1.318582	0.557218	-1.436277	1.410118	-0.536668
C	2.205019	1.420615	1.762799	-2.097226	1.591231	-1.769457
C	3.160503	2.421811	1.963591	-3.014717	2.622814	-1.947357
C	3.442773	3.356157	0.962624	-3.288591	3.519243	-0.905370
C	2.762730	3.295519	-0.251587	-2.642526	3.394890	0.329498
N	0.053929	-2.200727	3.548822	-0.039140	-2.071662	-3.628652
N	-0.442244	-1.185237	2.822989	0.394029	-1.040915	-2.882616
N	0.158459	-1.154434	1.669295	-0.185963	-1.084885	-1.724303
N	1.063350	-2.159465	1.621958	-1.015909	-2.153817	-1.688868
C	0.978286	-2.794649	2.803593	-0.904474	-2.752360	-2.888887
C	1.815771	-2.286403	0.417901	-1.732786	-2.360343	-0.479624
C	2.205037	-1.420603	-1.762790	-2.097207	-1.591261	1.769449
C	3.160534	-2.421789	-1.963575	-3.014678	-2.622861	1.947348
C	3.442805	-3.356133	-0.962607	-3.288528	-3.519300	0.905364
C	2.762752	-3.295503	0.251599	-2.642457	-3.394940	-0.329501
H	-0.609289	2.645853	1.616424	0.548793	2.710079	-1.545220
H	-5.046183	0.841678	0.589772	4.996930	0.898600	-0.521248
H	-4.894970	2.933454	1.897237	4.838315	3.023250	-1.747189
H	-2.622460	3.874109	2.432981	2.540014	3.967020	-2.286139
H	-0.609290	-2.645867	-1.616406	0.548831	-2.710068	1.545219

H	-2.622460	-3.874114	-2.432977	2.540069	-3.966976	2.286146
H	-4.894969	-2.933443	-1.897259	4.838357	-3.023170	1.747205
H	-5.046183	-0.841663	-0.589800	4.996942	-0.898517	0.521264
H	1.572500	3.648822	-3.084853	-1.437889	3.641447	3.184518
H	2.011348	0.714863	2.564457	-1.891102	0.917145	-2.593198
H	3.690584	2.472545	2.909989	-3.521688	2.736436	-2.899595
H	4.186168	4.129168	1.124410	-4.001859	4.322751	-1.051664
H	2.967277	4.014793	-1.037583	-2.854672	4.090117	1.133664
H	1.572489	-3.648834	3.084849	-1.437803	-3.641482	-3.184515
H	3.690622	-2.472517	-2.909969	-3.521652	-2.736490	2.899584
H	4.186210	-4.129135	-1.124387	-4.001780	-4.322822	1.051657
H	2.967301	-4.014774	1.037597	-2.854585	-4.090175	-1.133665
C	1.496120	-1.318579	-0.557215	-1.436255	-1.410139	0.536662
H	2.011365	-0.714853	-2.564450	-1.891100	-0.917167	2.593188
Ir	0.038543	-0.000002	0.000000	-0.102383	0.000000	-0.000001

Complex 3a

	State S ₀			State T ₁		
C	-0.921349	-1.594861	2.519928	-0.945051	-1.543836	2.521925
N	-0.460554	-1.670402	1.259986	-0.474705	-1.602169	1.255166
C	-0.256065	-2.888717	0.695550	-0.252675	-2.844729	0.665310
C	-0.520723	-4.061281	1.411423	-0.537069	-4.021529	1.418051
C	-0.997480	-3.978454	2.715950	-1.015637	-3.936955	2.701919
C	-1.201919	-2.722500	3.283630	-1.228519	-2.658706	3.283294
C	0.256080	-2.888715	-0.695550	0.252650	-2.844732	-0.665305
N	0.460562	-1.670399	-1.259986	0.474694	-1.602175	-1.255161
C	0.921355	-1.594855	-2.519928	0.945042	-1.543848	-2.521920
C	1.201931	-2.722491	-3.283631	1.228499	-2.658723	-3.283288
C	0.997499	-3.978447	-2.715951	1.015602	-3.936969	-2.701911
C	0.520743	-4.061277	-1.411425	0.537031	-4.021536	-1.418044
C	-2.745450	1.114893	0.174582	-2.770270	1.076421	0.132099
C	-4.033504	1.062801	-0.304473	-4.048325	0.995851	-0.374156
N	-4.044117	0.111117	-1.306416	-4.003274	0.084937	-1.406873
C	-2.792939	-0.391252	-1.419949	-2.731134	-0.368508	-1.516263
N	-1.989685	0.194775	-0.542564	-1.969296	0.215229	-0.605159
C	-2.018271	1.856790	1.196557	-2.091281	1.792443	1.195615
C	-0.634513	1.525480	1.287687	-0.693521	1.483682	1.321068
C	0.112432	2.207192	2.261988	0.023885	2.132602	2.348855
C	-0.472824	3.160007	3.104341	-0.595333	3.050272	3.191569
C	-1.832291	3.465421	2.995297	-1.960897	3.341951	3.041815
C	-2.605899	2.810672	2.037779	-2.708298	2.715121	2.046838
C	1.832274	3.465426	-2.995299	1.960922	3.341928	-3.041823
C	0.472808	3.160008	-3.104340	0.595355	3.050260	-3.191576
C	-0.112444	2.207193	-2.261985	-0.023870	2.132597	-2.348859
C	0.634506	1.525483	-1.287685	0.693532	1.483674	-1.321071

C	2.018263	1.856796	-1.196559	2.091295	1.792424	-1.195620
C	2.605887	2.810679	-2.037783	2.708319	2.715095	-2.046846
C	2.745446	1.114902	-0.174585	2.770278	1.076400	-0.132102
N	1.989684	0.194786	0.542567	1.969298	0.215217	0.605160
C	2.792942	-0.391241	1.419948	2.731134	-0.368527	1.516262
N	4.044121	0.111122	1.306404	4.003279	0.084904	1.406866
C	4.033503	1.062807	0.304461	4.048334	0.995818	0.374148
Ir	0.000000	0.072471	0.000001	0.000001	0.133087	0.000000
H	-1.060010	-0.593176	2.909467	-1.088500	-0.546720	2.922263
H	-0.358670	-5.031370	0.960198	-0.371762	-4.993217	0.967937
H	-1.205008	-4.882754	3.277646	-1.228343	-4.840099	3.265381
H	-1.571110	-2.609855	4.296266	-1.601967	-2.544987	4.293951
H	1.060011	-0.593168	-2.909466	1.088503	-0.546735	-2.922259
H	1.571120	-2.609844	-4.296267	1.601950	-2.545009	-4.293943
H	1.205030	-4.882745	-3.277649	1.228299	-4.840116	-3.265373
H	0.358695	-5.031368	-0.960200	0.371713	-4.993222	-0.967930
H	-4.925538	1.603095	-0.031025	-4.963759	1.493256	-0.096528
C	-5.203590	-0.285542	-2.100145	-5.133018	-0.324333	-2.240615
H	1.172644	1.996353	2.371568	1.079754	1.920982	2.481859
H	0.136958	3.667096	3.848117	-0.021816	3.546386	3.968875
H	-2.284725	4.205614	3.648643	-2.438294	4.056466	3.705077
H	-3.664858	3.040264	1.946103	-3.764501	2.942573	1.937084
H	2.284705	4.205620	-3.648647	2.438323	4.056438	-3.705087
H	-0.136978	3.667096	-3.848114	0.021842	3.546377	-3.968883
H	-1.172656	1.996351	-2.371562	-1.079740	1.920985	-2.481862
H	3.664845	3.040274	-1.946110	3.764523	2.942538	-1.937092
H	4.925537	1.603098	0.031006	4.963773	1.493213	0.096516
H	-5.599570	0.576976	-2.639912	-5.549540	0.545032	-2.752185
H	-4.896939	-1.046968	-2.816692	-4.781239	-1.043261	-2.979445
H	-5.979900	-0.694808	-1.450324	-5.902276	-0.788562	-1.621066
C	5.203587	-0.285504	2.100159	5.133015	-0.324352	2.240623
H	5.979993	-0.694570	1.450329	5.902347	-0.788439	1.621061
H	5.599421	0.576983	2.640086	5.549430	0.544991	2.752317
H	4.896984	-1.047081	2.816566	4.781264	-1.043400	2.979350
H	2.515524	-1.153405	2.130526	2.410531	-1.095171	2.245297
H	-2.515519	-1.153418	-2.130524	-2.410535	-1.095155	-2.245296

Complex 3b

	State S ₀			State T ₁		
C	-0.858380	-1.583956	2.541936	-1.056694	-1.530380	2.477590
N	-0.434650	-1.661582	1.269950	-0.531074	-1.589680	1.232024
C	-0.239717	-2.878932	0.701428	-0.280685	-2.831907	0.653803
C	-0.484020	-4.050812	1.424889	-0.593034	-4.008014	1.395269
C	-0.926123	-3.967061	2.741625	-1.128112	-3.923667	2.656444
C	-1.115622	-2.711344	3.314138	-1.370376	-2.645124	3.225574

C	0.239134	-2.878996	-0.701386	0.280073	-2.831996	-0.653686
N	0.434326	-1.661699	-1.269930	0.530757	-1.589848	-1.231951
C	0.858076	-1.584191	-2.541917	1.056411	-1.530719	-2.477511
C	1.115067	-2.711645	-3.314104	1.369843	-2.645565	-3.225447
C	0.925279	-3.967311	-2.741574	1.127267	-3.924030	-2.656276
C	0.483158	-4.050942	-1.424835	0.592152	-4.008204	-1.395105
C	-2.724221	1.125691	0.190840	-2.761728	1.076525	0.059624
C	-4.003674	1.040554	-0.322651	-4.009302	0.964384	-0.522660
N	-3.934301	0.089065	-1.290103	-3.845955	0.068078	-1.528480
N	-2.703601	-0.418678	-1.405997	-2.588779	-0.379117	-1.605258
N	-1.980529	0.212519	-0.511120	-1.944633	0.234978	-0.646985
C	-2.000434	1.871860	1.209050	-2.120609	1.794499	1.147676
C	-0.619830	1.530798	1.297571	-0.728306	1.484348	1.310059
C	0.130204	2.203185	2.274765	-0.040101	2.127039	2.360373
C	-0.452161	3.158754	3.115508	-0.683962	3.046281	3.184154
C	-1.808911	3.476230	3.004467	-2.041691	3.342401	2.992922
C	-2.587109	2.828207	2.047004	-2.762973	2.716248	1.974577
C	1.809613	3.475842	-3.004509	2.042373	3.341827	-2.993109
C	0.452804	3.158621	-3.115557	0.684582	3.045976	-3.184317
C	-0.129749	2.203171	-2.274807	0.040539	2.126908	-2.360485
C	0.620145	1.530662	-1.297595	0.728619	1.484128	-1.310144
C	2.000812	1.871468	-1.209058	2.120986	1.794004	-1.147783
C	2.587677	2.827690	-2.047024	2.763533	2.715580	-1.974735
C	2.724454	1.125153	-0.190850	2.761959	1.075969	-0.059684
N	1.980575	0.212128	0.511105	1.944693	0.234629	0.646976
N	2.703519	-0.419233	1.405966	2.588716	-0.379544	1.605280
N	3.934339	0.088214	1.290038	3.845986	0.067379	1.528467
C	4.003894	1.039726	0.322620	4.009512	0.963602	0.522601
Ir	0.000015	0.075188	-0.000005	0.000020	0.137502	-0.000006
H	-0.986624	-0.582674	2.935519	-1.218773	-0.534555	2.872937
H	-0.332652	-5.021162	0.970734	-0.403515	-4.979351	0.954230
H	-1.117797	-4.871176	3.309171	-1.361735	-4.826627	3.211640
H	-1.456103	-2.598125	4.336633	-1.787442	-2.530845	4.218909
H	0.986533	-0.582942	-2.935516	1.218733	-0.534949	-2.872894
H	1.455561	-2.598516	-4.336605	1.786952	-2.531422	-4.218780
H	1.116731	-4.871476	-3.309115	1.360683	-4.827066	-3.211436
H	0.331550	-5.021250	-0.970673	0.402399	-4.979481	-0.954033
H	-4.918950	1.559055	-0.088132	-4.958008	1.430714	-0.311644
C	-5.011211	-0.412853	-2.139225	-4.853326	-0.435658	-2.461096
H	1.187338	1.982628	2.392021	1.008258	1.907187	2.532099
H	0.159050	3.659512	3.861987	-0.133824	3.537849	3.980593
H	-2.255451	4.219458	3.657812	-2.537267	4.057588	3.641431
H	-3.644249	3.063163	1.953812	-3.814144	2.946838	1.832436
H	2.256308	4.218957	-3.657877	2.538092	4.056880	-3.641657
H	-0.158301	3.659468	-3.862064	0.134539	3.537618	-3.980776
H	-1.186923	1.982810	-2.392069	-1.007868	1.907265	-2.532191

H	3.644861	3.062449	-1.953827	3.814751	2.945964	-1.832613
H	4.919293	1.557993	0.088073	4.958313	1.429724	0.311556
H	-5.503449	0.424703	-2.634782	-5.358462	0.406094	-2.935337
H	-4.566351	-1.073732	-2.880654	-4.338129	-1.033067	-3.210447
H	-5.734350	-0.963526	-1.535032	-5.576511	-1.051014	-1.923822
C	5.011085	-0.413724	2.139360	4.853198	-0.436310	2.461280
H	5.735149	-0.963011	1.535020	5.577393	-1.050336	1.923855
H	5.502234	0.423656	2.636307	5.357139	0.405424	2.936837
H	4.566266	-1.075910	2.879645	4.338052	-1.035073	3.209585

Complex 3c

	State S ₀			State T ₁		
C	0.949865	1.599421	2.509350	1.169415	-1.536347	-2.426901
N	0.483504	1.677471	1.252151	0.589126	-1.597139	-1.203947
C	0.259699	2.894719	0.693265	0.309482	-2.840101	-0.640359
C	0.514676	4.066203	1.412761	0.650602	-4.015079	-1.369714
C	1.000496	3.982472	2.714109	1.241047	-3.929932	-2.605677
C	1.221878	2.727252	3.275724	1.511711	-2.650763	-3.160674
C	-0.263362	2.894398	-0.693233	-0.309040	-2.840187	0.640194
N	-0.485325	1.676877	-1.252248	-0.588907	-1.597302	1.203842
C	-0.951270	1.598238	-2.509563	-1.169225	-1.536677	2.426790
C	-1.224731	2.725728	-3.275923	-1.511333	-2.651192	3.160501
C	-1.005354	3.981225	-2.714140	-1.240429	-3.930285	2.605447
C	-0.519941	4.065565	-1.412678	-0.649953	-4.015263	1.369487
C	2.720905	-1.100641	0.067632	2.753363	1.049733	0.083833
N	3.961613	-1.076703	-0.409621	3.961079	0.994536	0.632140
N	3.884056	-0.141120	-1.361486	3.782333	0.116393	1.622260
N	2.694640	0.409497	-1.502596	2.560888	-0.369062	1.721715
N	1.950926	-0.193087	-0.602172	1.903987	0.220482	0.751356
C	2.061569	-1.858079	1.112175	2.189050	1.776501	-1.037747
C	0.687135	-1.517959	1.264953	0.808631	1.468756	-1.273829
C	-0.010253	-2.202497	2.272244	0.186833	2.115990	-2.361301
C	0.620239	-3.161873	3.072061	0.884044	3.036746	-3.140961
C	1.972322	-3.474794	2.894175	2.228784	3.328134	-2.872251
C	2.700616	-2.817142	1.907211	2.888814	2.694609	-1.815322
C	-1.968574	-3.476790	-2.894264	-2.229281	3.327543	2.872534
C	-0.616854	-3.162351	-3.072226	-0.884500	3.036321	3.141223
C	0.012632	-2.202354	-2.272359	-0.187158	2.115733	2.361481
C	-0.685447	-1.518692	-1.264955	-0.808860	1.468521	1.273943
C	-2.059491	-1.860339	-1.112106	-2.189323	1.776082	1.037889
C	-2.697528	-2.820032	-1.907189	-2.889220	2.694019	1.815548
C	-2.719610	-1.103633	-0.067523	-2.753526	1.049332	-0.083756
N	-1.950611	-0.195182	0.602188	-1.904024	0.220269	-0.751354
N	-2.694923	0.406545	1.502693	-2.560852	-0.369338	-1.721724
N	-3.883739	-0.145387	1.361654	-3.782334	0.116034	-1.622317

N	-3.960313	-1.081073	0.409808	-3.961239	0.993983	-0.632055
Ir	0.000070	-0.055076	-0.000017	-0.000012	0.122783	-0.000004
H	1.100366	0.599036	2.896808	1.352973	-0.541396	-2.813885
H	0.336634	5.036269	0.967980	0.437457	-4.986306	-0.939575
H	1.200585	4.886650	3.278523	1.495801	-4.832240	-3.152246
H	1.596931	2.614185	4.285956	1.972664	-2.535731	-4.134241
H	-1.100243	0.597658	-2.897108	-1.352970	-0.541780	2.813823
H	-1.599350	2.612187	-4.286263	-1.972323	-2.536291	4.134067
H	-1.206659	4.885155	-3.278520	-1.495024	-4.832665	3.151970
H	-0.343427	5.035856	-0.967778	-0.436627	-4.986430	0.939302
C	5.025038	0.244674	-2.183709	4.853514	-0.273962	2.534591
H	-1.061039	-1.992146	2.447611	-0.849141	1.901344	-2.600117
H	0.048815	-3.672190	3.842876	0.382912	3.532624	-3.966283
H	2.450161	-4.221871	3.519753	2.762719	4.043281	-3.489021
H	3.752343	-3.039211	1.751799	3.930003	2.914118	-1.603168
H	-2.445636	-4.224336	-3.519875	-2.763319	4.042560	3.489367
H	-0.044924	-3.671953	-3.843139	-0.383442	3.532193	3.966593
H	1.063163	-1.990782	-2.447782	0.848843	1.901200	2.600283
H	-3.749001	-3.043275	-1.751735	-3.930440	2.913399	1.603413
H	5.376570	-0.627270	-2.735978	5.194836	0.608528	3.076060
H	4.689087	1.019699	-2.869052	4.445725	-1.011490	3.222006
H	5.817214	0.623274	-1.537159	5.671061	-0.700401	1.953479
C	-5.025076	0.239113	2.183986	-4.853423	-0.274306	-2.534764
H	-5.817697	0.616946	1.537532	-5.670954	-0.700908	-1.953748
H	-5.375641	-0.633266	2.736185	-5.194812	0.608218	-3.076134
H	-4.689900	1.014423	2.869387	-4.445521	-1.011702	-3.222253

Complex 4a

	State S ₀			State T ₁		
C	-2.381257	-0.736166	1.903197	-2.368447	-0.915473	1.883116
N	-1.692306	-1.104139	0.804307	-1.633812	-1.232442	0.798652
C	-2.105296	-2.189803	0.123769	-1.970540	-2.325633	0.093091
C	-3.208943	-2.950924	0.509505	-3.044767	-3.147519	0.435925
C	-3.903316	-2.564719	1.650058	-3.791143	-2.810998	1.559250
C	-3.486337	-1.438245	2.361961	-3.451198	-1.676747	2.298601
N	-1.344133	-2.514867	-1.018429	-1.160604	-2.596672	-1.030672
N	-0.322291	-1.689953	-1.401057	-0.167922	-1.722660	-1.373146
C	0.206427	-2.236207	-2.491811	0.424042	-2.234232	-2.448237
C	-0.471673	-3.425854	-2.832257	-0.183487	-3.451851	-2.818532
C	-1.450006	-3.574790	-1.876862	-1.185740	-3.653678	-1.898051
C	-1.527245	2.471960	-0.268387	-1.689463	2.367408	-0.275254
C	-2.433851	3.410052	-0.780193	-2.655655	3.249758	-0.849119
C	-3.095833	3.161721	-1.975140	-3.274755	2.943407	-2.032562
C	-2.845235	1.969332	-2.658072	-2.938402	1.723628	-2.691964
C	-1.942088	1.070724	-2.110693	-1.988549	0.890107	-2.120557

N	-1.300721	1.307310	-0.948885	-1.365970	1.168825	-0.963779
C	-0.753214	2.610453	0.967541	-0.997048	2.549476	0.932720
C	0.119452	1.528274	1.266062	-0.030812	1.484904	1.299735
C	0.886997	1.625744	2.438073	0.682556	1.618152	2.502616
C	0.790510	2.735796	3.280906	0.496725	2.709295	3.344589
C	-0.078003	3.788836	2.973885	-0.429519	3.737369	2.975977
C	-0.848594	3.725201	1.817482	-1.150769	3.672351	1.810505
C	4.150494	1.483791	-2.184626	4.022248	1.745764	-2.222034
C	2.955019	2.104577	-2.563124	2.781926	2.265783	-2.608944
C	1.744414	1.736294	-1.971310	1.607098	1.822732	-1.998798
C	1.688064	0.736342	-0.987424	1.641804	0.848908	-0.988756
C	2.912202	0.121600	-0.609304	2.908243	0.329478	-0.603718
C	4.127818	0.493574	-1.207940	4.085333	0.780143	-1.221347
C	2.806498	-0.905713	0.428909	2.886889	-0.685715	0.453544
N	1.532203	-1.133675	0.870549	1.637316	-0.999606	0.908151
C	1.309126	-2.044470	1.838652	1.483300	-1.923731	1.875493
C	2.330901	-2.781409	2.417914	2.559699	-2.585727	2.447615
C	3.638705	-2.568549	1.975822	3.845628	-2.277679	1.998529
C	3.872625	-1.628924	0.980880	4.006526	-1.325825	0.999764
Ir	0.052561	0.001548	-0.056230	0.074341	0.027412	-0.032378
H	-2.010138	0.147314	2.408056	-2.053319	-0.027200	2.417635
H	-3.521900	-3.814062	-0.062811	-3.296029	-4.018506	-0.154469
H	-4.764412	-3.138324	1.974379	-4.632449	-3.430153	1.850103
H	-4.005761	-1.106641	3.252693	-4.011982	-1.384658	3.178058
H	1.041906	-1.755992	-2.979436	1.249631	-1.709618	-2.905770
H	-0.269787	-4.084170	-3.662425	0.077534	-4.093360	-3.645286
H	-2.193859	-4.343478	-1.744353	-1.896628	-4.457509	-1.796304
H	-2.613490	4.331476	-0.240211	-2.891991	4.172306	-0.330684
H	-3.796808	3.888710	-2.371634	-4.007079	3.616659	-2.464608
H	-3.335489	1.734859	-3.595352	-3.402785	1.438806	-3.628227
H	-1.707515	0.134063	-2.599861	-1.698719	-0.035747	-2.603947
H	1.571372	0.825984	2.703981	1.399636	0.853010	2.783001
H	1.396899	2.781515	4.181805	1.051205	2.793753	4.273253
H	-0.151333	4.650498	3.630041	-0.561169	4.589332	3.637419
H	-1.520979	4.544702	1.582405	-1.840957	4.470967	1.560070
H	5.089814	1.771598	-2.646390	4.933857	2.091295	-2.699172
H	2.967350	2.881310	-3.323392	2.732154	3.020061	-3.389324
H	0.834295	2.237167	-2.286744	0.656302	2.239384	-2.313970
H	5.057733	0.014486	-0.916747	5.052099	0.382232	-0.929319
H	0.279271	-2.167889	2.147505	0.466097	-2.118264	2.190698
H	2.100735	-3.500917	3.194514	2.387499	-3.319809	3.225497
H	4.464556	-3.126890	2.403961	4.712128	-2.773491	2.423089
H	4.880897	-1.448220	0.629452	4.997270	-1.075460	0.641746

Complex 4b

	State S ₀			State T ₁		
C	-2.387338	-0.758602	1.888986	-2.062419	-1.573365	1.724142
N	-1.704452	-1.110887	0.782650	-1.204665	-1.596262	0.669382
C	-2.126786	-2.185710	0.093710	-1.128203	-2.764440	-0.067425
C	-3.225078	-2.954503	0.466156	-1.894482	-3.905942	0.263328
C	-3.916146	-2.583028	1.615917	-2.743085	-3.850636	1.343178
C	-3.493524	-1.467887	2.339568	-2.834157	-2.649020	2.098911
N	-1.365006	-2.491421	-1.062531	-0.264648	-2.731897	-1.127759
N	-0.338743	-1.671384	-1.429119	0.386905	-1.548616	-1.433509
N	0.206857	-2.139701	-2.511449	1.212928	-1.753149	-2.471791
C	-0.459155	-3.273276	-2.866551	1.062432	-3.040492	-2.840888
C	-1.461706	-3.512036	-1.956703	0.150537	-3.691671	-2.031731
C	-1.511839	2.480284	-0.230596	-2.341162	1.741091	-0.333318
C	-2.408810	3.435320	-0.727151	-3.506531	2.276204	-0.890098
C	-3.055379	3.222979	-1.937448	-3.920990	1.866098	-2.152815
C	-2.797421	2.050875	-2.651879	-3.164166	0.922341	-2.847483
C	-1.905159	1.133713	-2.118042	-2.015038	0.418896	-2.251339
N	-1.282036	1.333539	-0.939310	-1.616032	0.818946	-1.031062
C	-0.747886	2.583989	1.014938	-1.782264	2.072664	0.981152
C	0.121049	1.493670	1.292018	-0.582414	1.379407	1.339200
C	0.881385	1.557125	2.470191	-0.011254	1.648712	2.600338
C	0.781282	2.645394	3.340857	-0.585636	2.578474	3.461522
C	-0.083219	3.707489	3.055693	-1.753817	3.257960	3.088037
C	-0.846740	3.675962	1.893250	-2.350984	3.006637	1.852152
C	4.162805	1.516646	-2.142796	3.499561	2.807046	-1.995804
C	2.970788	2.150649	-2.509268	2.189774	2.980724	-2.467421
C	1.757121	1.772517	-1.929862	1.150754	2.221003	-1.941877
C	1.696078	0.749053	-0.972053	1.389798	1.277043	-0.920805
C	2.915812	0.121929	-0.603497	2.734677	1.101116	-0.463896
C	4.134241	0.503873	-1.189748	3.771922	1.871184	-0.997229
C	2.804393	-0.927806	0.410848	2.924233	0.092170	0.581319
N	1.529038	-1.161422	0.846039	1.773031	-0.526050	0.976938
C	1.301579	-2.089756	1.796481	1.806147	-1.478674	1.925585
C	2.320095	-2.841596	2.361675	2.991253	-1.863757	2.539249
C	3.628858	-2.624846	1.924243	4.178818	-1.242840	2.152137
C	3.867232	-1.666077	0.948975	4.143255	-0.261583	1.167621
Ir	0.054750	-0.001159	-0.064217	0.059933	0.087064	-0.037555
H	-2.013550	0.115382	2.407962	-2.098476	-0.640404	2.274153
H	-3.536117	-3.810716	-0.117847	-1.809878	-4.803860	-0.337210
H	-4.775976	-3.160149	1.936615	-3.339015	-4.716517	1.610515
H	-4.008806	-1.148406	3.237134	-3.492579	-2.567210	2.954971
H	-0.184174	-3.842536	-3.740283	1.616062	-3.449309	-3.673849
H	-2.196119	-4.296331	-1.883278	-0.208617	-4.705595	-2.011370
H	-2.592214	4.342000	-0.164122	-4.083329	3.006915	-0.337271
H	-3.749116	3.962974	-2.322319	-4.824104	2.278765	-2.589225
H	-3.273312	1.845992	-3.603308	-3.451181	0.576645	-3.833167

H	-1.664310	0.213424	-2.634424	-1.383870	-0.313359	-2.738655
H	1.561637	0.749032	2.719940	0.890372	1.129956	2.907022
H	1.381922	2.666236	4.246376	-0.128804	2.780292	4.425365
H	-0.159032	4.551932	3.733501	-2.200442	3.981060	3.762652
H	-1.515988	4.502679	1.675505	-3.254519	3.542959	1.582631
H	5.104290	1.811822	-2.595323	4.308433	3.399642	-2.410535
H	2.987635	2.945224	-3.250686	1.989059	3.711118	-3.244994
H	0.849887	2.283652	-2.236160	0.145226	2.364885	-2.321114
H	5.061698	0.015096	-0.907273	4.791874	1.753515	-0.647185
H	0.271430	-2.215321	2.103400	0.856024	-1.927359	2.184637
H	2.086860	-3.575084	3.124081	2.973273	-2.633550	3.301176
H	4.452307	-3.194861	2.341423	5.121854	-1.519866	2.610674
H	4.876474	-1.481912	0.602350	5.055751	0.228459	0.852708

Complex 4c

	State S ₀			State T ₁		
C	-2.413741	-0.764982	1.866596	-2.080326	-1.566909	1.720019
N	-1.726925	-1.109240	0.760749	-1.237398	-1.589928	0.655945
C	-2.152114	-2.177423	0.065443	-1.184164	-2.745590	-0.092090
C	-3.250049	-2.950917	0.421925	-1.958940	-3.883830	0.228267
C	-3.945691	-2.586331	1.572355	-2.795673	-3.828055	1.318277
C	-3.524060	-1.477372	2.304942	-2.863810	-2.638662	2.088269
N	-1.381701	-2.471546	-1.093009	-0.331199	-2.707557	-1.159607
N	-0.351939	-1.658804	-1.453062	0.354165	-1.542896	-1.454260
N	0.173114	-2.143374	-2.530552	1.140959	-1.788962	-2.518304
N	-0.483603	-3.265640	-2.904653	0.954835	-3.046667	-2.910409
C	-1.437184	-3.458819	-2.014741	0.072394	-3.622634	-2.108238
C	-1.483579	2.503371	-0.199700	-2.307716	1.789337	-0.297754
C	-2.367359	3.477778	-0.681479	-3.465696	2.355270	-0.839045
C	-3.011931	3.295298	-1.897703	-3.892576	1.976421	-2.107308
C	-2.764884	2.133765	-2.632735	-3.155121	1.033107	-2.822996
C	-1.885859	1.196494	-2.112485	-2.012663	0.498411	-2.241631
N	-1.265326	1.366674	-0.927683	-1.601717	0.867412	-1.015302
C	-0.721721	2.576115	1.048935	-1.736509	2.088179	1.018832
C	0.133262	1.471528	1.309891	-0.545789	1.370046	1.357715
C	0.892635	1.503412	2.489276	0.039049	1.609255	2.618491
C	0.804269	2.578139	3.378050	-0.514624	2.533854	3.498423
C	-0.046094	3.655556	3.109571	-1.675086	3.236995	3.144984
C	-0.808157	3.653797	1.945758	-2.284853	3.015469	1.909636
C	4.176737	1.496959	-2.130211	3.542000	2.763463	-1.986452
C	2.992182	2.148936	-2.488318	2.231437	2.974076	-2.441165
C	1.774597	1.779020	-1.911426	1.181027	2.230640	-1.915906
C	1.704286	0.746025	-0.965440	1.410263	1.265749	-0.911690
C	2.916044	0.100482	-0.603943	2.755656	1.053657	-0.469987
C	4.137879	0.474524	-1.187862	3.803927	1.807422	-1.004163

C	2.793702	-0.958420	0.399595	2.932967	0.028450	0.561275
N	1.516001	-1.185156	0.831114	1.772620	-0.571249	0.958771
C	1.278982	-2.118677	1.774299	1.793959	-1.533122	1.898367
C	2.290303	-2.883835	2.334167	2.975926	-1.947857	2.498757
C	3.601232	-2.675131	1.899363	4.172635	-1.347302	2.108211
C	3.849342	-1.710492	0.932360	4.149150	-0.355331	1.134034
Ir	0.053728	0.001636	-0.069263	0.064823	0.088367	-0.040121
H	-2.041058	0.103111	2.396061	-2.097103	-0.640770	2.281995
H	-3.557794	-3.803712	-0.169403	-1.890324	-4.775650	-0.383132
H	-4.807288	-3.164621	1.885602	-3.399691	-4.689468	1.581778
H	-4.043092	-1.164133	3.202529	-3.513200	-2.559873	2.951290
H	-2.148329	-4.268898	-2.010139	-0.278405	-4.638649	-2.162526
H	-2.542028	4.375958	-0.102475	-4.026688	3.085669	-0.269873
H	-3.695531	4.050287	-2.271307	-4.790033	2.412889	-2.531957
H	-3.238907	1.951866	-3.589689	-3.451682	0.711215	-3.813858
H	-1.654884	0.284324	-2.647181	-1.398043	-0.234552	-2.748546
H	1.562437	0.683208	2.726194	0.935012	1.072906	2.910255
H	1.403680	2.575815	4.284484	-0.047333	2.713123	4.461638
H	-0.112168	4.489283	3.801421	-2.105723	3.955388	3.834777
H	-1.466309	4.492616	1.741221	-3.182217	3.569451	1.655820
H	5.120972	1.785561	-2.581113	4.359679	3.343370	-2.401697
H	3.017307	2.950979	-3.221263	2.039288	3.720239	-3.205697
H	0.873070	2.303602	-2.211102	0.175259	2.402988	-2.281920
H	5.059781	-0.028193	-0.912182	4.824576	1.661896	-0.667207
H	0.247731	-2.237392	2.080166	0.838048	-1.966043	2.162630
H	2.050018	-3.621072	3.090672	2.948188	-2.724587	3.253264
H	4.419166	-3.255747	2.312655	5.113398	-1.647894	2.556366
H	4.860614	-1.532005	0.588838	5.068725	0.119978	0.817250

Complex 2b'

	State S ₀			State T ₁		
C	1.620882	2.268668	-1.434651	-1.554905	-2.322026	-1.366949
N	1.699857	1.136471	-0.715749	-1.616860	-1.156858	-0.676431
C	2.917846	0.625435	-0.397856	-2.860628	-0.614729	-0.357584
C	4.088523	1.265428	-0.815386	-4.034664	-1.311318	-0.763583
C	4.003866	2.438241	-1.560002	-3.948313	-2.491274	-1.459199
C	2.748435	2.951776	-1.876407	-2.668746	-3.020012	-1.777091
C	2.917846	-0.625435	0.397856	-2.860628	0.614729	0.357584
N	1.699857	-1.136471	0.715749	-1.616860	1.156857	0.676431
C	1.620882	-2.268668	1.434651	-1.554905	2.322026	1.366949
C	2.748436	-2.951776	1.876407	-2.668746	3.020011	1.777091
C	4.003866	-2.438240	1.560003	-3.948313	2.491273	1.459199
C	4.088523	-1.265427	0.815386	-4.034664	1.311317	0.763584
N	-1.065748	2.208711	1.535962	1.016087	-2.203580	1.600972
N	-1.129785	2.986921	2.601064	1.034889	-2.962052	2.684185

C	-0.215790	2.480961	3.443052	0.168232	-2.375990	3.517526
C	0.401409	1.374704	2.850755	-0.378933	-1.237813	2.903442
N	-0.156055	1.221897	1.641166	0.177074	-1.152705	1.692883
C	-1.811337	2.293063	0.331044	1.728631	-2.367820	0.394882
C	-1.490935	1.292708	-0.609473	1.444710	-1.376723	-0.586341
C	-2.198023	1.353948	-1.818960	2.119054	-1.511585	-1.817971
C	-3.152792	2.349430	-2.056021	3.024746	-2.546150	-2.030138
C	-3.434499	3.317657	-1.087331	3.278054	-3.491166	-1.022616
C	-2.755700	3.297140	0.129909	2.626309	-3.409876	0.209679
C	-0.215790	-2.480960	-3.443052	0.168231	2.375990	-3.517526
C	0.401410	-1.374704	-2.850755	-0.378934	1.237813	-2.903442
N	-0.156055	-1.221897	-1.641166	0.177074	1.152705	-1.692883
N	-1.065747	-2.208711	-1.535962	1.016086	2.203580	-1.600972
N	-1.129784	-2.986921	-2.601063	1.034889	2.962052	-2.684185
C	-1.811336	-2.293063	-0.331044	1.728631	2.367821	-0.394882
C	-2.198023	-1.353948	1.818960	2.119053	1.511586	1.817971
C	-3.152792	-2.349430	2.056021	3.024745	2.546151	2.030138
C	-3.434499	-3.317657	1.087331	3.278053	3.491166	1.022616
C	-2.755700	-3.297141	-0.129909	2.626309	3.409876	-0.209679
H	0.620386	2.621059	-1.654240	-0.559235	-2.685407	-1.590406
H	5.058976	0.857536	-0.565694	-5.006418	-0.900420	-0.517550
H	4.907746	2.940555	-1.886590	-4.850174	-3.013000	-1.762603
H	2.634661	3.861663	-2.453561	-2.553390	-3.946152	-2.327008
H	0.620386	-2.621059	1.654240	-0.559235	2.685407	1.590406
H	2.634661	-3.861662	2.453561	-2.553391	3.946151	2.327008
H	4.907746	-2.940555	1.886590	-4.850174	3.012999	1.762604
H	5.058976	-0.857535	0.565695	-5.006419	0.900419	0.517551
H	-0.044523	2.920951	4.413122	-0.026149	-2.779082	4.499106
H	-2.002701	0.619582	-2.594470	1.932409	-0.796813	-2.611782
H	-3.681838	2.368380	-3.004517	3.541395	-2.626013	-2.980904
H	-4.176821	4.085926	-1.277151	3.983039	-4.296337	-1.199400
H	-2.946909	4.034739	0.901311	2.807561	-4.131765	0.997117
H	-0.044523	-2.920951	-4.413122	-0.026150	2.779082	-4.499106
H	-3.681838	-2.368381	3.004516	3.541395	2.626014	2.980904
H	-4.176821	-4.085926	1.277151	3.983038	4.296338	1.199400
H	-2.946908	-4.034740	-0.901311	2.807560	4.131766	-0.997117
C	-1.490935	-1.292708	0.609473	1.444709	1.376723	0.586341
H	-2.002701	-0.619582	2.594470	1.932409	0.796813	2.611782
Ir	-0.034065	0.000000	0.000000	0.101078	0.000000	0.000000
H	1.173299	0.713648	3.208979	-1.100146	-0.516262	3.250993
H	1.173300	-0.713648	-3.208979	-1.100146	0.516262	-3.250993

Complex 2b''

	State S ₀			State T ₁		
C	-1.619595	-2.283168	-1.412379	1.554260	2.321704	-1.364874

N	-1.697398	-1.143873	-0.704847	1.616505	1.158141	-0.671913
C	-2.915056	-0.629325	-0.391842	2.860356	0.616783	-0.353717
C	-4.086289	-1.272574	-0.803391	4.034421	1.316408	-0.754830
C	-4.002569	-2.452781	-1.536195	3.947760	2.496082	-1.450759
C	-2.747373	-2.970363	-1.847132	2.667923	3.021334	-1.773280
C	-2.915056	0.629326	0.391842	2.860356	-0.616781	0.353717
N	-1.697398	1.143874	0.704847	1.616505	-1.158140	0.671913
C	-1.619595	2.283168	1.412379	1.554261	-2.321703	1.364874
C	-2.747373	2.970363	1.847131	2.667924	-3.021333	1.773280
C	-4.002569	2.452782	1.536195	3.947762	-2.496080	1.450759
C	-4.086289	1.272575	0.803390	4.034422	-1.316406	0.754830
N	1.077425	-2.224704	1.546328	-1.029231	2.205337	1.630094
C	1.034239	-2.929483	2.693744	-0.943641	2.873367	2.801453
N	0.126916	-2.423659	3.525619	-0.080921	2.280034	3.616640
C	-0.389618	-1.377218	2.846387	0.369479	1.219422	2.908804
N	0.156698	-1.218892	1.643235	-0.180809	1.136596	1.702907
C	1.816910	-2.298629	0.331140	-1.738950	2.367271	0.415816
C	1.492455	-1.293961	-0.605473	-1.440560	1.388461	-0.574093
C	2.194383	-1.347441	-1.819067	-2.101197	1.528908	-1.812559
C	3.149139	-2.338372	-2.070067	-3.016688	2.553957	-2.027688
C	3.436422	-3.311574	-1.109359	-3.290595	3.484490	-1.014623
C	2.763335	-3.298490	0.111438	-2.649375	3.398238	0.223385
N	0.126916	2.423659	-3.525619	-0.080920	-2.280034	-3.616640
C	-0.389617	1.377217	-2.846387	0.369480	-1.219422	-2.908804
N	0.156698	1.218892	-1.643235	-0.180808	-1.136596	-1.702907
N	1.077426	2.224704	-1.546328	-1.029230	-2.205337	-1.630094
C	1.034240	2.929483	-2.693744	-0.943639	-2.873368	-2.801453
C	1.816911	2.298629	-0.331140	-1.738949	-2.367272	-0.415816
C	2.194383	1.347441	1.819067	-2.101196	-1.528909	1.812559
C	3.149140	2.338372	2.070067	-3.016687	-2.553958	2.027688
C	3.436422	3.311574	1.109359	-3.290593	-3.484491	1.014623
C	2.763335	3.298490	-0.111438	-2.649374	-3.398239	-0.223385
H	-0.619195	-2.637784	-1.629147	0.558658	2.684011	-1.590117
H	-5.056524	-0.861338	-0.558362	5.006216	0.907823	-0.505079
H	-4.906793	-2.957526	-1.858088	4.849388	3.020256	-1.750658
H	-2.634152	-3.886021	-2.415246	2.551988	3.947154	-2.323662
H	-0.619195	2.637784	1.629147	0.558659	-2.684011	1.590117
H	-2.634151	3.886021	2.415246	2.551990	-3.947153	2.323662
H	-4.906793	2.957527	1.858088	4.849389	-3.020254	1.750659
H	-5.056524	0.861339	0.558362	5.006216	-0.907821	0.505080
H	1.992949	-0.607778	-2.587891	-1.897739	0.822341	-2.609344
H	3.672695	-2.350211	-3.021692	-3.523757	2.636034	-2.983375
H	4.178017	-4.078728	-1.305899	-4.002798	4.283845	-1.188451
H	2.975004	-4.051029	0.864089	-2.862902	4.120950	1.002775
H	3.672695	2.350211	3.021692	-3.523756	-2.636035	2.983375
H	4.178017	4.078728	1.305899	-4.002796	-4.283847	1.188451

H	2.975005	4.051029	-0.864089	-2.862900	-4.120952	-1.002775
C	1.492455	1.293961	0.605473	-1.440559	-1.388462	0.574093
H	1.992949	0.607778	2.587891	-1.897739	-0.822342	2.609343
Ir	0.038769	0.000000	0.000000	-0.105410	0.000000	0.000000
H	-1.162384	-0.720838	3.216127	1.093642	0.500206	3.259597
H	-1.162383	0.720838	-3.216127	1.093642	-0.500206	-3.259597
H	1.663979	-3.785212	2.882716	-1.512452	3.765959	3.013003
H	1.663980	3.785211	-2.882716	-1.512450	-3.765960	-3.013003

Complex **3b'**

	State S ₀			State T ₁		
C	-1.050819	-1.611043	2.469347	-1.118947	-1.547878	2.450114
N	-0.525961	-1.686801	1.234700	-0.560464	-1.607412	1.217915
C	-0.289791	-2.904951	0.682042	-0.297261	-2.850580	0.646251
C	-0.585108	-4.077257	1.385359	-0.630936	-4.026350	1.378771
C	-1.127644	-3.994653	2.664065	-1.197627	-3.941382	2.626021
C	-1.365950	-2.739133	3.218803	-1.452386	-2.662550	3.189266
C	0.289861	-2.904943	-0.682046	0.297265	-2.850580	-0.646253
N	0.525998	-1.686787	-1.234705	0.560467	-1.607411	-1.217915
C	1.050851	-1.611014	-2.469352	1.118949	-1.547875	-2.450115
C	1.366011	-2.739095	-3.218809	1.452390	-2.662546	-3.189267
C	1.127741	-3.994622	-2.664071	1.197632	-3.941379	-2.626023
C	0.585209	-4.077241	-1.385364	0.630941	-4.026348	-1.378773
C	-2.737986	1.088704	0.030744	-2.765182	1.041990	-0.046798
N	-3.985092	1.108447	-0.412523	-3.997130	1.023229	-0.525949
N	-3.984225	0.171521	-1.404151	-3.922585	0.130563	-1.551056
C	-2.771090	-0.381776	-1.536877	-2.681436	-0.362352	-1.670558
N	-1.957196	0.176485	-0.644874	-1.924143	0.200478	-0.734271
C	-2.078949	1.843675	1.083993	-2.172044	1.771597	1.061541
C	-0.704431	1.511840	1.249055	-0.787615	1.469372	1.277830
C	-0.015654	2.205624	2.257499	-0.147152	2.126490	2.349246
C	-0.653746	3.164391	3.052116	-0.831855	3.047257	3.138697
C	-2.006758	3.467466	2.865537	-2.183803	3.330909	2.893831
C	-2.724218	2.802185	1.874678	-2.858667	2.691381	1.852158
C	2.006681	3.467516	-2.865528	2.183798	3.330914	-2.893829
C	0.653675	3.164415	-3.052107	0.831850	3.047261	-3.138694
C	0.015603	2.205632	-2.257491	0.147148	2.126492	-2.349244
C	0.704395	1.511860	-1.249050	0.787613	1.469374	-1.277829
C	2.078907	1.843722	-1.083988	2.172041	1.771601	-1.061539
C	2.724156	2.802247	-1.874671	2.858663	2.691386	-1.852157
C	2.737960	1.088761	-0.030742	2.765181	1.041994	0.046799
N	1.957191	0.176525	0.644875	1.924143	0.200480	0.734272
C	2.771098	-0.381723	1.536873	2.681437	-0.362351	1.670557
N	3.984222	0.171597	1.404146	3.922586	0.130565	1.551053
N	3.985068	1.108527	0.412520	3.997130	1.023232	0.525948

Ir	-0.000002	0.051381	0.000000	0.000000	0.120682	0.000000
H	-1.213859	-0.610370	2.851489	-1.292773	-0.551952	2.840120
H	-0.396246	-5.047048	0.944184	-0.432722	-4.997915	0.942043
H	-1.359532	-4.899088	3.215806	-1.447217	-4.844102	3.174498
H	-1.787009	-2.626508	4.210899	-1.895423	-2.547970	4.171222
H	1.213864	-0.610337	-2.851493	1.292774	-0.551948	-2.840120
H	1.787065	-2.626458	-4.210906	1.895427	-2.547965	-4.171223
H	1.359652	-4.899051	-3.215812	1.447223	-4.844098	-3.174500
H	0.396374	-5.047037	-0.944189	0.432729	-4.997914	-0.942046
C	-5.199061	-0.110121	-2.155399	-5.101229	-0.174219	-2.353309
H	1.036740	2.002597	2.433466	0.896467	1.921320	2.562465
H	-0.088838	3.681450	3.823663	-0.316872	3.550701	3.951151
H	-2.493636	4.213632	3.485821	-2.709193	4.046717	3.517672
H	-3.776080	3.019378	1.711342	-3.904795	2.905120	1.657906
H	2.493544	4.213693	-3.485811	2.709187	4.046723	-3.517669
H	0.088756	3.681464	-3.823651	0.316866	3.550705	-3.951147
H	-1.036786	2.002585	-2.433457	-0.896471	1.921322	-2.562463
H	3.776014	3.019461	-1.711336	3.904792	2.905126	-1.657905
H	-5.528306	0.794653	-2.668911	-5.453525	0.737056	-2.838403
H	-4.984801	-0.890187	-2.884884	-4.827415	-0.912241	-3.105840
H	-5.978796	-0.449163	-1.471546	-5.882586	-0.576058	-1.707053
C	5.199062	-0.110013	2.155397	5.101229	-0.174213	2.353309
H	5.978824	-0.448975	1.471536	5.882600	-0.576016	1.707047
H	5.528251	0.794752	2.668962	5.453502	0.737055	2.838432
H	4.984837	-0.890129	2.884839	4.827426	-0.912263	3.105817
H	2.520791	-1.147456	2.253760	2.371768	-1.087252	2.406294
H	-2.520766	-1.147501	-2.253766	-2.371765	-1.087251	-2.406297