Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information to: "A fluorescent receptor for halide recognition: clues for design of anion chemosensors"

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Contents:

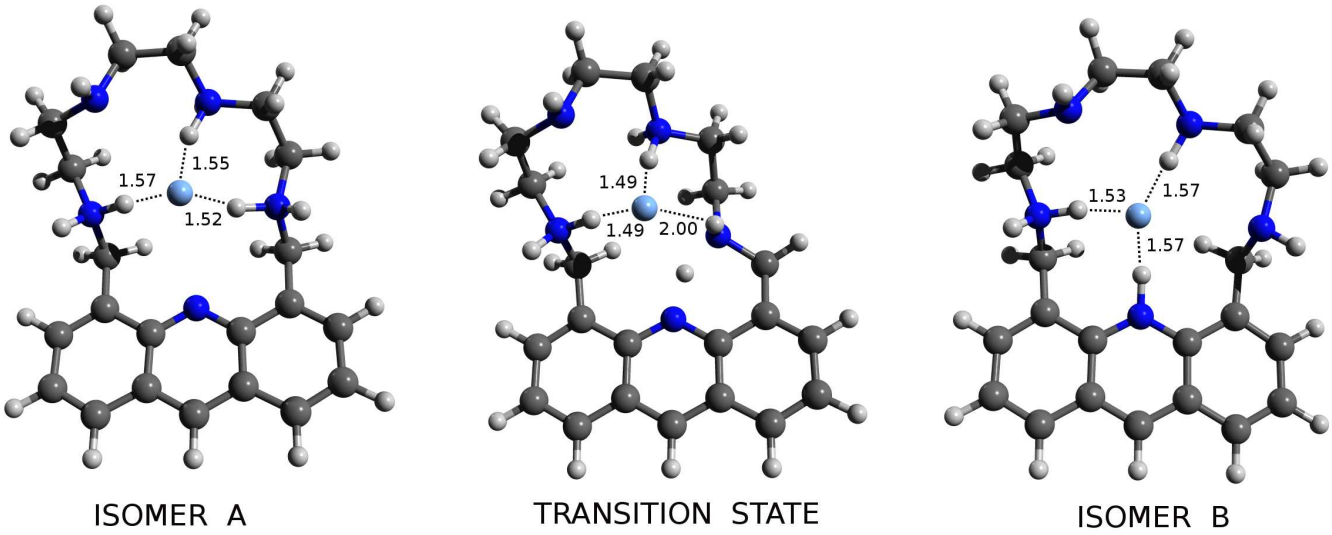

Figure 1: Graphical representations of S_0 optimized geometries of **Fluoride-LH$_3^{2+}$** complexes (Isomer A, Isomer B and Transition State). Calculations were performed by using DFT with B3-LYP exchange-correlation functional and 6-31++G(d,p) basis set. The shortest distances between the anion and the nitrogen atoms are displayed (in Å units). The atomic Cartesian coordinates are reported in Table 1 of this document.

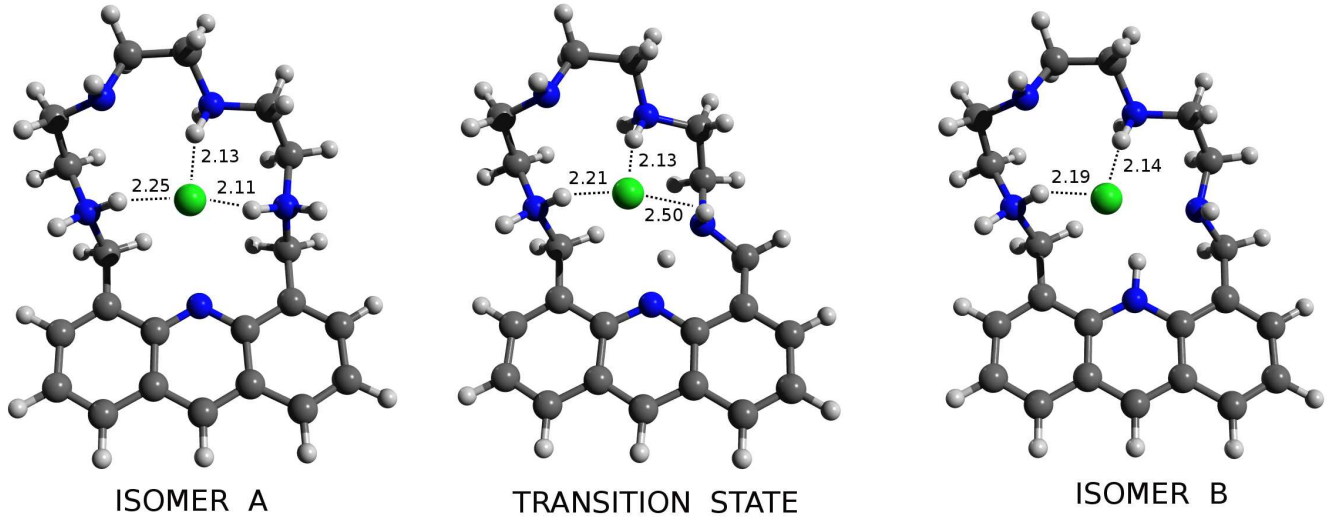

Figure 2: Graphical representations of S_0 optimized geometries of **Chloride-LH$_3^{2+}$** complexes (Isomer A, Isomer B and Transition State). Calculations were performed by using DFT with B3-LYP exchange-correlation functional and 6-31++G(d,p) basis set. The shortest distances between the anion and the nitrogen atoms are displayed (in Å units). The atomic Cartesian coordinates are reported in Table 2 of this document.

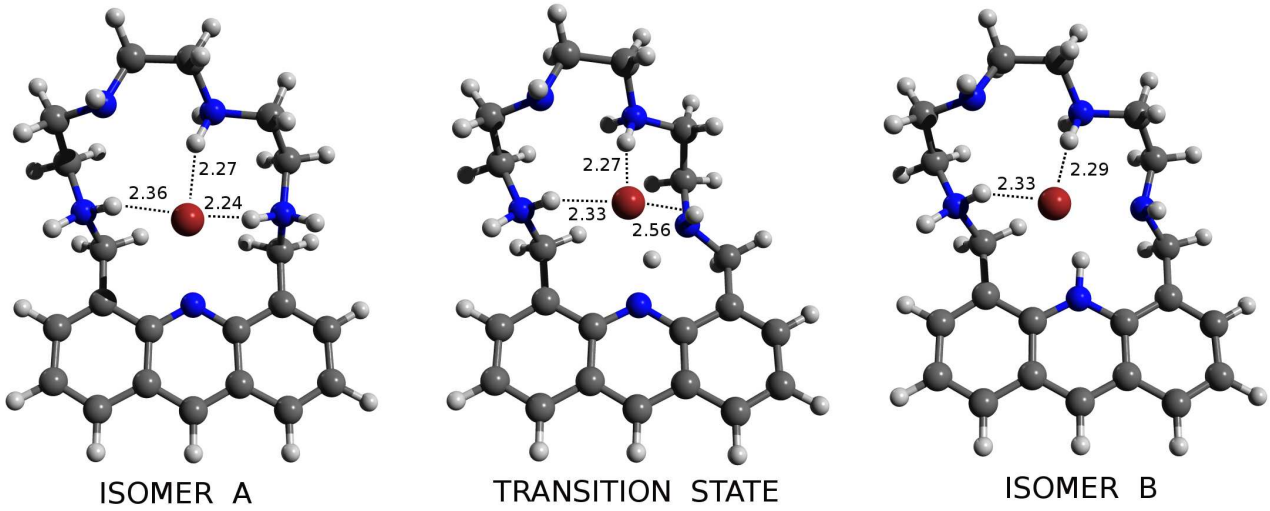

Figure 3: Graphical representations of S_0 optimized geometries of **Bromide-LH$_3^{2+}$** complexes (Isomer A, Isomer B and Transition State). Calculations were performed by using DFT with B3-LYP exchange-correlation functional and 6-31++G(d,p) basis set. The shortest distances between the anion and the nitrogen atoms are displayed (in Å units). The atomic Cartesian coordinates are reported in Table 3 of this document.

Table 1: S_0 optimized geometries of **Fluoride-LH$_3^{2+}$** complexes (Isomer A, Isomer B and Transition State). Calculations were performed by using DFT with B3-LYP exchange-correlation functional and 6-31++G(d,p) basis set. Atomic coordinates are in Å units.

ISOMER A				ISOMER B				TRANSITION STATE			
C	3.164740	1.722283	-0.323980	C	3.186143	1.623259	-0.339956	C	2.877767	1.950819	-0.111091
C	3.484177	3.095035	-0.554199	C	3.662419	2.945677	-0.574921	C	3.033154	3.367981	-0.153089
H	4.439093	3.339270	-1.010804	H	4.674608	3.073918	-0.944145	H	3.978318	3.773875	-0.499520
C	2.600548	4.079726	-0.196651	C	2.853802	4.021684	-0.321142	C	2.010366	4.187780	0.241115
H	2.840884	5.125033	-0.360076	H	3.202059	5.034534	-0.488717	H	2.119404	5.266428	0.226589
C	4.042937	0.687803	-0.662317	C	4.004887	0.511505	-0.558110	C	3.915611	1.113339	-0.530218
H	5.001370	0.921629	-1.118773	H	5.015711	0.664924	-0.924990	H	4.836413	1.555287	-0.900437
C	3.697374	-0.643393	-0.414626	C	3.566688	-0.788083	-0.297302	C	3.786274	-0.274383	-0.486785
C	4.178369	-3.023506	-0.470214	C	3.976931	-3.168453	-0.185258	C	4.628336	-2.513200	-0.867739
H	4.830766	-3.855368	-0.714087	H	4.624073	-4.031628	-0.295288	H	5.398035	-3.194398	-1.214018
C	4.558436	-1.735277	-0.743291	C	4.431603	-1.907880	-0.468403	C	4.815400	-1.157050	-0.931630
H	5.515894	-1.522832	-1.210176	H	5.446423	-1.733493	-0.810168	H	5.734243	-0.731793	-1.322444
N	1.564695	0.086838	0.536678	N	1.413081	0.121353	0.292360	N	1.540105	0.004878	0.429933
H	0.676513	4.535350	0.681383	H	0.959172	4.672742	0.469954	H	-0.015479	4.275016	0.971927
C	1.355446	3.734664	0.399363	C	1.559333	3.805403	0.210388	C	0.789035	3.611014	0.667772
C	0.987472	2.425385	0.629738	C	1.031653	2.545504	0.446399	C	0.569319	2.245322	0.711121
C	1.901258	1.364234	0.282447	C	1.846320	1.407741	0.134001	C	1.641393	1.358933	0.349397
C	-0.359653	2.134176	1.242998	C	-0.321752	2.476834	1.120432	C	-0.805656	1.787731	1.127662
H	-0.373288	1.171098	1.751515	H	-0.414968	1.621778	1.791256	H	-0.812001	0.778569	1.532402
H	-0.628761	2.921280	1.949022	H	-0.468637	3.385172	1.705504	H	-1.195011	2.456443	1.896777
N	-1.461994	2.089520	0.198123	N	-1.464824	2.378341	0.141868	N	-1.788984	1.821928	-0.030262
H	-1.442593	1.131324	-0.263916	H	-1.495347	1.354908	-0.155390	H	-1.658635	0.911917	-0.603378
H	-1.252162	2.777813	-0.529832	H	-1.272176	2.961712	-0.676259	H	-1.540690	2.599254	-0.647554
C	-2.827605	2.382976	0.758865	C	-2.799408	2.746439	0.718263	C	-3.215228	2.006311	0.418621
H	-2.776966	3.362362	1.241032	H	-2.745785	3.772728	1.088326	H	-3.287167	2.997075	0.873837
H	-3.025043	1.634801	1.529456	H	-2.970202	2.078471	1.565416	H	-3.402358	1.271929	1.204982
C	-3.909388	2.393121	-0.324849	C	-3.890471	2.609368	-0.344267	C	-4.229537	1.878068	-0.722312
H	-4.832557	2.763538	0.145420	H	-4.842337	2.923864	0.110914	H	-5.197644	2.214157	-0.319004
H	-3.638559	3.126987	-1.090962	H	-3.686735	3.309701	-1.160785	H	-3.964154	2.580177	-1.519055
N	-4.083005	1.091586	-0.971623	N	-3.933488	1.254445	-0.899521	N	-4.282197	0.535883	-1.296251
H	-4.232283	1.209941	-1.967646	H	-4.218855	1.295611	-1.873370	H	-4.442652	0.574733	-2.295184
C	-5.100249	0.200989	-0.409520	C	-4.797562	0.315514	-0.180442	C	-5.147624	-0.458527	-0.658210
H	-5.171434	0.378238	0.669601	H	-4.634457	0.429051	0.897158	H	-5.432778	-0.106822	0.340790
H	-6.105156	0.375091	-0.820825	H	-5.867463	0.511678	-0.353331	H	-6.084960	-0.617153	-1.207043
C	-4.735164	-1.263396	-0.661638	C	-4.521155	-1.127495	-0.593799	C	-4.440941	-1.815296	-0.528667
H	-5.496098	-1.938340	-0.263424	H	-5.343804	-1.775855	-0.284460	H	-5.055827	-2.527510	0.027093
H	-4.604447	-1.462185	-1.727746	H	-4.408008	-1.207470	-1.677452	H	-4.198782	-2.237172	-1.506377
N	-3.428010	-1.573365	0.009691	N	-3.267894	-1.686526	0.024105	N	-3.146642	-1.615901	0.201873
H	-3.532643	-1.394565	1.012208	H	-3.400971	-1.712954	1.039055	H	-3.347238	-1.057418	1.034348
H	-2.677822	-0.904048	-0.352054	H	-2.429419	-1.046941	-0.121918	H	-2.477979	-1.046231	-0.430779
C	-2.912108	-2.969591	-0.167325	C	-2.966407	-3.083561	-0.446473	C	-2.412806	-2.838473	0.659247
H	-2.738759	-3.127589	-1.233688	H	-2.788442	-3.026609	-1.522051	H	-2.172623	-3.437856	-0.222193
H	-3.687244	-3.663475	0.162787	H	-3.864865	-3.679623	-0.266039	H	-3.083792	-3.416300	1.298325
C	-1.657631	-3.221554	0.667684	C	-1.769759	-3.711824	0.266326	C	-1.157700	-2.472223	1.456962
H	-1.481397	-4.296765	0.723833	H	-1.816361	-4.786724	0.056094	H	-0.844839	-3.376639	1.983931
H	-1.787661	-2.850434	1.687396	H	-1.893042	-3.611629	1.352693	H	-1.393384	-1.730635	2.226884
N	-0.410053	-2.585656	0.116927	N	-0.476959	-3.157409	-0.161090	N	-0.007780	-1.985713	0.632352
H	-0.624171	-1.587903	-0.215561	H	0.041635	-3.868700	-0.666976	H	-0.288985	-1.934681	-0.351963
H	-0.115057	-3.105827	-0.713860	C	0.358495	-2.641420	0.936958	C	1.198330	-2.837510	0.800380
C	0.727075	-2.582468	1.119740	H	0.471008	-3.379098	1.748392	H	1.018637	-3.852321	0.431223
H	0.752595	-3.573686	1.575483	H	-0.138674	-1.770179	1.366138	H	1.386437	-2.904652	1.878547
H	0.462044	-1.841577	1.874424	C	2.210710	-0.981423	0.143538	C	2.560972	-0.809351	0.036702
C	2.417143	-0.897776	0.203683	C	1.749068	-2.301730	0.437642	C	2.405176	-2.229870	0.129007
C	2.047732	-2.265572	0.472195	C	2.648727	-3.343092	0.277926	C	3.419559	-3.039439	-0.336201
C	2.918518	-3.281141	0.141906	H	2.320881	-4.347083	0.534385	H	3.297357	-4.117486	-0.282055
H	2.641916	-4.310217	0.354936	F	-1.159762	-0.130040	0.007545	F	-1.342269	-0.432758	-1.166839
F	-1.298331	-0.346858	-0.770411	H	0.371825	-0.037668	0.353293	H	0.559842	-0.770355	0.699112

Table 2: S_0 optimized geometries of **Chloride-LH$_3^{2+}$** complexes (Isomer A, Isomer B and Transition State). Calculations were performed by using DFT with B3-LYP exchange-correlation functional and 6-31++G(d,p) basis set. Atomic coordinates are in Å units.

ISOMER A				ISOMER B				TRANSITION STATE			
C	-3.130542	1.817861	0.257415	C	-2.792291	2.089854	0.172777	C	-2.850912	2.013819	0.119956
C	-3.393071	3.198914	0.507439	C	-2.868940	3.504042	0.321593	C	-2.954346	3.432215	0.223554
H	-4.341369	3.476194	0.958657	H	-3.790772	3.937108	0.695131	H	-3.880570	3.855798	0.598447
C	-2.465544	4.151080	0.173488	C	-1.800244	4.290479	-0.021835	C	-1.910538	4.232566	-0.155118
H	-2.663385	5.203003	0.350351	H	-1.848744	5.369529	0.068231	H	-1.981479	5.312854	-0.097779
C	-4.058953	0.818118	0.564966	C	-3.885821	1.273219	0.485218	C	-3.924644	1.203308	0.500286
H	-5.012494	1.086925	1.012258	H	-4.792327	1.732403	0.869104	H	-4.826377	1.666324	0.891170
C	-3.769792	-0.522335	0.296802	C	-3.849338	-0.109365	0.297664	C	-3.856868	-0.183442	0.381739
C	-4.359456	-2.879071	0.300389	C	-4.887658	-2.293077	0.356359	C	-4.807923	-2.399186	0.621336
H	-5.053205	-3.684284	0.517759	H	-5.730606	-2.942290	0.565571	H	-5.614607	-3.061816	0.915402
C	-4.684543	-1.579685	0.591416	C	-4.971745	-0.943603	0.577410	C	-4.931763	-1.041795	0.762552
H	-5.638932	-1.332062	1.047150	H	-5.878413	-0.486598	0.959233	H	-5.836334	-0.596795	1.164526
N	-1.592651	0.127840	-0.610177	N	-1.564794	0.119515	-0.434991	N	-1.584336	0.038825	-0.494965
H	-0.521669	4.541025	-0.688499	H	0.190924	4.330457	-0.832425	H	0.090436	4.279412	-0.948485
C	-1.231501	3.762785	-0.417857	C	-0.625438	3.682988	-0.522464	C	-0.722962	3.630414	-0.634564
C	-0.915417	2.441897	-0.659334	C	-0.473556	2.310559	-0.651477	C	-0.549598	2.260156	-0.726859
C	-1.876421	1.414635	-0.339430	C	-1.581325	1.479587	-0.305833	C	-1.639685	1.393693	-0.371325
C	0.418435	2.098197	-1.273218	C	0.832619	1.800707	-1.217318	C	0.787339	1.777667	-1.228300
H	0.434572	1.078614	-1.653791	H	0.824696	0.741457	-1.469511	H	0.770519	0.740781	-1.550083
H	0.658560	2.792212	-2.080439	H	1.073591	2.351910	-2.128142	H	1.108391	2.385639	-2.075405
N	1.559543	2.209793	-0.271165	N	1.991340	2.012525	-0.264479	N	1.877771	1.918553	-0.173492
H	1.561727	1.367107	0.345691	H	1.976567	1.251912	0.460390	H	1.791115	1.139974	0.523856
H	1.376367	3.001204	0.352813	H	1.844432	2.880328	0.258516	H	1.705989	2.774491	0.362478
C	2.906128	2.404263	-0.922233	C	3.331115	2.084127	-0.955691	C	3.271210	1.991935	-0.754934
H	2.886074	3.382333	-1.407771	H	3.398776	3.060925	-1.438354	H	3.353132	2.954246	-1.264616
H	2.999888	1.638893	-1.694559	H	3.331897	1.317983	-1.732782	H	3.346209	1.205815	-1.509323
C	4.044975	2.322840	0.094211	C	4.468336	1.865288	0.041524	C	4.352381	1.841827	0.318498
H	4.968014	2.618333	-0.424541	H	5.416075	2.003018	-0.499594	H	5.316429	2.060325	-0.162317
H	3.882616	3.063415	0.883536	H	4.432964	2.636819	0.816535	H	4.210319	2.604311	1.090437
N	4.134583	0.994347	0.704275	N	4.343424	0.556409	0.680578	N	4.310611	0.522830	0.947313
H	4.305193	1.071880	1.701204	H	4.624655	0.603656	1.653847	H	4.419986	0.589061	1.952070
C	5.078058	0.054123	0.098074	C	4.995258	-0.567583	0.010260	C	5.153881	-0.535783	0.387981
H	5.073875	0.199000	-0.987962	H	4.934025	-0.420296	-1.073900	H	5.388951	-0.290006	-0.654056
H	6.116554	0.197396	0.430577	H	6.065356	-0.655774	0.250731	H	6.114112	-0.646268	0.908464
C	4.676903	-1.386698	0.414539	C	4.328916	-1.891874	0.376275	C	4.423680	-1.885162	0.426673
H	5.336519	-2.099355	-0.083421	H	4.824916	-2.721309	-0.131573	H	4.961231	-2.646461	-0.141755
H	4.678661	-1.584679	1.488623	H	4.353044	-2.072119	1.453396	H	4.263556	-2.240097	1.446189
N	3.271608	-1.628118	-0.072775	N	2.880078	-1.904025	-0.037275	N	3.066977	-1.689103	-0.194685
H	3.223652	-1.357304	-1.059100	H	2.809403	-1.583530	-1.006370	H	3.205502	-1.128049	-1.037207
H	2.637222	-0.982917	0.458824	H	2.346600	-1.218464	0.554292	H	2.498179	-1.120957	0.481927
C	2.764424	-3.035256	0.067099	C	2.210901	-3.247141	0.058541	C	2.288898	-2.907946	-0.589391
H	2.617088	-3.231954	1.130500	H	1.989634	-3.421006	1.114018	H	2.031722	-3.451917	0.321885
H	3.542165	-3.703541	-0.306108	H	2.930518	-3.996783	-0.274044	H	2.949700	-3.533350	-1.191849
C	1.506665	-3.276633	-0.762516	C	0.963566	-3.339336	-0.811610	C	1.056108	-2.556081	-1.425072
H	1.364041	-4.351183	-0.880688	H	0.639839	-4.392128	-0.771449	H	0.748593	-3.483015	-1.915954
H	1.611510	-2.843943	-1.760051	H	1.219512	-3.132016	-1.858250	H	1.312592	-1.853080	-2.223713
N	0.233100	-2.725467	-0.171234	N	-0.112131	-2.427664	-0.399686	N	-0.113647	-2.026615	-0.654665
H	0.395799	-1.815059	0.329658	H	-0.258238	-2.526006	0.604876	H	0.069939	-2.100826	0.351448
H	-0.099561	-3.363522	0.557498	C	-1.368237	-2.746804	-1.100753	C	-1.358081	-2.772982	-0.994766
C	-0.862321	-2.563936	-1.214524	H	-1.550863	-3.830577	-1.138852	H	-1.258546	-3.830200	-0.731643
H	-0.925862	-3.516314	-1.742756	H	-1.270353	-2.407566	-2.141267	H	-1.473599	-2.707519	-2.083069
H	-0.513218	-1.788205	-1.895655	C	-2.639142	-0.693527	-0.202602	C	-2.648803	-0.743121	-0.154351
C	-2.492449	-0.822908	-0.306292	C	-2.572038	-2.093480	-0.461529	C	-2.557925	-2.161516	-0.321161
C	-2.180823	-2.202093	-0.590295	C	-3.691225	-2.851133	-0.165909	C	-3.615472	-2.950237	0.077655
C	-3.102322	-3.182991	-0.295112	H	-3.657000	-3.919503	-0.356696	H	-3.541424	-4.027558	-0.039678
H	-2.870128	-4.219739	-0.523540	Cl	1.101442	-0.131304	1.920340	Cl	1.084565	-0.427065	1.913780
Cl	1.028932	-0.346522	1.709480	H	-0.682314	-0.380271	-0.609072	H	-0.606777	-0.784540	-0.708508

Table 3: S_0 optimized geometries of **Bromide-LH$_3^{2+}$** complexes (Isomer A, Isomer B and Transition State). Calculations were performed by using DFT with B3-LYP exchange-correlation functional and 6-31++G(d,p) basis set. Atomic coordinates are in Å units.

ISOMER A				ISOMER B				TRANSITION STATE			
C	-3.148758	1.860306	0.194115	C	-2.850327	2.091696	0.073738	C	-2.903439	2.024957	0.057547
C	-3.382251	3.241103	0.472182	C	-2.927482	3.504988	0.230452	C	-3.015239	3.440695	0.184353
H	-4.315569	3.526749	0.948605	H	-3.841570	3.933967	0.626899	H	-3.931628	3.850915	0.596431
C	-2.447552	4.183183	0.130171	C	-1.868124	4.295705	-0.131299	C	-1.989440	4.254943	-0.213081
H	-2.623155	5.235306	0.328064	H	-1.917431	5.374226	-0.035238	H	-2.066339	5.333627	-0.136345
C	-4.089950	0.872451	0.501617	C	-3.931711	1.269567	0.413225	C	-3.957641	1.200406	0.461502
H	-5.030707	1.151196	0.969375	H	-4.828962	1.723783	0.823875	H	-4.847047	1.650207	0.893873
C	-3.831984	-0.467775	0.202688	C	-3.895841	-0.111858	0.216994	C	-3.887568	-0.182978	0.310551
C	-4.470652	-2.811454	0.167178	C	-4.927351	-2.298500	0.287034	C	-4.823823	-2.407292	0.528050
H	-5.178063	-3.606579	0.377548	H	-5.762401	-2.951543	0.515234	H	-5.617175	-3.080175	0.834848
C	-4.764040	-1.512047	0.489860	C	-5.007436	-0.951367	0.523214	C	-4.944764	-1.054623	0.710369
H	-5.707182	-1.253917	0.963010	H	-5.903701	-0.499873	0.935022	H	-5.834834	-0.623219	1.157121
N	-1.661224	0.158693	-0.735535	N	-1.636250	0.129878	-0.584539	N	-1.653404	0.071774	-0.651737
H	-0.522628	4.556703	-0.777418	H	0.104787	4.345979	-0.983323	H	-0.012609	4.331236	-1.060591
C	-1.235011	3.783989	-0.497092	C	-0.702027	3.693756	-0.658669	C	-0.811760	3.669531	-0.735878
C	-0.947217	2.462553	-0.768231	C	-0.550376	2.322862	-0.798191	C	-0.633793	2.302595	-0.861194
C	-1.914277	1.445099	-0.434241	C	-1.649210	1.487670	-0.434919	C	-1.707408	1.422280	-0.488692
C	0.360743	2.105913	-1.430885	C	0.737297	1.814113	-1.406733	C	0.693389	1.836476	-1.404012
H	0.368017	1.070475	-1.766526	H	0.733825	0.746770	-1.620886	H	0.685200	0.794550	-1.708729
H	0.558359	2.765762	-2.277760	H	0.933560	2.338008	-2.344200	H	0.979506	2.437081	-2.268958
N	1.539697	2.267891	-0.484935	N	1.927788	2.069364	-0.508019	N	1.805778	2.010123	-0.379944
H	1.542675	1.466131	0.184849	H	1.925903	1.345401	0.251264	H	1.718892	1.254229	0.340791
H	1.394762	3.103141	0.089453	H	1.804393	2.964272	-0.026705	H	1.647526	2.883748	0.130707
C	2.870401	2.384158	-1.181613	C	3.254619	2.084169	-1.225728	C	3.195070	2.047417	-0.972336
H	2.873878	3.339366	-1.711035	H	3.343637	3.044439	-1.737265	H	3.299169	3.005215	-1.486305
H	2.917367	1.579720	-1.917653	H	3.223675	1.294042	-1.977781	H	3.246687	1.255067	-1.721998
C	4.025119	2.299843	-0.182524	C	4.391072	1.857502	-0.227902	C	4.271368	1.869697	0.103524
H	4.950989	2.534914	-0.725467	H	5.341675	1.949662	-0.772222	H	5.242718	2.056570	-0.374300
H	3.906225	3.078014	0.578114	H	4.381619	2.650640	0.525865	H	4.150797	2.639648	0.872000
N	4.068494	0.991394	0.475091	N	4.224198	0.567318	0.440261	N	4.189482	0.551890	0.731899
H	4.214035	1.094869	1.473638	H	4.448075	0.635314	1.427158	H	4.234613	0.615460	1.741802
C	4.999066	0.007876	-0.079182	C	4.899746	-0.577872	-0.166857	C	5.053658	-0.515244	0.223402
H	5.023631	0.121420	-1.168910	H	4.874859	-0.467582	-1.256806	H	5.335263	-0.280996	-0.809397
H	6.033262	0.134267	0.273267	H	5.961256	-0.654826	0.112949	H	5.988898	-0.624077	0.787887
C	4.556592	-1.413636	0.268700	C	4.224699	-1.891221	0.220392	C	4.316322	-1.861730	0.242155
H	5.216618	-2.152346	-0.188962	H	4.739699	-2.734093	-0.244347	H	4.868356	-2.627071	-0.306242
H	4.525752	-1.581231	1.347426	H	4.213365	-2.037927	1.302779	H	4.121017	-2.214201	1.256527
N	3.161294	-1.644288	-0.252386	N	2.790477	-1.920323	-0.241107	N	2.980462	-1.657793	-0.421297
H	3.137818	-1.378448	-1.240831	H	2.744893	-1.595351	-1.210426	H	3.139947	-1.075579	-1.246028
H	2.524377	-0.989961	0.263070	H	2.235708	-1.244870	0.338466	H	2.397445	-1.103001	0.251930
C	2.640196	-3.047088	-0.114816	C	2.133892	-3.270590	-0.167058	C	2.213805	-2.868282	-0.862866
H	2.483735	-3.240058	0.948206	H	1.922133	-3.466833	0.886709	H	1.958758	-3.447739	0.027095
H	3.416397	-3.721192	-0.480236	H	2.857039	-4.007307	-0.520309	H	2.881258	-3.464520	-1.487497
C	1.385224	-3.279987	-0.952362	C	0.878749	-3.351059	-1.027119	C	0.978962	-2.493870	-1.686481
H	1.248938	-4.352652	-1.091795	H	0.553379	-4.403750	-1.000318	H	0.669499	-3.406217	-2.202813
H	1.487418	-2.827088	-1.941143	H	1.124032	-3.126412	-2.072682	H	1.234492	-1.768393	-2.464861
N	0.109617	-2.747706	-0.348514	N	-0.186462	-2.441825	-0.586308	N	-0.185164	-1.984972	-0.895660
H	0.273585	-1.856181	0.184098	H	-0.329617	-2.567204	0.415756	H	0.011274	-2.071813	0.107761
H	-0.226723	-3.409244	0.357450	C	-1.452820	-2.725969	-1.283522	C	-1.434162	-2.728293	-1.221705
C	-0.985520	-2.539126	-1.383459	H	-1.645709	-3.806141	-1.357492	H	-1.323007	-3.791044	-0.987532
H	-1.073057	-3.477971	-1.932016	H	-1.367328	-2.349772	-2.312227	H	-1.582556	-2.634917	-2.303929
H	-0.622947	-1.756345	-2.049077	C	-2.699535	-0.688108	-0.323741	C	-2.699024	-0.723410	-0.285688
C	-2.569568	-0.781257	-0.424684	C	-2.638529	-2.085251	-0.599286	C	-2.611312	-2.137378	-0.491428
C	-2.290575	-2.161121	-0.740160	C	-3.746114	-2.848743	-0.276741	C	-3.650805	-2.939776	-0.073317
C	-3.227878	-3.128757	-0.450996	H	-3.715505	-3.914970	-0.479373	H	-3.578056	-4.013437	-0.220836
H	-3.019799	-4.165307	-0.702394	Br	0.934948	-0.077512	1.814308	Br	0.908207	-0.371686	1.796361
Br	0.871549	-0.262765	1.639754	H	-0.755877	-0.364941	-0.776878	H	-0.679773	-0.746015	-0.916517

Table 4: S_0 optimized geometries of **Fluoride-LH$_2^+$** complexes (Isomer A, Isomer B and Transition State). Calculations were performed by using DFT with B3-LYP exchange-correlation functional and 6-31++G(d,p) basis set. Atomic coordinates are in Å units.

ISOMER A			ISOMER B			TRANSITION STATE		
C	3.197952	1.663673 -0.306307	C	-3.345168	-1.411124 -0.283706	C	2.935345	1.885891 -0.038253
C	3.543114	3.030109 -0.539321	C	-3.937002	-2.688061 -0.511597	C	3.123768	3.299963 -0.046572
H	4.499744	3.256277 -1.001817	H	-4.980667	-2.732574 -0.805463	H	4.084298	3.694103 -0.363263
C	2.678186	4.031968 -0.182034	C	-3.194375	-3.827738 -0.345227	C	2.106045	4.132701 0.337231
H	2.938110	5.071845 -0.350902	H	-3.631237	-4.805985 -0.511935	H	2.240257	5.208786 0.342992
C	4.043591	0.605487 -0.656310	C	-4.079245	-0.226660 -0.406200	C	3.944698	1.014404 -0.463317
H	5.004090	0.812970 -1.121251	H	-5.127443	-0.281277 -0.686899	H	4.888988	1.426323 -0.808793
C	3.658207	-0.716984 -0.416423	C	-3.504912	1.023545 -0.159194	C	3.754813	-0.369691 -0.468555
C	4.046162	-3.112450 -0.510569	C	-3.670156	3.428056 0.026693	C	4.470397	-2.634761 -0.934499
H	4.663243	-3.964838 -0.775314	H	-4.240632	4.350080 -0.002874	H	5.203470	-3.342950 -1.305787
C	4.473862	-1.835975 -0.769503	C	-4.271640	2.223135 -0.225923	C	4.736915	-1.289539 -0.942395
H	5.433322	-1.654366 -1.245459	H	-5.327915	2.155461 -0.465027	H	5.680899	-0.903289 -1.313389
N	1.568137	0.071895 0.577017	N	-1.395508	-0.084302 0.210283	N	1.532491	-0.015289 0.448731
H	0.756992	4.528337 0.685461	H	-1.315104	-4.647024 0.325147	H	0.054926	4.262300 0.999133
C	1.424675	3.714503 0.414287	C	-1.854690	-3.729104 0.109094	C	0.854394	3.582282 0.717705
C	1.036129	2.413567 0.653824	C	-1.217385	-2.520297 0.332388	C	0.605229	2.222383 0.736218
C	1.932879	1.337324 0.312799	C	-1.959714	-1.317213 0.083307	C	1.674260	1.329892 0.390398
C	-0.317138	2.133921 1.258557	C	0.145194	-2.547523 0.995025	C	-0.790046	1.759408 1.083250
H	-0.320839	1.199158 1.818060	H	0.282399	-1.697071 1.665395	H	-0.816168	0.758651 1.512597
H	-0.605604	2.952849 1.919978	H	0.224650	-3.459134 1.589156	H	-1.219866	2.443221 1.818334
N	-1.399879	2.015097 0.204646	N	1.315283	-2.527728 0.045903	N	-1.703547	1.749225 -0.120527
H	-1.294388	1.056025 -0.298364	H	1.358036	-1.518452 -0.340232	H	-1.471817	0.818399 -0.736445
H	-1.240720	2.738393 -0.501243	H	1.142439	-3.169866 -0.731266	H	-1.467220	2.551287 -0.709243
C	-2.783453	2.195043 0.768998	C	2.609198	-2.886955 0.714295	C	-3.146969	1.867763 0.281759
H	-2.757382	3.081281 1.408272	H	2.524116	-3.907807 1.094988	H	-3.253262	2.814513 0.819342
H	-2.991355	1.323286 1.393418	H	2.719942	-2.209158 1.563683	H	-3.350059	1.044586 0.969750
C	-3.855296	2.379033 -0.309572	C	3.788294	-2.767533 -0.251396	C	-4.128077	1.837974 -0.892769
H	-4.739973	2.799281 0.197138	H	4.677477	-3.156806 0.273265	H	-5.061037	2.296684 -0.520501
H	-3.519883	3.140793 -1.022603	H	3.618438	-3.425254 -1.110927	H	-3.762589	2.486487 -1.696965
N	-4.154814	1.151435 -1.042455	N	3.957263	-1.399809 -0.736444	N	-4.346497	0.500700 -1.442932
H	-4.426461	1.373474 -1.993854	H	4.387547	-1.417843 -1.656568	H	-4.714345	0.581600 -2.383780
C	-5.152260	0.261776 -0.423005	C	4.742892	-0.522254 0.142814	C	-5.193874	-0.396120 -0.634343
H	-5.180247	0.467398 0.652632	H	4.358955	-0.612811 1.165120	H	-5.462796	0.105709 0.303725
H	-6.163498	0.447940 -0.814585	H	5.804285	-0.823441 0.170896	H	-6.133914	-0.614869 -1.157850
C	-4.787031	-1.211413 -0.615654	C	4.646431	0.941010 -0.287749	C	-4.493762	-1.718451 -0.295711
H	-5.562064	-1.837123 -0.153896	H	5.461672	1.500531 0.189281	H	-5.129939	-2.285185 0.396752
H	-4.780604	-1.451195 -1.696120	H	4.828743	0.998672 -1.379496	H	-4.391338	-2.329908 -1.211462
N	-3.502110	-1.478473 0.026960	N	3.376598	1.564124 0.097351	N	-3.204695	-1.458177 0.344103
H	-2.811410	-0.852403 -0.393123	H	2.599960	0.976476 -0.214886	H	-2.600304	-1.027899 -0.359534
C	-3.032971	-2.853930 -0.095369	C	3.236323	2.908133 -0.464890	C	-2.544385	-2.641064 0.891025
H	-2.847723	-3.165849 -1.140737	H	3.160167	2.892130 -1.568837	H	-2.338283	-3.417286 0.128898
H	-3.806442	-3.526658 0.294067	H	4.150831	3.467733 -0.223574	H	-3.210991	-3.098976 1.632059
C	-1.784162	-3.098047 0.748876	C	2.061085	3.712789 0.096352	C	-1.242738	-2.276342 1.606573
H	-1.605946	-4.168208 0.877075	H	2.171195	4.737808 -0.276541	H	-0.912047	-3.131207 2.202613
H	-1.910293	-2.640121 1.732427	H	2.150970	3.759989 1.193197	H	-1.433234	-1.449233 2.298578
N	-0.525801	-2.517534 0.153410	N	0.721576	3.229882 -0.299406	N	-0.128618	-1.892287 0.685499
H	-0.275790	-3.070880 -0.670280	H	0.170418	4.026935 -0.602031	H	-0.485502	-1.752549 -0.268600
C	0.628799	-2.558921 1.127766	C	-0.017555	2.537776 0.772678	C	1.006211	-2.846492 0.702266
H	0.626059	-3.552401 1.580515	H	0.009644	3.115793 1.713291	H	0.738562	-3.799660 0.232435
H	0.407933	-1.814830 1.893418	H	0.473174	1.586332 0.971966	H	1.227754	-3.055221 1.755534
C	2.379347	-0.935889 0.218365	C	-2.098636	1.083717 0.145946	C	2.503903	-0.867793 0.029524
C	1.956607	-2.290756 0.469850	C	-1.479071	2.349089 0.398763	C	2.256352	-2.277456 0.062640
C	2.783143	-3.332928 0.111474	C	-2.289676	3.470828 0.350316	C	3.229403	-3.118509 -0.434561
H	2.469129	-4.354624 0.307935	H	-1.850107	4.435940 0.589157	H	3.049185	-4.190023 -0.434170
F	-1.065222	-0.254805 -0.929097	F	0.981053	-0.108979 -0.511457	F	-1.058505	-0.284347 -1.378584
H	-0.691784	-1.514179 -0.220387	H	-0.319063	-0.035421 0.060565	H	0.557690	-0.703136 0.734491

Table 5: S_0 optimized geometries of **Chloride-LH$_2^+$** complexes (Isomer A, Isomer B and Transition State). Calculations were performed by using DFT with B3-LYP exchange-correlation functional and 6-31++G(d,p) basis set. Atomic coordinates are in Å units.

ISOMER A				ISOMER B				TRANSITION STATE			
C	-3.098239	1.826506	0.200963	C	-2.784448	2.053609	0.069371	C	-2.800256	2.041931	0.004735
C	-3.343784	3.214921	0.427572	C	-2.843695	3.475560	0.136911	C	-2.867494	3.466092	0.032454
H	-4.291915	3.512698	0.866051	H	-3.757871	3.941772	0.488978	H	-3.790131	3.935702	0.358366
C	-2.398478	4.148882	0.090919	C	-1.766284	4.227975	-0.253517	C	-1.788285	4.215819	-0.354331
H	-2.583514	5.205762	0.251865	H	-1.803921	5.310963	-0.223711	H	-1.832351	5.299199	-0.353128
C	-4.036804	0.840187	0.522931	C	-3.875484	1.259010	0.445562	C	-3.891057	1.261060	0.404716
H	-4.989509	1.125006	0.962228	H	-4.775264	1.741807	0.816245	H	-4.794331	1.752457	0.755552
C	-3.755542	-0.507784	0.283921	C	-3.839846	-0.133879	0.343969	C	-3.837065	-0.133067	0.361882
C	-4.345976	-2.863363	0.346178	C	-4.841859	-2.325065	0.562147	C	-4.789202	-2.333183	0.707891
H	-5.039562	-3.662393	0.586288	H	-5.669307	-2.970013	0.837096	H	-5.598352	-2.978427	1.032798
C	-4.671290	-1.557001	0.604645	C	-4.942159	-0.965082	0.703444	C	-4.915621	-0.969753	0.778791
H	-5.624915	-1.298389	1.055986	H	-5.845790	-0.500409	1.083510	H	-5.823065	-0.506490	1.152562
N	-1.575434	0.109402	-0.637245	N	-1.574057	0.052402	-0.458324	N	-1.565803	0.028003	-0.500684
H	-0.433955	4.499392	-0.744063	H	0.234503	4.204833	-1.048304	H	0.246689	4.180688	-1.062824
C	-1.161034	3.735898	-0.477462	C	-0.592555	3.583224	-0.714815	C	-0.595369	3.564742	-0.757596
C	-0.863249	2.407686	-0.698594	C	-0.459686	2.205685	-0.768292	C	-0.458172	2.188220	-0.777063
C	-1.845348	1.401070	-0.381656	C	-1.581415	1.410927	-0.386050	C	-1.591026	1.380956	-0.427060
C	0.474158	2.025567	-1.280298	C	0.840065	1.625706	-1.277323	C	0.882628	1.620937	-1.175750
H	0.470634	1.003026	-1.653260	H	0.798660	0.556589	-1.481792	H	0.855971	0.567661	-1.444023
H	0.748360	2.706656	-2.087813	H	1.127341	2.125900	-2.204195	H	1.275014	2.171728	-2.031848
N	1.597100	2.113295	-0.258365	N	1.980565	1.831329	-0.305340	N	1.918958	1.760864	-0.072604
H	1.542477	1.293519	0.391817	H	1.843460	1.188837	0.521156	H	1.777356	1.001565	0.638911
H	1.442645	2.934967	0.332969	H	1.923376	2.776487	0.084502	H	1.747858	2.632415	0.436704
C	2.956674	2.228008	-0.899340	C	3.329199	1.662370	-0.957809	C	3.328303	1.786029	-0.612584
H	2.947332	3.147650	-1.488554	H	3.415393	2.450189	-1.709572	H	3.415547	2.696693	-1.209137
H	3.056262	1.378130	-1.577555	H	3.316125	0.689624	-1.453822	H	3.421216	0.915071	-1.263541
C	4.087226	2.254253	0.128506	C	4.469745	1.740843	0.053728	C	4.384612	1.755476	0.489292
H	4.992489	2.593367	-0.401270	H	5.397431	1.882974	-0.525603	H	5.332248	2.068058	0.018348
H	3.871910	3.011681	0.889913	H	4.352286	2.633042	0.678450	H	4.152378	2.506266	1.252486
N	4.253530	0.959027	0.780987	N	4.502172	0.562322	0.913227	N	4.466931	0.446032	1.128813
H	4.579998	1.084584	1.733322	H	4.927011	0.792913	1.804056	H	4.866604	0.539341	2.055456
C	5.109229	-0.003815	0.071410	C	5.137618	-0.631326	0.328472	C	5.172401	-0.592857	0.356958
H	5.015434	0.179595	-1.004135	H	5.293914	-0.462817	-0.743461	H	5.391487	-0.207551	-0.645962
H	6.172728	0.119172	0.329617	H	6.129374	-0.803802	0.770112	H	6.138626	-0.836012	0.819399
C	4.673289	-1.443381	0.347240	C	4.295662	-1.897281	0.495178	C	4.352374	-1.878893	0.212391
H	5.326865	-2.124841	-0.211064	H	4.836956	-2.726109	0.021934	H	4.885711	-2.552310	-0.470011
H	4.807340	-1.674416	1.420146	H	4.205750	-2.146501	1.567465	H	4.288931	-2.394476	1.186775
N	3.292084	-1.632988	-0.100788	N	2.986425	-1.770401	-0.157443	N	3.025041	-1.595241	-0.347333
H	2.707225	-1.008199	0.456118	H	2.403575	-1.170528	0.427530	H	2.477199	-1.163420	0.398785
C	2.798644	-3.002076	0.011368	C	2.316734	-3.060355	-0.332247	C	2.328417	-2.788523	-0.826714
H	2.631466	-3.331535	1.052209	H	2.077037	-3.549200	0.632005	H	2.120055	-3.521065	-0.024122
H	3.552348	-3.677090	-0.409471	H	3.012230	-3.730285	-0.851033	H	2.981742	-3.294452	-1.546824
C	1.538337	-3.217238	-0.821802	C	1.049715	-2.996141	-1.180899	C	1.028555	-2.470822	-1.562374
H	1.338926	-4.281277	-0.963444	H	0.760902	-4.035086	-1.406166	H	0.704742	-3.379317	-2.079366
H	1.658507	-2.742657	-1.797355	H	1.263385	-2.501021	-2.135360	H	1.205548	-1.704534	-2.323759
N	0.282487	-2.638206	-0.208446	N	-0.075143	-2.294905	-0.522211	N	-0.090209	-2.019592	-0.673887
H	0.001464	-3.226379	0.581369	H	-0.022672	-2.459667	0.483501	H	0.184412	-2.095787	0.310645
C	-0.858675	-2.579636	-1.205843	C	-1.370267	-2.795258	-1.016037	C	-1.339556	-2.792462	-0.908769
H	-0.914446	-3.568303	-1.663714	H	-1.455368	-3.886959	-0.913306	H	-1.225084	-3.833941	-0.590907
H	-0.560020	-1.848659	-1.956918	H	-1.414360	-2.577934	-2.092426	H	-1.504541	-2.795926	-1.992884
C	-2.481358	-0.827870	-0.314926	C	-2.640750	-0.739444	-0.154048	C	-2.632444	-0.731596	-0.136294
C	-2.170484	-2.211801	-0.569614	C	-2.559799	-2.149967	-0.340394	C	-2.535614	-2.155241	-0.241102
C	-3.090118	-3.184546	-0.245007	C	-3.654859	-2.904012	0.035649	C	-3.597030	-2.917926	0.195600
H	-2.858731	-4.226964	-0.446612	H	-3.613770	-3.981610	-0.093104	H	-3.529819	-4.000355	0.133121
Cl	0.819714	-0.229805	1.846759	Cl	0.875779	0.185405	2.132266	Cl	0.819779	-0.334193	2.109480
H	0.445566	-1.697940	0.220761	H	-0.702150	-0.493701	-0.630582	H	-0.626922	-0.763595	-0.703310

Table 6: S_0 optimized geometries of **Bromide-LH$_2^+$** complexes (Isomer A, Isomer B and Transition State). Calculations were performed by using DFT with B3-LYP exchange-correlation functional and 6-31++G(d,p) basis set. Atomic coordinates are in Å units.

ISOMER A				ISOMER B				TRANSITION STATE			
C	-3.113972	1.847507	0.108610	C	-2.792092	2.092637	-0.067507	C	-2.785280	2.097636	-0.082103
C	-3.354776	3.234008	0.351123	C	-2.824791	3.515347	0.000354	C	-2.815344	3.522344	-0.032927
H	-4.291047	3.527768	0.816945	H	-3.727660	3.998639	0.358424	H	-3.719459	4.010759	0.316279
C	-2.419487	4.171429	-0.003282	C	-1.732787	4.246965	-0.388637	C	-1.720921	4.249385	-0.420154
H	-2.600950	5.226962	0.170133	H	-1.749340	5.330488	-0.357313	H	-1.735731	5.333403	-0.400280
C	-4.041713	0.857724	0.450190	C	-3.892026	1.316540	0.321196	C	-3.890573	1.338318	0.319834
H	-4.981516	1.137646	0.919390	H	-4.779524	1.814465	0.701394	H	-4.774489	1.846330	0.695637
C	-3.767074	-0.487660	0.189469	C	-3.877966	-0.077342	0.226534	C	-3.875560	-0.055453	0.245209
C	-4.361701	-2.842586	0.240325	C	-4.906541	-2.252833	0.472622	C	-4.884264	-2.236079	0.553874
H	-5.048957	-3.643207	0.493021	H	-5.736956	-2.885042	0.767625	H	-5.705669	-2.866223	0.877685
C	-4.673968	-1.539047	0.527218	C	-4.984428	-0.891170	0.611512	C	-4.969633	-0.871947	0.661759
H	-5.611413	-1.284033	1.013286	H	-5.873532	-0.412236	1.007836	H	-5.856636	-0.392816	1.063605
N	-1.623498	0.141010	-0.804240	N	-1.633299	0.074520	-0.637241	N	-1.622555	0.064069	-0.669293
H	-0.471942	4.529128	-0.873775	H	0.273064	4.190409	-1.165143	H	0.302844	4.175440	-1.153574
C	-1.194327	3.763154	-0.601083	C	-0.567806	3.580994	-0.843654	C	-0.550228	3.574032	-0.848815
C	-0.903949	2.437359	-0.843929	C	-0.463169	2.201822	-0.902333	C	-0.453190	2.195550	-0.899553
C	-1.879990	1.427995	-0.515946	C	-1.606822	1.429561	-0.537627	C	-1.604298	1.413519	-0.552449
C	0.424716	2.057044	-1.447407	C	0.823151	1.586277	-1.406442	C	0.859147	1.589249	-1.337040
H	0.426881	1.022909	-1.786676	H	0.781880	0.503470	-1.515164	H	0.815947	0.514275	-1.489120
H	0.674598	2.716276	-2.280795	H	1.085478	2.011673	-2.377222	H	1.196628	2.050580	-2.267038
N	1.562180	2.191797	-0.448110	N	1.987714	1.862059	-0.482240	N	1.959401	1.823213	-0.319645
H	1.515993	1.397327	0.230847	H	1.899473	1.228895	0.350312	H	1.839862	1.132941	0.459463
H	1.412995	3.035498	0.112725	H	1.912827	2.812250	-0.109291	H	1.831300	2.741906	0.112962
C	2.918253	2.276261	-1.098264	C	3.327717	1.711400	-1.154916	C	3.341295	1.755147	-0.919257
H	2.926859	3.191986	-1.693538	H	3.419490	2.527794	-1.874405	H	3.446262	2.626131	-1.569250
H	2.998390	1.418929	-1.769676	H	3.302835	0.759335	-1.688888	H	3.369872	0.843752	-1.519333
C	4.044312	2.278645	-0.064569	C	4.459482	1.728599	-0.130754	C	4.424647	1.725580	0.155611
H	4.964327	2.584596	-0.588337	H	5.402473	1.834757	-0.691532	H	5.381334	1.933429	-0.352256
H	3.846042	3.047805	0.689782	H	4.371521	2.615948	0.505406	H	4.266197	2.540217	0.870771
N	4.161652	0.981807	0.596562	N	4.412714	0.535410	0.708351	N	4.419078	0.456550	0.877854
H	4.459673	1.101822	1.558937	H	4.801062	0.734049	1.623321	H	4.813975	0.582667	1.802646
C	5.019748	0.001787	-0.085211	C	5.035485	-0.667621	0.129112	C	5.071023	-0.667771	0.181355
H	4.937697	0.167318	-1.164553	H	5.190466	-0.502004	-0.942983	H	5.309234	-0.361139	-0.843951
H	6.081384	0.125160	0.182304	H	6.026891	-0.849589	0.568943	H	6.023902	-0.926074	0.663514
C	4.577789	-1.432797	0.207272	C	4.180063	-1.924633	0.295055	C	4.193304	-1.921369	0.113183
H	5.238601	-2.119794	-0.335415	H	4.718213	-2.758841	-0.172256	H	4.713995	-2.666305	-0.501338
H	4.702518	-1.651682	1.283732	H	4.081224	-2.171510	1.366940	H	4.083593	-2.359762	1.120068
N	3.202834	-1.631629	-0.255751	N	2.875548	-1.785796	-0.365571	N	2.892913	-1.626773	-0.503750
H	2.599996	-1.042586	0.321049	H	2.284505	-1.214469	0.240878	H	2.318898	-1.184467	0.216593
C	2.735846	-3.014562	-0.214761	C	2.213863	-3.073417	-0.585318	C	2.200837	-2.816644	-1.000337
H	2.564803	-3.399016	0.806480	H	1.978601	-3.597289	0.361513	H	1.974578	-3.551702	-0.204770
H	3.507046	-3.652702	-0.660200	H	2.909955	-3.721534	-1.130534	H	2.864342	-3.322891	-1.710787
C	1.485460	-3.210382	-1.069599	C	0.942184	-2.981974	-1.425154	C	0.914085	-2.490019	-1.755069
H	1.314706	-4.267517	-1.282509	H	0.634371	-4.014223	-1.654384	H	0.583307	-3.399120	-2.266852
H	1.597522	-2.669290	-2.010750	H	1.158192	-2.484977	-2.378345	H	1.106954	-1.731839	-2.520639
N	0.216926	-2.702642	-0.422376	N	-0.164022	-2.265472	-0.751973	N	-0.203843	-2.016431	-0.878485
H	-0.068110	-3.362739	0.306630	H	-0.069507	-2.371993	0.258931	H	0.058270	-2.106163	0.108806
C	-0.921497	-2.549415	-1.412091	C	-1.476020	-2.784705	-1.173029	C	-1.472143	-2.753086	-1.125339
H	-1.006250	-3.505170	-1.931337	H	-1.555384	-3.871664	-1.024687	H	-1.381090	-3.802882	-0.828169
H	-0.605506	-1.778550	-2.114198	H	-1.564038	-2.609814	-2.254505	H	-1.642191	-2.729946	-2.208445
C	-2.514580	-0.801103	-0.456944	C	-2.700083	-0.701063	-0.299359	C	-2.699002	-0.674265	-0.293610
C	-2.216901	-2.183228	-0.740739	C	-2.640503	-2.114372	-0.476136	C	-2.643574	-2.097856	-0.431174
C	-3.127599	-3.157983	-0.397513	C	-3.736828	-2.851083	-0.070877	C	-3.717243	-2.841272	0.008199
H	-2.906004	-4.198327	-0.620638	H	-3.711263	-3.930357	-0.189267	H	-3.680315	-3.923497	-0.078254
Br	0.643542	-0.214872	1.734682	Br	0.693745	0.001086	1.925370	Br	0.664159	-0.267638	1.934548
H	0.369501	-1.803307	0.093447	H	-0.777485	-0.489274	-0.840679	H	-0.704750	-0.754059	-0.897082