

## Supporting Information

**A kinetic study on the reduction of CO<sub>2</sub> by frustrated Lewis pairs: from understanding to rational design**

Lei Liu, Nina Vankova, Thomas Heine

Department of Physics and Earth Science, Jacobs University Bremen

Campus Ring 1, 28759, Bremen, Germany

**Table S1.** The only one imaginary frequencies of the TSs for H<sub>2</sub> activation and H transfer computed at B97D/6-31G(d) level of theory. All values are given in cm<sup>-1</sup>.

	FLPs	TS <sup>a</sup>	TS <sup>b</sup>
TMP + B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> ( <b>1</b> )		-29.1	-111.9
btam + B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> ( <b>2</b> )		-38.3	-74.0
Lut + B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> ( <b>3</b> )		-69.1	-60.7
TMP + B( <i>p</i> -C <sub>6</sub> F <sub>2</sub> H <sub>3</sub> ) <sub>3</sub> ( <b>4</b> )		-63.4	-156.1
TMP + B(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> ( <b>5</b> )		-148.3	-162.5

### Cartesian coordinates

#### H<sub>2</sub>

H	-0.497242	-0.384892	-0.000051
H	-0.993299	-0.939246	0.018316

#### CO<sub>2</sub>

C	-2.317661	0.049843	0.035655
O	-3.467351	0.302441	0.007250
O	-1.167971	-0.202754	0.064060

#### HCOOH

C	-0.002146	-0.202687	0.382703
H	-0.009860	0.803483	0.864184
O	0.008671	-0.147356	-0.980661
H	0.006556	0.790163	-1.255880
O	-0.003222	-1.243603	0.989655

#### TMP

C	-0.032996	0.826565	0.525177
C	-1.471627	0.302790	0.311989
C	-1.511978	-1.258490	0.090451
N	-0.269245	-1.934141	0.547382
C	1.030363	-1.420809	0.013539
C	0.952035	0.085685	-0.391791
H	0.752512	-2.234385	-2.008329
H	3.080144	-1.357545	0.771682
C	2.069710	-1.589025	1.141962

H	1.847290	-0.913453	1.985607
H	2.059191	-2.626665	1.512725
C	1.478311	-2.281834	-1.185641
H	2.451407	-1.924723	-1.563899
H	1.579861	-3.333511	-0.875958
H	-1.694612	-2.660231	-1.571858
H	-2.503420	-1.695355	1.990217
C	-2.662008	-1.872766	0.912065
H	-3.620739	-1.409041	0.630066
H	-2.721112	-2.958517	0.740446
C	-1.763676	-1.575533	-1.399250
H	-2.770359	-1.228486	-1.683757
H	-1.041040	-1.067061	-2.052668
H	0.616877	0.182604	-1.438441
H	1.958783	0.532579	-0.339183
H	-1.916496	0.808840	-0.562176
H	-2.091616	0.578239	1.182135
H	-0.244731	-1.820315	1.564116
H	0.268758	0.662336	1.574526
H	0.004506	1.914121	0.352649

**TMPH+**

C	-0.270841	0.872955	-0.454570
C	-1.300992	0.192270	0.462378
C	-1.552406	-1.274310	0.040678
N	-0.203379	-1.837001	-0.547024
C	1.156804	-1.275527	-0.040173
C	1.143626	0.266859	-0.273964
H	2.081849	-1.776988	-1.965333
H	2.341474	-1.385218	1.743503
C	1.319755	-1.652000	1.438358
H	0.624688	-1.105246	2.086615
H	1.192454	-2.734618	1.596860
C	2.227617	-1.975996	-0.890964
H	3.213158	-1.579432	-0.609090
H	2.237334	-3.064515	-0.719230
H	-2.652656	-2.400230	-1.488277
H	-1.256171	-2.174203	2.024708
C	-1.986446	-2.169719	1.206283
H	-2.935681	-1.779815	1.600748
H	-2.164560	-3.204460	0.870425

C	-2.561690	-1.367561	-1.115396
H	-3.548812	-1.053282	-0.749677
H	-2.281884	-0.704320	-1.949572
H	1.759182	0.511078	-1.152635
H	1.631920	0.732281	0.594665
H	-2.266448	0.717167	0.421956
H	-0.957266	0.233944	1.506969
H	-0.198077	-2.859074	-0.425804
H	-0.230198	1.950489	-0.246398
H	-0.594245	0.774678	-1.505178
H	-0.220072	-1.675236	-1.562967

**btam**

N	-0.519316	-2.848639	-0.264323
H	-0.116008	-5.250336	1.146769
H	-0.898879	-2.307785	-1.046759
C	0.835129	-3.281017	-0.637527
C	-1.494735	-3.916225	0.069397
C	-2.826317	-3.199038	0.368232
H	-3.603387	-3.928231	0.646380
H	-2.693569	-2.480407	1.191227
H	-3.176563	-2.648630	-0.522098
C	-1.707254	-4.927739	-1.084514
H	-2.041846	-4.404218	-1.996208
H	-2.473964	-5.672242	-0.814542
H	-0.776996	-5.469308	-1.316985
C	-1.025705	-4.659400	1.336364
H	-0.815239	-3.937151	2.140147
H	-1.811747	-5.352451	1.674855
H	1.011194	-0.906167	0.687739
H	0.864071	-3.997009	-1.486935
H	1.264055	-3.811223	0.229706
C	1.708445	-2.083643	-0.976942
C	2.560164	-2.113294	-2.095438
C	3.388930	-1.020499	-2.396405
C	3.367393	0.121412	-1.581191
C	2.513096	0.162969	-0.465958
C	1.690368	-0.931710	-0.165811
H	2.570814	-3.000569	-2.734467
H	4.043933	-1.058967	-3.269773
H	4.007649	0.974943	-1.814779

H	2.489052	1.050726	0.170396
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**batmH<sup>+</sup>**

N	-0.482777	-2.905968	-0.400757
H	-0.301275	-4.968344	1.504154
H	-0.714558	-2.548150	-1.339232
C	1.006642	-3.301382	-0.422055
C	-1.550843	-3.965349	0.002166
C	-2.898391	-3.232193	-0.086969
H	-3.701142	-3.930418	0.187390
H	-2.939521	-2.378934	0.609084
H	-3.095733	-2.874969	-1.110532
C	-1.470763	-5.119823	-1.003498
H	-1.603752	-4.762721	-2.037435
H	-2.284575	-5.825335	-0.785582
H	-0.521868	-5.669188	-0.926121
C	-1.249073	-4.415835	1.436241
H	-1.224571	-3.560166	2.130127
H	-2.053238	-5.089422	1.763525
H	2.099506	-1.384011	1.186504
H	1.084372	-4.139135	-1.123914
H	1.241215	-3.640994	0.592880
C	1.813190	-2.104214	-0.843077
C	2.052236	-1.862184	-2.210447
C	2.744923	-0.709559	-2.606686
C	3.196049	0.204029	-1.639199
C	2.959999	-0.034131	-0.274745
C	2.267520	-1.185941	0.124252
H	1.717325	-2.584991	-2.959609
H	2.941146	-0.529597	-3.664275
H	3.740546	1.097221	-1.948119
H	3.322934	0.669439	0.475355
H	-0.571970	-2.095054	0.229291

**Lut**

C	0.335938	-2.794230	-0.322217
C	-0.882756	-3.476912	-0.420673
C	-0.864226	-4.877078	-0.571575
N	0.282643	-5.586976	-0.624989
C	1.455652	-4.925913	-0.529801
C	1.527580	-3.527618	-0.377284

H	-1.833858	-2.942598	-0.382266
H	-2.205173	-6.419808	0.126015
H	2.739806	-6.333899	-1.546356
H	2.498321	-3.033762	-0.304298
H	0.356646	-1.708295	-0.204502
C	-2.147210	-5.674473	-0.683713
H	-3.033527	-5.024177	-0.632295
H	-2.168674	-6.230925	-1.634724
C	2.707247	-5.776544	-0.596191
H	3.617625	-5.163999	-0.512016
H	2.704475	-6.523225	0.214370

**LutH<sup>+</sup>**

C	0.340799	-2.794580	-0.342388
C	-0.887475	-3.469726	-0.417174
C	-0.909091	-4.861751	-0.526686
N	0.298529	-5.506576	-0.556075
C	1.525606	-4.902839	-0.487042
C	1.547386	-3.510844	-0.377243
H	-1.832184	-2.929645	-0.391600
H	-2.209951	-6.402698	0.235897
H	2.773421	-6.356681	-1.476490
H	2.508418	-3.002903	-0.320453
H	0.357750	-1.707568	-0.256858
C	-2.151571	-5.700932	-0.612603
H	-3.042412	-5.061449	-0.594754
H	-2.164174	-6.290291	-1.544297
C	2.741297	-5.783251	-0.535285
H	3.651820	-5.175487	-0.468756
H	2.739664	-6.500996	0.301677
H	0.282653	-6.524844	-0.636457

**B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>**

F	1.495131	1.339995	0.432779
B	-0.600727	-0.659408	-0.028500
F	-2.235227	-0.069101	2.334716
F	0.827637	-2.983769	1.049181
C	-1.263354	-2.025418	0.385335
C	-2.653101	-2.249032	0.279349
C	-3.259889	-3.459378	0.633440
C	-2.464514	-4.501260	1.135724

C	-1.078238	-4.325303	1.268766
C	-0.506567	-3.106372	0.886734
F	-3.460490	-1.285711	-0.212142
F	-4.584652	-3.635635	0.499507
F	-3.028280	-5.663060	1.487959
F	-0.322533	-5.321960	1.758158
C	0.815112	-0.647762	-0.715169
C	1.212517	-1.642013	-1.634934
C	2.463277	-1.644193	-2.262665
C	3.381557	-0.626702	-1.959487
C	3.037492	0.380273	-1.044032
C	1.770034	0.357696	-0.451087
F	0.361389	-2.634003	-1.972609
F	2.793810	-2.600564	-3.145809
F	4.586043	-0.616812	-2.543471
F	3.922851	1.346624	-0.750261
C	-1.354237	0.694892	0.243799
C	-1.294184	1.781998	-0.654627
C	-1.965030	2.990469	-0.435411
C	-2.721342	3.149303	0.736429
C	-2.804980	2.100857	1.666026
C	-2.134495	0.901165	1.401918
F	-0.593819	1.675613	-1.803473
F	-1.895106	3.993382	-1.326119
F	-3.363044	4.301108	0.967503
F	-3.522566	2.260737	2.790115

**B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>H<sup>-</sup>**

F	0.978253	1.676160	-1.579313
B	-0.774374	-0.533972	-0.936488
F	0.707870	0.849709	1.397273
F	-0.459154	-1.788094	1.720023
C	-1.546661	-1.889312	-0.399809
C	-2.497199	-2.575898	-1.167058
C	-3.224265	-3.678954	-0.686836
C	-3.004347	-4.131673	0.618911
C	-2.061822	-3.478233	1.424860
C	-1.366031	-2.381340	0.901118
F	-2.761527	-2.201114	-2.443419
F	-4.135047	-4.313382	-1.467370
F	-3.693879	-5.193949	1.099951

F	-1.842887	-3.918383	2.688897
C	0.867140	-0.655586	-1.057206
C	1.634862	-1.822141	-0.922906
C	3.029132	-1.864577	-1.099246
C	3.718934	-0.695345	-1.433277
C	2.999904	0.496682	-1.589454
C	1.611483	0.485549	-1.405861
F	1.055707	-3.015042	-0.618887
F	3.715679	-3.025772	-0.954643
F	5.062087	-0.714859	-1.609863
F	3.658028	1.636123	-1.918731
C	-1.279636	0.689624	0.061986
C	-2.582806	1.190418	-0.093521
C	-3.132579	2.202319	0.707479
C	-2.359331	2.753791	1.736580
C	-1.058504	2.280413	1.942965
C	-0.554608	1.262585	1.117004
F	-3.393433	0.685364	-1.059385
F	-4.397161	2.651273	0.507163
F	-2.866095	3.732280	2.524878
F	-0.309510	2.806277	2.944137
H	-1.177954	-0.272252	-2.057619

**B(C<sub>6</sub>F<sub>2</sub>H<sub>3</sub>)<sub>3</sub>**

C	-1.176635	-5.818315	0.824501
C	-2.319113	-6.621523	1.068350
C	-2.827042	-6.730860	2.364646
C	-2.263876	-6.050384	3.450378
C	-1.144316	-5.251059	3.192146
C	-0.587553	-5.133124	1.916864
H	-2.802788	-7.166377	0.259043
F	-3.908115	-7.514590	2.588615
H	-2.678821	-6.139054	4.452708
F	-0.583321	-4.578507	4.224645
C	0.969373	-5.461632	-0.819064
C	1.902990	-5.984778	0.110703
C	3.270042	-5.780238	-0.088313
C	3.768553	-5.046637	-1.171063
C	2.834413	-4.525417	-2.073675
C	1.460248	-4.727279	-1.927963
H	1.570373	-6.556115	0.976119



F	4.153258	-6.299307	0.796899
H	4.836994	-4.888250	-1.305385
F	3.290474	-3.807761	-3.127282
C	-1.520435	-5.791234	-1.880312
C	-1.043277	-6.318055	-3.106906
C	-1.902134	-6.409057	-4.204342
C	-3.230961	-5.972268	-4.154563
C	-3.684341	-5.442862	-2.940799
C	-2.868063	-5.356601	-1.810972
H	-0.015506	-6.664607	-3.204502
F	-1.440297	-6.929888	-5.365604
H	-3.883872	-6.041250	-5.022689
F	-4.964621	-5.008511	-2.867776
H	0.778959	-4.306406	-2.665866
B	-0.575948	-5.690485	-0.624944
H	-3.275845	-4.944047	-0.889337
H	0.290029	-4.504218	1.774806

**B(C<sub>6</sub>F<sub>2</sub>H<sub>3</sub>)<sub>3</sub>H<sup>-</sup>**

C	-1.258726	-5.373803	0.840534
C	-1.794376	-6.682656	0.890102
C	-2.162124	-7.251566	2.111460
C	-2.031143	-6.580086	3.331508
C	-1.500711	-5.285691	3.267573
C	-1.120027	-4.683526	2.068606
H	-1.933776	-7.255733	-0.028040
F	-2.678649	-8.520259	2.134299
H	-2.328453	-7.035016	4.274880
F	-1.361525	-4.595552	4.443938
C	0.869963	-4.943914	-0.766222
C	1.529168	-6.090653	-0.263342
C	2.885100	-6.299829	-0.524966
C	3.658686	-5.410671	-1.278269
C	2.993866	-4.280079	-1.768948
C	1.641460	-4.036395	-1.531211
H	0.985174	-6.817669	0.341964
F	3.501680	-7.417437	-0.027266
H	4.716473	-5.584773	-1.468161
F	3.721715	-3.384282	-2.508737
C	-1.590024	-5.260785	-1.837208
C	-1.150202	-6.358559	-2.614188

C	-1.942773	-6.854359	-3.651940
C	-3.187778	-6.309584	-3.982961
C	-3.610081	-5.223383	-3.206480
C	-2.849059	-4.700601	-2.161370
H	-0.182550	-6.821979	-2.414819
F	-1.495706	-7.918095	-4.390547
H	-3.791080	-6.703655	-4.799070
F	-4.824317	-4.661072	-3.504738
H	1.179523	-3.136439	-1.940757
B	-0.739580	-4.675785	-0.555894
H	-3.232568	-3.852115	-1.592150
H	-0.712912	-3.671071	2.083510
H	-0.929710	-3.453919	-0.480902

**B(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>**

C	-1.207589	-5.814475	0.814939
C	-2.362830	-6.608570	1.037299
C	-2.916104	-6.758209	2.316156
C	-2.338670	-6.093011	3.410802
C	-1.201509	-5.289970	3.220854
C	-0.640600	-5.165236	1.942633
H	-2.819740	-7.122571	0.189371
H	-3.797079	-7.387608	2.461640
H	-2.773005	-6.200032	4.407580
H	-0.753441	-4.767234	4.069032
C	0.967586	-5.437106	-0.783801
C	1.895053	-5.977258	0.145011
C	3.276116	-5.791330	-0.003684
C	3.768543	-5.033903	-1.079772
C	2.874878	-4.476041	-2.009413
C	1.496843	-4.687294	-1.866516
H	1.517984	-6.561315	0.986823
H	3.968794	-6.230974	0.717667
H	4.844088	-4.879133	-1.193419
H	3.254337	-3.882197	-2.844163
C	-1.504685	-5.728263	-1.893306
C	-1.021456	-6.226715	-3.131334
C	-1.843037	-6.300627	-4.264252
C	-3.172653	-5.851747	-4.195030
C	-3.676799	-5.341671	-2.986818
C	-2.855333	-5.293910	-1.852370

H	0.013102	-6.570126	-3.192820
H	-1.449759	-6.702553	-5.200851
H	-3.813149	-5.899137	-5.078877
H	-4.708492	-4.986761	-2.931338
H	0.807634	-4.257199	-2.595842
B	-0.581665	-5.660026	-0.620585
H	-3.254521	-4.902595	-0.914549
H	0.247037	-4.545245	1.802097

**B(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>H<sup>-</sup>**

C	-1.252045	-5.356616	0.837504
C	-1.876337	-6.624396	0.918281
C	-2.271031	-7.193669	2.142300
C	-2.053370	-6.502149	3.344997
C	-1.436198	-5.239067	3.301506
C	-1.047831	-4.688687	2.069883
H	-2.062164	-7.172582	-0.010270
H	-2.752433	-8.178078	2.158512
H	-2.361846	-6.937480	4.301165
H	-1.261299	-4.685258	4.231028
C	0.888926	-4.977847	-0.774551
C	1.554643	-6.106335	-0.238553
C	2.917736	-6.359705	-0.473980
C	3.673382	-5.477424	-1.263291
C	3.044165	-4.344940	-1.810440
C	1.681702	-4.110704	-1.565505
H	0.983051	-6.798327	0.387392
H	3.393445	-7.245678	-0.038314
H	4.736184	-5.666109	-1.447158
H	3.620472	-3.645121	-2.426413
C	-1.579553	-5.273196	-1.849413
C	-1.148216	-6.351816	-2.658042
C	-1.929160	-6.865490	-3.708903
C	-3.186281	-6.307305	-3.992064
C	-3.645830	-5.233269	-3.208874
C	-2.852104	-4.735891	-2.163238
H	-0.167058	-6.792422	-2.456922
H	-1.555467	-7.701587	-4.310872
H	-3.797813	-6.699534	-4.811283
H	-4.623729	-4.784782	-3.418327
H	1.203134	-3.225475	-1.997289

B	-0.719538	-4.691443	-0.571459
H	-3.221194	-3.899574	-1.560379
H	-0.567863	-3.704660	2.049284
H	-0.892740	-3.460733	-0.512090

**FLP1**

C	0.269068	0.753556	-0.858854
C	-1.022472	0.200665	-0.238463
C	-1.032694	-1.351599	-0.294782
N	0.367473	-1.853767	-0.215282
C	1.354158	-1.102289	0.593729
C	1.498990	0.332150	-0.020908
H	2.972659	-1.940638	-0.598031
H	1.844142	-0.549753	2.659274
C	1.006737	-1.008341	2.106322
H	0.116144	-0.388647	2.280046
H	0.821125	-2.009618	2.523500
C	2.689809	-1.860861	0.461340
H	3.486955	-1.328695	1.004273
H	2.604221	-2.875123	0.886292
H	-1.489096	-2.900844	-1.764704
H	-1.566184	-1.678894	1.816033
C	-1.946070	-1.925447	0.815201
H	-2.967502	-1.519799	0.719989
H	-2.015924	-3.020490	0.724942
C	-1.581529	-1.811461	-1.663816
H	-2.645234	-1.539465	-1.768154
H	-1.006371	-1.350683	-2.480370
H	2.397776	0.375778	-0.657225
H	1.654497	1.053787	0.798287
H	-1.912219	0.580081	-0.766641
H	-1.102773	0.545826	0.805885
H	0.349222	-2.820805	0.106843
H	0.225233	1.851778	-0.939316
H	0.369167	0.355002	-1.880697
F	-4.873275	-4.677259	-2.969166
F	0.603955	-3.977056	-2.660892
B	-0.584073	-5.735066	-0.616906
F	-3.317074	-4.643971	-0.769511
F	0.347788	-4.357717	1.826473
C	-1.196089	-5.901754	0.826828

C	-2.306093	-6.737860	1.081723
C	-2.911023	-6.846955	2.339156
C	-2.410500	-6.088163	3.408806
C	-1.307204	-5.244101	3.210404
C	-0.714410	-5.188810	1.945759
F	-2.825561	-7.495725	0.094385
F	-3.958333	-7.664042	2.534143
F	-2.983680	-6.169890	4.614820
F	-0.830908	-4.508673	4.227773
C	0.950853	-5.453655	-0.803710
C	1.926609	-6.030332	0.039860
C	3.292978	-5.757790	-0.072869
C	3.727147	-4.854216	-1.055686
C	2.799804	-4.262665	-1.923605
C	1.443480	-4.577401	-1.797774
F	1.557786	-6.906708	0.998290
F	4.187006	-6.337341	0.745241
F	5.025301	-4.546318	-1.154671
F	3.218644	-3.361995	-2.827590
C	-1.527322	-5.790279	-1.876744
C	-1.108738	-6.368715	-3.094014
C	-1.913296	-6.405800	-4.238259
C	-3.192996	-5.831014	-4.192086
C	-3.653380	-5.237402	-3.006426
C	-2.827979	-5.243120	-1.877284
F	0.109703	-6.941281	-3.187679
F	-1.479589	-6.980456	-5.371961
F	-3.973654	-5.847060	-5.279198

## FLP2

N	-0.599820	0.290567	-1.328802
H	-0.265226	-2.339436	-2.004696
H	-1.026054	1.205875	-1.178856
C	0.618155	0.483502	-2.139538
C	-1.639020	-0.637285	-1.878093
C	-2.966336	-0.292963	-1.178298
H	-3.752293	-0.993792	-1.498179
H	-2.864656	-0.350117	-0.089579
H	-3.288787	0.726976	-1.450984
C	-1.858069	-0.518635	-3.406522
H	-2.115843	0.512254	-3.691290

H	-2.682954	-1.185234	-3.706609
H	-0.960576	-0.812145	-3.968840
C	-1.226682	-2.082452	-1.535759
H	-1.120980	-2.203898	-0.448870
H	-1.987669	-2.787476	-1.906794
H	0.964874	-0.503828	-2.475569
H	1.360023	0.031794	-4.740298
C	0.513265	1.432541	-3.330585
H	1.389403	0.878856	-1.464958
C	0.002866	2.734729	-3.165887
C	-0.081674	3.613027	-4.255890
C	0.354090	3.205145	-5.527396
C	0.880997	1.915667	-5.698193
C	0.958194	1.039621	-4.604833
H	-0.315761	3.073413	-2.177883
H	-0.481189	4.619226	-4.111207
H	0.287159	3.888701	-6.376235
H	1.226044	1.589724	-6.681897
F	2.732970	2.133486	2.174174
B	0.620588	0.131379	1.722232
F	-0.730778	0.684494	4.273345
F	2.061620	-2.345154	2.482551
C	-0.041426	-1.233731	2.162022
C	-1.440648	-1.395446	2.268556
C	-2.058747	-2.615337	2.560945
C	-1.261664	-3.739663	2.822343
C	0.135386	-3.624627	2.784209
C	0.713209	-2.389615	2.465642
F	-2.271071	-0.349239	2.062385
F	-3.397499	-2.716283	2.614078
F	-1.832346	-4.913683	3.119886
F	0.900540	-4.693323	3.062817
C	2.032479	0.152339	1.017810
C	2.428648	-0.819464	0.074232
C	3.644196	-0.773881	-0.614970
C	4.547527	0.263742	-0.343450
C	4.216355	1.242535	0.605057
C	2.979396	1.172200	1.258332
F	1.595630	-1.826062	-0.259142
F	3.943786	-1.699325	-1.543405
F	5.720218	0.320507	-0.987604

F	5.087236	2.228348	0.879390
C	-0.063134	1.502881	2.125910
C	-0.055245	2.633612	1.287445
C	-0.689116	3.838553	1.605878
C	-1.328946	3.964734	2.847904
C	-1.331956	2.882202	3.740160
C	-0.706922	1.685426	3.367259
F	0.571335	2.591458	0.086594
F	-0.681598	4.869985	0.742289
F	-1.931522	5.113986	3.180658
F	-1.929725	3.005525	4.937163

### FLP3

F	-2.941307	-6.558018	0.496164
F	-4.109481	-6.127366	2.882279
F	-2.872751	-4.561760	4.762831
F	-0.410606	-3.467091	4.238779
C	1.139631	-5.296775	-0.630491
C	2.050469	-5.896465	0.265059
C	-1.835192	-6.220271	-3.942527
C	3.438041	-5.787362	0.133133
C	3.963252	-5.042403	-0.935163
C	3.099957	-4.439353	-1.860966
C	-2.912842	-5.578160	2.615339
C	-2.992839	-5.428215	-4.000673
C	-3.357595	-4.645104	-2.895991
C	-2.563209	-4.673038	-1.745769
F	-1.493792	-6.981912	-4.995120
C	-2.279173	-4.783780	3.583614
C	-1.020367	-4.228834	3.313979
C	1.716990	-4.599917	-1.715485
C	-0.406864	-4.489813	2.084005
F	-3.747097	-5.421845	-5.107048
F	-4.447337	-3.858893	-2.958343
H	2.965553	-0.974855	1.008974
C	-1.372458	-5.420668	-1.650066
F	1.590757	-6.622202	1.306617
F	4.268823	-6.382018	1.006339
F	5.289120	-4.911725	-1.071020
C	-2.283561	-5.782938	1.382922
F	3.607895	-3.714897	-2.871512

C	-1.049200	-6.194145	-2.784938
F	0.056651	-6.967937	-2.782402
F	0.947174	-4.023278	-2.656044
B	-0.415596	-5.342366	-0.398375
F	-2.963799	-3.887499	-0.722699
F	0.818186	-3.955071	1.917392
C	-1.024618	-5.230821	1.050824
C	-1.135889	-0.985407	1.356294
C	-1.760273	-1.168701	0.114951
C	-0.965027	-1.476755	-1.003232
N	0.376351	-1.627229	-0.917504
C	0.974782	-1.451524	0.277613
C	0.254028	-1.115070	1.441178
H	-2.842208	-1.080093	0.008053
H	-2.650584	-1.810531	-2.334952
H	2.900679	-1.584504	-0.681399
H	0.773820	-0.994602	2.392897
H	2.685834	-2.700195	0.691137
H	-1.725212	-0.744885	2.244168
C	-1.567810	-1.627973	-2.383725
H	-1.398831	-0.710571	-2.973239
H	-1.078329	-2.452721	-2.918983
C	2.470769	-1.682606	0.325213

#### FLP4

C	0.270858	0.650846	-0.774613
C	-1.096392	0.095985	-0.348728
C	-1.125358	-1.450153	-0.491735
N	0.243828	-1.984789	-0.266651
C	1.145484	-1.307251	0.690056
C	1.377914	0.160579	0.187298
H	2.871204	-2.097529	-0.375131
H	1.401426	-0.860132	2.821155
C	0.633084	-1.291782	2.157251
H	-0.275252	-0.681643	2.259878
H	0.407980	-2.308840	2.512981
C	2.476776	-2.084136	0.650623
H	3.215500	-1.609285	1.315872
H	2.338306	-3.127783	0.981022
H	-1.425681	-2.915633	-2.087267
H	-1.954593	-1.826102	1.511401



C	-2.180612	-2.059517	0.461664
H	-3.185456	-1.669569	0.226142
H	-2.205608	-3.155555	0.353656
C	-1.496210	-1.826946	-1.944758
H	-2.528755	-1.517120	-2.178705
H	-0.806144	-1.340750	-2.650810
H	2.352482	0.229737	-0.322594
H	1.429118	0.830514	1.061703
H	-1.908838	0.524009	-0.958081
H	-1.296459	0.385106	0.696829
H	0.184374	-2.976239	-0.032551
H	0.254914	1.752519	-0.800461
H	0.492385	0.303659	-1.796044
F	-4.953649	-4.843049	-2.673164
H	0.824546	-4.019125	-2.484303
B	-0.498995	-5.632046	-0.594926
H	-3.231383	-4.924088	-0.732771
H	0.557008	-4.489414	1.708950
C	-1.039737	-5.728400	0.879555
C	-2.225805	-6.431362	1.205777
C	-2.697259	-6.422435	2.520409
C	-2.055392	-5.714410	3.544325
C	-0.886720	-5.024693	3.205329
C	-0.361476	-5.035688	1.913000
H	-2.776419	-6.984751	0.446544
F	-3.824286	-7.107486	2.824153
H	-2.448690	-5.703214	4.559116
F	-0.248319	-4.317959	4.169317
C	1.042747	-5.429435	-0.827889
C	1.987302	-6.069557	0.013939
C	3.351668	-5.857825	-0.190414
C	3.834196	-4.995098	-1.181590
C	2.887203	-4.351567	-1.984092
C	1.514812	-4.565675	-1.846055
H	1.663965	-6.730018	0.817493
F	4.247756	-6.491095	0.603201
H	4.900443	-4.818550	-1.309868
F	3.327857	-3.473722	-2.915864
C	-1.483499	-5.665394	-1.819565
C	-1.020797	-6.064959	-3.098716
C	-1.895831	-6.061912	-4.186635

C	-3.230020	-5.653782	-4.074114
C	-3.670636	-5.252917	-2.807764
C	-2.836980	-5.262809	-1.688513
H	0.011672	-6.377903	-3.245752
F	-1.445356	-6.456348	-5.400476
H	-3.895016	-5.644701	-4.935694

#### FLP5

C	0.359881	0.674840	-0.761304
C	-1.037659	0.135110	-0.420676
C	-1.075486	-1.412164	-0.563996
N	0.277508	-1.951667	-0.279213
C	1.123175	-1.298848	0.739173
C	1.402781	0.169738	0.263637
H	2.888145	-2.142979	-0.219182
H	1.258287	-0.915360	2.897200
C	0.516254	-1.289646	2.170824
H	-0.367591	-0.639311	2.231826
H	0.216721	-2.306684	2.468540
C	2.442754	-2.095071	0.784367
H	3.153331	-1.614756	1.476364
H	2.271334	-3.129051	1.126620
H	-1.334135	-2.881844	-2.163581
H	-2.015213	-1.760050	1.397512
C	-2.178594	-2.012208	0.340853
H	-3.171322	-1.633203	0.042532
H	-2.189422	-3.109402	0.250000
C	-1.384996	-1.790705	-2.030768
H	-2.398187	-1.459246	-2.314476
H	-0.651197	-1.323571	-2.705249
H	2.407123	0.230338	-0.186636
H	1.408643	0.835116	1.143513
H	-1.805594	0.573221	-1.078863
H	-1.298331	0.428001	0.610608
H	0.217460	-2.952920	-0.092932
H	0.358240	1.776988	-0.786320
H	0.637835	0.325021	-1.768005
H	-4.776000	-4.919340	-2.617186
H	0.769237	-4.098928	-2.575020
B	-0.507171	-5.579646	-0.570364
H	-3.221625	-4.889252	-0.682222

H	0.522981	-4.470180	1.765253
C	-1.033898	-5.710809	0.906389
C	-2.194518	-6.461530	1.226785
C	-2.670869	-6.551701	2.541688
C	-2.006836	-5.870812	3.576049
C	-0.855897	-5.117423	3.290804
C	-0.373653	-5.053944	1.977318
H	-2.719257	-6.987660	0.427108
H	-3.560411	-7.146246	2.761997
H	-2.383547	-5.929231	4.599786
H	-0.336872	-4.583534	4.090007
C	1.028410	-5.359350	-0.829675
C	2.006029	-5.931743	0.026077
C	3.376413	-5.751746	-0.201550
C	3.807658	-4.967769	-1.285311
C	2.864016	-4.374452	-2.139200
C	1.495649	-4.575980	-1.917130
H	1.675091	-6.534917	0.873916
H	4.108216	-6.215101	0.464057
H	4.875403	-4.815774	-1.459362
H	3.195249	-3.750864	-2.972407
C	-1.508078	-5.637558	-1.782018
C	-1.082660	-6.070065	-3.065518
C	-1.959971	-6.106926	-4.157245
C	-3.292180	-5.689794	-3.999007
C	-3.742884	-5.251020	-2.742866
C	-2.864420	-5.238010	-1.651942
H	-0.046847	-6.388109	-3.196813
H	-1.607666	-6.453864	-5.131303
H	-3.975652	-5.705591	-4.851122

**TS1a**

C	-0.645715	1.888532	-0.112033
C	-1.492792	0.977929	0.790428
C	-1.609074	-0.447363	0.165386
N	-0.376013	-0.815290	-0.599138
C	0.913794	-0.185392	-0.207104
C	0.815411	1.386353	-0.182436
H	1.646353	-0.303116	-2.265249
H	2.380693	-0.367581	1.380499
C	1.356201	-0.715225	1.172604

H	0.710527	-0.341424	1.979095
H	1.340962	-1.812624	1.188146
C	1.950940	-0.632245	-1.256456
H	2.928316	-0.176487	-1.033491
H	2.058225	-1.727007	-1.263777
H	-2.811574	-1.435772	-1.369760
H	-1.048036	-1.576307	1.967246
C	-1.881995	-1.501560	1.257445
H	-2.788359	-1.226524	1.822559
H	-2.038086	-2.486475	0.797751
C	-2.779131	-0.471905	-0.840980
H	-3.734326	-0.330978	-0.312922
H	-2.674064	0.336676	-1.583954
H	1.301790	1.808401	-1.077965
H	1.374737	1.768555	0.688176
H	-2.504424	1.391413	0.934256
H	-1.029468	0.920841	1.789518
H	0.037727	-2.784279	-0.748025
H	-0.669654	2.929911	0.245771
H	-1.085876	1.893633	-1.124539
H	-0.531628	-0.588695	-1.583841
F	1.842803	-4.684160	-2.481595
B	-0.163206	-5.592216	-0.536777
F	-2.429535	-3.877962	-1.283612
F	0.875332	-4.151684	1.786955
C	-0.957103	-5.337886	0.803445
C	-2.288584	-5.759559	0.995159
C	-3.025519	-5.463810	2.148384
C	-2.429215	-4.702955	3.165335
C	-1.103192	-4.270198	3.025549
C	-0.393551	-4.608791	1.869615
F	-2.910468	-6.496516	0.049760
F	-4.291982	-5.891772	2.289589
F	-3.126355	-4.388189	4.265663
F	-0.541640	-3.507301	3.980414
C	1.381815	-5.917719	-0.483870
C	1.947905	-6.695199	0.546409
C	3.313502	-6.998759	0.611813
C	4.172573	-6.503301	-0.380377
C	3.657577	-5.718112	-1.423295
C	2.283942	-5.454473	-1.463386

F	1.164377	-7.207629	1.520355
F	3.807372	-7.757112	1.605831
F	5.483553	-6.777641	-0.331868
F	4.483403	-5.236954	-2.368817
C	-0.928528	-5.634086	-1.919275
C	-0.565092	-6.512235	-2.960912
C	-1.202915	-6.525540	-4.208313
C	-2.247140	-5.621832	-4.454048
C	-2.646650	-4.727880	-3.448803
C	-1.998480	-4.763447	-2.210354
F	0.425603	-7.411681	-2.779803
F	-0.828149	-7.389316	-5.167332
F	-2.863582	-5.613711	-5.643823
F	-3.642594	-3.854540	-3.682304
H	0.283342	-3.502714	-0.841553

**TS2a**

C	3.148399	-4.111132	-1.625490
C	1.778863	-4.253554	-1.386982
H	-2.308468	-0.505463	1.045912
N	-0.481446	-1.128033	-0.803183
C	0.720884	-0.679870	-0.069269
F	1.790888	-6.820749	1.179808
F	-0.247944	-5.065905	4.828705
C	1.237496	-5.134127	-0.430517
F	-2.481370	-7.212050	0.305821
F	-3.382139	-7.964802	2.735091
F	-2.278483	-6.903123	5.010915
C	2.186065	-5.906127	0.269489
C	3.569108	-5.801744	0.057703
C	4.053925	-4.891605	-0.891183
F	-1.472150	-6.067145	-4.996829
C	-3.095062	-4.982166	-3.640166
C	-3.483864	-4.500881	-2.381314
C	-2.610930	-4.644804	-1.297987
F	0.209011	-6.285481	-2.897159
F	-3.920120	-4.862781	-4.691102
F	-4.676706	-3.897015	-2.230793
H	-0.548489	-3.447985	0.300817
F	4.431135	-6.564943	0.750596
F	5.371505	-4.775146	-1.106184

F	3.605279	-3.240491	-2.546826
C	-1.325003	-5.205942	-1.410281
H	-0.682254	-2.734015	-0.014719
C	-0.985775	-5.687921	-2.688173
C	-1.840566	-5.590114	-3.794432
H	-0.191875	-1.495411	-1.710662
F	0.957736	-3.468678	-2.134550
B	-0.331010	-5.240447	-0.172356
F	-3.037035	-4.161935	-0.107970
F	0.671041	-4.296394	2.401463
C	-0.868640	-5.709722	1.244817
C	-1.910388	-6.645449	1.391867
C	-2.392101	-7.059445	2.641564
C	-1.827340	-6.522023	3.806795
C	-0.787166	-5.584346	3.710795
C	-0.326433	-5.208497	2.444810
C	-1.636617	-0.210746	-1.009988
C	-1.301433	0.961869	-1.961688
H	-2.212540	1.547043	-2.167650
H	-0.545061	1.629685	-1.529027
H	-0.912279	0.579046	-2.918988
C	-2.744129	-1.077702	-1.644738
H	-2.389077	-1.525923	-2.588254
H	-3.624181	-0.457814	-1.874757
H	-3.046023	-1.884740	-0.965202
C	-2.122486	0.325408	0.347677
H	-1.391536	1.014253	0.798449
H	-3.061001	0.881767	0.203360
H	1.271698	-1.602229	0.183071
H	0.395533	-0.236604	0.881314
H	1.359171	1.918641	0.560308
C	1.641031	0.274011	-0.814077
C	2.289802	-0.153369	-1.988439
C	3.121731	0.721839	-2.700158
C	3.319733	2.035473	-2.242215
C	2.687885	2.465282	-1.064923
C	1.854533	1.585921	-0.355907
H	2.152363	-1.177393	-2.338972
H	3.622506	0.376629	-3.607124
H	3.968284	2.717009	-2.796305
H	2.843088	3.482536	-0.699185

**TS3a**

H	0.867416	1.185488	2.003362
F	-4.917049	-7.751418	-0.839343
F	-5.845023	-6.837154	1.576340
H	1.563814	-1.948500	2.012804
F	3.686994	-3.505728	1.619076
C	-0.297260	-5.111747	-1.850403
C	0.887825	-5.589401	-2.437953
C	1.175027	-5.444541	-3.803692
C	0.254812	-4.790374	-4.634766
C	-0.944586	-4.303193	-4.094134
C	-1.200746	-4.492460	-2.732608
F	1.813690	-6.232496	-1.693283
F	2.320714	-5.921860	-4.322189
F	0.520140	-4.627905	-5.940258
F	-4.294110	-5.159922	3.099022
C	0.597109	-5.322219	0.745204
C	0.638002	-6.283820	1.770615
C	1.671137	-6.349608	2.717376
C	2.711213	-5.411345	2.665608
C	2.716448	-4.441961	1.652794
C	1.683100	-4.431502	0.710889
F	-0.334625	-7.216322	1.876069
F	-1.821911	-3.649255	-4.878718
H	-0.936829	-3.568524	-0.070502
F	1.669018	-7.292249	3.676759
F	3.695612	-5.440417	3.577404
H	-0.692279	-2.794618	-0.128504
C	-3.839659	-5.603797	1.912830
C	-2.578708	-5.230793	1.435505
F	-2.480953	-7.010476	-1.731789
F	1.738699	-3.470649	-0.241296
B	-0.613477	-5.196312	-0.289177
F	-2.370871	-3.999588	-2.259621
F	-1.846494	-4.404446	2.223473
C	-2.062436	-5.656085	0.197744
C	-2.893241	-6.514426	-0.543764
C	-4.159146	-6.922294	-0.099096
C	-4.634684	-6.460248	1.135857
C	0.257637	1.577294	-0.048015

C	-0.213998	0.993320	-1.231643
C	-0.450594	-0.391127	-1.260755
N	-0.226941	-1.154460	-0.169381
C	0.243508	-0.614661	0.972750
C	0.492968	0.766951	1.068284
H	-0.400312	1.592802	-2.123465
H	-1.886298	-1.623656	-2.305996
H	0.442107	2.652291	0.001088
C	0.538514	-1.558266	2.115139
H	0.468743	-1.040318	3.082962
H	-0.150159	-2.413685	2.109057
C	-0.938807	-1.101688	-2.499742
H	-1.082764	-0.397361	-3.331051
H	-0.207607	-1.866432	-2.805014

#### **TS4a**

C	-0.764304	1.618904	-0.428660
C	-1.983682	0.754120	-0.074009
C	-1.835935	-0.676693	-0.675322
N	-0.388403	-1.088426	-0.713801
C	0.558411	-0.498494	0.282945
C	0.514346	1.071346	0.248004
H	2.218006	-0.705633	-1.130694
H	1.012981	-0.732039	2.388926
C	0.214956	-1.027725	1.690486
H	-0.729247	-0.613558	2.067918
H	0.139985	-2.124222	1.681165
C	1.961405	-1.008196	-0.100696
H	2.710310	-0.569812	0.576343
H	2.018701	-2.104807	-0.028605
H	-2.141308	-1.645884	-2.622833
H	-2.301106	-1.769734	1.173259
C	-2.657348	-1.694691	0.138758
H	-3.711402	-1.374481	0.158924
H	-2.606235	-2.698361	-0.305266
C	-2.333115	-0.677479	-2.135922
H	-3.416252	-0.487271	-2.160436
H	-1.832442	0.112257	-2.721317
H	1.401002	1.459583	-0.279662
H	0.571751	1.448815	1.282278
H	-2.914218	1.204040	-0.455409



H	-2.084767	0.696388	1.022258
H	-0.166434	-2.722477	-0.534588
H	-0.926543	2.666480	-0.131471
H	-0.633541	1.619147	-1.524572
H	-0.017370	-0.888924	-1.645725
H	2.341320	-4.502163	-1.336982
B	-0.234103	-5.150490	-0.422103
H	-2.038674	-3.819211	-2.098947
H	-0.509378	-4.300966	2.239050
C	-1.529976	-5.153502	0.508764
C	-2.783812	-5.596299	0.031637
C	-3.910082	-5.521883	0.857350
C	-3.858378	-5.007956	2.156519
C	-2.607485	-4.576956	2.614252
C	-1.456613	-4.650297	1.829549
H	-2.889878	-5.990592	-0.978001
F	-5.106152	-5.951868	0.383483
H	-4.746703	-4.947482	2.782242
F	-2.523898	-4.063509	3.868384
C	1.183662	-5.519723	0.209415
C	1.287880	-6.288555	1.390424
C	2.549132	-6.607060	1.904349
C	3.736904	-6.179581	1.303290
C	3.614837	-5.415739	0.136088
C	2.377013	-5.089339	-0.419484
H	0.397273	-6.642436	1.908103
F	2.632670	-7.352341	3.034702
H	4.709977	-6.429753	1.721543
F	4.749749	-4.982992	-0.469936
C	-0.420263	-5.275269	-2.002756
C	0.380848	-6.139024	-2.780840
C	0.193774	-6.200934	-4.166240
C	-0.750000	-5.415688	-4.836654
C	-1.529946	-4.561322	-4.048231
C	-1.394048	-4.490856	-2.663046
H	1.149821	-6.756735	-2.318409
F	0.965812	-7.041261	-4.899542
H	-0.869081	-5.465310	-5.917269
F	-2.445107	-3.763821	-4.661986
H	0.005241	-3.513580	-0.393212

**TS5a**

C	-0.621531	1.565025	-0.594317
C	-1.890236	0.776850	-0.233591
C	-1.785369	-0.693262	-0.732457
N	-0.343876	-1.157391	-0.687946
C	0.588118	-0.545158	0.320060
C	0.606471	1.016028	0.171140
H	2.293510	-0.913506	-1.001362
H	0.932639	-0.669675	2.451487
C	0.151321	-0.968159	1.735814
H	-0.784833	-0.480450	2.037699
H	0.018602	-2.057913	1.789227
C	1.978607	-1.141005	0.031932
H	2.716371	-0.694186	0.715663
H	1.981556	-2.232229	0.171154
H	-2.018345	-1.793680	-2.606128
H	-2.364835	-1.637143	1.167733
C	-2.664820	-1.632852	0.113004
H	-3.710182	-1.290585	0.053255
H	-2.610784	-2.667905	-0.249678
C	-2.215168	-0.785824	-2.209886
H	-3.291813	-0.577648	-2.296918
H	-1.670617	-0.049818	-2.825599
H	1.528155	1.331544	-0.344727
H	0.639173	1.463117	1.178293
H	-2.784516	1.237252	-0.682997
H	-2.036061	0.796717	0.858630
H	-0.266655	-2.618563	-0.485836
H	-0.749808	2.636248	-0.375579
H	-0.448924	1.484384	-1.681599
H	0.070707	-1.008721	-1.613027
H	2.203466	-4.205376	-1.313475
B	-0.332782	-4.947743	-0.401518
H	-2.407003	-3.968698	-2.011037
H	-0.588259	-4.183562	2.261133
C	-1.594106	-5.109017	0.583896
C	-2.812212	-5.703802	0.184903
C	-3.909287	-5.801200	1.057967
C	-3.816761	-5.296672	2.363806
C	-2.614112	-4.708111	2.793068
C	-1.525810	-4.626309	1.913863

H	-2.899496	-6.096891	-0.829982
H	-4.836335	-6.270218	0.717801
H	-4.669686	-5.365313	3.043555
H	-2.527678	-4.319625	3.811444
C	1.116903	-5.337960	0.177285
C	1.281694	-6.180871	1.299490
C	2.554383	-6.518607	1.789620
C	3.705865	-6.009045	1.170113
C	3.573662	-5.168441	0.051282
C	2.297445	-4.848881	-0.434049
H	0.392788	-6.577378	1.794653
H	2.647133	-7.177239	2.657222
H	4.697135	-6.264678	1.552586
H	4.464079	-4.768291	-0.441191
C	-0.577716	-5.127376	-1.982588
C	0.297955	-5.869260	-2.807444
C	0.084039	-5.997574	-4.190354
C	-1.019636	-5.376035	-4.794140
C	-1.913231	-4.636982	-3.999963
C	-1.691385	-4.526460	-2.619705
H	1.164996	-6.353243	-2.353411
H	0.780269	-6.582808	-4.796862
H	-1.186351	-5.470188	-5.870043
H	-2.783226	-4.156046	-4.455604
H	-0.179765	-3.481021	-0.323880

**[TMPH]<sup>+</sup>[HB(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>]<sup>-</sup>**

C	0.489783	0.947834	-0.808414
C	-0.911333	0.602535	-0.279514
C	-1.176293	-0.919076	-0.355225
N	0.157537	-1.666466	-0.049381
C	1.250576	-0.977789	0.783692
C	1.602153	0.384204	0.110130
H	2.824205	-2.075234	-0.267592
H	1.580850	-0.403621	2.826427
C	0.747658	-0.797585	2.226106
H	-0.079413	-0.079773	2.290346
H	0.429349	-1.753096	2.661329
C	2.454721	-1.935600	0.758767
H	3.265777	-1.494597	1.356710
H	2.193350	-2.914261	1.184490

H	-1.698942	-2.414405	-1.859215
H	-1.917493	-1.202020	1.688566
C	-2.229624	-1.395808	0.653088
H	-3.164994	-0.848433	0.464511
H	-2.425181	-2.469498	0.521428
C	-1.582929	-1.328162	-1.782507
H	-2.547667	-0.855120	-2.015576
H	-0.841112	-0.989020	-2.522107
H	2.530689	0.277008	-0.471425
H	1.813786	1.103235	0.916120
H	-1.687254	1.101198	-0.879322
H	-1.024658	0.966161	0.753360
H	-0.080239	-2.573200	0.390571
H	0.609181	2.036836	-0.902596
H	0.600900	0.532270	-1.823586
H	0.576866	-1.950688	-0.947742
F	1.006847	-3.228973	-2.239801
B	-0.686911	-5.106512	-0.691180
F	-3.349974	-4.115514	-1.289381
F	0.001113	-3.878430	1.841048
C	-1.135474	-5.706347	0.776798
C	-1.879358	-6.874614	1.005878
C	-2.267305	-7.302576	2.286693
C	-1.890227	-6.557784	3.413515
C	-1.128370	-5.394632	3.240909
C	-0.776169	-5.023569	1.939886
F	-2.257812	-7.660621	-0.027047
F	-2.989409	-8.428049	2.450012
F	-2.253307	-6.954659	4.647392
F	-0.746741	-4.660111	4.309102
C	0.935408	-5.260513	-0.942055
C	1.721271	-6.307955	-0.430664
C	3.117738	-6.367085	-0.561035
C	3.793520	-5.343711	-1.242324
C	3.052441	-4.296515	-1.800989
C	1.661024	-4.301189	-1.652066
F	1.138123	-7.332786	0.229728
F	3.820722	-7.389224	-0.037188
F	5.134270	-5.366520	-1.356635
F	3.681287	-3.267743	-2.418448
C	-1.614971	-5.641353	-1.927322

C	-1.260452	-6.657231	-2.826185
C	-2.086618	-7.079563	-3.879050
C	-3.343957	-6.483546	-4.047415
C	-3.752641	-5.475985	-3.163176
C	-2.888517	-5.091874	-2.129189
F	-0.071258	-7.297030	-2.700055
F	-1.693957	-8.056702	-4.722017
F	-4.153147	-6.874596	-5.050937
F	-4.964118	-4.898186	-3.314259
H	-0.905337	-3.906295	-0.618195

**[btamH]<sup>+</sup>[ B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>]<sup>-</sup>**

C	2.511705	-4.043116	-2.387423
C	1.161819	-4.129633	-2.024521
H	-0.747873	-1.345993	2.332347
N	-0.039022	-1.785469	-0.205891
C	1.428285	-1.499729	0.075756
F	1.296543	-6.482002	0.715375
F	-0.717113	-4.328205	4.260738
C	0.661849	-4.920058	-0.980673
F	-2.906189	-7.224226	0.153551
F	-3.587295	-7.781615	2.681375
F	-2.525277	-6.357204	4.777648
C	1.641655	-5.661084	-0.299861
C	3.011692	-5.601766	-0.608316
C	3.451891	-4.787439	-1.661701
F	-1.355135	-9.103774	-3.606636
C	-2.623204	-7.194499	-4.250858
C	-3.016213	-5.872537	-4.004271
C	-2.510704	-5.207135	-2.876040
F	-0.399345	-7.768171	-1.431594
F	-3.096446	-7.852207	-5.327246
F	-3.869216	-5.258073	-4.852427
H	-1.391727	-3.841002	-0.804657
F	3.909572	-6.323658	0.088202
F	4.757812	-4.722828	-1.976231
F	2.915811	-3.245617	-3.402091
C	-1.625166	-5.801534	-1.968820
H	-0.237492	-2.694467	0.245397
C	-1.256575	-7.121714	-2.261943
C	-1.734172	-7.830680	-3.370817

H	-0.158795	-1.976370	-1.210670
F	0.299902	-3.322025	-2.739693
B	-0.973559	-4.981134	-0.715634
F	-2.928771	-3.921362	-2.699455
F	0.026416	-3.774416	1.744661
C	-1.395348	-5.474723	0.800071
C	-2.314140	-6.488608	1.121455
C	-2.698712	-6.798916	2.438732
C	-2.160276	-6.078844	3.512537
C	-1.242519	-5.053430	3.249294
C	-0.895398	-4.801227	1.920042
C	-1.137202	-0.801366	0.255020
C	-1.141220	0.429836	-0.661757
H	-2.008657	1.050652	-0.392408
H	-0.231467	1.032260	-0.556055
H	-1.251411	0.131476	-1.716136
C	-2.463718	-1.573113	0.124272
H	-2.630039	-1.928395	-0.902682
H	-3.283589	-0.895733	0.405064
H	-2.482012	-2.448086	0.790014
C	-0.865361	-0.438515	1.720767
H	0.030995	0.190545	1.822362
H	-1.724592	0.130111	2.103712
H	1.932099	-2.435577	-0.199413
H	1.515061	-1.365292	1.158737
H	2.390150	0.844160	1.079359
C	1.964117	-0.321657	-0.693786
C	2.007835	-0.357360	-2.100539
C	2.478100	0.752271	-2.815339
C	2.917529	1.898494	-2.131986
C	2.892088	1.930863	-0.728828
C	2.414519	0.822920	-0.012848
H	1.682403	-1.248151	-2.637249
H	2.509771	0.717848	-3.905516
H	3.285856	2.760201	-2.691375
H	3.241757	2.815026	-0.193066
<b>[LutH]<sup>+</sup>[HB(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>]<sup>-</sup></b>			
F	-2.042813	-7.391222	0.124354
F	-3.075911	-8.000632	2.543332
F	-2.750795	-6.287192	4.666942

F	-1.364416	-3.930004	4.320221
C	1.075589	-5.194890	-0.654704
C	1.667008	-6.367055	-0.156215
C	-1.787613	-6.554656	-3.988049
C	3.051124	-6.599716	-0.159504
C	3.912566	-5.628410	-0.690843
C	3.367032	-4.457063	-1.228997
C	-2.403794	-6.844669	2.373637
C	-3.133830	-6.169568	-4.006765
C	-3.642639	-5.402028	-2.949759
C	-2.786245	-5.044113	-1.901615
F	-1.292417	-7.293856	-5.001692
C	-2.239291	-5.974976	3.460924
C	-1.533494	-4.778368	3.281893
C	1.977137	-4.289026	-1.221507
C	-1.015428	-4.486122	2.013460
F	-3.931804	-6.528423	-5.030854
F	-4.939078	-5.023937	-2.954732
H	-0.646286	-3.641589	-0.609213
C	-1.428552	-5.393686	-1.835918
F	0.892741	-7.349397	0.357871
F	3.565283	-7.739118	0.343033
F	5.245212	-5.818583	-0.683143
C	-1.860793	-6.500915	1.126288
F	4.177707	-3.484816	-1.713860
C	-0.969868	-6.166794	-2.912880
F	0.318577	-6.586799	-2.968190
F	1.520234	-3.122854	-1.784104
B	-0.531839	-4.872128	-0.565555
F	-3.342943	-4.310600	-0.891213
F	-0.334629	-3.294488	1.910053
C	-1.154888	-5.310713	0.892267
C	0.090665	1.400949	0.077566
C	-1.031403	0.798385	-0.509520
C	-1.076902	-0.592516	-0.640631
N	-0.010773	-1.308799	-0.188184
C	1.106518	-0.778735	0.376841
C	1.160721	0.613107	0.520711
H	-1.873841	1.389740	-0.864520
H	-2.651721	-2.056233	-0.515655
H	2.882387	-1.875862	-0.089834

H	2.042908	1.060176	0.976333
H	-0.093751	-2.352887	-0.285798
H	0.130807	2.485532	0.188153
C	-2.215273	-1.360789	-1.245912
H	-2.990454	-0.670024	-1.601858
H	-1.862142	-1.980242	-2.084643
C	2.219303	-1.704326	0.772227
H	2.808909	-1.256598	1.583605
H	1.828075	-2.677108	1.093232

[TMPH]<sup>+</sup>[B(C<sub>6</sub>F<sub>2</sub>H<sub>3</sub>)<sub>3</sub>]<sup>-</sup>

C	1.380957	-0.027863	-1.540076
C	-0.116128	0.233050	-1.764009
C	-0.953393	-1.036101	-1.470652
N	-0.238976	-1.831997	-0.337935
C	0.577932	-1.056903	0.716204
C	1.675297	-0.239614	-0.037414
H	1.892370	-2.762564	1.071500
H	0.199808	0.251298	2.376901
C	-0.369369	-0.164546	1.532606
H	-0.766392	0.675725	0.949729
H	-1.207014	-0.750720	1.941833
C	1.226175	-2.100209	1.637116
H	1.823414	-1.562222	2.388767
H	0.472076	-2.717527	2.144536
H	-1.460344	-2.912889	-2.481985
H	-2.422604	-0.100120	-0.125351
C	-2.388484	-0.702400	-1.041577
H	-2.852208	-0.116516	-1.849492
H	-2.985281	-1.613356	-0.903028
C	-0.979271	-1.952652	-2.706267
H	-1.559146	-1.448325	-3.492694
H	0.036501	-2.134218	-3.087255
H	2.644223	-0.749073	0.072401
H	1.763770	0.738101	0.461473
H	-0.316429	0.527391	-2.805088
H	-0.446069	1.068481	-1.126099
H	-0.910194	-2.463895	0.135913
H	1.980303	0.814353	-1.915340
H	1.695292	-0.916632	-2.110580
H	0.423356	-2.513015	-0.770838



H	0.470404	-4.093530	-2.140292
B	-0.606601	-5.142588	0.336596
H	-3.053357	-3.767869	0.352206
H	-0.333708	-5.552103	3.128605
C	-0.777186	-6.506389	1.218048
C	-1.084354	-7.747003	0.617063
C	-1.158276	-8.905001	1.394271
C	-0.937403	-8.905065	2.776492
C	-0.637494	-7.669358	3.357068
C	-0.558041	-6.487721	2.613705
H	-1.278834	-7.817599	-0.453757
F	-1.457924	-10.090030	0.794589
H	-1.002648	-9.816500	3.367489
F	-0.421630	-7.623963	4.701682
C	0.943950	-4.958582	-0.194029
C	2.037906	-5.302985	0.632687
C	3.336721	-4.920053	0.288708
C	3.637873	-4.170221	-0.860303
C	2.557376	-3.878701	-1.693149
C	1.247606	-4.273041	-1.399548
H	1.872810	-5.849602	1.561758
F	4.365881	-5.252247	1.108390
H	4.655321	-3.867513	-1.099087
F	2.779215	-3.147647	-2.829575
C	-1.723225	-5.008323	-0.845456
C	-1.593355	-5.626674	-2.111675
C	-2.579331	-5.456963	-3.088757
C	-3.722919	-4.674567	-2.883132
C	-3.846493	-4.083283	-1.623036
C	-2.886895	-4.237811	-0.619541
H	-0.715650	-6.228693	-2.349495
F	-2.424459	-6.052699	-4.299656
H	-4.473166	-4.539636	-3.659566
F	-4.927252	-3.284985	-1.383770
H	-0.797048	-4.176257	1.116960

**[TMPH]<sup>+</sup>[HB(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>]<sup>-</sup>**

C	1.193713	0.313622	-1.455114
C	-0.342182	0.361487	-1.470578
C	-0.943997	-1.051003	-1.262953
N	0.017445	-1.856130	-0.360849

C	0.860787	-1.123308	0.687418
C	1.716173	-0.039838	-0.043267
H	2.406575	-2.670273	0.591690
H	0.547261	-0.147407	2.577729
C	-0.072313	-0.517949	1.747561
H	-0.654030	0.327752	1.358837
H	-0.759171	-1.281862	2.142720
C	1.757243	-2.189711	1.336375
H	2.389880	-1.695025	2.089217
H	1.156271	-2.969139	1.824073
H	-1.366975	-2.847574	-2.440063
H	-2.329328	-0.512853	0.359701
C	-2.336281	-1.006956	-0.619785
H	-3.001814	-0.437743	-1.286518
H	-2.741898	-2.022949	-0.517890
C	-1.024382	-1.815233	-2.596742
H	-1.745990	-1.303037	-3.249503
H	-0.046889	-1.830069	-3.104684
H	2.758495	-0.385876	-0.116711
H	1.720404	0.867677	0.580945
H	-0.718149	0.750981	-2.428675
H	-0.695873	1.047059	-0.683554
H	-0.496620	-2.658405	0.115475
H	1.617632	1.276739	-1.775611
H	1.540705	-0.441347	-2.181525
H	0.685285	-2.376690	-0.959080
H	0.575895	-4.044619	-2.310628
B	-0.662857	-5.011910	0.111326
H	-3.297458	-4.121693	0.098123
H	-0.647476	-4.928418	2.943874
C	-0.928279	-6.188047	1.208606
C	-1.200812	-7.516421	0.808518
C	-1.374008	-8.551642	1.739971
C	-1.279609	-8.284318	3.116417
C	-1.014525	-6.974140	3.544955
C	-0.845317	-5.949161	2.598487
H	-1.287103	-7.736229	-0.259582
H	-1.586012	-9.567865	1.395262
H	-1.416586	-9.086985	3.845755
H	-0.945317	-6.751488	4.613920
C	0.912760	-4.953540	-0.371231

C	1.952134	-5.407528	0.475504
C	3.309553	-5.213478	0.173313
C	3.688755	-4.549468	-1.006340
C	2.688800	-4.121196	-1.894040
C	1.333639	-4.338534	-1.580176
H	1.679515	-5.912245	1.405222
H	4.077298	-5.574574	0.863353
H	4.744275	-4.391047	-1.240431
H	2.962151	-3.640693	-2.838608
C	-1.754823	-5.044479	-1.101045
C	-1.511271	-5.613621	-2.372989
C	-2.485349	-5.625382	-3.387610
C	-3.752825	-5.069686	-3.154817
C	-4.039928	-4.526170	-1.890755
C	-3.055790	-4.525878	-0.890572
H	-0.530212	-6.050500	-2.575874
H	-2.254645	-6.070183	-4.359830
H	-4.510815	-5.070200	-3.942112
H	-5.030597	-4.109681	-1.686568
H	-0.877154	-3.924081	0.757759

**TS1b**

C	-0.854464	2.425328	-1.652180
C	-2.141433	2.077690	-0.866728
C	-2.050774	0.766989	-0.028791
N	-0.945548	-0.122278	-0.609868
C	0.482237	0.446681	-0.794547
C	0.403568	1.988349	-0.886066
H	0.451610	0.233708	-2.976377
H	2.370051	0.337695	0.255886
C	1.341024	-0.027981	0.387338
H	0.957212	0.350643	1.345315
H	1.373819	-1.127722	0.425176
C	1.025745	-0.131237	-2.113926
H	2.076101	0.174310	-2.225721
H	0.983058	-1.223819	-2.128784
H	-3.341770	-0.908843	0.531298
H	-0.834899	1.634581	1.597475
C	-1.739465	1.029631	1.456061
H	-2.585798	1.576415	1.897653
H	-1.630052	0.077588	1.996377

C	-3.360744	-0.035613	-0.133180
H	-4.189515	0.615495	0.183085
H	-3.537070	-0.369090	-1.164706
H	1.314596	2.336322	-1.395996
H	0.407153	2.439174	0.118920
H	-2.981322	2.000113	-1.573508
H	-2.383857	2.895017	-0.169666
H	-0.884702	-0.944879	0.000793
H	-0.826585	3.505672	-1.856405
H	-0.874469	1.916846	-2.629128
H	-1.301787	-0.561916	-1.525578
F	1.081086	-3.530884	-2.704398
B	-0.970494	-4.596748	-0.900132
F	-3.394846	-4.999482	-2.441299
F	-1.218503	-2.393524	1.061222
C	-2.121375	-4.462579	0.223114
C	-3.116000	-5.436317	0.462094
C	-4.132387	-5.287625	1.420998
C	-4.179971	-4.134992	2.214870
C	-3.182706	-3.163771	2.057929
C	-2.193666	-3.363691	1.094398
F	-3.120351	-6.605522	-0.206028
F	-5.058630	-6.246070	1.589903
F	-5.149549	-3.971107	3.126931
F	-3.193254	-2.046175	2.818923
C	0.516729	-4.153114	-0.470542
C	1.012599	-4.269271	0.841636
C	2.298034	-3.854896	1.221684
C	3.157137	-3.308850	0.257999
C	2.721533	-3.202406	-1.069720
C	1.437085	-3.647529	-1.405120
F	0.247998	-4.809272	1.819024
F	2.716433	-3.981476	2.495055
F	4.384789	-2.886944	0.603811
F	3.529626	-2.659062	-2.000610
C	-1.133034	-5.665730	-2.063542
C	-0.096030	-6.509741	-2.506595
C	-0.234761	-7.390317	-3.587203
C	-1.452818	-7.443513	-4.278960
C	-2.517430	-6.626382	-3.875653
C	-2.337718	-5.766591	-2.789202

F	1.100503	-6.531589	-1.871108
F	0.782147	-8.190837	-3.961269
F	-1.600962	-8.282107	-5.317103
F	-3.688442	-6.675070	-4.536167
H	-1.385680	-3.291377	-1.908862
C	-1.651905	-2.629201	-2.958161
O	-1.882443	-1.416320	-2.709859
O	-1.626439	-3.311328	-3.965169

**TS2b**

C	-0.900867	-5.673879	-1.970451
C	-1.122953	1.911900	-2.417611
C	-1.805447	1.349112	-1.159391
N	-1.236758	-0.028953	-0.823952
C	0.116503	-0.155974	-0.174629
C	0.258178	-6.368216	-2.380915
H	-1.524276	-3.146561	-2.026937
F	1.391722	-6.297819	-1.645039
F	1.424195	-7.835960	-3.860348
F	-0.828293	-8.089772	-5.399024
F	-3.138998	-6.793290	-4.687635
C	-1.595346	-2.620170	-3.052204
O	-1.490629	-1.333473	-2.982699
O	-1.743039	-3.328870	-4.040401
H	-3.810704	0.694394	-0.556094
H	-0.570690	2.499446	0.231395
C	-1.633700	2.289256	0.041377
H	-2.136399	3.243614	-0.174937
H	-2.085669	1.861761	0.952076
C	-3.295538	1.084109	-1.451258
H	-3.784342	2.023536	-1.746790
H	-3.394345	0.355457	-2.269253
C	0.300724	-7.179068	-3.517579
C	-0.855186	-7.317894	-4.303367
H	-1.150250	1.171117	-3.228327
H	-1.677921	2.808407	-2.734676
H	-1.894254	-0.466017	-0.170384
C	-2.034577	-6.658389	-3.936086
C	-2.040744	-5.864182	-2.784658
H	-1.308704	-0.698138	-1.784501
F	1.147223	-3.560700	-2.487491

B	-0.931586	-4.715869	-0.728538
F	-3.207321	-5.267543	-2.471549
F	-1.946242	-2.334305	0.667862
C	-2.243898	-4.654739	0.170240
C	-3.057773	-5.782505	0.404588
C	-4.230939	-5.734868	1.171885
C	-4.635621	-4.518953	1.741527
C	-3.851955	-3.371363	1.549546
C	-2.682905	-3.476684	0.794229
F	-2.717618	-6.986685	-0.096104
F	-4.969280	-6.839374	1.369391
F	-5.758264	-4.452705	2.470318
F	-4.222521	-2.195746	2.093493
C	0.378377	-3.951362	-0.251477
C	0.674951	-3.731016	1.111315
C	1.815568	-3.044842	1.550254
C	2.735321	-2.565652	0.606477
C	2.507505	-2.788757	-0.758372
C	1.337199	-3.444760	-1.158344
F	-0.143547	-4.204420	2.077293
F	2.043745	-2.852194	2.862195
F	3.831347	-1.907810	1.007777
F	3.401393	-2.357336	-1.660991
H	-0.081741	2.197083	-2.225012
H	0.082465	0.354100	0.798081
H	0.799903	-0.838423	-2.751400
H	0.223855	-1.232327	0.012849
C	1.266440	0.359220	-1.005508
C	2.153391	1.299165	-0.452028
C	3.247463	1.768671	-1.194914
C	3.455480	1.302154	-2.501654
C	2.572927	0.360664	-3.056447
C	1.487299	-0.116408	-2.312123
H	1.986781	1.661128	0.565925
H	3.931673	2.496420	-0.754624
H	4.303739	1.667122	-3.083904
H	2.734522	-0.012626	-4.069058

**TS3b**

C	-3.573345	-2.953689	1.534440
C	-2.472554	-3.215984	0.717177

F	-2.932906	-6.742155	0.012231
F	-5.073592	-6.280114	1.583677
F	-5.527112	-3.777439	2.613273
F	-3.782108	-1.723236	2.052327
C	0.460309	-4.051150	-0.360585
F	1.231734	-6.537268	-1.612328
F	1.096079	-8.254203	-3.685841
F	-1.197821	-8.447645	-5.175037
F	-3.380300	-6.905932	-4.549869
C	0.796855	-3.796976	0.983675
C	1.973892	-3.140529	1.373839
C	2.889659	-2.742153	0.394515
C	2.628042	-3.022326	-0.951957
H	-1.371314	-3.269327	-1.945661
C	-1.673604	-2.634987	-2.903785
O	-1.903079	-1.404091	-2.643931
O	-1.709308	-3.269140	-3.950218
C	1.431672	-3.655959	-1.302146
F	-0.026159	-4.178905	1.984342
F	2.225613	-2.879764	2.670379
F	3.996106	-2.055349	0.734893
C	0.035430	-7.479379	-3.389062
C	-2.252455	-6.796979	-3.827223
F	3.508512	-2.614524	-1.892905
C	-2.171373	-5.911352	-2.747137
C	-1.006814	-5.750920	-1.965002
C	-1.139263	-7.584825	-4.149222
C	0.080117	-6.573867	-2.324207
F	1.209647	-3.839794	-2.621815
B	-0.941906	-4.678488	-0.811608
F	-3.279207	-5.196990	-2.468608
F	-1.621853	-2.184233	0.482370
C	-2.203907	-4.465551	0.137236
C	-3.115103	-5.485807	0.468339
C	-4.230620	-5.273866	1.292632
C	-4.464043	-3.997938	1.824977
C	1.756337	0.671268	0.507222
C	0.410326	0.834167	0.859203
C	-0.588493	0.445512	-0.042879
N	-0.215366	-0.081838	-1.236691
C	1.077703	-0.200156	-1.643970

C	2.094641	0.172848	-0.759287
H	0.122889	1.244306	1.826770
H	-2.646880	0.036822	-0.521286
H	0.982325	0.101925	-3.757261
H	3.132618	0.036469	-1.056194
H	2.543627	0.935115	1.214867
C	-2.063257	0.607956	0.211372
H	-2.324765	0.261359	1.219066
H	-2.332980	1.674207	0.129238
C	1.313744	-0.676124	-3.050178
H	2.377708	-0.877437	-3.211524
H	0.738423	-1.580217	-3.279838
H	-0.987226	-0.607242	-1.847555

#### **TS4b**

C	-1.105681	1.763700	-1.660537
C	-2.480512	1.459588	-1.014615
C	-2.442432	0.293960	0.022139
N	-1.187205	-0.539401	-0.269850
C	0.204250	0.135945	-0.201421
C	0.037986	1.612320	-0.643262
H	0.722280	-0.553077	-2.216210
H	1.767711	0.490204	1.222859
C	0.776024	0.013744	1.218204
H	0.151470	0.511035	1.968912
H	0.901209	-1.038247	1.509243
C	1.090864	-0.646859	-1.184754
H	2.113186	-0.245023	-1.136862
H	1.123921	-1.714981	-0.928898
H	-3.594242	-1.479543	0.582029
H	-1.662143	1.598714	1.613981
C	-2.401020	0.799261	1.473859
H	-3.390808	1.213171	1.717373
H	-2.184712	-0.018425	2.175988
C	-3.630378	-0.666319	-0.156026
H	-4.561952	-0.099489	-0.010681
H	-3.635075	-1.095316	-1.167276
H	0.993907	1.942652	-1.076803
H	-0.155987	2.252339	0.232425
H	-3.202435	1.219373	-1.808909
H	-2.853382	2.356582	-0.495779



H	-1.196590	-1.380329	0.342889
H	-1.114287	2.781248	-2.077660
H	-0.936395	1.073997	-2.501870
H	-1.319541	-0.919557	-1.232881
H	0.491970	-3.652685	-3.389309
B	-1.154493	-4.364958	-1.196744
H	-3.580441	-4.864707	-2.637155
H	-0.054871	-2.983422	1.093239
C	-1.819044	-3.954180	0.246325
C	-3.159871	-4.288733	0.545991
C	-3.746776	-3.879751	1.745851
C	-3.070923	-3.108991	2.703680
C	-1.744661	-2.796266	2.406522
C	-1.115082	-3.200712	1.223263
H	-3.747329	-4.886919	-0.149755
F	-5.031746	-4.222165	2.004842
H	-3.547653	-2.791979	3.628876
F	-1.046580	-2.017578	3.287225
C	0.465580	-4.279584	-1.297453
C	1.309654	-4.644517	-0.221884
C	2.701217	-4.587907	-0.361516
C	3.324196	-4.180726	-1.543844
C	2.477739	-3.851768	-2.609319
C	1.086075	-3.897852	-2.509852
H	0.895120	-4.983861	0.727389
F	3.484544	-4.931981	0.694796
H	4.407520	-4.136864	-1.636787
F	3.045622	-3.463258	-3.781387
C	-1.758150	-5.739248	-1.810410
C	-1.055944	-6.954860	-1.653265
C	-1.609569	-8.148507	-2.122098
C	-2.852181	-8.205440	-2.762378
C	-3.529200	-6.992037	-2.917749
C	-3.011897	-5.777113	-2.460393
H	-0.077179	-6.977135	-1.173238
F	-0.919799	-9.308969	-1.956795
H	-3.265591	-9.143135	-3.128498
F	-4.737847	-7.003583	-3.542102
H	-1.602397	-3.417279	-2.010681
C	-1.860031	-2.499451	-3.327769
O	-1.786453	-1.361328	-2.902480

O	-2.024327	-3.263437	-4.226929
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**TS5b**

C	-1.279775	1.749517	-1.717612
C	-2.649999	1.349055	-1.118632
C	-2.579262	0.178945	-0.088009
N	-1.273671	-0.590963	-0.334433
C	0.078667	0.164731	-0.254432
C	-0.159199	1.636712	-0.673076
H	0.654893	-0.444988	-2.275968
H	1.594953	0.630760	1.189245
C	0.651394	0.065125	1.166849
H	-0.022939	0.491940	1.919412
H	0.870259	-0.977455	1.433178
C	1.011317	-0.556927	-1.241935
H	2.017135	-0.118707	-1.165993
H	1.081171	-1.631579	-1.018997
H	-3.673632	-1.644653	0.430222
H	-1.882415	1.472228	1.554005
C	-2.610330	0.671977	1.367123
H	-3.613321	1.077724	1.566839
H	-2.430406	-0.163198	2.060850
C	-3.716249	-0.832028	-0.307692
H	-4.674555	-0.301675	-0.199789
H	-3.664966	-1.260298	-1.318259
H	0.789946	2.025615	-1.072190
H	-0.410280	2.247470	0.209125
H	-3.329359	1.072285	-1.937853
H	-3.095926	2.215105	-0.604467
H	-1.241653	-1.416363	0.302220
H	-1.336285	2.776606	-2.107404
H	-1.047661	1.094972	-2.570893
H	-1.360942	-0.991633	-1.290442
H	0.762937	-3.489750	-3.218051
B	-1.025177	-4.264621	-1.150842
H	-3.524247	-4.531359	-2.462832
H	0.184889	-2.981417	1.086981
C	-1.630792	-3.877427	0.329865
C	-2.963151	-4.184723	0.704259
C	-3.505497	-3.797634	1.939417
C	-2.730064	-3.075775	2.865232

C	-1.397907	-2.774988	2.544147
C	-0.868722	-3.176393	1.301333
H	-3.581801	-4.751851	0.006452
H	-4.538376	-4.059353	2.184660
H	-3.150168	-2.777696	3.828759
H	-0.764771	-2.245935	3.262454
C	0.601042	-4.319301	-1.224185
C	1.375354	-4.878443	-0.177848
C	2.774681	-4.982905	-0.251499
C	3.454173	-4.526724	-1.391555
C	2.715522	-3.984228	-2.455946
C	1.317536	-3.892239	-2.367440
H	0.864291	-5.239910	0.718412
H	3.333314	-5.422229	0.579783
H	4.542791	-4.600646	-1.453992
H	3.228918	-3.639479	-3.358010
C	-1.745629	-5.571615	-1.796544
C	-1.140722	-6.847932	-1.743417
C	-1.783221	-7.995198	-2.235730
C	-3.061887	-7.897244	-2.807413
C	-3.685662	-6.641406	-2.882706
C	-3.029712	-5.504672	-2.385315
H	-0.141130	-6.938640	-1.310555
H	-1.284069	-8.966663	-2.178235
H	-3.563276	-8.787005	-3.196975
H	-4.676418	-6.547920	-3.336490
H	-1.394154	-3.272389	-1.926964
C	-1.674063	-2.429724	-3.455680
O	-1.777981	-1.288698	-3.062953
O	-1.653328	-3.282925	-4.277635