Supplementary Material for PCCP

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Silyloxyazadienes: one intermediate and two competitive pericyclic reactions.

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The two competing mechanisms in the reaction of 3-trialkylsilyloxy-2-aza-1,3 dienes to form β-lactams through a [2+2] electrocyclic ring closure or tetrahydrooxazin-2-ones via a [4+2] hetero Diels-Alder reaction were studied using Density Functional computations. Although the [2+2] and [4+2] mechanisms are typical of dienes, their competition, starting from the same diene intermediate, has not yet been observed. The competition is governed by a delicate interplay between temperature and substituents at the diene and dienophile respectively. Clearly, entropy tends to favor the [4+2] hetero Diels-Alder at low temperatures and the [2+2] electrocyclic ring closure at high temperatures, but simple substituent modifications at the diene and dienophile, can make the [4+2] competitive at high temperatures and sometimes even trasform the [4+2] concerted mechanism into a two-step Mukaiyama-type process. A study of the global electrophilicity values showed that charge transfer in the hetero Diels-Alder transition states is driven by chemical hardness rather than by chemical potential.

Optimized geometries

DFT B3LYP 6-311+G(d,p)

Reactants

Acetone (2a)

E	-193.21818
E_0	-193.13506
$G_{198.15}$	-193.15240
$G_{298.15}$	-193.16358
$G_{398.15}$	-193.17577

C	-0.010956	-0.018487	0.000687
C	-0.000076	0.001088	1.517785
C	1.361758	0.018307	2.186430
O	-1.026075	0.003177	2.162209
H	-1.031777	0.075649	-0.367107
H	0.607643	0.789426	-0.401997
H	0.419626	-0.958975	-0.359284
H	1.249824	-0.082666	3.265109
H	1.994995	-0.785559	1.798913
H	1.871033	0.961555	1.961581

Acetone + BF_3 (2a + BF_3)

E	-517.89931
E_0	-517.80148
$G_{198.15}$	-517.82185
$G_{298.15}$	-517.83587
$G_{398.15}$	-517.85170

C	-0.002768	0.000191	-0.004499
O	0.008024	0.000021	1.233095
B	1.380673	-0.000562	2.224954
F	2.035627	1.151062	1.865171
F	2.034736	-1.152653	1.865057
F	0.834986	-0.000413	3.462774
C	-1.327599	0.000700	-0.695202
H	-1.395128	-0.876848	-1.346945
H	-2.144000	0.000875	0.024116
H	-1.394564	0.878444	-1.346738
C	1.249918	-0.000103	-0.822213
H	1.850187	0.873301	-0.553094
H	1.849610	-0.873985	-0.553356
H	1.035759	0.000125	-1.889526

Acetaldehyde (2b)

E	-153.88215
E_0	-153.82697
$G_{198.15}$	-153.84231

$G_{298.15}$	-153.85194
$G_{398.15}$	-153.86228

C	2.024372	-0.146607	-0.331837
O	1.035038	-0.032236	-1.011867
C	2.026798	-0.523312	1.124238
H	2.518079	0.265633	1.704413
H	1.011583	-0.679433	1.488789
H	2.621003	-1.433131	1.264257
H	3.029088	0.030351	-0.775031

Acetaldheyde + BF_3 (2b + BF_3)

E	-478.55847
E_0	-478.48881
$G_{198.15}$	-478.50870
$G_{298.15}$	-478.52210
$G_{398.15}$	-478.53702

C	1.972396	-0.338008	-0.336701
O	1.106517	0.300294	-0.923361
C	2.012680	-0.668451	1.109129
H	1.149267	-0.300542	1.654830
H	2.097923	-1.756830	1.208078
H	2.936947	-0.250197	1.525575
H	2.807738	-0.700628	-0.953814
B	-0.333960	1.004537	-0.186654
F	0.207351	1.849702	0.736528
F	-0.953178	-0.094264	0.332087
F	-0.914039	1.573653	-1.259360

Formaldehyde (2c)

E	-114.54176
E_0	-114.51526
$G_{198.15}$	-114.52862
$G_{298.15}$	-114.53692
$G_{398.15}$	-114.54567

O	-1.431455	-1.783127	3.055482
C	-2.388836	-2.458929	3.322440
H	-3.012584	-2.930818	2.537582
H	-2.701677	-2.648209	4.368409

Formaldehyde + BF_3 (2c + BF_3)

E	-439.21643
E_0	-439.17485
$G_{198.15}$	-439.19351
$G_{298.15}$	-439.20580
$G_{398.15}$	-439.21935

C	-0.059220	0.093130	1.045719
H	0.093416	-0.135666	-0.016664
H	0.596527	0.821718	1.539898
O	-0.949855	-0.462805	1.656484
B	-1.262085	-0.115597	3.468427
F	-2.517538	0.350933	3.382952
F	-0.283626	0.795070	3.703895
F	-1.072215	-1.350357	3.958513

Diene Reactants

Reactions A and D Uncalalyzed (1a)

E	-1118.34252
E_0	-1118.00139
$G_{198.15}$	-1118.03157
$G_{298.15}$	-1118.05494
$G_{398.15}$	-1118.08286

C	-2.053849	1.482432	0.209966
C	-1.337333	0.736274	-0.740347
C	-1.804208	0.691224	-2.062184
C	-2.962910	1.370143	-2.428717
C	-3.668132	2.104151	-1.476932
C	-3.209540	2.158066	-0.157451
C	-0.118105	0.003534	-0.392207
N	0.337421	-0.075133	0.802099
C	1.553620	-0.709795	1.060939
C	2.661668	-0.541628	0.294305
C	4.013674	-1.054625	0.482263
C	5.019087	-0.598749	-0.395607
C	6.332147	-1.040912	-0.290992
C	6.685795	-1.957464	0.699282
C	5.705595	-2.422961	1.575535
C	4.389064	-1.984430	1.473440
O	1.563987	-1.442017	2.196203
Si	0.425729	-1.534049	3.466871
C	-1.212938	-2.219336	2.857428
C	1.245761	-2.749193	4.637579
C	0.231765	0.147473	4.277646
H	0.394653	-0.496502	-1.223015
H	2.535664	0.117601	-0.556590

H	0.627455	-2.911871	5.526137
H	1.399272	-3.719418	4.156605
H	2.219891	-2.381189	4.971329
H	-1.876032	-2.422778	3.705095
H	-1.720607	-1.520568	2.189807
H	-1.067449	-3.160384	2.318674
H	-0.435143	0.083463	5.143831
H	1.196936	0.525126	4.627477
H	-0.183756	0.876753	3.579324
H	4.756771	0.115720	-1.169598
H	7.081181	-0.669891	-0.982191
H	7.709058	-2.305205	0.785010
H	5.968108	-3.139090	2.347078
H	3.640998	-2.357982	2.156441
H	-1.254172	0.119206	-2.802583
H	-3.314336	1.327537	-3.453237
H	-4.569851	2.635415	-1.759862
H	-3.756353	2.733128	0.581325
H	-1.685568	1.523320	1.227474

Reactions A and D Catalyzed (1a + BF_3)

E	-1443.02247
E_0	-1442.66628
$G_{198.15}$	-1442.69855
$G_{298.15}$	-1442.72443
$G_{398.15}$	-1442.75565

C	0.054194	-0.211424	0.096752
C	0.079773	0.184156	1.450712
C	1.244107	0.794249	1.956010
C	2.329256	1.011025	1.117839
C	2.279744	0.636971	-0.226199
C	1.137556	0.023333	-0.738382
C	-1.126353	-0.132588	2.200160
N	-1.525874	0.222450	3.382722
C	-2.836795	-0.256486	3.776943
O	-2.871996	-1.057917	4.835876
Si	-1.871946	-2.061021	5.803924
C	-0.378142	-2.637760	4.825365
C	-3.915182	0.157741	3.080626
C	-5.328293	-0.157405	3.280109
C	-5.822436	-1.024224	4.273082
C	-7.187642	-1.268143	4.386749
C	-8.096200	-0.660207	3.521031
C	-7.623732	0.202973	2.533085
C	-6.260924	0.449663	2.416710
C	-3.000839	-3.503344	6.210521
C	-1.393983	-1.120285	7.344262
B	-0.807467	1.319964	4.411727
F	-1.727282	1.564140	5.403108
F	0.349537	0.711426	4.904187
F	-0.530405	2.434673	3.642437
H	-1.815340	-0.781052	1.661589
H	-3.707057	0.866062	2.287723
H	-0.895227	-1.790405	8.052725
H	-0.718013	-0.295671	7.113352
H	-2.277840	-0.705363	7.836008
H	-0.664153	-3.112199	3.881806
H	0.305672	-1.812849	4.617420
H	0.169702	-3.382921	5.412117
H	-2.481963	-4.223933	6.850961
H	-3.893956	-3.170233	6.746529
H	-3.323737	-4.029925	5.308150
H	-5.904683	1.127303	1.647403
H	-8.317655	0.686715	1.854556
H	-9.158437	-0.854239	3.616772
H	-7.545237	-1.938099	5.161204
H	-5.133092	-1.498058	4.955487
H	-0.831080	-0.698250	-0.298642
H	1.095359	-0.275906	-1.778825
H	3.132821	0.817761	-0.870431
H	3.222194	1.477523	1.516813
H	1.305342	1.082198	2.992860

Diene Reaction B Uncatalyzed (1b)

E	-1232.90075
E_0	-1232.52734
$G_{198.15}$	- 1232.55921
$G_{298.15}$	-1232.58437
$G_{398.15}$	-1232.61457

C	-1.755561	0.656323	-2.055011
C	-1.292233	0.699044	-0.735549
C	-2.025969	1.449846	0.204518
C	-3.173828	2.119752	-0.166344
C	-3.628521	2.064310	-1.495595
C	-2.912211	1.328124	-2.444142
C	-0.078636	-0.026407	-0.377415
N	0.375730	-0.098633	0.819569
C	1.593861	-0.727448	1.079413
O	1.606609	-1.458450	2.216581
Si	0.463149	-1.554197	3.480898
C	1.284812	-2.761989	4.658816
O	-4.765881	2.759085	-1.757206

C	-5.285776	2.753082	-3.082646
C	2.702639	-0.559943	0.313443
C	4.054215	-1.074817	0.500218
C	4.431854	-1.999090	1.495879
C	5.747906	-2.439723	1.596216
C	6.726444	-1.981962	0.714017
C	6.370849	-1.070684	-0.280471
C	5.058236	-0.626581	-0.383371
C	0.254159	0.126833	4.289344
C	-1.169282	-2.252216	2.868213
H	0.438955	-0.530666	-1.203096
H	2.577022	0.099242	-0.537587
H	0.663122	-2.926977	5.544625
H	1.447084	-3.732091	4.180410
H	2.254958	-2.387120	4.996587
H	-1.834063	-2.457036	3.714304
H	-1.678462	-1.558879	2.196166
H	-1.015606	-3.194139	2.333206
H	-0.415992	0.059229	5.152821
H	1.215384	0.511162	4.642828
H	-0.162910	0.852361	3.588117
H	4.794933	0.083854	-1.160817
H	7.118215	-0.705062	-0.976473
H	7.749352	-2.331141	0.798539
H	6.011385	-3.151416	2.371636
H	3.685561	-2.366538	2.184146
H	-1.203364	0.086072	-2.795252
H	-3.239986	1.272229	-3.473085
H	-3.743413	2.701186	0.548598
H	-1.670709	1.497005	1.226414
H	-6.184991	3.365337	-3.050033
H	-4.573690	3.189704	-3.790479
H	-5.547396	1.739086	-3.402106

Diene Reaction B Catalyzed (1b + BF_3)

E	-1557.57899
E_0	-1557.19056
$G_{198.15}$	- 1557.22449
$G_{298.15}$	-1557.25215
$G_{398.15}$	-1557.28564

C	-6.216652	0.482472	2.363635
C	-5.292739	-0.126777	3.226855
C	-5.810861	-0.988260	4.217001
C	-7.171232	-1.220287	4.324944
C	-8.073856	-0.602564	3.450093
C	-7.587385	0.256527	2.461695
C	-3.876541	0.173280	3.039958
C	-2.809440	-0.238503	3.755421
O	-2.868608	-1.023282	4.828965
Si	-1.894322	-2.048679	5.795967
C	-1.406881	-1.124400	7.343655
N	-1.491069	0.226680	3.376344
B	-0.769459	1.312635	4.413334
F	-0.476376	2.428204	3.649845
C	-1.083746	-0.126639	2.195281
C	0.128504	0.187390	1.453993
C	0.108734	-0.202437	0.098239
C	1.198631	0.027905	-0.729647
C	2.342268	0.631210	-0.208548
C	2.386087	0.999248	1.137274
C	1.294336	0.787012	1.968172
C	-0.404358	-2.650069	4.825482
C	-3.048416	-3.474342	6.192741
F	-1.690935	1.565332	5.401104
F	0.379259	0.691677	4.910709
H	-1.771303	-0.771383	1.650784
H	-3.653791	0.871339	2.241761
H	-0.922289	-1.805851	8.051143
H	-0.716632	-0.309747	7.119449
H	-2.285918	-0.697088	7.833467
H	-0.692471	-3.115647	3.878130
H	0.296409	-1.837595	4.624980
H	0.125063	-3.407494	5.413464
H	-2.543991	-4.205653	6.832624
H	-3.938586	-3.129382	6.726232
H	-3.375624	-3.992460	5.286984
H	-5.855834	1.156846	1.593604
H	-8.255913	0.753400	1.771488
O	-9.391549	-0.899845	3.641416
H	-7.563467	-1.880954	5.089107
H	-5.135329	-1.470211	4.907581
H	-0.777430	-0.681751	-0.304321
H	1.160302	-0.267076	-1.771494
H	3.200482	0.808344	-0.846941
H	3.279943	1.457553	1.543691
H	1.351683	1.070277	3.006493
C	-10.355479	-0.290591	2.793632
H	-11.322521	-0.665194	3.125094
H	-10.337748	0.800628	2.887957
H	-10.198881	-0.568820	1.745677

Diene Reaction C Uncatalyzed (1c)

E	-1322.91046

E_0	-1322.56689
$G_{198.15}$	-1322.59916
$G_{298.15}$	-1322.62453
$G_{398.15}$	-1322.65490

C	4.391251	-1.935039	1.504183
C	4.010166	-1.033567	0.484336
C	5.009544	-0.616888	-0.425593
C	6.315609	-1.063284	-0.331676
C	6.651617	-1.948672	0.691635
C	5.697393	-2.386154	1.608461
C	2.668243	-0.513522	0.299775
C	1.560430	-0.682497	1.074835
O	1.574156	-1.414086	2.200845
Si	0.422650	-1.543752	3.469403
C	0.214548	0.125761	4.296968
N	0.349771	-0.042029	0.815944
C	-0.122067	0.005572	-0.374007
C	-1.337124	0.739283	-0.728749
C	-2.035161	1.518452	0.208834
C	-3.186296	2.197061	-0.166238
C	-3.657485	2.111595	-1.479750
C	-2.970873	1.343852	-2.418453
C	-1.816450	0.662054	-2.044709
C	-1.199498	-2.232190	2.825039
C	1.253711	-2.770597	4.616483
H	0.373808	-0.526519	-1.195076
H	2.540489	0.146154	-0.549758
H	0.631945	-2.960020	5.497192
H	1.423213	-3.728898	4.117489
H	2.219890	-2.396612	4.966233
H	-1.866111	-2.465347	3.662151
H	-1.712191	-1.522860	2.172568
H	-1.038807	-3.157888	2.264593
H	-0.458806	0.046039	5.156768
H	1.174244	0.504089	4.660586
H	-0.200403	0.862019	3.605740
H	4.744633	0.073724	-1.218717
H	7.075501	-0.740295	-1.029794
N	8.032376	-2.429122	0.802188
H	5.989572	-3.076074	2.388354
H	3.651045	-2.277435	2.210397
H	-1.280178	0.063637	-2.774178
H	-3.333356	1.277453	-3.437677
H	-4.556013	2.645058	-1.768471
H	-3.719847	2.798402	0.561007
H	-1.657097	1.582516	1.221562
O	8.299206	-3.209814	1.712253
O	8.849355	-2.024854	-0.021505

Diene Reaction C Catalyzed (1c + BF_3)

E	-1647,58812
E_0	-1647.22968
$G_{198.15}$	-1647.26434
$G_{298.15}$	-1647.29239
$G_{398.15}$	-1647.32626

C	-6.273003	0.494447	2.447408
C	-5.331092	-0.136737	3.287793
C	-5.815553	-1.030675	4.265092
C	-7.173375	-1.283003	4.390668
C	-8.069442	-0.643922	3.537676
C	-7.631042	0.249168	2.563031
C	-3.924316	0.179902	3.082347
C	-2.843206	-0.264837	3.760713
O	-2.877908	-1.100961	4.784155
Si	-1.863281	-2.072869	5.787120
C	-1.435217	-1.100175	7.320437
N	-1.533465	0.217591	3.367791
B	-0.830717	1.329466	4.401139
F	-0.563737	2.441925	3.628741
C	-1.128838	-0.142093	2.188158
C	0.083515	0.167143	1.449307
C	0.073890	-0.245169	0.099735
C	1.164708	-0.014071	-0.726132
C	2.296968	0.613732	-0.208791
C	2.330345	1.005461	1.130899
C	1.238281	0.791605	1.960158
C	-0.348319	-2.622187	4.828972
C	-2.976234	-3.528317	6.182943
F	-1.767330	1.559338	5.380484
F	0.325573	0.733964	4.903947
H	-1.816679	-0.788364	1.644795
H	-3.717832	0.908707	2.308522
H	-0.934331	-1.751598	8.044657
H	-0.772801	-0.264272	7.091887
H	-2.335902	-0.700043	7.793371
H	-0.613728	-3.111460	3.887076
H	0.320705	-1.785138	4.621878
H	0.208408	-3.350630	5.428192
H	-2.453648	-4.239129	6.831101
H	-3.879415	-3.208186	6.709859
H	-3.281051	-4.063733	5.279531
H	-5.925528	1.191851	1.693311
H	-8.350682	0.734210	1.918173
N	-9.508851	-0.916297	3.668471

H	-7.548874	-1.966818	5.139519
H	-5.120806	-1.522510	4.927818
H	-0.804131	-0.742043	-0.299257
H	1.136194	-0.326228	-1.763120
H	3.155620	0.792297	-0.846122
H	3.215827	1.483360	1.532734
H	1.286753	1.093205	2.993811
O	-10.272251	-0.340061	2.899898
O	-9.865940	-1.705458	4.537421

Diene Reactions E, F and G Uncatalyzed (1d)

E	-887.22663
E_0	-886.96693
$G_{198.15}$	-886.99364
$G_{298.15}$	-887.01371
$G_{398.15}$	-887.03734

C	-2.099355	1.360607	0.205248
C	-1.387633	0.732330	-0.744622
N	-1.757597	0.650554	-2.095137
C	-2.165248	1.695982	-2.706339
H	-3.016927	1.874999	-0.039765
H	-2.161783	2.674018	-2.208720
C	-2.651994	1.680629	-4.089832
C	-3.015436	2.890707	-4.696997
C	-3.479021	2.913960	-6.009745
C	-3.584782	1.725462	-6.729353
C	-3.226822	0.513418	-6.131835
C	-2.765356	0.488370	-4.822739
H	-2.933077	3.815472	-4.134878
H	-3.757136	3.855387	-6.469454
H	-3.946371	1.740121	-7.751378
H	-3.312639	-0.411038	-6.691757
H	-2.491306	-0.444811	-4.346484
O	-0.259522	0.050957	-0.435447
Si	0.591756	-1.151850	-1.285782
C	-0.534814	-2.613088	-1.637127
H	-0.964884	-3.007083	-0.711694
H	-1.356675	-2.328041	-2.297541
H	0.023166	-3.423955	-2.117084
C	1.344707	-0.462273	-2.863197
H	0.577258	-0.185925	-3.589092
H	2.000384	-1.206007	-3.328765
H	1.948742	0.425283	-2.652271
C	1.941374	-1.620323	-0.070407
H	2.574659	-0.759577	0.162081
H	1.516335	-1.985771	0.868478
H	2.582224	-2.408040	-0.479196
H	-1.786342	1.312360	1.238623

Diene Reactions E, F and G Catalyzed (1d + BF_3)

E	-1211.90791
E_0	-1211.63293
$G_{198.15}$	-1211.66173
$G_{298.15}$	-1211.68423
$G_{398.15}$	-1211.71109

C	-0.037684	-0.017721	0.054150
C	0.063231	0.236488	1.361184
N	1.304453	0.750932	1.915253
C	2.331179	-0.033708	1.820062
H	0.776536	0.206043	-0.618801
H	2.129829	-0.993702	1.347344
C	3.717262	0.134720	2.230664
C	4.599935	-0.855155	1.750702
C	5.951008	-0.823440	2.066979
C	6.439499	0.187435	2.893362
C	5.572777	1.159229	3.396641
C	4.223099	1.144115	3.071771
H	4.216945	-1.647630	1.116349
H	6.617135	-1.584856	1.679184
H	7.492200	0.214921	3.151408
H	5.952465	1.937243	4.048321
H	3.567670	1.897713	3.477484
B	1.272547	2.336734	2.434215
F	2.307169	2.971576	1.772658
F	1.463835	2.306265	3.817257
F	0.033949	2.820419	2.090531
O	-0.933907	0.076253	2.224497
Si	-1.268495	-0.168455	3.882220
C	0.243395	-0.847479	4.766514
H	0.626617	-1.753641	4.287389
H	1.045090	-0.108081	4.820171
H	-0.029141	-1.113941	5.793383
C	-1.839833	1.453193	4.610409
H	-1.032075	2.187240	4.619446
H	-2.186499	1.306501	5.638927
H	-2.668123	1.868813	4.030302
C	-2.649816	-1.436435	3.849232
H	-2.321061	-2.373841	3.391571

H	-3.505217	-1.065714	3.277694
H	-2.997033	-1.661289	4.862846
H	-0.969924	-0.386028	-0.350066

Transition States HDA

System A Uncatalyzed (1a +2a)

E	-1311.51794
E_0	-1311.09081
$G_{198.15}$	-1311.12287
$G_{298.15}$	-1311.14884
$G_{398.15}$	-1311.18036

C	-0.059195	-0.201762	-0.013312
N	-0.128658	-0.199457	1.315275
C	0.989923	-0.219394	2.031389
O	0.857573	-0.194256	3.363066
Si	-0.566521	0.026975	4.303391
C	2.282417	-0.419300	1.471949
O	1.029338	-1.780214	-0.496094
C	1.902333	-2.164421	0.377415
C	3.299095	-2.417919	-0.175448
C	1.439351	-3.166978	1.426090
C	-1.269932	-0.431500	-0.817689
H	0.713534	0.375743	-0.519093
C	3.527997	-0.446575	2.265260
H	2.407094	0.075636	0.514690
C	0.141289	0.160205	6.034830
C	-1.678435	-1.477970	4.163004
C	-1.433720	1.614568	3.811604
H	2.161141	-3.285682	2.236708
H	0.466468	-2.884755	1.829325
H	1.320593	-4.138182	0.931029
H	4.043655	-2.552067	0.610004
H	3.256359	-3.336497	-0.771385
H	3.605900	-1.606960	-0.837563
H	-2.518196	-1.393982	4.860949
H	-2.082950	-1.587051	3.155478
H	-1.133034	-2.393083	4.411394
H	-2.256679	1.824670	4.502964
H	-0.745616	2.464268	3.849168
H	-1.841837	1.550682	2.801492
H	-0.654688	0.321827	6.768733
H	0.675347	-0.751029	6.318481
H	0.842546	0.995667	6.110709
C	4.683800	0.140532	1.719668
C	5.901347	0.112223	2.392635
C	6.000971	-0.516692	3.632435
C	4.867469	-1.110383	4.186753
C	3.647545	-1.075901	3.517069
H	4.621186	0.631858	0.753918
H	6.772309	0.581022	1.947735
H	6.947711	-0.542787	4.159946
H	4.931889	-1.602653	5.151229
H	2.777937	-1.528739	3.971450
C	-1.217194	-0.222225	-2.201172
C	-2.341406	-0.438572	-2.992060
C	-3.532347	-0.865689	-2.405939
C	-3.593171	-1.076528	-1.027186
C	-2.468897	-0.863837	-0.237591
H	-0.285831	0.098106	-2.655363
H	-2.289738	-0.276346	-4.062687
H	-4.410162	-1.033478	-3.020037
H	-4.519273	-1.407547	-0.570523
H	-2.504911	-1.021548	0.832462

System A Catalyzed (1a + 2a-BF_3)

E	-1636.22620
E_0	-1635.78394
$G_{198.15}$	-1635.81873
$G_{298.15}$	-1635.84758
$G_{398.15}$	-1635.88279

C	-1.457696	0.181305	-2.204124
C	-1.501140	-0.086834	-0.824254
C	-2.743953	-0.311541	-0.200558
C	-3.912738	-0.258955	-0.941950
C	-3.858680	0.013476	-2.313873
C	-2.633822	0.231240	-2.942614
C	-0.256301	-0.112460	-0.086767
N	-0.219213	-0.346066	1.194387
C	0.953584	-0.440969	1.875913
O	0.825374	-0.481021	3.184059
Si	-0.597929	-0.308418	4.177766
C	0.159979	-0.322151	5.889155
C	2.252244	-0.605716	1.307123
C	3.478044	-0.314716	2.108069
C	3.701873	-0.761951	3.419670
C	4.895016	-0.472043	4.077521
C	5.890930	0.271534	3.446849
C	5.684450	0.720256	2.143933
C	4.495339	0.425199	1.483421
C	-1.717766	-1.788033	3.927228
C	-1.420760	1.332868	3.813329

O	1.434011	-2.355898	-0.496767
C	2.224287	-2.433833	0.569571
C	1.617198	-3.321042	1.641314
C	3.704094	-2.689200	0.332614
H	0.639461	0.129238	-0.658167
H	2.323706	-0.180806	0.312653
H	2.120833	-3.204641	2.601862
H	0.550003	-3.125658	1.750337
H	1.733089	-4.360839	1.318148
H	4.251943	-2.714796	1.273239
H	3.782792	-3.663856	-0.157156
H	4.151935	-1.953387	-0.331945
H	-2.559699	-1.739607	4.625857
H	-2.117252	-1.830564	2.912956
H	-1.182982	-2.721862	4.122033
H	-2.212956	1.522532	4.545236
H	-0.703261	2.155340	3.885764
H	-1.864529	1.353376	2.816737
H	-0.615774	-0.213021	6.653653
H	0.687703	-1.259738	6.084669
H	0.871840	0.497815	6.015508
H	4.350616	0.768995	0.464608
H	6.450053	1.297362	1.637529
H	6.817032	0.496119	3.963687
H	5.045944	-0.830106	5.090163
H	2.942780	-1.334599	3.932635
H	-0.498806	0.311168	-2.689826
H	-2.595338	0.428258	-4.007193
H	-4.775923	0.050197	-2.891149
H	-4.869246	-0.430748	-0.462001
H	-2.768661	-0.521377	0.860772
B	1.883313	-1.958619	-1.892322
F	0.721397	-1.891524	-2.652656
F	2.479085	-0.665326	-1.809211
F	2.787789	-2.881998	-2.393354

System B Uncatalyzed (1b + 2a)

E	-1426.07386
E_0	-1425.61456
$G_{198.15}$	-1425.64837
$G_{298.15}$	-1425.67618
$G_{398.15}$	-1425.71004

C	-2.492336	-0.805380	-0.261372
C	-1.276428	-0.410089	-0.832610
C	-1.204566	-0.214778	-2.217337
C	-2.326061	-0.408547	-3.017860
C	-3.533916	-0.798436	-2.440445
C	-3.614043	-0.994938	-1.060573
C	-0.068014	-0.204696	-0.018237
N	-0.147741	-0.201502	1.309653
C	0.966771	-0.236891	2.031794
C	2.260930	-0.445651	1.481445
C	3.503050	-0.480188	2.279416
C	4.674312	0.079726	1.731429
C	5.885971	0.051234	2.401721
C	5.976834	-0.555200	3.659368
C	4.833745	-1.124555	4.224786
C	3.618922	-1.081820	3.539757
O	0.824701	-0.223050	3.364326
Si	-0.606680	0.001290	4.290561
C	-1.456664	1.601256	3.808573
C	0.084403	0.112080	6.031173
C	-1.730756	-1.492605	4.128842
O	0.990338	-1.808634	-0.482506
C	1.869069	-2.187673	0.388549
C	1.412857	-3.189178	1.441534
C	3.263074	-2.442650	-0.171143
H	0.720309	0.355803	-0.518920
H	2.394284	0.046890	0.524141
H	2.137071	-3.300682	2.251290
H	0.439861	-2.909177	1.846184
H	1.297353	-4.163528	0.951815
H	4.012934	-2.568422	0.610719
H	3.219581	-3.365843	-0.759910
H	3.563665	-1.636089	-0.841633
H	-2.578226	-1.404516	4.816939
H	-2.123515	-1.593187	3.115826
H	-1.196701	-2.413901	4.379132
H	-2.283187	1.811433	4.495674
H	-0.761518	2.444483	3.859966
H	-1.857139	1.551070	2.794675
H	-0.717875	0.271728	6.758626
H	0.608704	-0.806134	6.310772
H	0.790577	0.941832	6.122840
H	4.627810	0.554418	0.756553
H	6.776238	0.493246	1.970377
O	7.210834	-0.537256	4.245800
H	4.870547	-1.599545	5.196239
H	2.746307	-1.515492	4.006743
H	-0.260411	0.076358	-2.664695
H	-2.259162	-0.257685	-4.089334
H	-4.409660	-0.948463	-3.062067
H	-4.553217	-1.296896	-0.610453
H	-2.543216	-0.952405	0.809581
C	7.363550	-1.138459	5.523445

H	8.410982	-1.007796	5.790884
H	6.734310	-0.648302	6.274573
H	7.128393	-2.208180	5.493702

System B Catalyzed (1b + 2a-BF_3)

E	-1750.78240
E_0	-1750.30801
$G_{198.15}$	-1750.34455
$G_{298.15}$	-1750.37525
$G_{398.15}$	-1750.41280

C	4.489484	0.390051	1.519929
C	3.450892	-0.334398	2.134812
C	3.664303	-0.768570	3.447352
C	4.852785	-0.493006	4.125716
C	5.864230	0.235802	3.496251
C	5.671193	0.677621	2.182485
C	2.232084	-0.617846	1.322297
C	0.927389	-0.454455	1.878061
O	0.786874	-0.509232	3.185559
Si	-0.647079	-0.341796	4.162660
C	-1.457708	1.308588	3.811812
N	-0.239223	-0.348264	1.188338
C	-0.263821	-0.115916	-0.093733
C	-1.503702	-0.073177	-0.839159
C	-1.447996	0.192438	-2.219074
C	-2.618778	0.259763	-2.964726
C	-3.850802	0.062324	-2.343324
C	-3.917189	-0.207534	-0.971463
C	-2.753756	-0.277664	-0.223006
C	0.090257	-0.380232	5.883422
C	-1.772955	-1.812109	3.885159
C	2.199463	-2.439367	0.582966
C	3.679685	-2.701530	0.353061
O	1.415299	-2.361142	-0.489803
B	1.876290	-1.968651	-1.881572
F	2.778334	-2.898263	-2.376526
C	1.585201	-3.329409	1.648651
F	0.720313	-1.894915	-2.651113
F	2.480085	-0.678832	-1.796904
H	0.638925	0.111536	-0.659516
H	2.313957	-0.188180	0.330587
H	2.080142	-3.211645	2.613714
H	0.516703	-3.136446	1.749029
H	1.706238	-4.368969	1.326689
H	4.222431	-2.728744	1.296565
H	3.756849	-3.676392	-0.136423
H	4.134069	-1.967429	-0.308943
H	-2.622494	-1.765017	4.574651
H	-2.161040	-1.842718	2.866069
H	-1.246095	-2.751038	4.077092
H	-2.258103	1.491790	4.536435
H	-0.737075	2.126251	3.904818
H	-1.888618	1.345548	2.810090
H	-0.694387	-0.280078	6.640033
H	0.613741	-1.321614	6.072278
H	0.801762	0.436818	6.029445
H	4.364806	0.730777	0.497437
H	6.460987	1.240144	1.699356
O	7.058699	0.562192	4.068911
H	4.972335	-0.850777	5.139728
H	2.898363	-1.329265	3.963397
H	-0.484301	0.306692	-2.699091
H	-2.570664	0.454798	-4.029302
H	-4.763853	0.112758	-2.926189
H	-4.879102	-0.363655	-0.496925
H	-2.788266	-0.485833	0.838374
C	7.322614	0.118042	5.392615
H	8.320986	0.479088	5.633872
H	6.604219	0.536530	6.106095
H	7.307105	-0.975369	5.457777

System C Uncatalyzed (1c + 2a)

E	-1516.08431
E_0	-1515.65475
$G_{198.15}$	-1515.68886
$G_{298.15}$	-1515.71679
$G_{398.15}$	-1515.75074

C	-2.446701	-0.933159	-0.234006
C	-1.268008	-0.449376	-0.814557
C	-1.233701	-0.206476	-2.193077
C	-2.357266	-0.441439	-2.979321
C	-3.527912	-0.921347	-2.393141
C	-3.570074	-1.165411	-1.019270
C	-0.057663	-0.199236	-0.014833
N	-0.126053	-0.203136	1.318315
C	0.987067	-0.213237	2.035312
C	2.285957	-0.397684	1.471865
C	3.522407	-0.438073	2.264588
C	4.690227	0.134437	1.719949
C	5.904698	0.091144	2.386542
C	5.967836	-0.545375	3.623187
C	4.839549	-1.129489	4.194243

C	3.629751	-1.072520	3.518798
O	0.861134	-0.183982	3.364651
Si	-0.561842	0.047277	4.315654
C	-1.422007	1.633085	3.810381
C	0.158743	0.188287	6.039636
C	-1.672637	-1.457881	4.181982
O	1.058602	-1.714559	-0.527160
C	1.913771	-2.134186	0.347112
C	1.424476	-3.141010	1.377656
C	3.310222	-2.398095	-0.197508
H	0.687671	0.420771	-0.512099
H	2.410195	0.113656	0.523392
H	2.137538	-3.284641	2.191843
H	0.452452	-2.850849	1.776536
H	1.295536	-4.102251	0.866297
H	4.041775	-2.577188	0.591316
H	3.255200	-3.295611	-0.823375
H	3.643144	-1.573967	-0.829712
H	-2.507987	-1.373046	4.884963
H	-2.084408	-1.566869	3.177418
H	-1.126813	-2.373284	4.428186
H	-2.242517	1.852007	4.501787
H	-0.731330	2.480947	3.839668
H	-1.833704	1.562235	2.802172
H	-0.632467	0.357557	6.776859
H	0.690288	-0.722972	6.327801
H	0.862635	1.022186	6.107350
H	4.637087	0.629678	0.756779
H	6.795845	0.538983	1.968837
N	7.249601	-0.600426	4.340040
H	4.922869	-1.616783	5.156057
H	2.753702	-1.513271	3.970571
H	-0.318237	0.156421	-2.647618
H	-2.321057	-0.252134	-4.046007
H	-4.405245	-1.103546	-3.003672
H	-4.480864	-1.536614	-0.562983
H	-2.469529	-1.114499	0.832634
O	7.274771	-1.170488	5.426642
O	8.224665	-0.074142	3.812191

System C Catalyzed (1c + 2a-BF_3)

E	-1840.79042
E_0	-1840.34582
$G_{198.15}$	-1840.38281
$G_{298.15}$	-1840.41370
$G_{398.15}$	-1840.45142

C	4.496935	0.400050	1.489991
C	3.470882	-0.338676	2.106409
C	3.683824	-0.799008	3.417525
C	4.867085	-0.524201	4.089766
C	5.853027	0.220498	3.450393
C	5.682762	0.687697	2.151387
C	2.248369	-0.617108	1.302438
C	0.949655	-0.436835	1.881092
O	0.831710	-0.456821	3.188088
Si	-0.588667	-0.266308	4.194575
C	-1.417664	1.362269	3.794324
N	-0.218714	-0.348956	1.200272
C	-0.262102	-0.094760	-0.078438
C	-1.502589	-0.101581	-0.818446
C	-1.466911	0.207467	-2.190577
C	-2.641701	0.224575	-2.931845
C	-3.856630	-0.067967	-2.313927
C	-3.902921	-0.381666	-0.950292
C	-2.735844	-0.400526	-0.205600
C	0.186157	-0.240610	5.896805
C	-1.696702	-1.758544	3.975032
C	2.217213	-2.420112	0.543639
C	3.695069	-2.697638	0.314146
O	1.439056	-2.313858	-0.529591
B	1.909464	-1.878674	-1.908909
F	2.815949	-2.790397	-2.422960
C	1.586416	-3.319688	1.592174
F	0.758604	-1.779985	-2.680194
F	2.511468	-0.591072	-1.775098
H	0.626323	0.193834	-0.640151
H	2.321050	-0.172720	0.316419
H	2.084918	-3.235458	2.558940
H	0.522092	-3.108089	1.698751
H	1.685883	-4.353632	1.246543
H	4.234906	-2.756160	1.258382
H	3.761202	-3.662927	-0.195067
H	4.162615	-1.957833	-0.332286
H	-2.535157	-1.704229	4.677286
H	-2.102208	-1.821494	2.964214
H	-1.154228	-2.684943	4.183306
H	-2.200744	1.569988	4.531049
H	-0.702107	2.188528	3.835716
H	-1.875142	1.354729	2.803778
H	-0.583514	-0.117273	6.665224
H	0.718116	-1.171918	6.109852
H	0.895309	0.584844	6.000599
H	4.360516	0.751968	0.473654
H	6.467999	1.261458	1.678821
N	7.106148	0.520492	4.167457

H	5.035933	-0.876750	5.097982
H	2.919604	-1.371589	3.921103
H	-0.513718	0.394801	-2.668532
H	-2.609931	0.453588	-3.990115
H	-4.772828	-0.057434	-2.893836
H	-4.852052	-0.611229	-0.480242
H	-2.754028	-0.640746	0.849381
O	7.953503	1.184420	3.582055
O	7.227478	0.089056	5.308914

System D Uncatalyzed (1a + 2c)

E	-1232.86098
E_0	-1232.48958
$G_{198.15}$	-1232.52068
$G_{298.15}$	-1232.54525
$G_{398.15}$	-1232.57478

C	-0.000238	-0.253715	-0.011893
C	-0.084946	-0.116854	1.381272
C	1.095415	-0.046804	2.134019
C	2.336387	-0.108479	1.509101
C	2.410576	-0.239402	0.122812
C	1.239664	-0.310995	-0.635421
C	-1.370646	-0.053511	2.074949
N	-2.506202	-0.008410	1.410480
C	-3.673086	-0.189864	2.039045
C	-3.780482	-0.610412	3.390491
C	-5.060257	-0.866200	4.087863
C	-5.174687	-0.494651	5.437805
C	-6.331853	-0.757202	6.164859
C	-7.402930	-1.413255	5.560685
C	-7.299756	-1.802317	4.225882
C	-6.145137	-1.533294	3.495868
O	-4.774118	-0.125208	1.289129
Si	-4.927861	0.189927	-0.399280
C	-4.168902	1.849975	-0.825425
C	-6.790382	0.235639	-0.604871
C	-4.185558	-1.228465	-1.376346
O	-1.504259	-2.008678	3.004721
C	-2.713955	-2.287603	3.294942
H	-3.334324	-2.834183	2.564587
H	-2.954675	-2.540893	4.337867
H	-1.313261	0.230366	3.123850
H	-3.032415	-0.161651	4.036498
H	-4.355975	-1.081006	-2.448071
H	-3.110433	-1.314527	-1.210215
H	-4.647706	-2.179850	-1.097119
H	-4.381974	2.106476	-1.868580
H	-4.587458	2.642946	-0.198594
H	-3.086441	1.842306	-0.687356
H	-7.060397	0.442701	-1.645351
H	-7.245690	-0.718793	-0.326341
H	-7.237882	1.014246	0.018837
H	-4.344586	0.011809	5.920540
H	-6.395680	-0.451008	7.203222
H	-8.305648	-1.621588	6.123689
H	-8.124869	-2.319112	3.747815
H	-6.086494	-1.835110	2.459408
H	1.032878	0.038811	3.213334
H	3.243672	-0.058315	2.100091
H	3.376994	-0.287360	-0.366572
H	1.298576	-0.413570	-1.713179
H	-0.914281	-0.308745	-0.588692

System D Catalyzed (1a + 2c-BF_3)

E	-1557.57125
E_0	-1557.18523
$G_{198.15}$	-1557.22034
$G_{298.15}$	-1557.24862
$G_{398.15}$	-1557.28269

C	-1.34456	-0.11224	-2.47368
C	-1.41084	-0.4711	-1.11336
C	-2.68308	-0.66027	-0.5436
C	-3.83387	-0.51284	-1.3149
C	-3.74964	-0.16728	-2.66193
C	-2.49578	0.03383	-3.23842
C	-0.13541	-0.57506	-0.38396
C	0.1152	-1.26773	0.80118
O	-0.89067	-1.61074	1.59425
Si	-0.87881	-2.52916	3.07148
C	-0.34474	-4.28322	2.69032
N	1.35387	-1.65891	1.24545
C	2.44353	-1.04598	0.91639
C	3.75913	-1.51007	1.32868
C	4.86716	-0.68961	1.05651
C	6.14486	-1.0962	1.42746
C	6.32706	-2.32171	2.0658
C	5.22907	-3.14424	2.34084
C	3.9524	-2.74206	1.97928
C	-2.68944	-2.46347	3.54771
C	0.18724	-1.68472	4.3575
C	-0.11044	1.41749	0.60069
H	-0.35731	1.8249	-0.37837

O	0.99484	1.72599	1.14867
B	2.09674	2.45833	0.29274
F	1.66309	3.74881	0.10041
H	-0.92831	1.12914	1.25765
F	3.25427	2.34417	1.03128
F	2.18013	1.74361	-0.9142
H	2.43711	-0.13914	0.31516
H	0.73801	-0.42123	-1.00453
H	0.04825	-2.16812	5.33044
H	1.24707	-1.73094	4.10195
H	-0.08794	-0.63225	4.47136
H	-0.43627	-4.90784	3.58497
H	-0.97432	-4.72455	1.91245
H	0.69181	-4.32188	2.35177
H	-2.86165	-3.01783	4.47571
H	-3.02314	-1.43494	3.71113
H	-3.3228	-2.90667	2.77439
H	-0.37421	0.05123	-2.93092
H	-2.41394	0.3072	-4.28436
H	-4.64956	-0.05235	-3.25513
H	-4.80419	-0.66768	-0.85586
H	-2.76845	-0.93263	0.49763
H	4.71204	0.27186	0.57994
H	6.99538	-0.45676	1.22282
H	7.32333	-2.63931	2.35275
H	5.37791	-4.09669	2.83657
H	3.09421	-3.36968	2.1841

System E Uncatalyzed (1d + 2a)

E	-1080.41012
E_0	-1080.06395
$G_{198.15}$	-1080.09278
$G_{298.15}$	-1080.11549
$G_{398.15}$	-1080.14277

C	0.073596	-0.167618	-0.042292
C	-0.024499	-0.078247	1.354053
C	1.148424	-0.036567	2.120583
C	2.395304	-0.080835	1.505973
C	2.482872	-0.164674	0.116809
C	1.319442	-0.206997	-0.655191
C	-1.316392	-0.035182	2.035872
N	-2.446463	-0.009288	1.366328
C	-3.600375	-0.231698	2.013799
C	-3.687203	-0.716567	3.329230
H	-4.688452	-0.924166	3.688551
O	-4.722586	-0.181533	1.287519
Si	-4.932628	0.161358	-0.385363
C	-4.246240	1.859387	-0.789892
C	-6.800352	0.140460	-0.544200
C	-4.162703	-1.195357	-1.427534
O	-1.406618	-2.023620	3.007676
C	-2.597878	-2.400950	3.295575
C	-3.313607	-3.283494	2.269236
C	-2.834269	-2.829451	4.751152
H	-1.276230	0.218728	3.092760
H	-3.019803	-0.281450	4.061475
H	-4.381986	-3.389162	2.472685
H	-3.169230	-2.889717	1.262624
H	-2.855952	-4.278766	2.303081
H	-3.893312	-2.954655	4.988796
H	-2.334172	-3.792713	4.900139
H	-2.385397	-2.111738	5.439514
H	-4.371317	-1.021644	-2.488600
H	-3.080101	-1.239946	-1.295920
H	-4.577273	-2.172901	-1.165169
H	-4.494664	2.133076	-1.820772
H	-4.676259	2.621517	-0.133202
H	-3.160750	1.888729	-0.679054
H	-7.106819	0.351064	-1.573763
H	-7.209454	-0.834781	-0.266045
H	-7.259860	0.893172	0.102394
H	1.074239	0.011092	3.201351
H	3.296905	-0.053795	2.107140
H	3.454040	-0.198263	-0.364373
H	1.388992	-0.271932	-1.735252
H	-0.835156	-0.198795	-0.629407

System E Catalyzed (1d + 2a-BF_3)

E	-1405,12190
E_0	-1404.76107
$G_{198.15}$	-1404.79362
$G_{298.15}$	-1404.81987
$G_{398.15}$	-1404.85150

C	-1.680203	0.167273	-2.065027
C	-1.676904	-0.058064	-0.691657
N	-2.753960	-0.043526	0.164475
C	-3.963108	-0.132122	-0.293169
H	-2.538453	0.648775	-2.510488
H	-4.169282	-0.258671	-1.353475
C	-5.130576	-0.080808	0.569157
C	-5.036713	0.193407	1.946320
C	-6.183365	0.246220	2.723052

C	-7.435276	0.019477	2.139735
C	-7.537586	-0.260394	0.778183
C	-6.391579	-0.309389	-0.009194
H	-4.061503	0.367765	2.383193
H	-6.112078	0.463722	3.782616
H	-8.329367	0.059856	2.752022
H	-8.507452	-0.443340	0.330976
H	-6.455647	-0.547809	-1.065173
O	-0.518686	-0.347976	-0.115423
14	-0.131554	-0.629663	1.552455
C	1.701491	-0.996245	1.438357
C	-0.448453	0.939541	2.525220
C	-1.073308	-2.110639	2.206477
H	1.892960	-1.876685	0.818722
H	2.248317	-0.154672	1.004396
H	2.120299	-1.190647	2.430782
H	0.090557	1.785559	2.089207
H	-0.099929	0.821771	3.556567
H	-1.510499	1.189144	2.549559
H	-0.718361	-2.362269	3.211614
H	-2.145987	-1.918048	2.261586
H	-0.916247	-2.989976	1.575180
C	-2.016693	-1.706454	-3.026241
O	-3.251790	-2.016789	-2.770132
B	-4.480767	-1.553344	-3.576110
F	-4.427361	-0.144633	-3.654927
F	-4.440610	-2.134503	-4.830524
F	-5.572364	-1.955592	-2.820926
C	-1.020191	-2.604944	-2.335374
H	-0.024381	-2.165285	-2.293015
H	-1.358609	-2.857403	-1.331076
H	-0.966882	-3.534631	-2.914730
C	-1.639630	-1.240010	-4.417889
H	-2.262832	-0.415842	-4.758104
H	-1.815803	-2.083033	-5.094708
H	-0.586919	-0.961957	-4.465155
H	-0.715369	0.392868	-2.499025
C	1.097987	-0.073570	1.938741
C	2.368639	-0.344165	1.410403
C	-1.155059	-0.257431	-0.917658
C	-1.026612	-0.215949	-2.313229
C	-2.134039	-0.415788	-3.130425
C	-3.383675	-0.657153	-2.560690
C	-3.521456	-0.701448	-1.171175
C	-2.415670	-0.506541	-0.353960
H	-0.049361	-0.045025	-2.751062
H	-2.024098	-0.387646	-4.208409
H	-4.248495	-0.812339	-3.196126
H	-4.493568	-0.890066	-0.729659
H	-2.509873	-0.538082	0.723826
H	0.915220	0.293153	-0.629743
O	0.961687	-0.071118	3.268571
14	-0.474551	-0.097461	4.217912
C	-1.512257	1.427577	3.878571
C	-1.405423	-1.696687	3.912156
C	0.223335	-0.049593	5.957258
H	-1.920638	1.417701	2.866545
H	-2.345635	1.484737	4.586812
H	-0.916812	2.337941	3.995743
H	-1.726389	-1.781402	2.872380
H	-2.293316	-1.749781	4.551007
H	-0.779046	-2.563009	4.144014
H	-0.580126	-0.067387	6.700501
H	0.811018	0.857853	6.121916
H	0.873317	-0.908381	6.146321
H	2.635139	0.120596	0.469737
H	3.173214	-0.419190	2.132311
C	2.098382	-2.112379	0.532551
O	1.243278	-1.942711	-0.396358
C	3.541487	-2.422049	0.136462
H	3.896735	-1.718115	-0.619433
H	3.557665	-3.423556	-0.305931
H	4.217008	-2.415232	0.995460
H	1.777295	-2.662459	1.436542

System F Uncatalyzed (1d + 2b)

E	-1041.08179
E_0	-1040.76354
$G_{198.15}$	-1040.79215
$G_{298.15}$	-1040.81438
$G_{398.15}$	-1040.84086

C	0.031082	-0.044356	-0.093203
N	-0.035166	-0.022604	1.215207

System F Catalyzed (1d + 2b-BF_3)

E	-1365.79163
E_0	-1365.45892
$G_{198.15}$	-1365.49120
$G_{298.15}$	-1365.51695
$G_{398.15}$	-1365.54779

C	2.032570	-0.222925	-0.390687
C	1.088699	0.621366	-0.972668

C	0.083332	1.200799	-0.191003
C	0.021200	0.935505	1.168699
C	0.972791	0.089744	1.765368
C	1.979685	-0.488037	0.974443
C	0.958771	-0.212920	3.189636
N	-0.003410	0.145666	3.971227
C	0.049612	-0.100741	5.326385
O	-1.131433	-0.289306	5.910697
14	-2.731902	-0.194876	5.255890
C	-3.067992	1.570292	4.724532
C	1.184663	-0.171022	6.105381
C	-3.764263	-0.662546	6.747042
C	-2.946975	-1.434287	3.867979
C	1.482987	-2.416398	6.163625
O	1.718858	-2.816493	4.975895
B	3.148676	-2.922326	4.337824
F	2.910160	-3.153803	2.998672
F	3.760802	-1.675933	4.539989
F	3.820501	-3.945182	4.973239
C	2.522088	-2.437410	7.245242
H	0.441718	-2.511925	6.469921
H	1.057468	-0.087616	7.175653
H	1.812971	-0.779083	3.556651
H	2.141652	0.104133	5.686934
H	-4.001241	-1.487859	3.576044
H	-2.363276	-1.163160	2.986485
H	-2.641606	-2.436712	4.181732
H	-4.105792	1.675804	4.391745
H	-2.913724	2.266049	5.554290
H	-2.414303	1.869095	3.903232
H	-4.831577	-0.621459	6.507918
H	-3.538403	-1.677612	7.085370
H	-3.582870	0.018616	7.582916
H	2.698145	-1.157530	1.434705
H	2.806833	-0.675781	-0.998698
H	1.132194	0.830181	-2.035845
H	-0.646560	1.858311	-0.649376
H	-0.749878	1.378958	1.786395
H	2.137604	-1.993992	8.162879
H	2.762332	-3.491089	7.432668
H	3.443905	-1.946843	6.937461

System G Uncatalyzed (1d + 2c)

E	-1001.75157
E_0	-1001.46123
$G_{198.15}$	-1001.48890
$G_{298.15}$	-1001.51015
$G_{398.15}$	-1001.53534

C	0.031082	-0.044356	-0.093203
N	-0.035166	-0.022604	1.215207
C	1.097987	-0.073570	1.938741
C	2.368639	-0.344165	1.410403
C	-1.155059	-0.257431	-0.917658
C	-1.026612	-0.215949	-2.313229
C	-2.134039	-0.415788	-3.130425
C	-3.383675	-0.657153	-2.560690
C	-3.521456	-0.701448	-1.171175
C	-2.415670	-0.506541	-0.353960
H	-0.049361	-0.045025	-2.751062
H	-2.024098	-0.387646	-4.208409
H	-4.248495	-0.812339	-3.196126
H	-4.493568	-0.890066	-0.729659
H	-2.509873	-0.538082	0.723826
H	0.915220	0.293153	-0.629743
O	0.961687	-0.071118	3.268571
Si	-0.474551	-0.097461	4.217912
C	-1.512257	1.427577	3.878571
C	-1.405423	-1.696687	3.912156
C	0.223335	-0.049593	5.957258
H	-1.920638	1.417701	2.866545
H	-2.345635	1.484737	4.586812
H	-0.916812	2.337941	3.995743
H	-1.726389	-1.781402	2.872380
H	-2.293316	-1.749781	4.551007
H	-0.779046	-2.563009	4.144014
H	-0.580126	-0.067387	6.700501
H	0.811018	0.857853	6.121916
H	0.873317	-0.908381	6.146321
H	2.635139	0.120596	0.469737
H	3.173214	-0.419190	2.132311
C	2.098382	-2.112379	0.532551
O	1.243278	-1.942711	-0.396358
C	3.541487	-2.422049	0.136462
H	3.896735	-1.718115	-0.619433
H	3.557665	-3.423556	-0.305931
H	4.217008	-2.415232	0.995460
H	1.777295	-2.662459	1.436542

System G Catalyzed (1d + 2c-BF_3)

EC

E	-1326.45261
E_0	-1326.14862

$G_{198.15}$	-1326.18371
$G_{298.15}$	-1326.21088
$G_{398.15}$	-1326.24300

C	-7.476045	-0.206497	2.146155
C	-6.433309	-1.137228	2.185206
C	-5.290773	-0.937167	1.423639
C	-5.176275	0.202327	0.610140
C	-6.228130	1.129525	0.576389
C	-7.372984	0.926304	1.341212
C	-3.991978	0.450351	-0.210303
N	-2.963075	-0.313710	-0.215271
C	-1.913856	-0.051311	-1.101161
O	-0.686040	-0.222788	-0.595212
Si	-0.117137	-0.527129	0.997234
C	1.731630	-0.321846	0.797965
C	-2.078249	0.216517	-2.421449
C	-0.565005	-2.279967	1.492398
C	-0.821504	0.741063	2.187208
C	-1.900405	-2.233497	-3.061041
O	-2.363069	-2.299870	-4.208034
B	-1.454841	-1.859324	-5.519188
F	-0.146728	-1.961171	-5.089833
F	-1.855874	-0.566631	-5.745405
F	-1.813694	-2.761152	-6.471845
H	-3.066170	0.338054	-2.841257
H	1.983002	0.691085	0.472157
H	2.129275	-1.019589	0.056011
H	2.249052	-0.508680	1.744288
H	-0.142808	-3.008622	0.794297
H	-1.647964	-2.418836	1.519094
H	-0.169305	-2.509303	2.487327
H	-0.637442	1.759857	1.833821
H	-1.897093	0.615931	2.327824
H	-0.341620	0.641203	3.166491
H	-4.021190	1.352676	-0.833066
H	-6.145597	2.008904	-0.054031
H	-8.181662	1.646904	1.308657
H	-8.367210	-0.367920	2.741980
H	-6.519153	-2.018605	2.810278
H	-4.477856	-1.652319	1.442045
H	-2.543384	-2.518456	-2.228537
H	-0.835761	-2.067880	-2.894452
H	-1.224193	0.418154	-3.051716

TS1 (1d + 2c-BF_3)

E	-1326.45202
E_0	-1326.14746

$G_{198.15}$	-1326.18106
$G_{298.15}$	-1326.20708
$G_{398.15}$	-1326.23789

C	-7.471828	-0.164922	2.220490
C	-6.395102	-1.052000	2.317791
C	-5.270438	-0.872164	1.526058
C	-5.209613	0.202987	0.623140
C	-6.294823	1.087868	0.532690
C	-7.421568	0.904203	1.327923
C	-4.050403	0.423986	-0.235101
N	-2.998760	-0.310712	-0.207516
C	-1.975502	-0.097206	-1.122401
O	-0.745160	-0.186941	-0.642191
Si	-0.109463	-0.532424	0.929920
C	1.723625	-0.294348	0.660669
C	-2.173925	0.015364	-2.477723
C	-0.532566	-2.303563	1.370308
C	-0.794116	0.697241	2.168633
C	-2.114775	-2.089856	-3.043763
O	-2.350118	-2.119113	-4.285658
B	-1.179863	-1.831293	-5.325105
F	-0.010447	-2.296034	-4.731620
F	-1.169492	-0.450359	-5.471710
F	-1.535111	-2.510671	-6.457233
H	-3.172303	0.187847	-2.854971
H	1.948685	0.732158	0.359037
H	2.097312	-0.961494	-0.120547
H	2.281753	-0.504940	1.578316
H	-0.131527	-3.001282	0.629764
H	-1.612779	-2.451930	1.431283
H	-0.099235	-2.567108	2.340687
H	-0.640104	1.726189	1.830795
H	-1.861798	0.549508	2.343617
H	-0.277868	0.586347	3.127960
H	-4.115154	1.280573	-0.916506
H	-6.251995	1.917905	-0.164918
H	-8.256844	1.590151	1.251788
H	-8.348934	-0.310628	2.840668
H	-6.440853	-1.883105	3.011909
H	-4.431593	-1.554043	1.588633
H	-2.930475	-2.381731	-2.384295
H	-1.089679	-2.196472	-2.689491
H	-1.342195	0.269852	-3.119553

M1 (1d + 2c-BF_3)

E	-1326.45723

E_0	-1326.15017
$G_{198.15}$	-1326.18304
$G_{298.15}$	-1326.20862
$G_{398.15}$	-1326.23898

C	-7.526317	-0.187139	2.150782
C	-6.400345	-0.987977	2.372302
C	-5.264192	-0.818203	1.597654
C	-5.244201	0.159490	0.585256
C	-6.379830	0.959992	0.371742
C	-7.516417	0.785916	1.152070
C	-4.089929	0.354526	-0.268374
N	-2.991241	-0.310992	-0.146196
C	-1.988992	-0.226274	-1.064120
O	-0.772784	-0.293510	-0.630897
Si	-0.032287	-0.562658	0.943109
C	1.776621	-0.417820	0.523546
C	-2.205127	-0.289539	-2.488699
C	-0.526203	-2.282008	1.484339
C	-0.614624	0.784951	2.103701
C	-2.206663	-1.876724	-2.964198
O	-2.386328	-1.951637	-4.296870
B	-1.212040	-1.645930	-5.183585
F	-0.061373	-2.264926	-4.647223
F	-1.008774	-0.236208	-5.179368
F	-1.514279	-2.105515	-6.450771
H	-3.174662	0.100303	-2.794213
H	2.016879	0.577707	0.141219
H	2.062397	-1.146889	-0.238952
H	2.394067	-0.595392	1.409602
H	-0.228205	-3.026731	0.741494
H	-1.603927	-2.364348	1.638913
H	-0.028798	-2.535561	2.426151
H	-0.413162	1.778127	1.692311
H	-1.683009	0.709226	2.316918
H	-0.077077	0.710350	3.054748
H	-4.183896	1.134169	-1.031653
H	-6.366803	1.711507	-0.410560
H	-8.391032	1.402192	0.982929
H	-8.412442	-0.325048	2.759743
H	-6.418636	-1.742671	3.149521
H	-4.386358	-1.431993	1.755611
H	-3.038248	-2.356238	-2.435488
H	-1.244229	-2.280568	-2.626290
H	-1.390225	0.154983	-3.056721

TS2 (1d + 2c-BF_3)

E	-1326.45704
E_0	-1326.15006
$G_{198.15}$	-1326.18153
$G_{298.15}$	-1326.20604
$G_{398.15}$	-1326.23523

C	-7.577676	0.795511	1.546617
C	-7.452456	-0.008931	2.678776
C	-6.279956	-0.738852	2.905100
C	-5.231989	-0.665960	2.002118
C	-5.347486	0.143004	0.855488
C	-6.529731	0.872936	0.637787
C	-4.290441	0.234618	-0.128021
N	-3.159066	-0.383315	-0.020503
C	-2.261847	-0.396949	-1.045526
C	-2.629355	-0.534245	-2.433608
C	-2.716065	-2.141747	-2.805527
O	-3.448414	-2.325542	-3.922807
B	-2.978339	-1.689161	-5.197980
F	-3.524140	-2.390835	-6.255193
O	-1.006769	-0.472618	-0.735251
Si	-0.143883	-0.592015	0.795352
C	-0.616545	0.873656	1.857785
C	1.626679	-0.513105	0.218083
C	-0.591255	-2.242811	1.549194
F	-1.562385	-1.700876	-5.218054
F	-3.416200	-0.336717	-5.190808
H	-3.620141	-0.146577	-2.658542
H	1.837430	0.432619	-0.288081
H	1.850737	-1.324012	-0.479699
H	2.313096	-0.599721	1.066142
H	-0.348790	-3.064402	0.869869
H	-1.654006	-2.302091	1.791948
H	-0.023201	-2.397753	2.472243
H	-0.466914	1.815759	1.322718
H	-1.657417	0.823601	2.183546
H	0.015344	0.901579	2.751609
H	-4.486590	0.890042	-0.982347
H	-6.622023	1.491644	-0.248425
H	-8.488618	1.355616	1.374063
H	-8.269662	-0.070974	3.388315
H	-6.193934	-1.363170	3.786464
H	-4.319829	-1.226908	2.161430
H	-3.189497	-2.656084	-1.961345
H	-1.666167	-2.447866	-2.899583
H	-1.884574	-0.120994	-3.109000

Transition State 2+2EC

System H Uncatalyzed (da 1a)

E	-1118.29687
E_0	-1117.95685
$G_{198.15}$	-1117.98637
$G_{298.15}$	-1118.00915
$G_{398.15}$	-1118.03638

C	0.018522	-0.083149	-0.040780
N	-0.071554	-0.220570	1.340755
C	1.193683	-0.132747	1.668821
O	1.720824	-0.593149	2.806438
Si	0.901593	-1.414107	4.076570
C	1.967618	0.530642	0.640616
C	-0.910227	0.758567	-0.783872
H	0.484656	-0.887898	-0.599036
H	1.603223	1.524604	0.410203
C	3.352566	0.273026	0.274688
C	2.297169	-1.817136	5.260502
C	-0.347979	-0.253138	4.853318
C	0.096364	-2.968303	3.402935
H	1.919388	-2.336879	6.146719
H	3.044152	-2.461253	4.788256
H	2.803824	-0.907865	5.595499
H	-0.370299	-3.536758	4.214250
H	-0.676048	-2.722805	2.671165
H	0.831243	-3.620776	2.922166
H	-0.825859	-0.723734	5.718881
H	0.131526	0.667898	5.197396
H	-1.127216	0.013555	4.135692
C	4.046107	1.204267	-0.524344
C	5.352503	0.969091	-0.935183
C	6.006814	-0.203852	-0.556171
C	5.336439	-1.138181	0.235150
C	4.027378	-0.908696	0.641725
H	3.545250	2.120461	-0.820432
H	5.864747	1.702661	-1.548106
H	7.027362	-0.387222	-0.872445
H	5.838554	-2.051455	0.535562
H	3.521189	-1.638554	1.260990
C	-0.989552	0.661998	-2.184682
C	-1.869263	1.463868	-2.901101
C	-2.688468	2.374721	-2.230349
C	-2.618467	2.480450	-0.840304
C	-1.731678	1.686825	-0.121125
H	-0.356652	-0.050130	-2.704613
H	-1.922370	1.379073	-3.980712
H	-3.376446	2.999373	-2.788960
H	-3.254779	3.187179	-0.319215
H	-1.667285	1.762223	0.957783

System H Catalyzed (da 1a-BF_3)

E	-1442.99404
E_0	-1442.63941
$G_{198.15}$	-1442.67157
$G_{298.15}$	-1442.69721
$G_{398.15}$	-1442.72812

C	-1.830498	1.789940	-0.363268
C	-1.022598	0.853418	-1.035768
C	-0.917518	0.922462	-2.438776
C	-1.609589	1.891006	-3.151793
C	-2.415959	2.808593	-2.475070
C	-2.524180	2.753057	-1.084358
C	-0.260528	-0.156325	-0.335225
N	-0.483179	-0.531070	0.991330
C	0.752003	-0.571672	1.505751
C	1.613765	0.260045	0.723830
C	3.029942	0.059038	0.458938
C	3.798905	1.137586	-0.019960
C	5.143305	0.976113	-0.331865
C	5.752781	-0.268764	-0.173814
C	5.004572	-1.349641	0.296183
C	3.659742	-1.192786	0.607725
O	1.140915	-1.363048	2.473228
Si	1.114219	-1.481923	4.199646
C	0.385831	-3.151228	4.601906
C	2.919913	-1.387175	4.700037
C	0.139850	-0.037184	4.874162
H	0.288794	-0.865694	-0.940575
H	1.240882	1.266762	0.581775
H	3.020533	-1.487646	5.785838
H	3.504130	-2.188203	4.238451
H	3.368927	-0.433160	4.410246
H	0.401542	-3.323688	5.683185
H	-0.645321	-3.211682	4.251113
H	0.958228	-3.954165	4.128467
H	0.090005	-0.108430	5.965930
H	0.617471	0.916554	4.629923
H	-0.880405	-0.018014	4.486002
H	3.329189	2.107536	-0.146352
H	5.717365	1.820067	-0.697219
H	6.801545	-0.396723	-0.416080
H	5.473405	-2.319666	0.418048
H	3.089997	-2.037134	0.974672

H	-0.294271	0.204685	-2.961867
H	-1.527431	1.931406	-4.231753
H	-2.959629	3.564079	-3.031039
H	-3.155062	3.462363	-0.561401
H	-1.926269	1.743400	0.714219
B	-1.909103	-0.846195	1.697105
F	-2.815621	-1.062063	0.675961
F	-1.720707	-1.968545	2.498010
F	-2.242519	0.270175	2.476292

System I Uncatalyzed (da 1b)

E	-1232.85454
E_0	-1232.48232
$G_{198.15}$	-1232.51363
$G_{298.15}$	-1232.53827
$G_{398.15}$	-1232.56786

C	-1.713320	1.693349	-0.056732
C	-0.902907	0.765949	-0.726755
C	-1.005766	0.687774	-2.130651
C	-1.884455	1.492655	-2.829667
C	-2.697202	2.407366	-2.141559
C	-2.609855	2.502990	-0.747923
C	0.026921	-0.083703	-0.002650
N	-0.057368	-0.240457	1.380662
C	1.208156	-0.144143	1.701421
C	1.971616	0.525728	0.669188
C	3.352283	0.265968	0.286877
C	4.041284	1.199222	-0.513884
C	5.341783	0.961277	-0.941777
C	5.995932	-0.216903	-0.578985
C	5.330319	-1.153270	0.213887
C	4.027120	-0.920745	0.637678
O	1.744218	-0.606794	2.835335
Si	0.938717	-1.447816	4.099000
C	0.148756	-3.005860	3.415661
C	2.341184	-1.845543	5.277003
C	-0.322838	-0.309920	4.891593
H	0.482967	-0.887180	-0.571080
H	1.610481	1.524453	0.454421
H	1.971839	-2.379976	6.158043
H	3.095884	-2.474313	4.796409
H	2.836525	-0.933393	5.621026
H	-0.308859	-3.586458	4.223533
H	-0.628331	-2.762565	2.688122
H	0.889460	-3.645719	2.926935
H	-0.790749	-0.793937	5.755219
H	0.146375	0.614339	5.241272
H	-1.108170	-0.047404	4.179088
H	3.541294	2.119715	-0.798064
H	5.849669	1.697097	-1.555776
H	7.011823	-0.402565	-0.908654
H	5.831577	-2.070961	0.502318
H	3.525499	-1.653082	1.257862
H	-0.385191	-0.020414	-2.670279
H	-1.968987	1.434412	-3.908069
O	-3.530836	3.154002	-2.915885
H	-3.226712	3.201298	-0.198385
H	-1.640636	1.764604	1.022041
C	-4.392049	4.095588	-2.286421
H	-4.958321	4.562190	-3.090536
H	-5.082573	3.602810	-1.594078
H	-3.821584	4.862192	-1.751672

System I Catalyzed (da 1b-BF_3)

E	-1557.55194
E_0	-1557.16506
$G_{198.15}$	-1557.19891
$G_{298.15}$	-1557.22635
$G_{398.15}$	-1557.25954

C	3.655025	-1.149863	0.683684
C	3.010901	0.090103	0.530584
C	3.788934	1.174877	0.070340
C	5.133409	1.031871	-0.213616
C	5.757815	-0.213129	-0.047657
C	5.008030	-1.306255	0.403882
C	1.591764	0.276317	0.768883
C	0.725409	-0.563886	1.538148
O	1.110690	-1.353192	2.511884
Si	1.053866	-1.456405	4.236820
C	0.057885	-0.013503	4.883389
N	-0.499752	-0.541290	1.002269
B	-1.931409	-0.877220	1.681057
F	-2.298708	0.234616	2.452625
C	-0.255093	-0.162285	-0.320885
C	-1.016032	0.840267	-1.034300
C	-1.844643	1.768333	-0.375614
C	-2.534362	2.726598	-1.107346
C	-2.402119	2.786664	-2.495687
C	-1.575265	1.877430	-3.158732
C	-0.887359	0.913583	-2.435066
C	0.332031	-3.127510	4.644906
C	2.850118	-1.344886	4.769561

F	-2.816610	-1.110617	0.644985
F	-1.741959	-1.995135	2.489700
H	0.307095	-0.869514	-0.916790
H	1.210473	1.279297	0.622477
H	2.932114	-1.435969	5.857747
H	3.447447	-2.145950	4.324927
H	3.297589	-0.390151	4.479725
H	0.329665	-3.288046	5.728154
H	-0.692031	-3.200045	4.276101
H	0.919057	-3.930938	4.190490
H	-0.014328	-0.078213	5.974291
H	0.534562	0.941599	4.642660
H	-0.954221	-0.003134	4.473970
H	3.319431	2.143796	-0.064020
H	5.727133	1.867236	-0.564311
O	7.081732	-0.256684	-0.348851
H	5.465611	-2.277073	0.538415
H	3.091057	-2.004626	1.035496
H	-0.248672	0.202419	-2.948600
H	-1.473882	1.920263	-4.237053
H	-2.942664	3.538210	-3.059975
H	-3.181166	3.428695	-0.594036
H	-1.959882	1.718970	0.699867
C	7.780339	-1.489251	-0.206111
H	8.808190	-1.281249	-0.497205
H	7.760130	-1.839989	0.830837
H	7.365262	-2.259989	-0.863603

System L Uncatalyzed (da 1c)

E	-1322.86089
E_0	-1322.51868
$G_{198.15}$	-1322.55046
$G_{298.15}$	-1322.57533
$G_{398.15}$	-1322.60512

C	-1.765168	1.653768	-0.116914
C	-0.917515	0.752088	-0.787809
C	-0.974359	0.681177	-2.193366
C	-1.851679	1.476784	-2.911332
C	-2.684382	2.352251	-2.214395
C	-2.655115	2.447478	-0.824192
C	0.014080	-0.085153	-0.048362
N	-0.071263	-0.216497	1.332445
C	1.193506	-0.135427	1.664102
C	1.977013	0.529785	0.640132
C	3.358048	0.266389	0.275877
C	4.061293	1.204597	-0.507060
C	5.367737	0.965080	-0.913469
C	6.009530	-0.218583	-0.546148
C	5.329151	-1.160000	0.228503
C	4.020253	-0.926519	0.631067
O	1.718837	-0.591018	2.799552
Si	0.904712	-1.408455	4.081950
C	0.094769	-2.960323	3.410828
C	2.309176	-1.807814	5.254510
C	-0.336410	-0.238591	4.856549
H	0.489304	-0.882246	-0.609495
H	1.613358	1.523138	0.406196
H	1.937451	-2.323366	6.145628
H	3.051307	-2.455341	4.779406
H	2.819542	-0.898080	5.582359
H	-0.369603	-3.527099	4.224539
H	-0.681113	-2.715509	2.682492
H	0.826379	-3.615135	2.928349
H	-0.807926	-0.701745	5.729492
H	0.146701	0.684286	5.190271
H	-1.122264	0.023573	4.144510
H	3.568883	2.128575	-0.792481
H	5.889722	1.702225	-1.513283
H	7.030266	-0.405384	-0.859516
H	5.823555	-2.080682	0.517992
H	3.504423	-1.660668	1.237070
H	-0.323940	-0.009372	-2.719004
H	-1.908289	1.431469	-3.990008
N	-3.621667	3.200605	-2.971123
H	-3.319805	3.138396	-0.324176
H	-1.718190	1.709557	0.963402
O	-4.339335	3.966289	-2.336570
O	-3.630606	3.092406	-4.192912

System L Catalyzed (da 1c-BF_3)

E	-1647.55668
E_0	-1647.19986
$G_{198.15}$	-1647.23443
$G_{298.15}$	-1647.26226
$G_{398.15}$	-1647.29583

C	3.721837	-1.027981	0.731381
C	3.075942	0.186119	0.414151
C	3.822450	1.184438	-0.247173
C	5.154651	0.990964	-0.573768
C	5.757469	-0.218862	-0.238045

C	5.053840	-1.231960	0.410494
C	1.670958	0.423095	0.686338
C	0.826172	-0.304253	1.586126
O	1.268749	-0.927514	2.637486
Si	1.060140	-1.499530	4.267697
C	-0.060637	-0.331000	5.194248
N	-0.426243	-0.308128	1.107225
B	-1.839300	-0.516019	1.877393
F	-2.082238	0.641841	2.618929
C	-0.258546	-0.093083	-0.261470
C	-1.030423	0.849048	-1.033615
C	-1.776151	1.882115	-0.432123
C	-2.482015	2.777624	-1.223239
C	-2.449766	2.666713	-2.615024
C	-1.707134	1.651830	-3.222753
C	-1.000597	0.751462	-2.439245
C	0.485635	-3.274656	4.196946
C	2.815964	-1.403298	4.920460
F	-2.792709	-0.734912	0.902648
F	-1.668573	-1.620384	2.712169
H	0.266290	-0.867260	-0.806308
H	1.297317	1.407031	0.433928
H	2.853284	-1.747822	5.959168
H	3.497446	-2.032065	4.340723
H	3.198512	-0.379279	4.896120
H	0.473918	-3.696621	5.207661
H	-0.517268	-3.351940	3.777629
H	1.166959	-3.884237	3.595973
H	-0.098327	-0.633361	6.246634
H	0.322676	0.692943	5.160508
H	-1.075724	-0.332089	4.797867
H	3.343610	2.122992	-0.502970
H	5.731963	1.754296	-1.076835
N	7.174729	-0.433625	-0.579357
H	5.556397	-2.158669	0.651031
H	3.173029	-1.809897	1.238473
H	-0.425697	-0.041359	-2.906142
H	-1.685456	1.565277	-4.302699
H	-3.003600	3.370300	-3.226204
H	-3.063386	3.563722	-0.756028
H	-1.812073	1.963513	0.647177
O	7.679567	-1.506704	-0.268491
O	7.765807	0.473539	-1.154470

System M Uncatalyzed (da 1d-BF_3)

E	-887.17725
E_0	-886.91830
$G_{198.15}$	-886.94422
$G_{298.15}$	-886.96360
$G_{398.15}$	-886.98643

C	0.076915	-0.005536	-0.034937
C	-0.038861	-0.192338	1.351705
C	1.126554	-0.212762	2.135378
C	2.376636	-0.059400	1.548013
C	2.481006	0.113688	0.166291
C	1.329696	0.136416	-0.622144
C	-1.350759	-0.356770	1.976670
N	-2.479003	-0.629411	1.225952
C	-3.340663	0.178048	1.814422
C	-2.684966	1.248404	2.494654
H	-3.141262	1.743368	3.350143
O	-4.665873	0.009927	1.819246
Si	-5.552667	-1.324627	1.200108
C	-4.967586	-2.903408	2.028412
C	-7.312247	-0.902637	1.686628
C	-5.344200	-1.393228	-0.661110
H	-1.343992	-0.659835	3.018012
H	-2.034352	1.871179	1.895314
H	-8.010204	-1.670259	1.337694
H	-7.413145	-0.826341	2.772837
H	-7.621151	0.052798	1.253651
H	-5.585031	-3.750387	1.711311
H	-3.930432	-3.123815	1.767012
H	-5.040079	-2.829788	3.117538
H	-5.953595	-2.195281	-1.090474
H	-5.652490	-0.453059	-1.127649
H	-4.299751	-1.578165	-0.922706
H	1.043404	-0.350692	3.208781
H	3.270126	-0.077318	2.161853
H	3.456011	0.232778	-0.292926
H	1.411285	0.270847	-1.694995
H	-0.825530	0.013995	-0.634093

System M Catalyzed (da 1d-BF_3)

E	-1211.87548
E_0	-1211.60174
$G_{198.15}$	-1211.63026
$G_{298.15}$	-1211.65244
$G_{398.15}$	-1211.67888

C	-1.501723	1.958793	-0.771450
C	-0.928350	0.695424	-1.018690

N	-1.073142	0.387380	-2.325821
C	-1.176019	1.644739	-2.910526
H	-2.516258	2.126270	-1.104305
O	-0.283475	0.000499	-0.119771
Si	1.183125	-0.900435	0.102973
C	1.877166	-0.128870	1.667678
H	2.112774	0.929951	1.526432
H	1.165447	-0.208291	2.494188
H	2.798462	-0.636223	1.972130
C	0.713781	-2.681165	0.397035
H	0.005109	-2.760454	1.226474
H	1.601771	-3.264532	0.662678
H	0.259914	-3.120586	-0.491480
C	2.335726	-0.608485	-1.342488
H	3.308284	-1.063195	-1.125105
H	1.950209	-1.050394	-2.261600
H	2.509302	0.459544	-1.507258
B	-1.258705	-1.059919	-3.030864
F	-0.307664	-1.902164	-2.452960
F	-1.040384	-0.871069	-4.385082
F	-2.552073	-1.501576	-2.753663
C	-2.152112	2.009614	-3.918488
C	-3.334402	1.276152	-4.125255
C	-4.242140	1.685230	-5.093825
C	-3.992525	2.826222	-5.857919
C	-2.826623	3.567031	-5.653872
C	-1.914950	3.163531	-4.688802
H	-3.525735	0.384865	-3.541384
H	-5.146514	1.110893	-5.256718
H	-4.706170	3.139045	-6.611827
H	-2.632565	4.452137	-6.248295
H	-1.006872	3.735174	-4.527633
H	-0.297760	2.273700	-2.843622
H	-1.151648	2.581013	0.047043