Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Supporting Information for

Domino Synthesis of 1,3,5-Trisubstituted Hydantoins: a DFT Study

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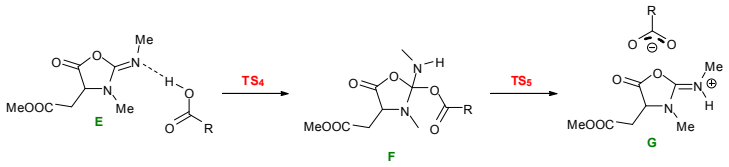

Scheme S1 Calculated mechanism for the formal protonation of imino-oxazolidinone **5**

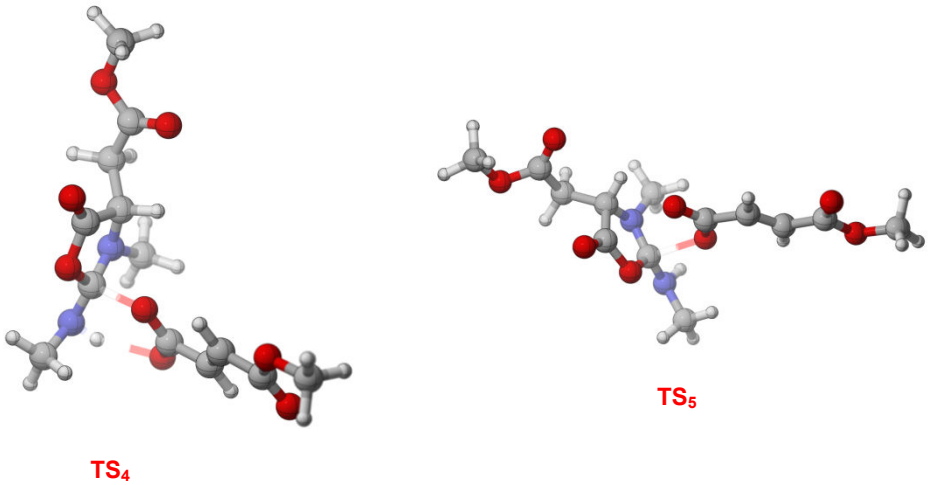

Fig. S1 Transition states for the formal protonation of imino-oxazolidinone **5**

The following pages contain the coordinates and energies for all structures. Alternative stationary points with higher energy than those described in the main text are labeled with one or more prime symbols (e.g **D″**).

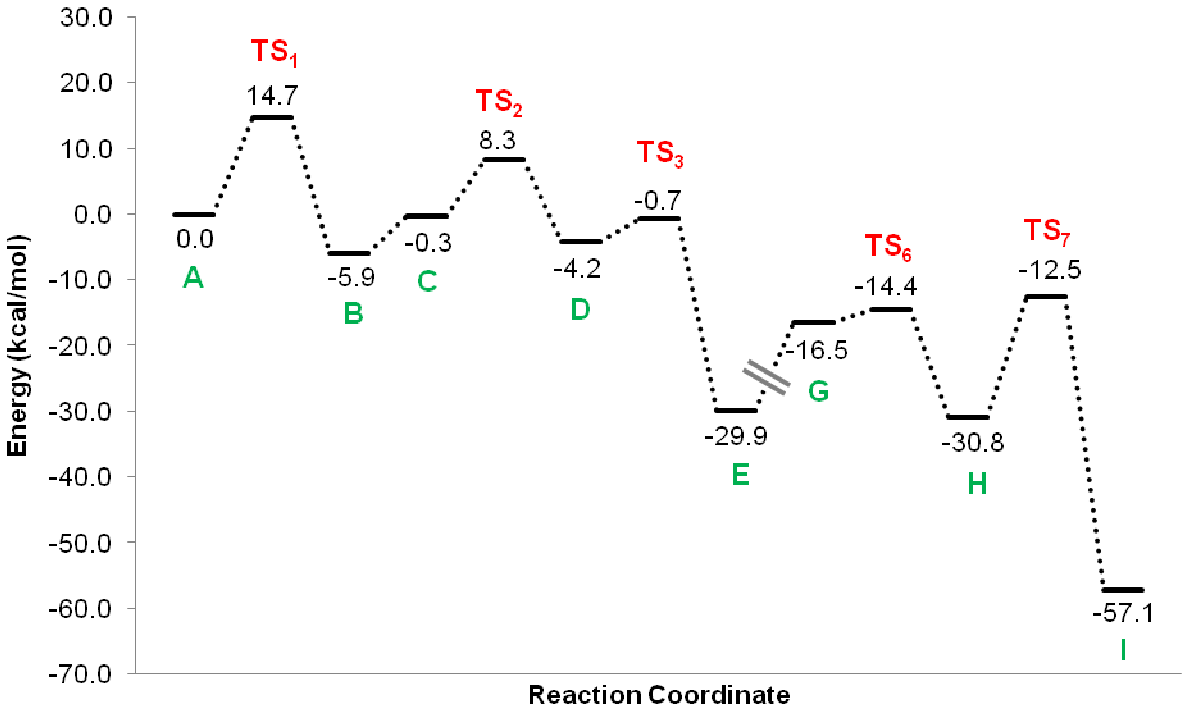

Fig. S2 MPW1K potential energy profile for Pathway A

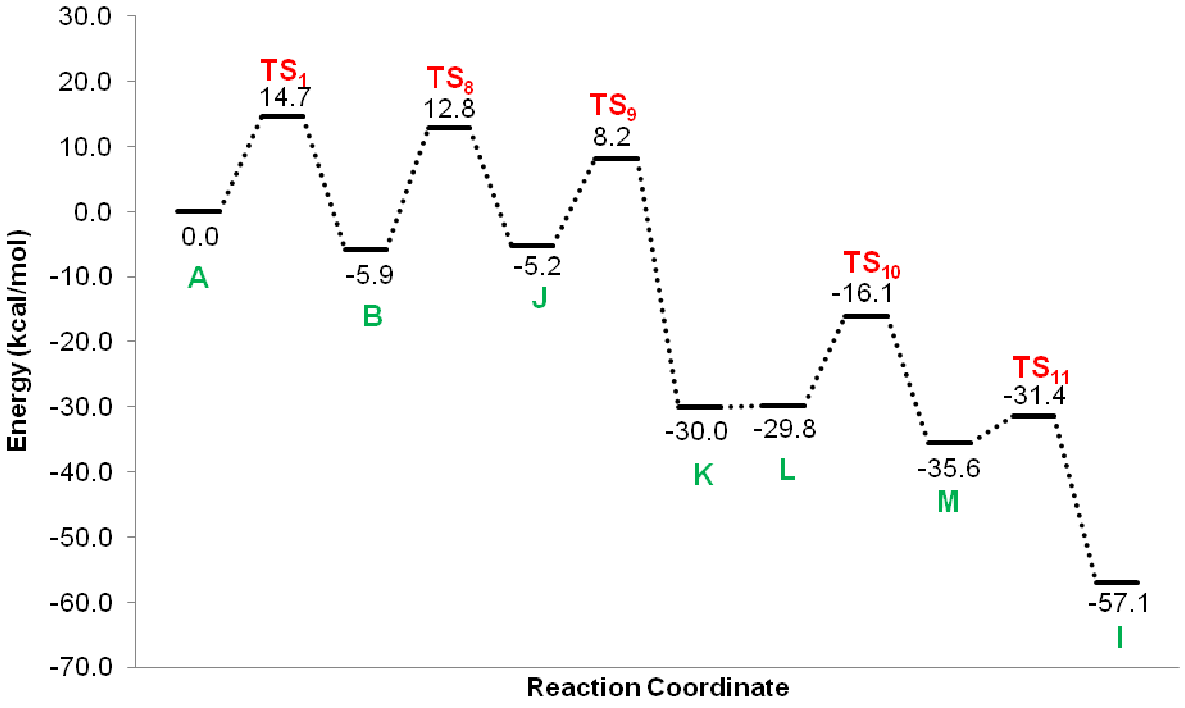

Fig. S3 MPW1K potential energy profile for Pathway B

1a

***B3LYP* [Hartree]: -495.213665181**
***MPW1K* [Hartree]: -495.024736409**
***ZPE* [kcal/mol]: 69.6**
***CPCM* [kcal/mol]: -10.4**

C	0.025927	0.110047	0.808862
O	0.104893	0.197079	-0.399108
O	-0.016584	1.189390	1.625422
H	0.028503	1.970110	1.047899
C	-0.037171	-1.153305	1.584782
H	-0.106787	-1.094510	2.666121
C	-0.008686	-2.336776	0.963045
H	0.060940	-2.395828	-0.118339
C	-0.071725	-3.602635	1.738478
O	-0.150719	-3.685399	2.947348
O	-0.028126	-4.667237	0.909015
C	-0.082503	-5.949933	1.555642
H	0.761946	-6.070318	2.238646
H	-0.037263	-6.686252	0.754153
H	-1.010643	-6.053432	2.123035

2

***B3LYP* [Hartree]: -227.473596927**
***MPW1K* [Hartree]: -227.386463848**
***ZPE* [kcal/mol]: 56.7**
***CPCM* [kcal/mol]: -2.9**

H	0.826896	0.362216	0.411766
C	0.040270	-0.227655	0.892585
H	-0.716900	-0.445516	0.132737
H	0.474227	-1.173138	1.237964
N	-0.560076	0.559309	1.958926
C	-0.625614	0.258590	3.145068
N	-0.636755	0.131681	4.363977
C	-1.678363	-0.493314	5.164959
H	-2.522888	-0.863570	4.572294
H	-2.054404	0.232733	5.892560
H	-1.250392	-1.329335	5.727164

3

***B3LYP* [Hartree]: -722.763256672**
***MPW1K* [Hartree]: -722.516808067**
***ZPE* [kcal/mol]: 130.7**
***CPCM* [kcal/mol]: -8.9**

O	-0.105526	3.919889	2.493791
C	-0.059781	1.063706	0.517736
C	-0.083554	3.120464	1.577473
O	0.029316	-0.134262	0.329453
N	-0.034339	1.717611	1.729037
C	0.087646	1.069200	3.022540
H	1.014325	1.371362	3.517214
H	0.094508	-0.006737	2.846598
H	-0.755223	1.340718	3.662222
N	-0.093816	3.376614	0.225116
C	-0.419368	4.689506	-0.295289
H	-0.370962	5.394682	0.535207
H	-1.428480	4.711100	-0.727213
H	0.297433	4.997391	-1.063426
C	-0.189515	2.152039	-0.555135
H	-1.173446	2.058396	-1.037138
C	0.886731	1.998638	-1.642365
H	1.877943	1.854298	-1.208016
H	0.913991	2.912329	-2.247858
C	0.536241	0.854964	-2.579151
O	-0.575132	0.655163	-3.020187
O	1.618386	0.120079	-2.888491
C	1.373127	-0.988624	-3.774076
H	0.672106	-1.689507	-3.315768
H	2.343070	-1.460204	-3.927585
H	0.959320	-0.638815	-4.722687

A

***B3LYP* [Hartree]: -722.699228603**
***MPW1K* [Hartree]: -722.424356599**
***ZPE* [kcal/mol]: 127.2**
***CPCM* [kcal/mol]: -6.6**

C	-0.812375	-3.265845	4.218332
O	-0.634316	-1.957687	3.652024
C	-0.522512	-1.924972	2.304542
O	-0.565239	-2.913170	1.599394
C	-0.342192	-0.529804	1.831559
C	-0.209020	-0.256789	0.529520
C	-0.027032	1.143048	0.053930
O	0.081317	1.197788	-1.275850
O	0.016017	2.113614	0.794465
C	0.172238	4.616563	-1.115447
N	0.630584	3.847868	-1.972010
C	1.812736	4.137463	-2.786501
N	-0.437044	5.342148	-0.357328
C	-0.325954	5.456345	1.092219
H	-0.231148	-1.051003	-0.209856
H	-0.320783	0.265957	2.568911
H	-1.724541	-3.729635	3.834756
H	-0.882621	-3.113751	5.294946
H	0.037241	-3.908608	3.974845
H	0.377626	6.256356	1.344251
H	0.000998	4.516394	1.541985
H	-1.303725	5.731459	1.492954
H	2.593474	3.402791	-2.566876
H	2.212773	5.141286	-2.612878
H	1.548866	4.041477	-3.843561
H	0.214841	2.146721	-1.553912

TS_1

***B3LYP* [Hartree]: -722.672346486**
***MPW1K* [Hartree]: -722.396884023**
***ZPE* [kcal/mol]: 125.5**
***CPCM* [kcal/mol]: -7.5**

C	0.456235	-0.883767	-0.131845
O	0.942790	0.288250	-0.103940
O	1.138383	-1.955281	-0.201502
C	-1.029926	-1.047904	-0.082028
H	-1.405914	-2.066615	-0.096455
C	-1.873137	-0.011395	-0.025134
H	-1.501381	1.007390	-0.013726
C	-3.339938	-0.220030	0.023116
O	-3.909907	-1.293076	0.018317
O	-3.988133	0.969421	0.075847
C	-5.419823	0.879885	0.125840
H	-5.805382	0.368125	-0.759601
H	-5.779349	1.908112	0.160982
H	-5.740865	0.330172	1.014342
C	3.056013	0.452356	-0.149597
N	3.303926	1.618039	-0.339513
C	2.695798	2.851313	0.106470
H	3.132916	3.165070	1.060273
H	1.620539	2.705215	0.229573
H	2.882923	3.632938	-0.632210
N	3.342110	-0.794446	-0.035826
C	4.655357	-1.241545	0.437866
H	4.517273	-1.997686	1.214926
H	5.224876	-0.405545	0.849287
H	5.222491	-1.683891	-0.387096
H	2.441078	-1.476433	-0.150821

B

***B3LYP* [Hartree]: -722.701133123**
***MPW1K* [Hartree]: -722.437562215**
***ZPE* [kcal/mol]: 128.9**
***CPCM* [kcal/mol]: -6.0**

C	-0.744604	-2.739266	4.388016
O	-0.514701	-1.533203	3.638749
C	-0.502142	-1.683457	2.297574
O	-0.669423	-2.742684	1.728711
C	-0.257573	-0.375792	1.631369
C	-0.209711	-0.299072	0.296140
C	0.040273	0.942451	-0.471992
O	0.136121	0.949221	-1.684718
O	0.140590	2.033557	0.329273
C	0.368197	3.361680	-0.135315
N	1.182316	3.452041	-1.230498
C	1.427788	4.771318	-1.794313
N	-0.074537	4.353899	0.510873
C	-0.819686	4.206957	1.744382
H	-0.343787	-1.189572	-0.309716
H	-0.120344	0.494934	2.262170
H	-1.711270	-3.174628	4.124014
H	-0.729186	-2.441664	5.435721
H	0.039974	-3.471560	4.183082
H	-0.202773	4.532738	2.591737
H	-1.171804	3.189010	1.949284
H	-1.689662	4.871728	1.713737
H	2.114311	4.661388	-2.636580
H	1.887146	5.413454	-1.040243
H	0.507997	5.263593	-2.135772
H	1.083304	2.682238	-1.881543

C

***B3LYP* [Hartree]: -1217.919153750**
***MPW1K* [Hartree]: -1217.467990330**
***ZPE* [kcal/mol]: 199.4**
***CPCM* [kcal/mol]: -13.6**

C	0.312563	-1.875961	3.266573
N	0.699727	-2.588234	0.252379
C	-0.586747	-2.671633	0.735469
O	-1.008215	-1.438174	1.259672
C	-0.435875	-0.917456	2.405878
C	1.240550	-3.699482	-0.517921
N	-1.293999	-3.718912	0.691269
C	-2.604294	-3.763707	1.314337
O	-0.609034	0.246205	2.660877
C	1.050526	-1.425489	4.290436
C	1.798078	-2.328272	5.195583
O	1.631124	-3.631037	4.927047
C	2.340029	-4.547577	5.782982
O	2.507916	-1.938226	6.114536
O	3.277414	0.516055	7.107340
C	2.811444	1.556512	6.411689
O	2.098126	1.462923	5.425077
C	3.268274	2.850558	6.986645
C	2.896519	4.013510	6.441669
C	3.352512	5.303911	7.016709
O	4.075997	5.432887	7.984063
O	2.848882	6.341297	6.310983
C	3.227168	7.643575	6.784689
H	0.682373	-3.880933	-1.445211
H	1.192097	-4.609695	0.082290
H	2.283891	-3.482951	-0.756738
H	0.959031	-1.660487	-0.056832
H	-3.354980	-3.995481	0.550408
H	-2.902149	-2.835922	1.817024
H	-2.631824	-4.583022	2.042075
H	0.238971	-2.936439	3.055698
H	1.152925	-0.364099	4.505680
H	3.416344	-4.374230	5.718000
H	2.086016	-5.541035	5.416370
H	2.020528	-4.424223	6.819964
H	4.313004	7.763175	6.753175
H	2.887458	7.791681	7.812758
H	2.742957	8.352938	6.114293
H	2.252793	4.035548	5.568350
H	3.910667	2.826190	7.861034
H	2.957995	-0.320995	6.690370

C′

***B3LYP* [Hartree]: -1217.916069890**
***MPW1K* [Hartree]: -1217.464855940**
***ZPE* [kcal/mol]: 199.2**
***CPCM* [kcal/mol]: -9.9**

N	-2.896889	-5.610419	-1.971742
C	-0.613017	-4.189244	-0.517741
C	-0.855178	-5.497335	0.170523
O	-1.292915	-6.546851	-0.595251
C	-1.721673	-6.323785	-1.923743
C	-0.131880	-3.169545	0.205634
C	0.149224	-1.846710	-0.392020
O	-0.004284	-1.526114	-1.561216
O	-0.646804	-5.682052	1.345650
N	-1.081808	-6.714310	-2.941905
C	0.254918	-7.266458	-2.826048
C	-4.058027	-5.969236	-1.164132
O	0.616306	-0.996203	0.535003
C	0.925795	0.332205	0.073046
O	-0.692772	-1.704160	-4.226420
C	-1.482821	-2.715504	-4.591335
O	-1.901251	-3.567393	-3.821924
C	-1.784186	-2.677933	-6.046613
C	-2.479873	-3.656818	-6.634219
C	-2.773390	-3.613946	-8.089363
O	-2.425074	-2.738452	-8.855748
O	-3.495032	-4.695314	-8.458101
C	-3.836296	-4.756029	-9.852654
H	0.036287	0.805447	-0.348492
H	1.706716	0.297272	-0.689897
H	1.270645	0.872669	0.953213
H	0.064385	-3.289754	1.265770
H	-0.829718	-4.073056	-1.574692
H	0.621613	-7.375082	-1.798203
H	0.955613	-6.634984	-3.385454
H	0.272047	-8.253237	-3.302028
H	-3.079548	-5.275951	-2.909802
H	-4.597873	-6.842661	-1.557024
H	-4.745611	-5.120493	-1.130318
H	-3.743970	-6.195453	-0.143953
H	-2.933223	-4.789923	-10.467107
H	-4.417370	-5.669554	-9.974019
H	-4.425592	-3.882411	-10.141774
H	-2.839777	-4.505493	-6.062117
H	-1.414703	-1.836628	-6.623950
H	-0.515093	-1.760194	-3.258819

TS_2

***B3LYP* [Hartree]: -1217.883903270**
***MPW1K* [Hartree]: -1217.443153480**
***ZPE* [kcal/mol]: 196.6**
***CPCM* [kcal/mol]: -12.31**

H	-1.706009	-4.609320	0.457631
C	-2.747697	-4.516063	0.138072
H	-2.800066	-4.688756	-0.939919
H	-3.366785	-5.243390	0.664750
O	-3.289210	-3.237130	0.485609
C	-2.655934	-2.150520	-0.019124
O	-1.654234	-2.339318	-0.817646
C	-3.168620	-0.920917	0.334560
H	-4.036266	-0.851853	0.976291
C	-2.601574	0.262073	-0.295660
H	-2.084632	-0.022121	-1.222116
C	-3.548802	1.405261	-0.615514
O	-4.675848	1.379825	-0.998142
O	-2.875974	2.626070	-0.436838
C	-1.638642	2.452443	0.125932
N	-0.761803	3.313242	0.347272
C	-0.974566	4.704543	-0.028462
H	-1.933304	4.896910	-0.520181
H	-0.159711	5.007361	-0.692733
H	-0.901532	5.320800	0.872977
N	-1.464913	1.047425	0.492442
H	-0.503194	0.667743	0.122648
C	-1.470731	0.847662	1.970705
H	-0.606855	1.372413	2.376968
H	-1.411912	-0.223766	2.158012
H	-2.394479	1.240386	2.399424
H	7.549279	0.151334	-0.886261
C	7.163006	0.739517	-0.050124
H	7.525033	1.765859	-0.103401
H	7.477272	0.268333	0.884507
O	5.730781	0.828588	-0.114485
C	5.078583	-0.355970	-0.060380
O	5.638481	-1.429375	0.038263
C	3.611239	-0.145632	-0.136885
H	3.241590	0.870870	-0.219518
C	2.766681	-1.182212	-0.107694
H	3.139205	-2.198379	-0.027632
C	1.286610	-1.005680	-0.187063
O	0.815094	0.155007	-0.296009
O	0.622663	-2.099828	-0.129443
H	-0.531958	-2.126834	-0.440099

TS_2'

***B3LYP* [Hartree]:** **-1217.876527320**
***MPW1K* [Hartree]:** **-1217.435096410**
***ZPE* [kcal/mol]:** **196.9**
***CPCM* [kcal/mol]:** **-12.9**

H	2.259402	-1.723210	1.793631
C	1.787855	-2.474392	2.425062
H	1.395508	-3.287499	1.811905
H	2.488175	-2.860879	3.163824
N	0.670912	-1.828924	3.170606
H	1.131538	-1.072960	3.792634
C	-0.353564	-1.234670	2.312755
N	-0.076234	-0.583994	1.283968
C	-1.130530	-0.001185	0.464245
H	-1.006994	1.086141	0.469240
H	-2.144187	-0.248600	0.794412
H	-0.991367	-0.337479	-0.567384
O	-1.589576	-1.521317	2.824952
C	-1.538230	-2.431001	3.894446
O	-2.537915	-2.817253	4.411744
C	-0.095019	-2.781962	4.215663
H	0.121612	-3.800064	3.878515
C	0.323927	-2.521688	5.582957
H	-0.079208	-1.653023	6.087365
C	1.513836	-3.026341	6.072134
O	2.198508	-2.501297	7.018584
O	2.013207	-4.151161	5.472801
C	3.250697	-4.651136	5.994587
H	4.035759	-3.891967	5.953108
H	3.510214	-5.502383	5.363275
H	3.135620	-4.976886	7.031491
C	2.879950	6.239865	3.624101
H	3.862056	6.467225	4.046147
H	2.117235	6.747563	4.219941
H	2.827132	6.557224	2.582922
O	2.651022	4.822239	3.611089
C	2.683741	4.224748	4.826668
O	2.887799	4.823578	5.863497
C	2.438247	2.767886	4.695929
H	2.269720	2.363776	3.703464
C	2.426813	1.970153	5.769213
H	2.598497	2.374517	6.761709
C	2.182258	0.497687	5.665484
O	1.991363	-0.011400	4.535692
O	2.201004	-0.099167	6.803324
H	2.159220	-1.272767	6.893302

D

***B3LYP* [Hartree]:** **-1217.911075420**
***MPW1K* [Hartree]:** **-1217.474033400**
***ZPE* [kcal/mol]:** **200.2**
***CPCM* [kcal/mol]:** **-9.0**

C	-0.033051	-0.291167	4.388239
O	-0.203078	0.673746	3.353688
C	-0.465221	0.042082	2.186147
C	-0.348466	-1.464386	2.391511
N	-0.339825	-1.519450	3.857761
O	-0.754920	0.641907	1.175952
C	-1.424911	-2.204584	1.679162
C	-1.181421	-3.250611	0.859147
O	0.018852	-3.869298	0.855355
C	0.365955	-4.651360	-0.296803
C	-0.021262	-2.742944	4.566058
N	0.310107	-0.023490	5.568897
C	0.527856	1.347474	5.996050
O	-2.080861	-3.781829	0.017181
O	-3.418671	-1.556782	-0.829448
C	-3.069779	-0.592056	-1.504261
O	-2.088203	0.245227	-1.198399
C	-3.722745	-0.216135	-2.784739
C	-4.755148	-0.917485	-3.264606
C	-5.406075	-0.532142	-4.543945
O	-6.429610	-1.367265	-4.822922
C	-7.136647	-1.083072	-6.042310
O	-5.076051	0.398993	-5.249709
H	0.628810	-1.778819	1.986308
H	-0.625209	-3.552258	4.149944
H	-0.261095	-2.609187	5.621235
H	1.042246	-3.008345	4.479409
H	0.435920	2.091495	5.196287
H	1.527740	1.432052	6.436351
H	-0.189388	1.599909	6.785949
H	-2.437501	-1.824814	1.732211
H	-2.717682	-3.075036	-0.227650
H	1.384344	-4.994908	-0.113101
H	0.336754	-4.048577	-1.209716
H	-0.302907	-5.506907	-0.409701
H	-6.462886	-1.150198	-6.899904
H	-7.566704	-0.079163	-6.009857
H	-7.921079	-1.835914	-6.109530
H	-5.141284	-1.778793	-2.729709
H	-3.340741	0.648368	-3.317639
H	-1.668625	0.061951	-0.322716

D′

***B3LYP* [Hartree]:** **-1217.904777190**
***MPW1K* [Hartree]:** **-1217.468427230**
***ZPE* [kcal/mol]:** **200.0**
***CPCM* [kcal/mol]:** **-10.7**

C	0.347885	-2.708676	3.577261
N	0.136743	-1.779908	2.471067
C	-0.996988	-2.115783	1.756006
O	-1.725473	-3.053197	2.504696
C	-0.999138	-3.443764	3.604412
C	1.246838	-1.124898	1.804162
N	-1.341022	-1.656548	0.633455
C	-2.592026	-2.066784	0.019677
O	-1.410015	-4.230308	4.408427
C	0.688708	-2.070203	4.896426
C	1.470554	-2.714588	5.818796
O	2.073811	-3.866681	5.503422
C	3.049847	-4.402862	6.412583
O	1.730207	-2.273004	7.045410
O	1.542816	0.379360	7.014412
C	2.050830	0.971319	6.061492
O	2.284808	0.414211	4.877483
C	2.449680	2.391106	6.171796
C	2.961137	3.100526	5.158927
C	3.333913	4.528261	5.354039
O	3.219693	5.148149	6.391259
O	3.822044	5.047103	4.208688
C	4.213917	6.429739	4.279465
H	0.842208	-0.522312	0.991363
H	1.957642	-1.851937	1.383705
H	1.777760	-0.475657	2.503832
H	1.878411	-0.502410	4.841330
H	-3.251882	-1.196577	-0.080241
H	-3.131642	-2.846399	0.569691
H	-2.392781	-2.431480	-0.994459
H	1.116939	-3.459405	3.332343
H	0.002475	-1.317612	5.273238
H	3.872689	-3.700077	6.566613
H	3.414165	-5.310244	5.931743
H	2.593738	-4.643228	7.374808
H	4.996236	6.566756	5.029665
H	3.358070	7.055652	4.542975
H	4.583619	6.681203	3.286269
H	3.116830	2.665618	4.177913
H	2.298069	2.846119	7.144898
H	1.514250	-1.304528	7.116064

D″

***B3LYP* [Hartree]:** **-1217.903814860**
***MPW1K* [Hartree]:** **-1217.467252770**
***ZPE* [kcal/mol]:** **200.4**
***CPCM* [kcal/mol]:** **-10.1**

N	-1.446373	-5.099623	-1.785831
C	-0.216052	-4.265741	-1.539543
C	0.861636	-5.344589	-1.452846
O	0.246665	-6.583394	-1.444803
C	-1.136931	-6.443081	-1.490429
C	-0.229770	-3.355928	-0.360848
C	-0.448294	-2.022316	-0.467612
O	-0.753187	-1.323803	-1.570343
O	2.049207	-5.222258	-1.397132
N	-1.976219	-7.362833	-1.321789
C	-1.538730	-8.725952	-1.064683
C	-2.746384	-4.613398	-1.297208
O	-0.342189	-1.258275	0.635000
C	-0.720146	0.121083	0.552526
O	-1.610963	-2.539697	-3.898110
C	-1.867349	-3.409621	-4.729587
O	-1.886952	-4.709996	-4.472507
C	-2.186374	-3.051453	-6.130956
C	-2.498105	-3.947641	-7.074572
C	-2.809635	-3.503237	-8.460217
O	-2.811854	-2.352182	-8.845747
O	-3.093693	-4.565551	-9.242312
C	-3.409877	-4.253019	-10.610307
H	-1.762228	0.232124	0.239660
H	-0.078556	0.668752	-0.142203
H	-0.591694	0.510201	1.562858
H	-0.025953	-3.747285	0.627832
H	-0.010639	-3.690124	-2.447684
H	-0.453762	-8.841150	-0.966434
H	-1.887104	-9.372160	-1.878177
H	-2.016083	-9.083665	-0.146239
H	-1.697318	-4.887379	-3.498210
H	-3.508417	-5.327275	-1.608082
H	-2.945732	-3.638380	-1.744089
H	-2.761204	-4.519243	-0.207642
H	-2.567409	-3.750851	-11.091810
H	-3.613496	-5.209358	-11.090393
H	-4.285216	-3.601107	-10.660677
H	-2.533270	-5.010498	-6.862251
H	-2.157675	-1.992145	-6.363166
H	-1.003797	-1.882405	-2.334600

TS_3

***B3LYP* [Hartree]:** **-1217.897327750**
***MPW1K* [Hartree]:** **-1217.460285430**
***ZPE* [kcal/mol]:** **196.8**
***CPCM* [kcal/mol]:** **-10.7**

N	0.610953	-1.392903	1.303915
C	1.267324	-1.150702	0.029722
H	1.468093	-0.080569	-0.128166
H	0.644016	-1.520937	-0.786241
H	2.217028	-1.684912	0.033944
C	1.362630	-1.543371	2.453530
N	2.595743	-1.792091	2.520393
C	3.245590	-1.981404	3.805482
H	2.595551	-1.810062	4.671333
H	4.105380	-1.305646	3.876663
H	3.639146	-3.003023	3.866882
O	0.505089	-1.392756	3.558987
C	-0.737188	-0.996235	3.135307
O	-1.662268	-0.836834	3.881107
C	-0.693642	-0.825843	1.613702
C	-1.855457	-1.502380	0.910810
H	-1.952286	-2.565362	1.138287
C	-3.106943	-0.845894	0.888885
O	-3.184848	0.418447	1.268552
C	-4.432130	1.118739	1.069915
H	-5.223648	0.654341	1.660051
H	-4.710675	1.115351	0.014451
H	-4.242596	2.133295	1.416363
O	-4.183283	-1.384305	0.411476
H	-3.946786	-2.209722	-0.218444
H	-0.724283	0.257059	1.406299
O	-2.040459	-5.307020	-5.553625
C	-3.019035	-5.403382	-4.840977
O	-4.052369	-6.237954	-5.085968
C	-3.926138	-7.035828	-6.275123
H	-4.830741	-7.641137	-6.320483
H	-3.039237	-7.671455	-6.217279
H	-3.844580	-6.397218	-7.158025
C	-3.256517	-4.635052	-3.591268
H	-4.178075	-4.811161	-3.046761
C	-2.353933	-3.751322	-3.151433
H	-1.433890	-3.578007	-3.699828
C	-2.563376	-2.963880	-1.909074
O	-3.591839	-3.151724	-1.211175
O	-1.628382	-2.114777	-1.638474
H	-1.695939	-1.723367	-0.517711

TS_3'

***B3LYP* [Hartree]:** **-1217.893654710**
***MPW1K* [Hartree]:** **-1217.456318050**
***ZPE* [kcal/mol]:** **196.3**
***CPCM* [kcal/mol]:** **-11.1**

C	0.665448	-0.720572	1.883922
O	1.384168	-0.641085	0.929016
O	0.481783	0.311531	2.771354
C	-0.180931	-1.905805	2.351790
H	0.521583	-2.656970	2.756457
N	-0.965558	-1.296679	3.413070
C	-1.638937	-2.104757	4.412935
H	-2.340731	-2.788125	3.927629
H	-2.187359	-1.437532	5.077235
H	-0.929243	-2.694141	5.012559
C	-0.439138	-0.064987	3.761652
N	-0.736015	0.614453	4.779752
C	-0.142220	1.922645	4.995771
H	0.616735	2.202549	4.256178
H	0.314420	1.950022	5.991571
H	-0.930237	2.684840	4.986533
C	-1.029376	-2.503220	1.233775
H	-2.056419	-2.724699	1.523318
C	-0.464682	-3.505712	0.413229
O	-1.104772	-4.094108	-0.542105
H	-1.973261	-3.521087	-0.842577
O	0.813368	-3.813360	0.569304
C	1.444344	-4.645237	-0.427486
H	2.488815	-4.703406	-0.125859
H	1.354913	-4.187413	-1.414044
H	0.990193	-5.637665	-0.440774
O	-5.598221	1.005894	-3.597588
C	-5.599072	-0.207634	-3.640156
O	-6.439457	-0.934658	-4.409389
C	-7.361962	-0.167004	-5.200281
H	-6.823189	0.494179	-5.883344
H	-8.005073	0.439617	-4.557977
H	-7.951293	-0.895970	-5.755439
C	-4.695411	-1.100995	-2.870345
H	-4.803271	-2.172847	-2.996907
C	-3.774268	-0.593679	-2.043784
H	-3.665679	0.479057	-1.922362
C	-2.851837	-1.459183	-1.263807
O	-2.970261	-2.713213	-1.327699
O	-1.979432	-0.829416	-0.559158
H	-1.439466	-1.545628	0.225032

E

***B3LYP* [Hartree]: -1217.946915670**
***MPW1K* [Hartree]: -1217.510013840**
***ZPE* [kcal/mol]: 200.5**
***CPCM* [kcal/mol]: -12.5**

N	0.076158	-0.529426	2.448863
C	-0.440151	-0.754939	1.108010
C	-1.210345	0.534464	0.858607
O	-0.934454	1.400761	1.896757
C	-0.085670	0.780734	2.810318
O	-1.956718	0.807690	-0.035353
C	-1.349303	-1.985697	0.964810
C	-1.565711	-2.323974	-0.501297
O	-2.797501	-2.814482	-0.712919
C	-3.086148	-3.187516	-2.075049
N	0.426347	1.371776	3.811860
C	0.094632	2.768232	4.084958
C	1.124913	-1.351068	3.042503
O	-0.719279	-2.199710	-1.360085
O	3.847269	0.415063	3.673976
C	3.699457	0.650514	4.864157
C	4.823255	0.681047	5.843585
C	6.083130	0.459452	5.454271
C	7.200249	0.492250	6.430421
O	8.377120	0.237773	5.813795
C	9.529428	0.246100	6.671219
O	2.530677	0.902635	5.453471
O	7.096769	0.713449	7.620563
H	0.361352	-0.834214	0.357989
H	2.124618	-0.972715	2.805946
H	1.015667	-2.374347	2.678809
H	1.004642	-1.358456	4.128081
H	-0.854202	-2.848966	1.424885
H	-2.304657	-1.845344	1.474182
H	-2.999956	-2.318646	-2.730836
H	-4.108805	-3.562080	-2.063946
H	-2.394353	-3.961673	-2.414525
H	-0.282472	3.304410	3.209386
H	0.992806	3.272832	4.450940
H	-0.660380	2.825472	4.877883
H	1.783036	0.940026	4.775355
H	4.592841	0.890790	6.883276
H	6.311854	0.251864	4.414060
H	9.650013	1.224405	7.143160
H	10.378739	0.024130	6.025778
H	9.431856	-0.510865	7.453393

E′

***B3LYP* [Hartree]: -1217.944836760**
***MPW1K* [Hartree]: -1217.507648940**
***ZPE* [kcal/mol]: 200.5**
***CPCM* [kcal/mol]: -11.2**

C	-0.294221	-0.059591	3.690757
O	0.368898	0.215400	2.477983
C	0.524319	-0.935801	1.759437
C	-0.050170	-2.090615	2.572457
N	-0.676485	-1.388606	3.672344
O	1.033297	-0.976828	0.673052
C	-1.020999	-2.947192	1.735364
C	-0.352140	-3.610624	0.550933
O	0.787827	-4.225583	0.889325
C	1.525834	-4.830426	-0.193132
C	-1.087481	-2.060823	4.890152
N	-0.502108	0.770650	4.612052
C	-0.086436	2.156145	4.478664
O	-0.796924	-3.634002	-0.585024
O	-2.831185	-2.313068	-1.848405
C	-3.570012	-1.512296	-1.078533
O	-3.405175	-1.360281	0.123142
C	-4.645088	-0.797070	-1.812760
C	-4.861691	-0.913297	-3.127968
C	-5.960579	-0.156620	-3.781368
O	-5.989304	-0.415904	-5.108384
C	-7.017118	0.268883	-5.842294
O	-6.735157	0.593715	-3.222703
H	0.788717	-2.721534	2.907788
H	-1.847987	-2.814468	4.667255
H	-1.512485	-1.313056	5.559028
H	-0.240536	-2.548169	5.394926
H	0.477457	2.372592	3.564126
H	0.529694	2.430550	5.342088
H	-0.971352	2.802581	4.499947
H	-1.423939	-3.743293	2.373005
H	-2.129777	-2.749335	-1.302925
H	2.407919	-5.271532	0.268779
H	1.810020	-4.067727	-0.920542
H	0.922272	-5.595610	-0.685095
H	-6.898258	1.351286	-5.750229
H	-8.005807	-0.008705	-5.468458
H	-6.896974	-0.043889	-6.879060
H	-4.247973	-1.554604	-3.750587
H	-5.269046	-0.147579	-1.207622
H	-1.855345	-2.345488	1.366362

TS_4

***B3LYP* [Hartree]:** **-1217.918973550**
***MPW1K* [Hartree]:** **-1217.485705070**
***ZPE* [kcal/mol]:** **201.0**
***CPCM* [kcal/mol]:** **-11.8**

C	0.456457	0.496539	1.363021
O	0.611972	0.729630	0.202140
C	0.203404	-0.829230	2.067168
H	1.151888	-1.383836	2.110695
O	0.425508	1.493418	2.326626
C	0.290020	0.901066	3.555623
N	-0.107611	1.714117	4.571882
N	-0.225793	-0.367976	3.386115
C	-0.325415	-1.308910	4.492788
H	0.649504	-1.711957	4.786934
H	-0.985970	-2.126948	4.197134
H	-0.772305	-0.811433	5.353745
C	-0.837634	-1.670085	1.318776
H	-1.184711	-2.480165	1.970841
H	-1.710289	-1.077352	1.038257
C	-0.217443	-2.324813	0.094604
O	0.917868	-2.745808	0.047400
O	-1.104393	-2.414803	-0.910116
C	-0.613667	-3.047044	-2.108657
H	0.231571	-2.485977	-2.512670
H	-1.450328	-3.038757	-2.806001
H	-0.295245	-4.070680	-1.898842
C	0.295777	3.124460	4.508242
H	1.384831	3.247241	4.478387
H	-0.097077	3.620500	5.396803
H	-0.137314	3.594864	3.624974
C	2.529248	0.420323	5.039109
O	2.122752	0.595010	3.814529
O	1.802106	0.371023	6.047012
H	0.183763	1.282131	5.454442
C	4.009188	0.272437	5.212737
H	4.349390	0.107220	6.230793
C	4.887923	0.336349	4.205911
H	4.560713	0.501910	3.185339
C	6.342483	0.182275	4.454415
O	6.865717	-0.007244	5.534621
O	7.034795	0.280659	3.294730
C	8.458177	0.142559	3.420746
H	8.864376	0.920290	4.072449
H	8.855039	0.242844	2.410828
H	8.714725	-0.833852	3.839474

F

***B3LYP* [Hartree]:** **-1217.919184150**
***MPW1K* [Hartree]:** **-1217.492986830**
***ZPE* [kcal/mol]:** **201.2**
***CPCM* [kcal/mol]:** **-13.6**

C	0.900552	0.390766	3.138983
N	0.116337	-0.799271	2.979919
C	0.067222	-1.166168	1.570492
C	0.664274	0.050123	0.882914
O	1.140238	0.908395	1.840695
C	0.271043	-1.874493	3.949806
C	-1.358487	-1.450450	1.064873
C	-1.329659	-2.083386	-0.314760
O	-0.584069	-2.983530	-0.635979
O	0.705031	0.301112	-0.288270
N	0.238356	1.349987	3.931961
C	0.964328	2.528530	4.391643
O	-2.259096	-1.546035	-1.126597
C	-2.293417	-2.089119	-2.458998
O	2.965875	-1.281166	2.148780
C	3.169108	-0.598965	3.133721
C	4.493611	-0.553059	3.801921
C	4.789072	0.202210	4.866249
C	6.155231	0.174783	5.452450
O	7.079818	-0.504728	5.056491
O	2.241714	0.171711	3.750376
O	6.234368	1.020552	6.503211
C	7.519623	1.078509	7.145572
H	0.708548	-2.026303	1.339950
H	1.171088	-2.480288	3.774293
H	-0.602532	-2.530749	3.900536
H	0.317674	-1.461727	4.960532
H	-1.828048	-2.174920	1.740802
H	-1.970210	-0.546558	1.066856
H	-1.338790	-1.918506	-2.961464
H	-3.096656	-1.559693	-2.970416
H	-2.494391	-3.162728	-2.432058
H	1.727671	2.319882	5.152943
H	0.243235	3.240860	4.800534
H	1.450856	3.000734	3.535156
H	-0.343487	0.907800	4.630902
H	5.250103	-1.190775	3.355272
H	4.055743	0.852503	5.328742
H	7.800533	0.094816	7.529306
H	7.409116	1.792673	7.960762
H	8.284542	1.413166	6.440751

F′

***B3LYP* [Hartree]: -1217.919639660**
***MPW1K* [Hartree]: -1217.492727590**
***ZPE* [kcal/mol]: 201.6**
***CPCM* [kcal/mol]: -12.1**

N	-0.098437	-0.450586	3.336007
C	0.229444	-0.926357	1.995683
C	0.563096	0.367822	1.273804
O	0.700677	1.354990	2.214484
C	0.547574	0.816701	3.504857
O	0.670825	0.571412	0.097905
C	-0.917906	-1.672253	1.300891
C	-0.426684	-2.371112	0.045019
O	-1.352327	-2.337152	-0.929319
C	-0.976654	-2.990739	-2.156153
N	-0.125411	1.728458	4.331591
C	0.448063	3.074403	4.433697
C	-0.031300	-1.440795	4.403348
O	0.648642	-2.922621	-0.054479
O	2.029785	0.609342	3.883693
C	2.409795	0.494484	5.165860
C	3.884211	0.389544	5.324361
C	4.763205	0.438571	4.316496
C	6.221371	0.325542	4.585185
O	6.920196	0.402855	3.432393
C	8.347433	0.303274	3.572973
O	1.659843	0.472159	6.130839
O	6.728589	0.182982	5.679301
H	1.123320	-1.571705	1.977283
H	0.954579	-1.924930	4.471866
H	-0.782501	-2.212566	4.216295
H	-0.251464	-0.979713	5.365372
H	-1.297312	-2.450702	1.973258
H	-1.747904	-1.001890	1.071441
H	-0.088707	-2.517199	-2.580502
H	-1.830335	-2.873816	-2.822678
H	-0.766607	-4.048218	-1.979591
H	1.445977	3.101640	4.892247
H	-0.227570	3.680498	5.040673
H	0.506514	3.517847	3.438934
H	-0.242247	1.318097	5.252146
H	4.227115	0.268309	6.347143
H	4.445489	0.561859	3.287257
H	8.726906	1.109376	4.205549
H	8.748602	0.384970	2.563486
H	8.622003	-0.654857	4.020831

TS_5

***B3LYP* [Hartree]: -1217.913455530**
***MPW1K* [Hartree]: -1217.477819980**
***ZPE* [kcal/mol]: 200.7**
***CPCM* [kcal/mol]: -16.4**

C	0.276852	0.671227	3.239457
N	-0.267709	-0.566145	3.097224
C	-0.045382	-1.031722	1.725805
C	0.490397	0.222127	1.055065
O	0.567604	1.227774	2.051638
C	-0.315545	-1.503234	4.212503
C	-1.335908	-1.524206	1.048221
C	-1.016157	-2.245306	-0.252029
O	-0.142266	-3.075819	-0.366891
O	0.674931	0.468061	-0.092998
N	-0.040993	1.514204	4.247427
C	0.676511	2.791218	4.351411
O	-1.844176	-1.867740	-1.240842
C	-1.606701	-2.501444	-2.513220
O	2.765998	-0.652191	1.975616
C	3.029178	-0.232853	3.118021
C	4.463349	-0.290141	3.568120
C	4.877890	0.101500	4.778677
C	6.303624	0.017390	5.168702
O	7.215079	-0.398555	4.480975
O	2.179350	0.244930	3.962774
O	6.479718	0.477734	6.434915
C	7.832658	0.439845	6.909693
H	0.734896	-1.796370	1.672946
H	0.689316	-1.673281	4.612116
H	-0.737997	-2.444824	3.859557
H	-0.973309	-1.126227	5.001766
H	-1.820048	-2.254455	1.707265
H	-2.040754	-0.708031	0.878703
H	-0.599479	-2.271204	-2.866617
H	-2.355691	-2.089684	-3.188440
H	-1.716446	-3.584943	-2.427964
H	1.741940	2.625107	4.530783
H	0.234179	3.360410	5.170339
H	0.546075	3.350933	3.425125
H	-0.135768	1.032516	5.132384
H	5.173213	-0.681766	2.845091
H	4.174538	0.490935	5.506542
H	8.213479	-0.584837	6.911510
H	7.802402	0.838246	7.923928
H	8.481809	1.050740	6.276988

G

***B3LYP* [Hartree]:** **-1217.915728550**
***MPW1K* [Hartree]:** **-1217.479209220**
***ZPE* [kcal/mol]:** **201.0**
***CPCM* [kcal/mol]:** **-18.9**

N	-0.286357	-0.544500	3.182327
C	0.037443	-1.027551	1.836030
C	0.626378	0.215432	1.185838
O	0.457352	1.289621	2.154990
C	0.076530	0.740566	3.295662
O	0.886326	0.457265	0.054900
C	-1.204388	-1.524635	1.073635
C	-0.791950	-2.277256	-0.182269
O	-1.540134	-1.919420	-1.238644
C	-1.211256	-2.583021	-2.475541
N	-0.166454	1.527596	4.345171
C	0.548055	2.805918	4.472139
C	-0.348227	-1.436643	4.336844
O	0.083812	-3.113314	-0.209728
O	2.270356	0.253293	4.255374
C	3.040332	-0.113966	3.314996
C	4.515039	-0.230167	3.610929
C	5.034367	0.023627	4.817930
C	6.484699	-0.099511	5.078901
O	6.766769	0.218680	6.371357
C	8.152799	0.132168	6.726020
O	2.695034	-0.402305	2.135595
O	7.338095	-0.434055	4.280311
H	0.808888	-1.799187	1.863080
H	0.611002	-1.407107	4.864095
H	-0.545771	-2.448372	3.981963
H	-1.169602	-1.151492	5.001781
H	-1.742781	-2.235400	1.711629
H	-1.886918	-0.707537	0.831500
H	-0.179396	-2.363653	-2.757312
H	-1.905846	-2.184330	-3.213715
H	-1.332286	-3.663849	-2.373875
H	1.611269	2.616580	4.641694
H	0.111860	3.355508	5.307012
H	0.414747	3.384202	3.558422
H	-0.263525	1.017578	5.213317
H	5.157214	-0.536328	2.789920
H	4.391576	0.329207	5.636570
H	8.526645	-0.885595	6.585493
H	8.209028	0.417537	7.776800
H	8.753130	0.809455	6.112728

TS_6

***B3LYP* [Hartree]:** **-1217.914693850**
***MPW1K* [Hartree]:** **-1217.477094090**
***ZPE* [kcal/mol]:** **200.8**
***CPCM* [kcal/mol]:** **-18.0**

N	-0.370525	-0.494886	3.222701
C	0.045525	-1.009135	1.914274
C	0.771532	0.182449	1.292003
O	0.457466	1.329274	2.241294
C	-0.011299	0.794463	3.336524
O	0.992587	0.428943	0.151584
C	-1.148676	-1.433892	1.042564
C	-0.674804	-2.264181	-0.139381
O	-1.353494	-1.962415	-1.258178
C	-0.965778	-2.706089	-2.429602
N	-0.271113	1.566773	4.394092
C	0.445851	2.836584	4.562309
C	-0.514996	-1.371549	4.379782
O	0.183323	-3.116647	-0.065319
O	2.221561	0.214928	4.302567
C	2.966589	-0.042876	3.323503
C	4.453107	-0.150903	3.541812
C	5.009182	0.001077	4.749042
C	6.471428	-0.111170	4.946581
O	6.792473	0.082904	6.252757
C	8.191910	-0.006870	6.551169
O	2.602689	-0.241239	2.114994
O	7.299612	-0.343478	4.087870
H	0.746088	-1.838956	2.018057
H	0.430656	-1.416808	4.930022
H	-0.786028	-2.367423	4.027778
H	-1.324562	-1.024436	5.029541
H	-1.813270	-2.071383	1.638425
H	-1.727097	-0.572953	0.702356
H	0.084638	-2.520503	-2.663267
H	-1.608364	-2.343608	-3.230946
H	-1.112609	-3.776874	-2.270302
H	1.499872	2.643964	4.780898
H	-0.022875	3.387479	5.378670
H	0.362217	3.420053	3.646112
H	-0.444598	1.056719	5.248981
H	5.068627	-0.362551	2.672563
H	4.389969	0.211500	5.614609
H	8.581122	-0.994419	6.289719
H	8.278059	0.166177	7.624034
H	8.755704	0.746861	5.995112

H

***B3LYP* [Hartree]: -1217.943515090**
***MPW1K* [Hartree]: -1217.508976980**
***ZPE* [kcal/mol]: 200.9**
***CPCM* [kcal/mol]: -14.5**

N	0.363239	-0.332729	3.236323
C	0.489328	-1.024103	1.958984
C	1.670206	-0.517272	1.126643
O	0.426574	1.652926	2.120739
C	0.223925	1.046419	3.173960
O	1.674395	-0.432481	-0.066103
C	-0.786239	-0.994068	1.098111
C	-0.775334	-2.094767	0.055469
O	-1.511325	-1.760308	-1.019837
C	-1.573386	-2.756609	-2.055450
N	-0.092605	1.688408	4.348032
C	-0.331203	3.124196	4.336335
C	0.127802	-1.110230	4.446299
O	-0.214430	-3.163208	0.186298
O	2.961216	-1.973658	3.182499
C	3.350441	-0.874272	2.849831
C	4.482272	-0.141283	3.468351
C	5.189783	-0.696128	4.458868
C	6.322517	0.034107	5.085415
O	6.894408	-0.719921	6.048584
C	8.009561	-0.110514	6.721408
O	2.837443	-0.143397	1.819559
O	6.692318	1.150985	4.785848
H	0.725435	-2.069272	2.176118
H	0.595942	-0.620517	5.305195
H	0.603807	-2.084837	4.337177
H	-0.940584	-1.262624	4.661205
H	-1.646921	-1.178874	1.752949
H	-0.922971	-0.019998	0.629353
H	-0.572703	-2.970322	-2.437629
H	-2.199024	-2.327629	-2.837575
H	-2.012597	-3.682128	-1.675057
H	-0.143415	3.530506	5.333402
H	-1.354876	3.379959	4.033690
H	0.355683	3.581540	3.624822
H	-0.525216	1.158534	5.087857
H	4.720196	0.849387	3.095981
H	4.953520	-1.690540	4.823578
H	8.806300	0.119267	6.009911
H	8.347030	-0.843030	7.453647
H	7.700051	0.814198	7.214412

TS_7

***B3LYP* [Hartree]: -1217.918394170**
***MPW1K* [Hartree]: -1217.482811840**
***ZPE* [kcal/mol]: 201.1**
***CPCM* [kcal/mol]: -12.8**

H	-3.144746	1.678197	1.035974
C	-3.208001	2.737680	0.774898
H	-4.188970	3.137844	1.029304
H	-3.012954	2.846902	-0.294858
O	-2.265716	3.504062	1.540559
C	-0.969642	3.166375	1.361287
O	-0.600724	2.279691	0.616486
C	-0.086178	4.020528	2.198141
H	-0.547429	4.789541	2.810928
C	1.240080	3.835788	2.172200
H	1.681254	3.076057	1.534354
C	2.193562	4.657362	2.958570
O	3.413308	4.581316	2.734159
O	1.654113	5.410761	3.888890
C	2.350714	6.878762	4.335651
O	2.264014	7.738997	3.481790
C	1.791952	7.023034	5.771110
H	1.916369	8.081328	6.035503
N	2.668363	6.193900	6.602285
C	2.404361	5.943564	8.010845
H	2.267509	6.888717	8.548600
H	3.262145	5.413779	8.424169
H	1.507891	5.330164	8.138192
C	3.842122	5.812304	6.045444
O	4.758919	5.196166	6.545129
N	3.875295	6.304255	4.653694
H	3.981811	5.509551	3.961004
C	4.921760	7.324755	4.404095
H	5.902975	6.858905	4.499378
H	4.825051	8.141429	5.121805
H	4.759833	7.708186	3.396685
C	0.303069	6.662047	5.911398
H	-0.032612	6.921940	6.921793
H	0.149555	5.598747	5.739794
C	-0.560205	7.427024	4.921756
O	-1.291573	6.923846	4.099027
O	-0.419023	8.756924	5.094258
C	-1.089239	9.579467	4.120770
H	-0.660106	9.404454	3.131888
H	-0.916132	10.607728	4.436571
H	-2.157775	9.355921	4.098471

I

***B3LYP* [Hartree]:** -1217.989343150
***MPW1K* [Hartree]:** -1217.555588340
***ZPE* [kcal/mol]:** 201.2
***CPCM* [kcal/mol]:** -11.8

N	3.768223	7.434907	4.719208
C	2.829362	8.403935	5.015189
C	1.855415	7.763961	6.012870
N	2.458619	6.454915	6.236144
C	3.516441	6.243318	5.411626
O	1.303642	4.666045	3.856605
C	1.809288	3.606398	3.511482
O	3.033420	3.207043	3.857968
O	2.773253	9.526014	4.554630
C	0.427077	7.691662	5.432227
C	-0.171583	9.058273	5.146465
O	-0.025636	9.882307	6.208153
C	-0.502902	11.225088	6.010020
C	1.858107	5.397434	7.025778
O	4.181490	5.214557	5.279938
C	4.848048	7.589113	3.759478
C	1.127460	2.600780	2.652591
C	-0.106290	2.816356	2.184380
C	-0.781880	1.809824	1.326713
O	-0.312167	0.743991	0.982467
O	-2.012526	2.240672	0.971270
C	-2.757071	1.340852	0.134040
O	-0.740081	9.364253	4.124795
H	-2.916147	0.386744	0.642572
H	-3.707730	1.836819	-0.058765
H	-2.222279	1.155887	-0.800769
H	-0.638004	3.732322	2.420402
H	1.660392	1.685974	2.413865
H	1.844073	8.357623	6.933898
H	1.585514	5.779500	8.014315
H	2.598779	4.605647	7.142500
H	0.974191	4.980846	6.532541
H	3.462339	3.909984	4.413448
H	5.815428	7.445336	4.246259
H	4.778511	8.600479	3.358612
H	4.745648	6.860313	2.952052
H	-0.220867	7.188762	6.159712
H	0.416164	7.104694	4.512287
H	0.050303	11.703310	5.198770
H	-0.325114	11.742503	6.952369
H	-1.567620	11.222921	5.766145

TS_8

***B3LYP* [Hartree]:** -722.672456485
***MPW1K* [Hartree]:** -722.405558809
***ZPE* [kcal/mol]:** 127.5
***CPCM* [kcal/mol]:** -6.0

H	-1.144877	0.305569	0.180006
C	-0.251858	0.371001	0.806366
H	0.606460	0.604256	0.171470
H	-0.377521	1.130960	1.576836
O	-0.037926	-0.863496	1.510011
C	0.137977	-1.949641	0.725066
O	0.122185	-1.917202	-0.488986
C	0.349066	-3.162550	1.555533
H	0.340024	-3.055722	2.635246
C	0.545574	-4.356475	0.985626
H	0.554092	-4.463985	-0.093840
C	0.754849	-5.575491	1.813563
O	0.780168	-5.559435	3.037219
O	0.908984	-6.649326	1.024943
C	1.211001	-8.053327	1.466756
N	0.878075	-8.248973	2.774871
H	0.791337	-7.411463	3.343286
C	1.210488	-9.515456	3.398284
H	0.756015	-10.341303	2.842948
H	0.809459	-9.519909	4.413937
H	2.293663	-9.694006	3.445910
N	1.630425	-8.819793	0.621461
C	2.108033	-9.707709	-0.356411
H	2.430474	-10.674057	0.059751
H	2.959034	-9.278599	-0.903296
H	1.328797	-9.913869	-1.102556

J

***B3LYP* [Hartree]:** -722.693920140
***MPW1K* [Hartree]:** -722.431298763
***ZPE* [kcal/mol]:** 128.8
***CPCM* [kcal/mol]:** -9.1

C	0.021734	-2.860354	-0.712739
N	0.329432	-1.995106	0.420547
C	-0.371120	-2.001378	1.598507
O	-1.242730	-3.064997	1.647911
C	-1.688246	-3.544722	2.875646
C	-0.670950	-3.662862	3.948392
C	-1.030953	-4.066005	5.173111
C	-0.011528	-4.236841	6.236761
O	-0.593413	-4.626293	7.393385
C	0.307229	-4.823054	8.494948
N	-0.310416	-1.183410	2.574522
C	0.634946	-0.085325	2.486322
O	-2.823577	-3.937955	2.953185
O	1.183730	-4.059687	6.107721
H	-0.027385	-3.899162	-0.384680
H	0.827670	-2.766891	-1.443900
H	-0.929255	-2.607960	-1.198254
H	0.768694	-1.113079	0.204229
H	0.379495	0.623599	1.680863
H	1.669385	-0.422993	2.316150
H	0.619561	0.477112	3.422678
H	0.367248	-3.446438	3.731132
H	-2.068083	-4.270950	5.415333
H	1.041280	-5.597031	8.257404
H	-0.316434	-5.129955	9.333977
H	0.837042	-3.896057	8.727775

J′

***B3LYP* [Hartree]: -722.690618454**
***MPW1K* [Hartree]: -722.426577321**
***ZPE* [kcal/mol]: 129.0**
***CPCM* [kcal/mol]: -8.2**

C	-0.240742	0.360518	0.951432
O	-0.308666	-0.956294	1.524705
C	0.280302	-1.930231	0.798402
C	0.148591	-3.241581	1.484906
C	0.665288	-4.350411	0.943649
C	0.537230	-5.659316	1.630723
O	1.136574	-6.615006	0.889539
C	1.285029	-7.994500	1.213185
N	1.841444	-8.635068	0.275640
C	1.906724	-10.083974	0.295649
O	0.836288	-1.744154	-0.264803
O	-0.038043	-5.820228	2.695618
N	0.807024	-8.374744	2.441553
C	1.510472	-9.347196	3.275951
H	-0.736624	0.380160	-0.022062
H	0.799653	0.668738	0.823044
H	-0.751859	1.014819	1.656624
H	-0.376205	-3.275183	2.433961
H	1.189652	-4.319200	-0.005360
H	0.338079	-7.626470	2.941493
H	1.395055	-10.369738	2.911470
H	1.074972	-9.300104	4.275976
H	2.582707	-9.127926	3.357989
H	2.063780	-10.435626	-0.728192
H	0.986716	-10.550234	0.675569
H	2.747710	-10.458260	0.894737

K

***B3LYP* [Hartree]: -722.730259228**
***MPW1K* [Hartree]: -722.470382747**
***ZPE* [kcal/mol]: 129.6**
***CPCM* [kcal/mol]: -10.2**

C	0.545856	-3.230717	-0.631817
N	0.184021	-2.213952	0.344390
C	-0.212566	-2.586588	1.600708
O	-0.358374	-3.756277	1.927242
C	-0.625662	-1.653954	3.864088
C	-0.090879	-2.888366	4.505789
C	-0.412373	-3.157641	5.777206
C	0.152955	-4.345149	6.462256
O	-0.346356	-4.450107	7.716455
C	0.139761	-5.568760	8.473759
N	-0.483095	-1.499017	2.470640
C	-0.798782	-0.176266	1.919323
O	-1.109802	-0.750338	4.533369
O	0.955753	-5.125419	5.990608
H	-0.131563	-4.077290	-0.520293
H	1.571511	-3.594857	-0.495029
H	0.444963	-2.815072	-1.637044
H	0.529383	-1.278386	0.197494
H	-1.457397	-0.273576	1.053951
H	0.110365	0.364898	1.627114
H	-1.298820	0.391077	2.701459
H	0.560107	-3.555684	3.958199
H	-1.087499	-2.517383	6.334222
H	-0.104804	-6.508371	7.972061
H	-0.358369	-5.509119	9.441106
H	1.224298	-5.508925	8.595523

TS_9

***B3LYP* [Hartree]: -722.670573880**
***MPW1K* [Hartree]: -722.404984114**
***ZPE* [kcal/mol]: 127.9**
***CPCM* [kcal/mol]: -11.4**

H	0.076490	-4.051414	-0.430549
C	0.307154	-3.068106	-0.840124
H	1.280394	-3.110300	-1.335471
H	-0.459874	-2.810015	-1.580310
N	0.361450	-2.111375	0.257943
H	0.728447	-1.190722	0.068886
C	-0.392948	-2.240658	1.373335
N	-0.537931	-1.394559	2.359676
C	0.156424	-0.144986	2.556309
H	-0.110282	0.597865	1.789591
H	1.250636	-0.260164	2.562416
H	-0.139431	0.271681	3.522138
O	-1.065570	-3.333318	1.614677
C	-1.545804	-2.761528	3.145892
O	-2.713525	-2.570615	3.303788
C	-0.579001	-3.364837	4.096579
H	0.431801	-3.559209	3.757237
C	-0.942103	-3.648079	5.352238
H	-1.952222	-3.461559	5.700502
C	0.034011	-4.232349	6.301568
O	1.200598	-4.477258	6.062428
O	-0.548545	-4.466033	7.500816
C	0.313216	-5.037876	8.496551
H	0.698845	-6.004523	8.162855
H	-0.303610	-5.158295	9.386763
H	1.158384	-4.375771	8.701270

L

***B3LYP* [Hartree]: -1217.958116500**
***MPW1K* [Hartree]: -1217.510399300**
***ZPE* [kcal/mol]: 200.0**
***CPCM* [kcal/mol]: -11.7**

N	1.590716	1.024240	0.265599
C	4.229824	0.268307	-0.281212
C	3.509016	-1.033528	-0.449800
N	2.341647	-1.216073	0.273854
C	1.551077	-0.186678	0.884285
C	4.850424	0.822308	-1.326766
C	5.458657	2.162226	-1.285621
O	5.963419	2.503760	-0.096038
C	6.495052	3.841196	0.003695
O	3.977739	-1.923956	-1.148736
C	1.816240	-2.583862	0.359134
O	0.891553	-0.411453	1.887932
C	0.823789	2.129171	0.818560
O	5.476460	2.916844	-2.255041
O	3.499167	2.765105	-4.128828
C	2.316040	2.368097	-3.667326
O	2.105444	1.977912	-2.525412
C	1.229269	2.420478	-4.677748
C	1.394635	2.831348	-5.940282
C	0.243678	2.849409	-6.881520
O	0.634106	3.292020	-8.096291
C	-0.404550	3.353374	-9.088447
O	-0.894108	2.522358	-6.611135
H	7.318231	3.974976	-0.700696
H	6.845897	3.935803	1.030097
H	5.717198	4.577091	-0.209856
H	4.811611	0.355061	-2.304690
H	4.209088	0.765977	0.681710
H	1.157591	-2.630799	1.224422
H	2.647164	-3.280177	0.470561
H	1.264925	-2.847727	-0.549310
H	1.870017	1.107111	-0.702473
H	-0.247985	1.905571	0.844760
H	0.994618	3.005607	0.191443
H	1.145537	2.347565	1.840612
H	2.359260	3.159126	-6.311492
H	0.253797	2.095589	-4.330623
H	4.189454	2.755549	-3.415288
H	-0.834493	2.362635	-9.254498
H	0.075398	3.721381	-9.994457
H	-1.198813	4.032636	-8.769315

L′

***B3LYP* [Hartree]: -1217.957896050**
***MPW1K* [Hartree]: -1217.510114480**
***ZPE* [kcal/mol]: 199.9**
***CPCM* [kcal/mol]: -11.7**

N	1.562785	1.013358	0.260142
C	4.200726	0.269566	-0.267070
C	3.507619	-1.053470	-0.391067
N	2.331220	-1.224548	0.321504
C	1.528643	-0.186523	0.900462
C	4.805125	0.810504	-1.330185
C	5.407564	2.154856	-1.312746
O	5.916237	2.512866	-0.129545
C	6.449764	3.850150	-0.048862
O	4.006360	-1.954611	-1.054281
C	1.822258	-2.590775	0.497060
O	0.851230	-0.405288	1.893616
C	0.744743	2.107814	0.761841
O	5.424942	2.896587	-2.292310
O	3.453713	2.787994	-4.145912
C	2.269822	2.392586	-3.685186
O	2.061395	1.993749	-2.545809
C	1.179193	2.466430	-4.689593
C	1.345571	2.885197	-5.949458
C	0.192600	2.922803	-6.887605
O	0.586313	3.362934	-8.102402
C	-0.453167	3.437924	-9.092672
O	-0.948198	2.606871	-6.616913
H	7.268281	3.975003	-0.760523
H	6.808161	3.956406	0.973820
H	5.671451	4.585116	-0.265322
H	4.758765	0.326024	-2.299601
H	4.194079	0.781563	0.688847
H	1.473279	-2.697937	1.523509
H	2.630104	-3.286701	0.280729
H	0.991189	-2.787745	-0.187688
H	1.868998	1.082082	-0.704022
H	-0.324393	1.873952	0.706430
H	0.951419	2.990491	0.155003
H	0.988527	2.316987	1.806173
H	2.312958	3.204445	-6.320698
H	0.201250	2.150202	-4.341626
H	4.146015	2.757911	-3.433500
H	-0.894144	2.452334	-9.260273
H	0.029509	3.802480	-9.998704
H	-1.239382	4.125294	-8.771119

TS_{10}

***B3LYP* [Hartree]: -1217.923142970**
***MPW1K* [Hartree]: -1217.484316320**
***ZPE* [kcal/mol]: 197.6**
***CPCM* [kcal/mol]: -11.9**

O	5.451492	-5.500842	-2.308667
C	6.472909	-5.391045	-3.313358
H	6.235093	-4.588772	-4.016147
H	6.490838	-6.354479	-3.821836
H	7.441761	-5.179667	-2.854173
C	5.262969	-4.392331	-1.557309
O	5.896368	-3.365540	-1.696750
C	4.187686	-4.618229	-0.558267
H	3.700339	-5.587177	-0.538587
C	3.827583	-3.650621	0.291804
H	4.313757	-2.680830	0.267263
C	2.744551	-3.844223	1.297672
O	2.164101	-4.952001	1.377669
O	2.516824	-2.802791	2.021358
H	1.580979	-2.718561	2.678446
H	-1.488016	-0.766527	3.391421
C	-1.059692	-0.607228	4.384920
H	-0.148265	-0.012587	4.279455
H	-1.775032	-0.085916	5.022580
O	-0.798471	-1.848150	5.045887
C	0.083363	-2.687406	4.445394
O	0.552954	-2.321167	3.307588
C	0.331947	-3.870567	5.120972
H	-0.178646	-4.075910	6.051289
C	1.261626	-4.825793	4.557615
H	2.108012	-4.351659	4.050802
C	1.807748	-5.882776	5.504399
O	2.326535	-5.699043	6.578188
N	1.642977	-7.157738	4.928119
C	2.085267	-8.386054	5.579700
H	2.791307	-8.916188	4.937186
H	1.229504	-9.034178	5.780236
H	2.566938	-8.097046	6.513154
C	0.967355	-7.176341	3.738168
O	0.628031	-8.139161	3.097094
N	0.689854	-5.783647	3.350296
H	1.296140	-5.501053	2.497676
C	-0.728002	-5.562075	2.956194
H	-1.002381	-6.340989	2.245082
H	-0.790173	-4.576964	2.496866
H	-1.365120	-5.591723	3.839598

TS_{10}'

***B3LYP* [Hartree]: -1217.915989730**
***MPW1K* [Hartree]: -1217.476891520**
***ZPE* [kcal/mol]: 197.6**
***CPCM* [kcal/mol]: -13.8**

C	4.943074	2.187490	-1.296650
O	5.134930	2.873314	-2.359162
O	5.228709	2.780947	-0.093642
C	5.762165	4.108705	-0.155065
H	6.736953	4.117782	-0.649703
H	5.868845	4.428601	0.882793
H	5.092419	4.783042	-0.694683
C	4.431030	0.903661	-1.258418
H	4.233573	0.429831	-2.211600
C	3.737805	0.411026	-0.081565
H	4.192500	0.730631	0.860303
C	3.460212	-1.086405	-0.048034
O	4.270551	-1.977871	-0.098812
N	2.069839	-1.301279	0.062039
C	1.474805	-2.632143	0.132488
H	0.937851	-2.753292	1.075675
H	2.291430	-3.350307	0.066749
H	0.778424	-2.774810	-0.696327
C	1.313223	-0.166222	0.158248
O	0.129219	-0.072290	0.355856
N	2.222659	0.987624	-0.007551
H	2.063302	1.436694	-0.975781
C	1.986137	2.062335	0.996053
H	0.948715	2.387240	0.921435
H	2.667000	2.879317	0.762108
H	2.188916	1.680193	1.998475
C	0.156427	2.889362	-6.775826
O	-1.025552	2.739552	-6.536819
O	0.642664	3.160973	-8.009196
C	1.261282	2.804164	-5.788331
H	2.275453	2.957516	-6.140195
C	1.008303	2.543913	-4.500741
H	-0.011840	2.394779	-4.161140
C	2.071550	2.441799	-3.455962
O	1.694390	2.221412	-2.282530
O	3.279088	2.592478	-3.876651
H	4.164396	2.684120	-3.135366
C	-0.345502	3.264128	-9.045924
H	-0.898287	2.326538	-9.145081
H	0.207040	3.482034	-9.959455
H	-1.053701	4.066420	-8.824017

M

***B3LYP* [Hartree]: -1217.957481430**
***MPW1K* [Hartree]: -1217.523416700**
***ZPE* [kcal/mol]: 200.9**
***CPCM* [kcal/mol]: -10.2**

C	-1.210318	-1.078159	0.294169
N	0.022548	-0.584000	0.579298
C	0.255843	0.668524	-0.072852
N	-0.876842	0.957177	-0.769561
C	-1.949366	-0.022848	-0.535952
C	1.050315	-1.280787	1.333334
O	1.294015	1.298444	0.007746
C	-1.074364	2.199016	-1.485719
C	-2.601423	-0.629469	-1.730359
C	-3.886714	-0.388856	-2.066822
O	-4.587225	-1.108449	-2.958170
O	-1.631484	-2.183177	0.630178
O	-4.566214	0.647006	-1.527261
C	-5.999840	0.595058	-1.559065
O	-3.688105	-3.614020	-2.336362
C	-3.913154	-4.272629	-1.323163
O	-3.489287	-3.980009	-0.104894
C	-4.708961	-5.529144	-1.333821
C	-5.209174	-6.021143	-2.472128
C	-6.000085	-7.279026	-2.474278
O	-6.391836	-7.588757	-3.729234
C	-7.166251	-8.794001	-3.848554
O	-6.266563	-7.946571	-1.495490
H	1.914583	-0.618803	1.386907
H	1.325077	-2.214592	0.835206
H	0.689064	-1.511065	2.338229
H	-0.107563	2.696081	-1.572158
H	-1.772706	2.860430	-0.957526
H	-1.474711	1.993077	-2.482398
H	-2.722485	0.430770	0.101872
H	-2.072921	-1.402705	-2.273542
H	-6.373847	0.625297	-2.584466
H	-6.330814	1.480078	-1.014751
H	-6.376265	-0.306130	-1.065223
H	-4.229719	-2.023179	-2.948796
H	-5.045588	-5.514704	-3.417685
H	-4.868364	-6.039723	-0.389822
H	-2.903446	-3.176417	-0.056072
H	-6.594068	-9.653655	-3.491399
H	-7.390943	-8.895360	-4.909687
H	-8.086898	-8.716930	-3.265014

M′

***B3LYP* [Hartree]: -1217.949318650**
***MPW1K* [Hartree]: -1217.515855690**
***ZPE* [kcal/mol]: 200.9**
***CPCM* [kcal/mol]: -12.2**

N	1.636170	0.455362	0.472255
C	3.069094	0.673658	0.261830
C	3.655392	-0.707152	0.633961
N	2.598929	-1.477256	1.063178
C	1.371641	-0.779082	1.009713
C	3.453211	1.108744	-1.126844
C	4.546660	1.904026	-1.344886
O	5.199868	2.452891	-0.313996
C	6.207576	3.440155	-0.585773
O	4.815887	-1.056840	0.558928
C	2.709807	-2.854633	1.506407
O	0.298378	-1.223029	1.378089
C	0.655908	1.522010	0.510670
O	5.029850	2.232075	-2.541074
O	3.010938	2.147212	-4.281516
C	1.953738	2.666721	-3.921779
O	1.593908	2.828510	-2.653632
C	0.938372	3.183075	-4.868386
C	1.135150	3.130470	-6.190301
C	0.106933	3.654464	-7.128858
O	0.509162	3.494697	-8.406123
C	-0.413168	3.968661	-9.403376
O	-0.948591	4.157831	-6.802633
H	7.025601	3.011532	-1.168092
H	6.567709	3.752580	0.394069
H	5.788449	4.294327	-1.124041
H	3.139514	0.474155	-1.950974
H	3.459251	1.400434	0.988323
H	1.721613	-3.170143	1.841442
H	3.426928	-2.929366	2.327637
H	3.048579	-3.496254	0.688020
H	2.252511	2.377486	-2.044378
H	-0.294457	1.084688	0.819005
H	0.532915	1.983726	-0.472904
H	0.942087	2.299980	1.231123
H	2.043748	2.706072	-6.604625
H	0.028475	3.607587	-4.457407
H	4.353110	2.051102	-3.245058
H	-1.366012	3.440015	-9.324023
H	0.061572	3.765303	-10.362336
H	-0.591819	5.039413	-9.279716

TS_{11}

***B3LYP* [Hartree]: -1217.939296930**
***MPW1K* [Hartree]: -1217.505255440**
***ZPE* [kcal/mol]: 196.6**
***CPCM* [kcal/mol]: -13.1**

N	0.037021	-0.915640	0.572514
C	1.126381	-1.607250	1.236426
H	2.046291	-1.076204	0.991478
H	1.188374	-2.642762	0.890923
H	0.971788	-1.609516	2.318533
C	0.228489	0.215783	-0.255660
O	1.302572	0.746931	-0.476809
N	-1.004850	0.566469	-0.735333
C	-1.215378	1.751601	-1.537341
H	-0.239034	2.200209	-1.724565
H	-1.854040	2.475186	-1.017040
H	-1.683113	1.501852	-2.496004
C	-2.076826	-0.280438	-0.203432
H	-2.712098	0.299610	0.479944
C	-1.283902	-1.290098	0.646420
O	-1.731585	-2.234406	1.266026
C	-2.952528	-0.955994	-1.237310
H	-2.403200	-1.495724	-2.010908
C	-4.080047	-0.273659	-1.756809
O	-4.455317	0.871791	-1.189974
C	-5.733975	1.422925	-1.569204
H	-5.741104	1.679190	-2.630073
H	-5.849423	2.316976	-0.958049
H	-6.534840	0.710333	-1.362903
O	-4.829750	-0.745760	-2.687200
H	-4.717394	-1.861485	-2.782138
C	-5.647768	-7.347133	-2.497122
O	-5.493006	-8.015216	-1.495233
O	-6.121704	-7.835254	-3.664527
C	-5.351194	-5.896421	-2.623786
H	-5.540339	-5.416400	-3.577951
C	-4.862702	-5.205834	-1.587409
H	-4.675269	-5.688031	-0.633779
C	-4.560537	-3.755561	-1.676190
O	-4.710316	-3.159372	-2.784296
O	-4.157806	-3.210260	-0.589100
H	-3.640387	-2.147283	-0.753368
C	-6.441786	-9.236604	-3.656310
H	-5.554661	-9.830771	-3.424006
H	-6.803533	-9.461589	-4.658988
H	-7.212509	-9.449188	-2.911448

TS_{11}'

***B3LYP* [Hartree]: -1217.939914970**
***MPW1K* [Hartree]: -1217.505745540**
***ZPE* [kcal/mol]: 197.1**
***CPCM* [kcal/mol]: -12.6**

N	0.204109	-0.381006	2.736455
C	-0.908777	-1.188300	2.233243
C	-2.085122	-0.204835	2.345883
N	-1.553241	0.999575	2.732555
C	-0.159736	0.914819	2.980612
O	-3.259169	-0.447359	2.139921
C	-1.184997	-2.479788	2.984633
C	-0.698961	-3.701606	2.469635
O	-0.932999	-4.849552	3.013371
C	-2.326016	2.206131	2.962922
O	0.541754	1.842338	3.342215
C	1.579155	-0.826975	2.788079
O	0.119840	-3.686659	1.423900
C	0.735409	-4.930016	1.024387
O	-1.413774	-4.596877	5.402874
C	-0.856271	-3.648885	6.017842
O	-0.312204	-2.620747	5.463903
C	-0.796799	-3.667919	7.502083
C	-1.267291	-4.694802	8.218560
C	-1.186107	-4.684471	9.702381
O	-1.722859	-5.814303	10.212810
C	-1.698126	-5.909163	11.646981
O	-0.707887	-3.795456	10.377244
H	-1.623979	2.993665	3.237134
H	-3.047590	2.052455	3.770234
H	-2.869202	2.485317	2.056738
H	1.936343	-1.133484	1.797202
H	1.690104	-1.668136	3.480597
H	2.183272	0.007736	3.145515
H	-0.755730	-1.392977	1.162703
H	-2.211752	-2.570229	3.341976
H	1.384763	-4.668842	0.190146
H	-0.024209	-5.647378	0.709126
H	1.314860	-5.351964	1.847548
H	-1.232578	-4.736617	4.046966
H	-0.670104	-5.872440	12.015551
H	-2.158813	-6.866887	11.886452
H	-2.262027	-5.087348	12.094908
H	-1.718327	-5.554517	7.734670
H	-0.345315	-2.810257	7.989732
H	-0.614929	-2.521905	4.316403

AcOH

***B3LYP* [Hartree]:** **-229.172238162**
***ZPE* [kcal/mol]:** **38.9**
***CPCM* [kcal/mol]:** **-7.4**

H	0.084696	-0.019084	0.025524
C	-0.021065	-0.027601	1.109326
H	0.963916	0.018969	1.582888
H	-0.582602	0.851533	1.438572
C	-0.737043	-1.283876	1.534998
O	-1.139069	-2.158994	0.802105
O	-0.890755	-1.334245	2.883169
H	-1.356379	-2.167602	3.067018

A_{Ph}

***B3LYP* [Hartree]:** **-1109.921356880**
***ZPE* [kcal/mol]:** **237.8**
***CPCM* [kcal/mol]:** **-8.9**

C	0.038990	-3.983376	3.793064
O	0.160680	-2.613651	3.377233
C	-0.128942	-2.379805	2.077211
C	0.028433	-0.938108	1.760233
C	-0.213512	-0.475508	0.529350
C	-0.056049	0.970067	0.208790
O	0.298256	1.812352	1.017507
O	-0.469115	-3.244604	1.294811
O	-0.350156	1.220292	-1.071006
N	0.275060	3.855301	-1.759032
C	1.458053	3.847227	-2.645409
C	-0.112128	4.786956	-1.051422
N	-0.658028	5.680279	-0.423319
C	-0.580832	6.032536	0.940900
H	-0.530945	-1.145670	-0.263018
H	0.344342	-0.266914	2.552229
H	-0.984974	-4.337985	3.651607
H	0.307056	-3.995674	4.849038
H	0.713941	-4.620963	3.216700
H	-0.223303	2.189856	-1.257748
C	-0.992105	7.320204	1.301490
C	-0.943860	7.712999	2.637841
C	-0.499113	6.822367	3.616432
C	-0.103479	5.532616	3.251759
C	-0.140223	5.128296	1.919032
H	-1.340630	7.996115	0.527871
H	-1.258703	8.714923	2.914206
H	-0.466955	7.128320	4.657854
H	0.233780	4.831827	4.009917
H	0.146146	4.119588	1.634588
C	2.466696	4.961687	-2.337851
H	1.942687	2.876998	-2.474035
C	3.666665	4.901770	-3.296567
H	1.962757	5.933060	-2.439957
H	2.799726	4.881505	-1.296648
C	3.220174	4.942615	-4.765529
H	4.352979	5.728234	-3.080331
H	4.229420	3.975683	-3.113942
C	2.199018	3.836212	-5.068916
H	2.767997	5.921157	-4.979465
H	4.088984	4.848882	-5.427134
C	0.998415	3.896975	-4.111931
H	1.849313	3.910855	-6.104711
H	2.687255	2.855877	-4.976348
H	0.441416	4.830258	-4.269873
H	0.301856	3.074250	-4.305035

A_{Cy}

***B3LYP* [Hartree]:** **-1109.921843750**
***ZPE* [kcal/mol]:** **237.6**
***CPCM* [kcal/mol]:** **-8.3**

C	-0.937719	-3.369685	4.166311
O	-0.744286	-2.055649	3.618578
C	-0.540950	-2.014336	2.282230
C	-0.353793	-0.613744	1.827658
C	-0.139312	-0.333000	0.538153
C	0.049377	1.070733	0.079267
O	0.022811	2.041873	0.819220
O	-0.516662	-2.999423	1.571967
O	0.248646	1.131980	-1.241108
N	0.844269	3.793381	-1.920663
C	1.909328	4.094755	-2.803496
C	0.349583	4.562812	-1.075122
N	-0.291453	5.253374	-0.319248
C	-0.203345	5.454777	1.135713
H	-0.097984	-1.124716	-0.203048
H	-0.395372	0.178622	2.567820
H	-1.812760	-3.847243	3.718564
H	-1.084958	-3.224275	5.236031
H	-0.061980	-3.996166	3.979667
H	0.395825	2.081721	-1.500427
C	-1.389212	6.307816	1.600665
H	-0.265266	4.459512	1.592102
C	-1.319610	6.574883	3.111892
H	-1.371875	7.258692	1.051378
H	-2.325850	5.805711	1.335892
C	0.016654	7.218727	3.510102
H	-2.157776	7.212999	3.413675
H	-1.440164	5.626524	3.654101
C	1.205344	6.371599	3.033000
H	0.083148	8.220736	3.063345
H	0.062749	7.357142	4.596474
C	1.137223	6.101287	1.521747
H	2.152305	6.866983	3.276069
H	1.207830	5.413727	3.571120
H	1.242909	7.044839	0.969471
H	1.960796	5.448988	1.209537
C	2.384171	5.399707	-3.000625
C	3.428928	5.630819	-3.892152
C	4.008464	4.571866	-4.594885
C	3.531855	3.274725	-4.399346
C	2.486140	3.032702	-3.510523
H	1.929924	6.224950	-2.459445
H	3.790018	6.644587	-4.039204
H	4.822247	4.757313	-5.288880
H	3.974278	2.443982	-4.940981
H	2.111779	2.026398	-3.351803

B_{Ph}

***B3LYP* [Hartree]: -1109.922182000**
***ZPE* [kcal/mol]: 239.1**
***CPCM* [kcal/mol]: -8.0**

C	-1.525793	-2.769208	4.179141
O	-1.207722	-1.562589	3.464212
C	-0.257892	-1.689890	2.515283
C	-0.012512	-0.382869	1.846152
C	0.890410	-0.298862	0.860969
C	1.222095	0.940585	0.125400
O	0.445752	1.985656	0.520731
C	0.537353	3.324902	0.075450
N	-0.019237	4.248398	0.754200
C	-0.853459	4.030477	1.859995
O	0.308681	-2.731326	2.252881
O	2.091852	0.987262	-0.724492
N	1.190999	3.520517	-1.093738
C	1.386821	4.861889	-1.647088
H	1.449502	-1.175940	0.550981
H	-0.582098	0.476587	2.183386
H	-1.899857	-3.532736	3.492798
H	-2.293259	-2.489751	4.899778
H	-0.640061	-3.156233	4.688452
H	1.803555	2.768815	-1.390372
C	1.604033	4.758501	-3.163800
H	0.459516	5.412133	-1.453474
C	1.814859	6.144622	-3.792591
H	2.489645	4.134608	-3.356901
H	0.750277	4.248974	-3.624581
C	2.962493	6.908846	-3.115279
H	2.005766	6.039431	-4.866785
H	0.887381	6.726352	-3.697402
C	2.750447	7.002865	-1.596994
H	3.911087	6.391021	-3.316817
H	3.056701	7.910985	-3.549891
C	2.546557	5.615347	-0.969221
H	3.599950	7.507311	-1.122260
H	1.866973	7.623606	-1.391989
H	3.464419	5.020356	-1.080021
H	2.339832	5.699296	0.102076
C	-0.633186	4.794691	3.017949
C	-1.466448	4.662511	4.126531
C	-2.549680	3.781584	4.098367
C	-2.791360	3.035863	2.942979
C	-1.956138	3.156028	1.832930
H	0.203226	5.486361	3.028790
H	-1.271654	5.256793	5.015073
H	-3.202528	3.685230	4.960562
H	-3.640256	2.358729	2.900508
H	-2.161924	2.587707	0.931442

B_{Cy}

***B3LYP* [Hartree]: -1109.917598160**
***ZPE* [kcal/mol]: 239.1**
***CPCM* [kcal/mol]: -7.4**

C	-1.262951	-2.791841	4.058500
O	-0.970050	-1.562880	3.369936
C	-0.610291	-1.700057	2.077067
C	-0.329284	-0.369014	1.472910
C	0.052068	-0.280265	0.193233
C	0.373917	0.980315	-0.512584
O	0.181464	2.073062	0.268535
C	0.384075	3.449100	-0.068421
N	0.022873	4.340157	0.751550
C	-0.615760	4.036757	2.025862
O	-0.529844	-2.764569	1.499535
O	0.770173	0.989789	-1.664756
N	0.990913	3.645472	-1.276664
C	1.338114	4.859130	-1.900973
H	0.160343	-1.176302	-0.409642
H	-0.441316	0.505515	2.103309
H	1.131336	2.799381	-1.819572
H	-1.535500	-2.502321	5.072534
H	-2.088418	-3.315449	3.570644
H	-0.385984	-3.443476	4.065280
C	1.878573	4.759294	-3.195658
C	2.261193	5.901072	-3.890740
C	2.113536	7.163352	-3.311037
C	1.578210	7.259760	-2.027494
C	1.188837	6.124750	-1.314786
H	1.996311	3.779822	-3.653098
H	2.675635	5.801783	-4.889844
H	2.411271	8.055488	-3.853147
H	1.457143	8.234648	-1.563451
H	0.770932	6.200887	-0.321581
C	-1.663152	5.123452	2.323814
H	-1.133008	3.065709	1.992014
C	-2.321455	4.923039	3.696394
H	-1.161861	6.099786	2.288745
H	-2.416349	5.129728	1.527773
C	-1.274396	4.859419	4.817971
H	-3.038069	5.730287	3.887957
H	-2.902136	3.989321	3.691119
C	-0.220198	3.779881	4.531185
H	-0.776365	5.835487	4.902763
H	-1.758806	4.670672	5.783440
C	0.433349	3.977671	3.154350
H	0.549640	3.779324	5.311960
H	-0.699390	2.790759	4.568797
H	1.003756	4.915679	3.141316
H	1.147954	3.172303	2.946760

$TS_{2\text{-}Ph}$

***B3LYP* [Hartree]: -1339.055159670**
***ZPE* [kcal/mol]: 276.3**
***CPCM* [kcal/mol]: -10.5**

C	-1.188650	-0.101950	-0.576031
N	0.184438	-0.059554	-0.082523
C	1.070947	-0.372546	-1.353157
C	0.062773	-1.101451	-2.223238
O	-1.227081	-0.815164	-1.749436
C	0.455577	-0.960770	1.117316
C	2.365892	-1.020191	-1.161378
C	3.508523	-0.258437	-1.208255
O	4.684526	-0.930559	-1.208211
C	5.879880	-0.142749	-1.200790
O	0.225383	-1.789812	-3.181758
N	-2.133986	0.455452	0.030100
C	-3.493997	0.492142	-0.338604
O	3.557541	1.038021	-1.301166
O	2.967995	2.503182	0.495590
C	1.813473	2.904359	0.849770
C	1.784396	4.187622	1.659017
O	0.711026	2.347325	0.586411
H	5.910597	0.528566	-0.338225
H	5.967292	0.453959	-2.112344
H	6.697545	-0.862571	-1.144876
H	2.447318	-2.098435	-1.136068
H	1.222748	0.624908	-1.788096
H	0.443629	0.988963	0.212871
H	3.170214	1.674774	-0.431066
H	0.792690	4.363842	2.075769
H	2.532416	4.140545	2.454565
H	2.058237	5.024708	1.008623
C	-0.054795	-2.391350	0.909874
H	1.550919	-0.977289	1.152369
C	0.311780	-3.264534	2.123738
H	-1.146128	-2.379913	0.789463
H	0.369555	-2.829733	0.000193
C	-0.207018	-2.660613	3.436338
H	-0.087624	-4.274092	1.978297
H	1.404325	-3.365596	2.174900
C	0.281625	-1.216215	3.613423
H	-1.305773	-2.673708	3.432498
H	0.110380	-3.277186	4.284929
C	-0.095424	-0.339708	2.407073
H	-0.138892	-0.778202	4.525282
H	1.373037	-1.213461	3.741307
H	-1.184856	-0.254775	2.334394
H	0.291934	0.676005	2.525262
C	-4.284061	1.382341	0.406853
C	-5.645395	1.510042	0.147305
C	-6.240477	0.738335	-0.852457
C	-5.463141	-0.157302	-1.589867
C	-4.097225	-0.285149	-1.344827
H	-3.801222	1.967580	1.182235
H	-6.241930	2.207256	0.727844
H	-7.303181	0.831590	-1.054980
H	-5.922066	-0.762464	-2.366136
H	-3.507551	-0.981749	-1.926107

$TS_{2\text{-}Ph}'$

***B3LYP* [Hartree]: -1339.046663590**
***ZPE* [kcal/mol]: 276.8**
***CPCM* [kcal/mol]: -10.9**

C	-0.137453	0.065702	2.628120
C	-1.227439	0.121680	1.577596
N	-0.379374	0.325144	0.256226
C	1.003812	0.014393	0.625200
O	1.110390	-0.034384	1.991220
C	-2.077522	-1.067274	1.483485
C	-3.334718	-0.974091	0.936293
O	-3.969996	-1.949806	0.375717
C	-0.596836	1.688993	-0.404946
N	1.894096	-0.186553	-0.233742
C	3.250155	-0.505874	-0.017150
O	-0.217705	0.086593	3.816324
O	-3.954881	0.240685	0.960558
C	-5.210318	0.332766	0.276973
O	-2.420136	-3.168591	-1.022147
C	-1.548682	-2.543029	-1.709645
C	-0.889810	-3.333754	-2.828726
O	-1.197168	-1.338583	-1.568165
H	-0.744212	-0.429833	-0.453814
H	-1.821601	1.025015	1.717916
H	-1.614919	-2.046012	1.495854
H	-5.110094	0.059676	-0.776818
H	-5.515406	1.376231	0.370267
H	-5.957642	-0.317509	0.737876
H	-3.214034	-2.547661	-0.249224
H	0.195076	-3.207547	-2.780593
H	-1.153433	-4.390252	-2.774565
H	-1.219887	-2.928990	-3.791336
C	-0.113322	1.702074	-1.860687
H	-1.689812	1.777576	-0.401216
C	-0.458262	3.055239	-2.505954
H	0.969479	1.543957	-1.885240
H	-0.570904	0.871623	-2.404742
C	0.133137	4.228934	-1.711929
H	-0.090970	3.067412	-3.537778
H	-1.550042	3.166938	-2.564440
C	-0.311049	4.187345	-0.242948
H	1.229835	4.182833	-1.760035
H	-0.160162	5.182680	-2.164828
C	0.013478	2.832534	0.412775
H	0.166845	4.990118	0.328720
H	-1.393664	4.364456	-0.183275
H	1.102612	2.702798	0.456903
H	-0.356365	2.824678	1.444699
C	3.971343	-0.834703	-1.176635
C	5.320856	-1.166905	-1.102550
C	5.972940	-1.164648	0.131849
C	5.264265	-0.830934	1.287909
C	3.911001	-0.504538	1.225600
H	3.445693	-0.827011	-2.125618
H	5.863362	-1.424098	-2.007233
H	7.026438	-1.420186	0.193727
H	5.767303	-0.826346	2.250330
H	3.375950	-0.251469	2.131229

$TS_{2\text{-}Cy}$

***B3LYP* [Hartree]: -1339.048369680**
***ZPE* [kcal/mol]: 275.6**
***CPCM* [kcal/mol]: -10.9**

C	-1.149511	-0.191306	-0.521675
N	0.225286	-0.143910	-0.032074
C	1.143244	-0.164705	-1.428888
C	0.117630	-0.783246	-2.359424
O	-1.163193	-0.665093	-1.815263
C	0.572855	-1.171895	0.942974
C	2.442423	-0.779271	-1.376349
C	3.562279	0.006383	-1.194458
O	4.754477	-0.617041	-1.332345
C	5.929117	0.172942	-1.118472
O	0.282223	-1.284542	-3.429222
N	-2.125751	0.162081	0.170397
C	-3.490478	0.137204	-0.360591
O	3.578027	1.279980	-0.957873
O	2.796007	2.334498	1.039280
C	1.606413	2.772137	1.229991
C	1.491821	3.995127	2.116962
O	0.557359	2.274745	0.747436
H	5.930213	0.624854	-0.122941
H	6.012457	0.967860	-1.864074
H	6.764096	-0.521814	-1.216860
H	2.560410	-1.838770	-1.556343
H	1.207260	0.912510	-1.622563
H	0.406543	0.871372	0.372110
H	3.091084	1.717123	0.004942
H	2.104601	3.861435	3.012102
H	1.890314	4.862821	1.580970
H	0.452860	4.181711	2.388289
C	1.599143	-0.895567	1.846700
C	1.981209	-1.878347	2.760569
C	1.352091	-3.122970	2.765136
C	0.336369	-3.390795	1.845729
C	-0.054113	-2.418653	0.926498
H	2.097461	0.067571	1.834177
H	2.776222	-1.665507	3.468225
H	1.652163	-3.882913	3.479831
H	-0.155477	-4.358387	1.840441
H	-0.845191	-2.632013	0.215000
C	-4.077456	1.556810	-0.262794
H	-3.505319	-0.180543	-1.413029
C	-5.553287	1.581857	-0.687438
H	-3.976382	1.899111	0.774904
H	-3.484704	2.241277	-0.879930
C	-6.391342	0.583849	0.125031
H	-5.951347	2.596769	-0.575056
H	-5.630514	1.335093	-1.755742
C	-5.803299	-0.832315	0.041480
H	-6.415676	0.903787	1.176193
H	-7.429656	0.584410	-0.226393
C	-4.327030	-0.856732	0.465731
H	-6.378151	-1.523795	0.668166
H	-5.891726	-1.201114	-0.990011
H	-4.233554	-0.587556	1.525687
H	-3.912400	-1.865905	0.357269

$TS_{2\text{-}Cy}'$

***B3LYP* [Hartree]: -1339.042397390**
***ZPE* [kcal/mol]: 276.5**
***CPCM* [kcal/mol]: -10.9**

C	-1.429859	0.327303	1.481553
N	-0.525865	0.533970	0.149184
C	0.854400	0.337176	0.617664
O	0.894959	0.468319	1.986289
C	-0.382243	0.563504	2.552043
C	-0.730190	1.806323	-0.555445
N	1.795690	0.090215	-0.161269
C	3.157947	-0.132103	0.329817
O	-0.525739	0.775489	3.716494
C	-2.022713	-1.001967	1.491742
C	-3.270069	-1.220831	0.952139
O	-4.139419	-0.184118	0.902460
C	-5.349975	-0.387028	0.161360
O	-3.673213	-2.355497	0.473994
O	-1.843305	-3.341137	-0.788826
C	-1.151033	-2.599162	-1.552024
O	-1.111470	-1.332536	-1.536641
C	-0.298854	-3.301750	-2.596706
H	-0.790802	-0.305235	-0.520535
H	-2.168935	1.126983	1.471610
H	-1.376772	-1.864430	1.600413
H	-5.137135	-0.667725	-0.873510
H	-5.871639	0.570179	0.193920
H	-5.963998	-1.165604	0.619529
H	-2.815793	-2.830032	-0.061205
H	0.737496	-2.962869	-2.508593
H	-0.353482	-4.385379	-2.490181
H	-0.645642	-3.013556	-3.594289
C	-1.313281	1.775012	-1.821174
C	-1.555230	2.982137	-2.478630
C	-1.221219	4.196270	-1.877870
C	-0.635289	4.208945	-0.610347
C	-0.387008	3.012178	0.059828
H	-1.553051	0.820515	-2.276684
H	-2.004291	2.968483	-3.466810
H	-1.412856	5.130775	-2.395833
H	-0.369462	5.150149	-0.139684
H	0.075883	3.025338	1.042019
C	4.098105	0.900160	-0.317466
H	3.211786	-0.022656	1.422442
C	5.563379	0.632975	0.060933
H	3.972818	0.844708	-1.406409
H	3.798987	1.910464	-0.015038
C	5.987787	-0.798590	-0.297738
H	6.211234	1.361719	-0.439513
H	5.695228	0.790412	1.140607
C	5.044291	-1.832307	0.334294
H	5.974546	-0.916636	-1.390297
H	7.019884	-0.979731	0.023915
C	3.579829	-1.564606	-0.043987
H	5.324435	-2.846039	0.026340
H	5.150065	-1.799620	1.427692
H	3.440099	-1.692689	-1.125138
H	2.915466	-2.282819	0.449754

$TS_{9\text{-}Ph}$

***B3LYP* [Hartree]: -1109.894440230**
***ZPE* [kcal/mol]: 238.4**
***CPCM* [kcal/mol]: -12.2**

C	0.278765	-4.089878	-0.296270
N	0.493779	-2.772962	-0.913337
C	1.566755	-2.502587	-1.686346
O	2.337196	-3.451075	-2.132786
C	3.303952	-2.327897	-3.015757
C	2.772481	-2.391445	-4.397273
C	3.569623	-2.155257	-5.444942
C	3.028564	-2.205268	-6.824159
O	4.003619	-1.952152	-7.727376
C	3.585516	-1.979884	-9.100778
N	2.000857	-1.332492	-2.111939
C	1.412621	-0.064860	-2.047820
O	4.435137	-2.206313	-2.656668
O	1.874915	-2.440205	-7.126435
H	0.053587	-1.972522	-0.477427
H	1.722815	-2.618182	-4.541630
H	4.621844	-1.928282	-5.312097
H	3.180907	-2.961426	-9.360013
H	4.479980	-1.766963	-9.685546
H	2.817369	-1.224401	-9.284526
C	-1.217335	-4.294618	-0.020725
H	0.607416	-4.824815	-1.038520
C	-1.481554	-5.659551	0.634616
H	-1.569527	-3.496277	0.650440
H	-1.780895	-4.196125	-0.955221
C	-0.646059	-5.851346	1.909117
H	-2.549797	-5.761731	0.856444
H	-1.235683	-6.454404	-0.082983
C	0.849898	-5.641634	1.631324
H	-0.977620	-5.131792	2.671085
H	-0.819697	-6.849788	2.326483
C	1.115726	-4.274868	0.982051
H	1.428697	-5.732014	2.557321
H	1.210100	-6.435232	0.962015
H	0.859244	-3.473939	1.690487
H	2.176834	-4.161274	0.736944
C	2.254727	1.048498	-1.886253
C	1.720079	2.332782	-1.847205
C	0.340919	2.531053	-1.959216
C	-0.499415	1.429910	-2.127208
C	0.026820	0.139237	-2.183908
H	3.322463	0.881220	-1.789743
H	2.382831	3.184164	-1.721840
H	-0.072840	3.534076	-1.921985
H	-1.571168	1.574082	-2.231462
H	-0.628308	-0.709017	-2.358469

$TS_{9\text{-}Cy}$

***B3LYP* [Hartree]: -1109.887386870**
***ZPE* [kcal/mol]: 238.2**
***CPCM* [kcal/mol]: -12.4**

C	0.111173	-4.238258	-0.428045
N	0.546259	-2.965810	-0.868611
C	1.648991	-2.616990	-1.586175
O	2.534945	-3.486621	-1.986503
C	3.442805	-2.281206	-2.789345
C	3.029700	-2.389604	-4.209910
C	3.893973	-2.115403	-5.193141
C	3.472097	-2.213358	-6.610751
O	4.507841	-1.937843	-7.436297
C	4.207063	-2.011373	-8.838614
N	1.971747	-1.417639	-1.992609
C	1.261093	-0.165567	-1.801101
O	4.526711	-2.048197	-2.348442
O	2.356806	-2.498640	-7.001426
H	-0.063868	-2.196540	-0.632427
H	2.012925	-2.689830	-4.433860
H	4.915467	-1.821068	-4.977958
H	3.873072	-3.016450	-9.108045
H	5.135847	-1.765343	-9.352535
H	3.421362	-1.298694	-9.101671
C	-1.133296	-4.294360	0.216646
C	-1.628851	-5.507510	0.685737
C	-0.892662	-6.680834	0.517594
C	0.344819	-6.620039	-0.123373
C	0.857521	-5.412569	-0.597223
H	-1.714687	-3.384357	0.347839
H	-2.594383	-5.531787	1.182034
H	-1.278091	-7.627945	0.881284
H	0.930017	-7.524741	-0.259627
H	1.818926	-5.375827	-1.090429
C	1.583569	0.796684	-2.957261
H	0.170743	-0.355173	-1.829712
C	0.883837	2.151787	-2.778065
H	2.671638	0.939035	-2.989413
H	1.296627	0.334067	-3.907728
C	1.220233	2.790559	-1.422497
H	1.164552	2.823447	-3.597253
H	-0.204108	2.011569	-2.852619
C	0.904067	1.834764	-0.262695
H	2.288805	3.045362	-1.398450
H	0.671331	3.731442	-1.299469
C	1.607225	0.481010	-0.443202
H	1.198686	2.281610	0.693776
H	-0.183282	1.678494	-0.209048
H	2.695719	0.611751	-0.400884
H	1.345704	-0.203547	0.373345

K_{Ph}

***B3LYP* [Hartree]: -1109.944438300**
***ZPE* [kcal/mol]: 239.5**
***CPCM* [kcal/mol]: -12.1**

C	-0.218988	0.738630	-2.054093
C	0.994504	0.073924	-1.860758
C	1.847280	0.451173	-0.820048
C	1.480578	1.493418	0.030754
C	0.268018	2.159715	-0.158633
C	-0.579720	1.782823	-1.201548
N	1.360766	-1.012621	-2.740242
C	1.204105	-2.367456	-2.315266
O	1.764205	-3.297968	-2.880418
C	2.034188	-0.641746	-3.927576
O	2.405535	0.513088	-4.068598
N	0.374666	-2.531850	-1.246976
C	0.213207	-3.837672	-0.606102
C	-1.172038	-3.929620	0.050395
C	-1.372732	-5.286548	0.743269
C	-0.253878	-5.581735	1.753471
C	1.130864	-5.484952	1.095483
C	1.333174	-4.125157	0.410750
C	2.190904	-1.655235	-5.009033
C	3.048338	-1.415180	-6.009060
C	3.188740	-2.374342	-7.130760
O	2.546393	-3.394224	-7.282799
O	4.146871	-1.957348	-7.992763
C	4.364505	-2.815958	-9.122261
H	0.005069	-1.717392	-0.779245
H	1.613438	-2.569001	-4.991395
H	3.657348	-0.517902	-6.023443
H	4.671115	-3.812628	-8.794833
H	5.155391	-2.343453	-9.704332
H	3.452304	-2.908528	-9.717203
H	0.279877	-4.579127	-1.409082
H	-1.269598	-3.125701	0.796260
H	-1.949641	-3.760619	-0.703214
H	-2.350856	-5.308543	1.237278
H	-1.391418	-6.078228	-0.018360
H	-0.313072	-4.859341	2.580016
H	-0.397614	-6.574348	2.195863
H	1.920182	-5.651983	1.837291
H	1.233457	-6.283509	0.347707
H	1.338241	-3.326388	1.166495
H	2.298617	-4.090090	-0.104488
H	2.791876	-0.067321	-0.691493
H	2.145064	1.788927	0.836858
H	-0.013948	2.972704	0.503535
H	-1.521088	2.301681	-1.354474
H	-0.865115	0.438526	-2.872944

K_{Cy}

***B3LYP* [Hartree]: -1109.940539270**
***ZPE* [kcal/mol]: 240.0**
***CPCM* [kcal/mol]: -11.2**

C	2.553243	0.625051	-0.853608
C	1.346414	-0.060144	-1.523887
C	0.362496	0.960391	-2.121404
C	-0.095591	1.961993	-1.047802
C	1.098554	2.652206	-0.372309
C	2.075658	1.622858	0.214282
N	1.756522	-1.113732	-2.504408
C	1.662870	-2.491330	-2.117711
O	2.596860	-3.267338	-2.225856
C	2.485049	-0.750408	-3.641484
O	2.805191	0.415739	-3.843187
N	0.419376	-2.818749	-1.635748
C	-0.004894	-4.029894	-1.041715
C	-1.342068	-4.093869	-0.621262
C	-1.836761	-5.247426	-0.020474
C	-1.004472	-6.351064	0.173438
C	0.324154	-6.283210	-0.246187
C	0.835159	-5.136885	-0.855192
C	2.766289	-1.811407	-4.655654
C	3.530657	-1.521482	-5.714949
C	3.792219	-2.542108	-6.759030
O	3.335150	-3.667692	-6.783685
O	4.622106	-2.048536	-7.706897
C	4.944101	-2.959034	-8.769627
H	-0.303153	-2.125295	-1.763228
H	2.356162	-2.807896	-4.553232
H	3.972617	-0.537999	-5.831954
H	5.436134	-3.851668	-8.375296
H	5.614140	-2.412859	-9.432998
H	4.039664	-3.263842	-9.302192
H	-1.994456	-3.235274	-0.765215
H	-2.874593	-5.280095	0.297444
H	-1.387868	-7.251792	0.642394
H	0.980981	-7.136635	-0.105129
H	1.861026	-5.093688	-1.191168
H	0.820442	-0.604325	-0.732462
H	0.853573	1.489878	-2.942012
H	-0.502939	0.436240	-2.548221
H	-0.762453	2.704656	-1.500269
H	-0.688024	1.437585	-0.283611
H	1.624907	3.269660	-1.112674
H	0.746716	3.332223	0.412169
H	2.941828	2.126911	0.657582
H	1.580754	1.079742	1.032589
H	3.138124	1.143644	-1.616584
H	3.199147	-0.138571	-0.405270

L_{Ph}

***B3LYP* [Hartree]: -1339.122581240**
***ZPE* [kcal/mol]: 279.9**
***CPCM* [kcal/mol]: -10.0**

C	0.530430	2.196135	-1.442438
C	1.533722	1.560280	-0.462205
C	2.674099	2.536722	-0.121995
C	3.371380	3.055113	-1.388423
C	2.370184	3.692735	-2.362126
C	1.233416	2.718639	-2.705200
N	0.876493	1.126746	0.774133
C	-1.433530	-1.143352	-0.447985
C	-0.096045	-1.819701	-0.479956
N	0.907863	-1.186362	0.248859
C	0.528578	-0.114500	1.170741
C	-2.491686	-1.735948	-1.014091
C	-3.823610	-1.094880	-1.001468
O	-4.702544	-1.794729	-1.736162
C	-6.040116	-1.265588	-1.786786
O	0.092913	-2.835903	-1.134926
C	2.231361	-1.720660	0.365727
C	2.885147	-1.660269	1.603990
C	4.194914	-2.122454	1.722278
C	4.857372	-2.660310	0.618781
C	4.197890	-2.730269	-0.609459
C	2.893141	-2.259880	-0.746559
O	-0.073097	-0.369053	2.203807
O	-4.127909	-0.062556	-0.418212
O	-3.531597	0.989678	2.084117
C	-2.444807	1.744940	2.253218
C	-2.113692	1.967440	3.706061
O	-1.772003	2.173875	1.326227
H	-3.649748	0.780118	1.128637
H	-6.040592	-0.273117	-2.243286
H	-6.460268	-1.194590	-0.781057
H	-6.608272	-1.968800	-2.394047
H	-2.392120	-2.699172	-1.502677
H	-1.550976	-0.171943	0.020167
H	0.403365	1.845622	1.315570
H	-1.638333	2.941651	3.830720
H	-2.997011	1.884407	4.340437
H	-1.395316	1.191465	3.990901
H	2.360393	-1.273039	2.470332
H	4.691335	-2.071389	2.686723
H	5.875045	-3.025970	0.715581
H	4.701933	-3.150820	-1.474617
H	2.381920	-2.325872	-1.697233
H	1.968860	0.670853	-0.926047
H	2.255869	3.385920	0.437656
H	3.389294	2.039711	0.542370
H	4.151686	3.773944	-1.113727
H	3.881169	2.218987	-1.887359
H	1.946339	4.597883	-1.904941
H	2.882391	4.014902	-3.276167
H	0.501005	3.200550	-3.362761
H	1.644501	1.869342	-3.269302
H	0.011338	3.018436	-0.932865
H	-0.239294	1.462594	-1.705383

L_{Ph}'

***B3LYP* [Hartree]: -1339.117248620**
***ZPE* [kcal/mol]: 280.0**
***CPCM* [kcal/mol]: -10.0**

C	-0.436730	2.647785	-0.165108
C	0.746053	1.790056	0.319565
C	1.666547	2.594779	1.256694
C	2.143395	3.898158	0.597880
C	0.961836	4.752584	0.117354
C	0.044008	3.952745	-0.818511
N	0.266693	0.582567	0.995191
C	-0.892835	-0.770333	-1.873780
C	0.577109	-1.060220	-1.770411
N	1.211212	-0.965292	-0.539329
C	0.462687	-0.712214	0.690414
C	-1.881250	-1.162109	-1.056659
C	-3.303532	-0.838395	-1.304408
O	-4.177225	-0.947868	-0.451751
O	1.169550	-1.335309	-2.805730
C	2.605240	-1.298626	-0.390458
C	3.011808	-2.136507	0.654220
C	4.367966	-2.414553	0.828051
C	5.318218	-1.877044	-0.039571
C	4.904793	-1.050753	-1.086298
C	3.555254	-0.753029	-1.262998
O	0.055312	-1.647488	1.372014
O	-3.560035	-0.395741	-2.543087
C	-4.926511	-0.025046	-2.807482
O	-3.525012	-1.505713	2.180561
C	-2.655577	-0.653730	2.724423
C	-2.075422	-1.163423	4.017684
O	-2.338966	0.407616	2.202756
H	-5.587611	-0.881754	-2.661131
H	-4.942080	0.300797	-3.846543
H	-5.237669	0.783815	-2.142749
H	-1.698227	-1.696065	-0.132030
H	-1.138822	-0.269972	-2.805910
H	-0.417007	0.707723	1.743754
H	-3.789257	-1.188231	1.281642
H	-1.827055	-0.323437	4.668137
H	-2.754540	-1.853742	4.519741
H	-1.151665	-1.694353	3.764409
H	2.266748	-2.563592	1.314541
H	4.676873	-3.063742	1.642003
H	6.371831	-2.102414	0.095112
H	5.636098	-0.629585	-1.769800
H	3.235189	-0.120910	-2.081259
H	1.331903	1.466838	-0.545820
H	1.112280	2.829214	2.176607
H	2.518194	1.971483	1.550405
H	2.764776	4.462926	1.302167
H	2.788249	3.656030	-0.258759
H	0.383253	5.092652	0.987720
H	1.325975	5.654613	-0.387868
H	-0.820636	4.557128	-1.115813
H	0.588958	3.716261	-1.743662
H	-1.080307	2.876724	0.695234
H	-1.048110	2.065950	-0.862872

$TS_{10\text{-}Ph}$

***B3LYP* [Hartree]: -1339.085909930**
***ZPE* [kcal/mol]: 276.9**
***CPCM* [kcal/mol]: -11.0**

N	-0.256530	0.192675	0.494057
C	-0.428880	-0.701397	-0.855537
C	1.015974	-0.776833	-1.322361
N	1.861436	-0.325674	-0.273070
C	1.180786	0.206332	0.804482
C	-1.415492	-0.277789	-1.827145
C	-2.725666	-0.720511	-1.748881
O	-3.268164	-1.468682	-0.858716
O	1.414031	-1.187228	-2.382393
C	3.295341	-0.420052	-0.313227
O	1.639776	0.630399	1.834453
C	-0.894784	1.569981	0.455937
O	-3.538224	-0.279828	-2.745164
C	-4.893308	-0.733804	-2.720430
O	-2.479822	-2.807585	0.953003
C	-1.991063	-2.404680	2.071775
O	-1.409971	-1.312236	2.272293
C	-2.153748	-3.374393	3.223681
H	-2.737472	-2.062715	0.079013
H	-5.404684	-0.416282	-1.807310
H	-4.950164	-1.823556	-2.789457
H	-5.365767	-0.278552	-3.592206
H	-1.129170	0.352845	-2.657550
H	-0.677998	-1.675897	-0.419894
H	-0.770954	-0.389221	1.258431
H	-1.569792	-3.051590	4.085337
H	-3.212114	-3.428366	3.498624
H	-1.852584	-4.376916	2.909031
C	3.985397	-0.943429	0.783161
C	5.375427	-1.031838	0.735131
C	6.070139	-0.613754	-0.400857
C	5.369925	-0.099604	-1.492665
C	3.980185	0.005376	-1.454039
H	3.442949	-1.264657	1.664049
H	5.913629	-1.432995	1.588182
H	7.152645	-0.688982	-0.434984
H	5.903789	0.225479	-2.380136
H	3.432363	0.398100	-2.301147
C	-0.066411	2.579809	-0.345480
H	-1.827032	1.382827	-0.088798
C	-0.804116	3.928927	-0.411206
H	0.909147	2.725525	0.136132
H	0.114032	2.203396	-1.358164
C	-1.148769	4.455029	0.989661
H	-0.188646	4.654340	-0.954430
H	-1.727044	3.804261	-0.993495
C	-1.947879	3.418747	1.793414
H	-0.219694	4.691596	1.526612
H	-1.712418	5.391678	0.911393
C	-1.211325	2.070714	1.871422
H	-2.141641	3.786458	2.807011
H	-2.929487	3.270791	1.322191
H	-0.279910	2.185729	2.436277
H	-1.817728	1.327967	2.399543

$TS_{10\text{-}Ph}'$

***B3LYP* [Hartree]: -1339.074645620**
***ZPE* [kcal/mol]: 277.0**
***CPCM* [kcal/mol]: -12.9**

N	-0.211529	0.446502	-0.005101
C	-0.114295	-0.525503	-1.260586
C	1.384600	-0.554973	-1.504473
N	2.030622	-0.049089	-0.344842
C	1.150985	0.459357	0.589078
C	-0.703425	-1.825838	-0.931908
C	-2.025576	-2.104200	-1.194513
O	-2.627753	-1.421213	-2.214332
C	-4.028084	-1.658799	-2.398040
O	1.954772	-0.963902	-2.483328
C	3.449703	-0.122445	-0.124513
O	1.390280	0.848474	1.701656
C	-0.791973	1.837113	-0.302245
O	-2.745735	-2.947983	-0.541294
O	-2.353936	-2.725136	1.826186
C	-2.146361	-1.589506	2.378015
O	-1.860812	-0.509714	1.798596
C	-2.302903	-1.565748	3.889082
H	-4.217238	-2.702350	-2.660604
H	-4.328082	-1.006520	-3.219776
H	-4.596560	-1.417614	-1.495830
H	-0.219236	-2.431077	-0.174556
H	-0.615416	-0.041413	-2.096737
H	-0.878387	-0.033201	0.707127
H	-2.501577	-2.835914	0.622978
H	-1.576639	-0.881171	4.331943
H	-3.303823	-1.191544	4.131980
H	-2.199356	-2.566974	4.309174
C	3.942245	-0.606025	1.090380
C	5.320404	-0.676947	1.285925
C	6.198365	-0.282250	0.275462
C	5.694494	0.190737	-0.936600
C	4.318411	0.278504	-1.142466
H	3.258224	-0.912062	1.872080
H	5.705549	-1.047945	2.230513
H	7.270881	-0.344728	0.431657
H	6.371740	0.496059	-1.728029
H	3.922399	0.637578	-2.083823
C	-0.683544	2.783154	0.904118
H	-0.198613	2.230305	-1.138993
C	-1.334531	4.141726	0.587364
H	-1.182580	2.310039	1.758107
H	0.358275	2.934444	1.191401
C	-2.792225	3.995825	0.136334
H	-1.265668	4.781687	1.473716
H	-0.758367	4.644936	-0.202288
C	-2.897392	3.029481	-1.049045
H	-3.394781	3.612365	0.970669
H	-3.207960	4.974312	-0.129732
C	-2.261137	1.667973	-0.726436
H	-3.944579	2.875760	-1.331429
H	-2.401624	3.469254	-1.926209
H	-2.798115	1.191515	0.102258
H	-2.353199	0.998359	-1.585469