

Opposing Auxiliary Conformations Produce the Same Torquoselectivity in an Oxazolidinone-Directed Nazarov Cyclization

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SUPPORTING INFORMATION

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Computational Methods and Data

Geometries listed below were optimized at the B3LYP/6-31G(d) level in the gas phase. Thermochemical corrections were obtained from frequency calculations at the same level and are unscaled. Single-point energies were then computed at the M06-2X/6-311+G(d,p) level on the B3LYP geometries and used in conjunction with the B3LYP thermochemical corrections to obtain gas-phase free energies. Free energies in solution were obtained by addition of solvation free energies computed by the SMD method at the M06-2X/6-31G(d) level. For **TSA–TSD**, solvation free energies were also computed by the CPCM method at the M06-2X/6-31G(d) level.

For benchmarking purposes, transition states **TSA–TSD** were also optimized at the M06-2X/6-31G(d) level. The M06-2X optimizations were carried out using the ultrafine integration grid of Gaussian 09. Subsequent single-point calculations were carried out at the M06-2X/6-311+G(d,p) level in the gas phase and at the M06-2X/6-31G(d) level in solution.

Transition states **TSA–TSD** were also fully optimized in implicit dichloromethane using the SMD model at the B3LYP/6-31G(d) level. The solvent-optimized geometries of **TSA–TSD** are given at the end of the series of data below.

A table comparing the relative energies of **TSA–TSD** computed by these different methods is provided on page S57.

Underneath the coordinates for the species optimized in the gas phase below are listed the following energies:

B3LYP/6-31G(d) electronic potential energy (E),
B3LYP/6-31G(d) zero-point energy (ZPE),
B3LYP/6-31G(d) enthalpy at 298.15 K (H),
B3LYP/6-31G(d) free energy at 298.15 K and 1 mol/L (G),
M06-2X/6-311+G(d,p) single-point electronic potential energy ($E_{M06-2X,LBS}$),
M06-2X/6-31G(d) single-point electronic potential energy ($E_{M06-2X,SBS}$),
Sum of M06-2X/6-31G(d) potential energy and free energy of solvation in dichloromethane at 298.15 K and 1 mol/L (E_{solv}), and
for **TSA–TSD**: Sum of M06-2X/6-31G(d) potential energy and free energy of solvation in toluene at 298.15 K and 1 mol/L by the SMD method ($E_{solv,toluene}$), and
Sum of M06-2X/6-31G(d) potential energy and free energy of solvation in dichloromethane at 298.15 K and 1 mol/L by the CPCM method ($E_{solv,CPCM}$).

For species optimized in solution, the following energies are listed:

B3LYP/6-31G(d) electronic potential energy in solution ($E_{solv-optd}$),
B3LYP/6-31G(d) zero-point energy in solution (ZPE),
B3LYP/6-31G(d) free energy in solution at 298.15 K and 1 mol/L (G_{solv}),
M06-2X/6-311+G(d,p) single-point electronic potential energy in the gas phase ($E_{M06-2X,LBS}$), and
B3LYP/6-31G(d) single-point electronic potential energy in the gas phase (E_{gas})

All energies are given in Hartree.

Hydroxypentadienyl cation 2a-syn, S-conformer

C	1.921291	1.023446	-0.296679
C	1.394773	0.004002	0.629479
C	2.173738	2.389491	0.135903
O	2.188668	0.724118	-1.508157
C	1.758983	0.061500	1.935000
C	2.830746	3.261360	-0.651784
H	3.218250	2.970430	-1.623535
H	2.991764	4.286904	-0.334376
H	1.784645	2.694441	1.100293
H	2.312205	0.939349	2.257276
C	1.526570	-0.974651	2.979054
H	2.433585	-1.098354	3.581235
H	1.245614	-1.943612	2.561490
H	0.741366	-0.645732	3.675740
N	0.569884	-1.053007	0.136620
C	0.825991	-1.809283	-0.973682
O	-0.117701	-2.716993	-1.167472
C	-1.082553	-2.655844	-0.081465
C	-0.827349	-1.295239	0.615953
O	1.785957	-1.671577	-1.744756
H	-0.892770	-3.507131	0.576930
H	-2.075810	-2.733816	-0.521358
H	-0.820572	-1.432259	1.698762
C	-1.777815	-0.171665	0.259598
C	-2.412378	0.544313	1.280759
C	-3.299113	1.579010	0.975506
C	-3.554100	1.906844	-0.355992
C	-2.924601	1.196320	-1.382496
C	-2.041738	0.162141	-1.078088
H	-2.225203	0.285832	2.320997
H	-3.791383	2.122490	1.776426
H	-4.246021	2.708538	-0.596171
H	-3.128052	1.443147	-2.420240
H	-1.571795	-0.390599	-1.888935
H	2.104926	-0.343443	-1.704184

0 imaginary frequencies

E = -861.392957

ZPE = 0.283932

H = -861.090923

G = -861.158316

E_{M06-2X,LBS} = -861.267840

E_{M06-2X,SBS} = -861.029445

E_{solv} = -861.112975

Hydroxypentadienyl cation 2a-syn, U-conformer

C	-1.932429	-0.740252	-0.935707
C	-1.536546	-0.602475	0.403731
C	-2.319082	0.167312	1.272551
C	-3.481451	0.791832	0.813880
C	-3.866882	0.652065	-0.519609
C	-3.091435	-0.116003	-1.393400
C	-0.276722	-1.264309	0.921983
N	0.959581	-0.756446	0.253492
C	1.433167	-1.675737	-0.642264
O	0.817904	-2.840565	-0.504818
C	-0.110487	-2.774920	0.611583
C	1.397271	0.600727	0.346964
C	1.801617	1.135336	1.525802
C	1.976678	0.414770	2.817814
O	2.298098	-1.474257	-1.504414
C	1.501866	1.416357	-0.879343

O	1.923747	0.902085	-1.967972
C	1.181911	2.833175	-0.938598
C	0.280463	3.423318	-0.133258
H	-0.250088	2.880129	0.642753
H	0.020919	4.469081	-0.267910
H	1.634518	3.369298	-1.768667
H	2.065242	2.188749	1.523777
H	2.925142	0.713671	3.278040
H	1.966207	-0.671037	2.703781
H	1.188541	0.704849	3.527786
H	0.334288	-3.325968	1.443689
H	-1.036656	-3.253802	0.296437
H	-0.200111	-1.099650	1.998952
H	-2.031216	0.265368	2.317395
H	-4.087174	1.377024	1.499470
H	-4.773142	1.131628	-0.877176
H	-3.394320	-0.235058	-2.429368
H	-1.347261	-1.345606	-1.624947
H	2.202426	-0.138836	-1.853602

0 imaginary frequencies
E = -861.391160
ZPE = 0.284183
H = -861.088929
G = -861.155927
E_{M06-2X,LBS} = -861.267233
E_{M06-2X,SBS} = -861.028878
E_{solv} = -861.113084

Hydroxypentadienyl cation 2a-syn, S-conformer, H-bond isomer

C	-2.067303	0.111522	-1.063509
C	-1.770274	-0.205975	0.271035
C	-2.406518	0.495448	1.301399
C	-3.330026	1.500114	1.006645
C	-3.618782	1.812121	-0.321817
C	-2.986234	1.116622	-1.356739
C	-0.786149	-1.300527	0.616900
N	0.603695	-1.013691	0.109712
C	0.850310	-1.783813	-0.956382
O	-0.039439	-2.723149	-1.151391
C	-1.016235	-2.673702	-0.062894
C	1.418721	0.059219	0.623054
C	1.815250	0.069802	1.911245
C	1.633412	-0.992246	2.944573
O	1.823162	-1.680150	-1.776821
C	1.887911	1.105341	-0.335407
O	2.144511	0.780476	-1.509847
C	2.072483	2.486775	0.127919
C	2.672280	3.397547	-0.654831
H	3.050252	3.129817	-1.637236
H	2.795043	4.426237	-0.330833
H	1.685917	2.755127	1.105457
H	2.369808	0.947664	2.233996
H	2.579448	-1.150802	3.474530
H	1.309152	-1.948734	2.528724
H	0.908469	-0.669455	3.704899
H	-0.806329	-3.519605	0.595129
H	-2.001882	-2.775960	-0.513661
H	-0.741484	-1.423366	1.699626
H	-2.190408	0.250523	2.339063
H	-3.823293	2.033632	1.813453

H	-4.338222	2.591767	-0.553306
H	-3.213241	1.353999	-2.391642
H	-1.591365	-0.425713	-1.881396
H	2.143322	-0.686201	-1.757449

0 imaginary frequencies
E = -861.394287
ZPE = 0.285017
H = -861.091080
G = -861.158753
E_{M06-2X,LBS} = -861.269377
E_{M06-2X,SBS} = -861.031431
E_{solv} = -861.113041

Hydroxypentadienyl cation 2a-syn, U-conformer, H-bond isomer

C	1.505928	1.453076	-0.911171
C	1.407644	0.636654	0.339966
C	1.145579	2.874586	-0.945994
O	1.941535	0.917582	-1.946246
C	1.844043	1.112724	1.522469
C	0.276536	3.457029	-0.105738
H	-0.205697	2.913921	0.701448
H	-0.004200	4.498501	-0.230566
H	1.564088	3.416258	-1.790325
H	2.123417	2.162923	1.537870
C	2.037885	0.365348	2.800618
H	3.023211	0.605291	3.216231
H	1.970199	-0.718302	2.682204
H	1.303266	0.687936	3.551365
N	0.950542	-0.725857	0.211257
C	1.414526	-1.658576	-0.628504
O	0.839267	-2.826197	-0.496228
C	-0.112781	-2.757098	0.612637
C	-0.281170	-1.243822	0.904497
O	2.317947	-1.517343	-1.519280
H	0.326030	-3.308584	1.446660
H	-1.029215	-3.239823	0.277171
H	-0.179478	-1.057871	1.974858
C	-1.548971	-0.594339	0.397057
C	-2.336567	0.155139	1.278896
C	-3.514610	0.759040	0.834483
C	-3.909028	0.619783	-0.496364
C	-3.127204	-0.126993	-1.382907
C	-1.953189	-0.732359	-0.939671
H	-2.038625	0.256451	2.320355
H	-4.123652	1.330566	1.528359
H	-4.826370	1.085832	-0.843193
H	-3.435238	-0.241845	-2.417679
H	-1.360911	-1.316699	-1.641070
H	2.357671	-0.507049	-1.780098

0 imaginary frequencies
E = -861.392559
ZPE = 0.285081
H = -861.089331
G = -861.156648
E_{M06-2X,LBS} = -861.268756
E_{M06-2X,SBS} = -861.030715
E_{solv} = -861.113065

Hydroxypentadienyl cation 2a-anti, S-conformer

C	0.721752	1.834677	-0.338617
O	0.010015	1.605468	-1.399634
C	0.857259	3.210616	0.078649

H	1.377448	3.411866	1.006750
C	0.350486	4.224701	-0.649666
H	-0.178426	4.055019	-1.582486
H	0.462608	5.252791	-0.319985
C	1.309619	0.680779	0.315619
C	2.261024	0.813589	1.281823
C	3.018455	-0.272487	1.947333
H	4.036737	-0.289882	1.528959
H	3.124005	-0.058848	3.017167
H	2.587055	-1.264716	1.809867
H	2.542710	1.821576	1.575589
N	0.909181	-0.567818	-0.253014
C	1.940848	-1.402920	-0.784545
O	3.021985	-1.027131	-1.145191
O	1.498044	-2.671579	-0.805280
C	0.129370	-2.745815	-0.354629
H	-0.515908	-2.853708	-1.229879
H	0.026937	-3.625849	0.280855
C	-0.125753	-1.426931	0.406249
H	0.145745	-1.549393	1.462687
C	-1.535590	-0.884562	0.324603
C	-2.192371	-0.496477	1.498444
C	-3.491938	0.012139	1.451369
C	-4.146086	0.143249	0.226357
C	-3.499597	-0.239598	-0.952031
C	-2.204336	-0.752987	-0.903376
H	-1.728101	-1.068203	-1.830347
H	-4.008455	-0.150257	-1.907169
H	-5.158333	0.534311	0.188174
H	-3.991988	0.300057	2.371249
H	-1.690667	-0.603247	2.457576
H	0.005160	0.621310	-1.542550

0 imaginary frequencies

E = -861.383091

ZPE = 0.285696

H = -861.079003

G = -861.146930

E_{M06-2X,LBS} = -861.259559

E_{M06-2X,SBS} = -861.020812

E_{solv} = -861.110426

TSA

C	-2.128226	-1.146546	-0.627954
C	-2.006871	-2.547630	-0.638682
C	-0.939361	-3.094037	0.080459
C	-1.327766	-0.543564	0.412933
C	-1.010675	-1.438003	1.471808
H	-2.768677	-3.163447	-1.110356
H	-1.004049	-4.116922	0.450082
H	0.074518	-2.726403	-0.040207
O	-2.866532	-0.530304	-1.519838
C	0.055112	-1.292213	2.516513
H	-1.847936	-2.039259	1.805962
N	-0.857898	0.776057	0.302844
C	-1.701205	1.835084	-0.045449
O	-1.034731	2.984568	0.006457
C	0.376730	2.737305	0.180514
C	0.487356	1.275376	0.692753
O	-2.884439	1.746079	-0.325674
H	0.764217	3.467838	0.890269
H	0.863884	2.862542	-0.789548
H	0.580217	1.276065	1.782884

C	1.644174	0.517530	0.071218
C	1.564252	-0.002083	-1.229288
C	2.666689	-0.640755	-1.799044
C	3.860560	-0.755112	-1.082372
C	3.949733	-0.229251	0.207207
C	2.844939	0.400846	0.783466
H	0.649169	0.103912	-1.806934
H	2.596204	-1.038229	-2.807268
H	4.718503	-1.247408	-1.530036
H	4.876416	-0.309244	0.767341
H	2.922628	0.809780	1.788858
H	-3.079525	0.397848	-1.202515
H	0.150367	-2.226461	3.076320
H	1.031539	-1.023806	2.111793
H	-0.249217	-0.523631	3.241398

1 imaginary frequency

E = -861.355255

ZPE = 0.285762

H = -861.052535

G = -861.116393

E_{M06-2X,LBS} = -861.230402

E_{M06-2X,SBS} = -860.993181

E_{solv} = -861.081094

E_{solv,toluene} = -861.053277

E_{solv,CPCM} = -861.059291

TSB

C	-2.091762	-0.346047	-0.936144
C	-1.784237	-0.122410	0.418022
C	-2.711028	0.550560	1.228093
C	-3.924543	0.988392	0.699176
C	-4.223469	0.767514	-0.647559
C	-3.306209	0.104142	-1.463366
C	-0.505963	-0.655420	1.051001
N	0.688745	-0.633886	0.169659
C	0.850166	-1.906300	-0.454025
O	0.031579	-2.779558	0.151404
C	-0.564461	-2.180775	1.320782
C	1.523675	0.422680	-0.124729
C	2.917581	0.217068	-0.367284
H	3.344761	0.733465	-1.220462
O	1.575416	-2.142730	-1.381798
C	1.081738	1.784442	-0.167027
C	2.131564	2.713174	-0.055096
C	3.327529	2.276169	0.496048
O	-0.161849	2.214761	-0.306965
C	3.721717	-0.926677	0.151144
H	2.028556	3.697984	-0.504322
H	4.255847	2.799513	0.272749
H	3.358841	1.654905	1.383113
H	-0.790397	1.498745	-0.550038
H	-0.290174	-0.112420	1.974958
H	-1.581578	-2.559257	1.410512
H	0.025484	-2.467839	2.196847
H	-2.482168	0.734607	2.275234
H	-4.631980	1.510033	1.336514
H	-5.166361	1.113674	-1.059486
H	-3.533987	-0.074204	-2.509847
H	-1.399643	-0.877761	-1.584016
H	4.755252	-0.603926	0.316541
H	3.321404	-1.343542	1.079517
H	3.749983	-1.725616	-0.600767

1 imaginary frequency
 E = -861.360817
 ZPE = 0.285220
 H = -861.058446
 G = -861.122703
 E_{M06-2X,LBS} = -861.236817
 E_{M06-2X,SBS} = -860.999284
 E_{solv} = -861.086733
 E_{solv,toluene} = -861.059047
 E_{solv,CPCM} = -861.064640

TSC

C	2.094118	-0.722745	0.984623
O	1.993128	0.039060	2.067097
C	2.949054	-1.810104	0.789045
C	3.065680	-2.286940	-0.516978
H	3.361956	-3.319660	-0.694122
H	3.209199	-1.617749	-1.356457
H	3.388568	-2.342343	1.630177
C	1.163701	-0.524772	-0.098279
C	0.893867	-1.657800	-0.902966
H	0.750407	-2.604757	-0.392580
C	0.370481	-1.585314	-2.300481
H	0.660706	-2.483729	-2.854548
H	-0.728414	-1.568201	-2.291197
H	0.729831	-0.704071	-2.838482
N	0.646938	0.719053	-0.328754
C	1.454956	1.887138	-0.173299
O	0.677540	2.962345	-0.348358
C	-0.713639	2.578716	-0.412192
H	-1.162199	2.742180	0.571386
H	-1.203569	3.208202	-1.154557
C	-0.714352	1.077503	-0.796470
O	2.637104	1.886080	0.036558
C	-1.834520	0.278120	-0.168013
C	-2.896484	-0.160385	-0.968609
C	-3.972724	-0.846418	-0.402443
C	-3.990659	-1.105761	0.968280
C	-2.932952	-0.673203	1.772889
C	-1.861398	0.019017	1.210572
H	-1.046755	0.356931	1.846987
H	-2.946055	-0.869492	2.840944
H	-0.761379	0.982276	-1.887174
H	-2.892013	0.046947	-2.036787
H	-4.826234	-1.640251	1.410086
H	-4.793767	-1.175531	-1.032188
H	2.818204	0.053677	2.583333

1 imaginary frequency
 E = -861.359965
 ZPE = 0.285260
 H = -861.057340
 G = -861.121902
 E_{M06-2X,LBS} = -861.236972
 E_{M06-2X,SBS} = -860.998585
 E_{solv} = -861.089227
 E_{solv,toluene} = -861.059521
 E_{solv,CPCM} = -861.066763

Transition state analogous to TSC but containing an OH...O=C hydrogen bond

C	-2.211147	-0.728751	-0.865756
O	-2.515202	0.038270	-1.899364
C	-2.821571	-1.992089	-0.727824
C	-2.829078	-2.597936	0.516590
H	-2.978038	-3.672898	0.607878
H	-3.008382	-2.030747	1.422841
H	-3.200064	-2.497617	-1.613635
C	-1.223231	-0.467203	0.143265
C	-0.805497	-1.593253	0.912317
H	-0.548932	-2.496909	0.371471
C	-0.299733	-1.525630	2.316387
H	-0.562918	-2.451457	2.839890
H	0.797500	-1.477406	2.326005
H	-0.704293	-0.678974	2.876182
N	-0.669330	0.785185	0.366173
C	-1.344557	1.994765	0.115752
O	-0.544401	3.023210	0.375726
C	0.814249	2.572469	0.576660
H	1.376522	2.792691	-0.333824
H	1.233549	3.126630	1.416032
C	0.719015	1.047628	0.843342
O	-2.485814	2.091310	-0.289127
C	1.793558	0.241535	0.143820
C	2.879750	-0.236841	0.887489
C	3.923652	-0.916693	0.257242
C	3.884461	-1.130760	-1.120965
C	2.802833	-0.657899	-1.869109
C	1.764280	0.029407	-1.242460
H	0.932187	0.399323	-1.837282
H	2.770909	-0.819025	-2.942513
H	0.767729	0.866469	1.920996
H	2.921583	-0.064175	1.961190
H	4.694341	-1.661278	-1.612438
H	4.764002	-1.276575	0.843058
H	-2.488944	0.990835	-1.627429

1 imaginary frequency

E = -861.359203

ZPE = 0.285118

H = -861.056942

G = -861.121314

E_{M06-2X,LBS} = -861.234386

E_{M06-2X,SBS} = -860.996882

E_{solv} = -861.085006

E_{solv,toluene} = -861.057073

E_{solv,CPCM} = -861.063087

TSD

C	-0.533592	1.579935	-1.194286
O	-0.073054	1.079298	-2.342089
C	-0.476357	2.918338	-0.785998
C	-0.683475	3.177073	0.564021
H	-1.027659	4.157564	0.887985
H	-0.229347	2.566099	1.334482
H	-0.409194	3.724360	-1.514654
C	-1.221054	0.716592	-0.282700
C	-2.110750	1.350843	0.631182
H	-2.743443	2.135068	0.228129
C	-2.526746	0.800504	1.950109
H	-2.728899	1.620784	2.647181

H	-3.461893	0.238390	1.829286
H	-1.781424	0.127718	2.382585
N	-0.996063	-0.632865	-0.263683
C	-2.059786	-1.569040	-0.103883
O	-1.545626	-2.804471	-0.162732
C	-0.102380	-2.756220	-0.190673
H	0.269713	-2.945680	0.820080
H	0.248510	-3.535538	-0.866643
C	0.249222	-1.332504	-0.679290
O	-3.219686	-1.288078	0.032370
C	1.515984	-0.752150	-0.091804
C	2.607338	-0.490140	-0.928501
C	3.801020	0.007471	-0.401769
C	3.909610	0.258388	0.966424
C	2.823916	0.003003	1.808997
C	1.635270	-0.503026	1.284226
H	0.803718	-0.717182	1.952153
H	2.908349	0.185677	2.876318
H	0.311282	-1.321358	-1.771501
H	2.528827	-0.690010	-1.994695
H	4.837614	0.644313	1.377515
H	4.644325	0.195343	-1.059722
H	0.539564	1.696118	-2.779442

1 imaginary frequency

E = -861.361683

ZPE = 0.285319

H = -861.059038

G = -861.123585

E_{M06-2X,LBS} = -861.238604

E_{M06-2X,SBS} = -861.000140

E_{solv} = -861.091419

E_{solv,toluene} = -861.061216

E_{solv,CPCM} = -861.069518

Cyclic oxyallyl cation (β)-3a-syn

C	-2.479177	-0.438881	-0.881304
O	-3.134431	0.485553	-1.573700
C	-2.752692	-1.779758	-1.030849
H	-3.501855	-2.134882	-1.732003
C	-1.911463	-2.662439	-0.194604
H	-2.513438	-3.365281	0.395345
H	-1.254463	-3.283076	-0.821671
C	-1.104294	-1.680228	0.679954
C	-1.378891	-0.332660	0.050966
C	-1.583841	-1.724671	2.156222
H	-2.668278	-1.587064	2.210475
H	-1.337103	-2.701423	2.581341
H	-0.032144	-1.899200	0.640341
H	-1.115534	-0.959009	2.780472
N	-0.636793	0.738076	0.389285
C	-0.886457	2.110655	0.027098
O	0.035721	2.877884	0.582000
C	0.878425	2.137466	1.494083
C	0.677292	0.652384	1.115660
O	-1.785439	2.520461	-0.664777
H	1.902740	2.475913	1.346668
H	0.546247	2.365599	2.510086
H	0.546156	0.059204	2.020362
C	1.785344	0.057035	0.267308
C	2.602655	-0.936312	0.822014
C	3.668902	-1.462409	0.089909
C	3.920582	-1.002125	-1.202581

C	3.108466	-0.011008	-1.761026
C	2.046972	0.520415	-1.030559
H	1.434278	1.298625	-1.479493
H	3.305087	0.352945	-2.764865
H	4.748384	-1.410801	-1.773970
H	4.298608	-2.229245	0.530591
H	2.417045	-1.292278	1.833511
H	-2.795929	1.387472	-1.364120

0 imaginary frequencies
E = -861.414279
ZPE = 0.288557
H = -861.108634
G = -861.173792

E_{M06-2X,LBS} = -861.290346
E_{M06-2X,SBS} = -861.054097
E_{solv} = -861.141547

Cyclic oxyallyl cation (β)-3a-*anti*

C	1.575347	-1.532888	-0.764417
O	0.645918	-1.981168	-1.636702
C	2.721662	-2.135012	-0.343840
H	3.045415	-3.120740	-0.667381
C	3.513786	-1.274805	0.574388
H	3.750688	-1.792666	1.511998
H	4.479900	-1.014275	0.119313
C	2.626655	-0.028453	0.801493
C	1.502825	-0.205449	-0.195034
C	2.076065	0.029035	2.251872
H	1.546546	-0.895260	2.504700
H	2.918395	0.145712	2.939167
H	3.163198	0.903097	0.605897
H	1.407526	0.878941	2.390727
N	0.595079	0.711088	-0.498574
C	0.730045	2.122972	-0.127317
O	-0.235167	2.798946	-0.740410
C	-0.964602	1.975453	-1.680155
C	-0.709954	0.522793	-1.232249
O	1.570068	2.578454	0.591542
H	-2.014358	2.257528	-1.619971
H	-0.573185	2.184090	-2.679608
H	-0.544951	-0.123892	-2.090288
C	-1.780216	-0.060889	-0.326680
C	-2.373324	-1.282967	-0.663620
C	-3.385358	-1.818601	0.135076
C	-3.805705	-1.140788	1.279299
C	-3.219015	0.080786	1.620191
C	-2.214468	0.622260	0.820400
H	-1.786296	1.584226	1.091503
H	-3.549503	0.616880	2.504694
H	-4.592613	-1.557506	1.900725
H	-3.845796	-2.762629	-0.140652
H	-2.048912	-1.814031	-1.553418
H	0.869376	-2.877637	-1.939267

0 imaginary frequencies
E = -861.413495
ZPE = 0.288516
H = -861.107723
G = -861.172601

$E_{M06-2X,LBS} = -861.293380$
 $E_{M06-2X,SBS} = -861.057117$
 $E_{solv} = -861.144169$

Cyclic oxyallyl cation (α)-3a-syn

C	-2.877870	-0.354141	-0.281453
O	-3.641258	0.639428	-0.728987
C	-3.394011	-1.594870	0.007862
C	-2.402657	-2.532181	0.584202
C	-1.061802	-1.780865	0.430137
C	-1.491441	-0.363150	0.136014
H	-4.444685	-1.827806	-0.135908
H	-2.632178	-2.737837	1.640295
H	-2.409897	-3.505009	0.078167
C	-0.241474	-2.369701	-0.753156
H	0.068758	-3.384850	-0.490063
H	-0.860984	-2.417454	-1.654132
H	0.651079	-1.782264	-0.968088
H	-0.453098	-1.830488	1.338633
N	-0.667435	0.684180	0.306034
C	-0.885731	2.019337	-0.196550
O	-0.030869	2.842896	0.386567
C	0.701568	2.180028	1.443959
C	0.607503	0.672703	1.107481
O	-1.672986	2.332470	-1.054575
H	0.222699	2.433687	2.393598
H	1.723408	2.554250	1.421521
H	0.427615	0.101065	2.020098
C	1.820656	0.124940	0.384985
C	2.611716	-0.833724	1.029307
C	3.771210	-1.316816	0.419726
C	3.360246	0.113789	-1.485941
C	4.143953	-0.846654	-0.839556
C	2.206495	0.604080	-0.876367
H	1.616256	1.357532	-1.392098
H	2.330045	-1.201100	2.013947
H	4.379203	-2.058039	0.929326
H	5.043864	-1.222779	-1.316453
H	3.650470	0.486170	-2.463641
H	-3.089785	1.390674	-1.045359

0 imaginary frequencies

E = -861.411652

ZPE = 0.288593

H = -861.106052

G = -861.170566

$E_{M06-2X,LBS} = -861.289499$

$E_{M06-2X,SBS} = -861.053139$

$E_{solv} = -861.140268$

Cyclic oxyallyl cation (α)-3a-anti

C	1.197919	-1.719017	-0.528188
O	0.247176	-2.009794	-1.440633
C	2.073656	-2.543674	0.108520
C	2.989136	-1.804676	1.019344
C	2.685169	-0.310399	0.745077
C	1.416462	-0.362220	-0.075627
H	2.100930	-3.622204	-0.021358
H	2.790018	-2.067455	2.068098
H	4.038562	-2.062609	0.833869
C	3.846276	0.370583	-0.027407
H	4.737751	0.361072	0.605444

H	4.071226	-0.172528	-0.951200
H	3.616162	1.409870	-0.264364
H	2.508533	0.255355	1.662128
N	0.631233	0.668080	-0.349378
C	0.849177	2.015903	0.190687
O	-0.032043	2.828538	-0.378319
C	-0.792326	2.164233	-1.414042
C	-0.672521	0.657732	-1.097275
O	1.663606	2.310663	1.015007
H	-0.349842	2.429639	-2.378231
H	-1.816979	2.526992	-1.354487
H	-0.548900	0.082381	-2.012344
C	-1.820893	0.097920	-0.276488
C	-2.703626	-0.802910	-0.884340
C	-3.813749	-1.281528	-0.187585
C	-3.166048	0.025202	1.738795
C	-4.044506	-0.871127	1.125904
C	-2.061692	0.513425	1.041246
H	-1.400622	1.220004	1.536932
H	-2.525756	-1.128851	-1.905865
H	-4.494855	-1.975461	-0.671092
H	-4.906395	-1.245306	1.670065
H	-3.343126	0.351236	2.759255
H	0.180137	-2.970633	-1.571363

0 imaginary frequencies
E = -861.413816
ZPE = 0.288377
H = -861.108113
G = -861.173472
E_{M06-2X,LBS} = -861.294289
E_{M06-2X,SBS} = -861.057756
E_{solv} = -861.144892

Transition states for Nazarov cyclization of 1b, analogous to TSA–TSD:

TSA

C	2.770753	-0.251711	-1.044249
C	1.691535	-0.460564	-0.176829
C	1.765982	0.011205	1.142148
C	2.904258	0.687923	1.580484
C	3.979662	0.891060	0.710608
C	3.913329	0.417690	-0.600048
C	0.488841	-1.241298	-0.666299
N	-0.830967	-0.709868	-0.225271
C	-1.684493	-1.776249	0.110442
O	-1.004938	-2.915177	0.114098
C	0.405428	-2.666512	-0.074213
C	-1.264705	0.580325	-0.529606
C	-0.552069	1.396419	-1.424805
H	0.458038	1.135903	-1.723240
O	-2.881068	-1.714203	0.328551
C	-2.359425	1.261116	0.147219
O	-3.388563	0.734973	0.750394
C	-2.198043	2.661314	0.114982
C	-0.934817	3.177710	-0.164938
H	-3.064748	3.305532	0.241097
H	-0.839063	4.188531	-0.560066
H	-0.031529	2.784762	0.289315
H	-1.081236	2.041476	-2.112288
H	0.797869	-3.433492	-0.741244
H	0.895142	-2.730508	0.900303
H	0.495112	-1.287420	-1.763663

H	0.940802	-0.154457	1.831003
H	2.956174	1.047630	2.603880
H	4.866743	1.412901	1.056491
H	4.747326	0.568085	-1.278753
H	2.725799	-0.620399	-2.067052
H	-3.410532	-0.264768	0.607405

1 imaginary frequency

E = -822.041736

ZPE = 0.257402

H = -821.768942

G = -821.829779

E_{M06-2X,LBS} = -821.924054

E_{M06-2X,SBS} = -821.697848

E_{solv} = -821.784786

TSB

C	0.585088	2.148932	1.382881
C	0.360308	0.649987	1.057353
N	-0.841024	0.779845	0.201953
C	-0.915001	2.101108	-0.341954
O	0.007239	2.856481	0.266722
C	1.563057	0.011300	0.372620
C	1.813671	0.176041	-1.001100
C	2.971847	-0.359998	-1.572186
C	3.888953	-1.052810	-0.781437
C	3.645640	-1.219885	0.584614
C	2.488940	-0.694864	1.158447
C	-1.748382	-0.191904	-0.154475
C	-1.485798	-1.606678	-0.037726
O	-0.303473	-2.193971	-0.018017
O	-1.666400	2.461182	-1.206604
C	-3.037578	0.149160	-0.601503
H	-3.442754	1.135956	-0.410033
C	-2.650670	-2.386780	0.069495
C	-3.835444	-1.776830	0.452210
H	-3.505682	-0.400333	-1.407050
H	-2.622765	-3.428480	-0.241098
H	-4.790923	-2.234548	0.201847
H	-3.879236	-1.017774	1.224092
H	0.431738	-1.591278	-0.277431
H	0.110401	0.099185	1.968559
H	1.638427	2.418305	1.441834
H	0.062677	2.455919	2.293897
H	2.303174	-0.833930	2.221083
H	4.352489	-1.765545	1.202105
H	4.788492	-1.465481	-1.227652
H	3.156321	-0.226104	-2.633662
H	1.118089	0.724972	-1.630392

1 imaginary frequency

E = -822.036896

ZPE = 0.257099

H = -821.764104

G = -821.825530

E_{M06-2X,LBS} = -821.920443

E_{M06-2X,SBS} = -821.693708

E_{solv} = -821.781682

TSC

C	-1.975705	-0.032447	1.121022
C	-1.832190	0.266995	-0.242755
C	-2.803472	-0.176427	-1.149001
C	-3.908582	-0.902370	-0.700922

C	-4.044640	-1.197355	0.655778
C	-3.075499	-0.763400	1.565359
C	-0.672944	1.094638	-0.744503
N	0.660457	0.653981	-0.263020
C	1.519551	1.785881	-0.087597
O	0.770520	2.891270	-0.164020
C	-0.634600	2.552874	-0.235321
C	1.137974	-0.618329	-0.227522
C	0.653998	-1.652289	-1.037394
H	0.022182	-1.423716	-1.891100
O	2.709880	1.735096	0.057937
C	2.243039	-0.966186	0.649963
C	3.015622	-2.020118	0.160789
C	2.871183	-2.347257	-1.189826
O	2.339068	-0.370529	1.826477
H	3.101587	-3.356007	-1.528934
H	2.850795	-1.594774	-1.967769
H	3.601785	-2.646513	0.829999
H	0.577970	-2.664026	-0.660946
H	-1.064263	2.645784	0.765639
H	-1.115627	3.255602	-0.914860
H	-1.228348	0.302636	1.836607
H	-3.180684	-0.989850	2.622206
H	-0.667694	1.095721	-1.841904
H	-2.705240	0.057839	-2.206956
H	-4.903520	-1.761853	1.006152
H	-4.659523	-1.234892	-1.411131
H	3.229230	-0.455773	2.212568

1 imaginary frequency

E = -822.036944

ZPE = 0.256949

H = -821.764084

G = -821.826009

E_{M06-2X,LBS} = -821.921555

E_{M06-2X,SBS} = -821.693855

E_{solv} = -821.784982

Transition state analogous to TSC but containing an OH...O=C hydrogen bond

C	-0.824721	2.105932	-1.427194
C	-0.652994	0.595048	-1.137576
N	0.662408	0.625382	-0.433196
C	0.912918	1.927069	0.041210
O	0.015809	2.766860	-0.456285
C	-1.773800	-0.034051	-0.329806
C	-1.969151	0.278504	1.023294
C	-3.047747	-0.266371	1.718710
C	-3.942669	-1.121818	1.070768
C	-3.756382	-1.433312	-0.276717
C	-2.674261	-0.893428	-0.973196
C	1.359137	-0.530656	-0.100243
C	2.685149	-0.591242	0.504584
O	3.286609	0.296801	1.247470
O	1.775648	2.274847	0.826384
C	0.836108	-1.789940	-0.450263
C	3.333475	-1.811095	0.222352
C	2.896968	-2.575788	-0.853270
H	0.025560	-1.873582	-1.165489
H	3.111967	-3.643372	-0.883081
H	2.648608	-2.140601	-1.814350
H	4.114721	-2.162933	0.891824
H	0.907265	-2.622903	0.234018

H	-1.845220	2.454971	-1.277168
H	-0.470657	2.383870	-2.423393
H	-1.288564	0.948065	1.543544
H	-3.192023	-0.018897	2.766044
H	-0.536859	0.064604	-2.086659
H	-2.538662	-1.134503	-2.026094
H	-4.782860	-1.541999	1.615165
H	-4.449526	-2.095776	-0.786196
H	2.742685	1.144186	1.307742

1 imaginary frequency
E = -822.040257
ZPE = 0.257291
H = -821.767463
G = -821.829239

E_{M06-2X,LBS} = -821.922061
E_{M06-2X,SBS} = -821.695495
E_{solv} = -821.783670

TSD

C	-1.536382	-0.595904	-1.212035
C	-1.307887	-0.772003	0.161374
C	-2.357431	-0.553965	1.061822
C	-3.618241	-0.170939	0.599903
C	-3.836499	0.008517	-0.766698
C	-2.793158	-0.203912	-1.672068
C	0.035825	-1.237224	0.679777
N	1.195184	-0.512742	0.102066
C	2.263706	-1.411934	-0.198863
O	1.837783	-2.659106	0.020000
C	0.414823	-2.682398	0.269844
C	1.372513	0.839573	0.027461
C	2.244880	1.418347	-0.907780
H	2.588325	0.848895	-1.763723
O	3.359008	-1.087197	-0.571035
C	0.653284	1.756262	0.874756
C	0.507848	3.043783	0.341829
C	0.677065	3.210509	-1.026351
O	0.251325	1.347195	2.074147
H	0.938735	4.186543	-1.430402
H	0.302020	2.492174	-1.744557
H	0.383751	3.903655	0.997914
H	2.831206	2.290903	-0.651067
H	-0.088144	-2.990282	-0.650518
H	0.223549	-3.410268	1.057861
H	-0.736532	-0.776790	-1.926908
H	-2.962284	-0.076533	-2.737334
H	0.064236	-1.139607	1.768900
H	-2.192871	-0.698473	2.127291
H	-4.816777	0.305586	-1.127108
H	-4.427890	-0.016166	1.306920
H	-0.380621	1.970151	2.475542

1 imaginary frequency
E = -822.036667
ZPE = 0.257116
H = -821.763650
G = -821.825525
E_{M06-2X,LBS} = -821.921138
E_{M06-2X,SBS} = -821.693444
E_{solv} = -821.785969

Transition states for Nazarov cyclization of 1c, analogous to TSA–TSD:

TSA

C	3.035633	-1.063777	0.644454
C	2.072701	-0.279868	-0.004117
C	1.645525	-0.642727	-1.289706
C	2.168052	-1.779625	-1.908209
C	3.128255	-2.556794	-1.255553
C	3.564456	-2.194884	0.019685
C	1.577099	0.986375	0.666891
N	0.173777	1.347199	0.348333
C	0.063833	2.702322	0.044515
O	1.268231	3.272865	0.051244
C	2.294180	2.263362	0.150567
C	-0.964774	0.529764	0.515748
C	-1.166750	-0.387414	1.579590
C	-0.157720	-0.907027	2.560265
O	-0.972112	3.308392	-0.174465
C	-2.003733	0.491457	-0.471086
O	-2.296088	1.430387	-1.349800
C	-2.740025	-0.714977	-0.470500
C	-2.122399	-1.792437	0.209951
C	-4.083197	-0.787273	-1.132040
C	-2.869195	-2.966689	0.764680
H	-1.075323	-1.986391	-0.005669
H	-2.176723	-0.399373	1.969523
H	3.063713	2.625378	0.832192
H	2.718315	2.111839	-0.845293
H	1.703516	0.909689	1.751467
H	0.917093	-0.031220	-1.816430
H	1.833613	-2.051237	-2.905237
H	3.537468	-3.437286	-1.741596
H	4.314635	-2.790994	0.530483
H	3.381528	-0.786528	1.638221
H	-1.930326	2.309250	-1.035708
H	-0.580594	-1.756853	3.104257
H	0.780932	-1.219259	2.101160
H	0.057132	-0.135184	3.313093
H	-4.663734	-1.646559	-0.790253
H	-4.654963	0.132091	-0.976386
H	-3.946332	-0.892768	-2.217420
H	-2.295946	-3.442520	1.566907
H	-3.861737	-2.706795	1.141559
H	-2.990613	-3.727556	-0.019848

1 imaginary frequency

E = -940.006140

ZPE = 0.341671

H = -939.644055

G = -939.715900

E_{M06-2X,LBS} = -939.861476

E_{M06-2X,SBS} = -939.603143

E_{solv} = -939.688528

TSB

C	-1.654701	2.201226	-1.261909
C	-1.122924	0.762910	-1.035052
N	0.005574	1.083850	-0.128406
C	-0.234062	2.323186	0.525381
O	-1.282308	2.919700	-0.068807
C	-2.178535	-0.165821	-0.451148
C	-2.575591	-0.083433	0.895445

C	-3.592473	-0.912573	1.379399
C	-4.226116	-1.818318	0.527670
C	-3.838944	-1.900105	-0.811979
C	-2.818757	-1.082467	-1.297147
C	1.131701	0.327328	0.148659
C	1.133504	-1.098620	0.161749
O	0.080855	-1.892956	0.335145
O	0.378007	2.753853	1.465446
C	2.394035	0.942020	0.381082
C	2.799085	2.294362	-0.100784
C	2.404750	-1.690813	0.001708
C	3.386693	-0.877136	-0.590141
H	2.982259	0.549699	1.202801
C	2.650184	-3.086398	0.503914
C	4.861534	-1.088057	-0.452373
H	3.096373	-0.264663	-1.437122
H	-0.727478	-1.400357	0.595300
H	-0.736855	0.346659	-1.969442
H	-2.738747	2.244974	-1.356806
H	-1.179776	2.684697	-2.121597
H	-2.517257	-1.158512	-2.339366
H	-4.324860	-2.606688	-1.477989
H	-5.016953	-2.458631	0.906102
H	-3.892190	-0.839711	2.420493
H	-2.109759	0.630476	1.569926
H	3.877387	2.308027	-0.296181
H	2.267479	2.601003	-1.005963
H	2.603512	3.039433	0.680740
H	3.713366	-3.329641	0.535778
H	2.211192	-3.241368	1.494303
H	2.164244	-3.802136	-0.172290
H	5.394834	-0.138803	-0.571244
H	5.147113	-1.537697	0.501638
H	5.218372	-1.742220	-1.261357

1 imaginary frequency

E = -940.010163

ZPE = 0.341270

H = -939.648340

G = -939.720490

E_{M06-2X,LBS} = -939.866389

E_{M06-2X,SBS} = -939.607544

E_{solv} = -939.692893

TSC

C	-2.194410	-0.395662	1.245610
C	-2.309649	-0.150977	-0.130985
C	-3.204392	-0.915249	-0.889862
C	-3.976810	-1.908540	-0.284590
C	-3.854048	-2.149901	1.083942
C	-2.960586	-1.393017	1.846914
C	-1.534322	0.963694	-0.798669
N	-0.114146	1.068133	-0.388560
C	0.275606	2.429057	-0.243346
O	-0.813069	3.198819	-0.382270
C	-2.006141	2.386033	-0.404257
C	0.786879	0.053474	-0.188377
C	0.885977	-1.092140	-1.005072
C	0.316554	-1.196109	-2.383691
O	1.399578	2.816312	-0.065644
C	1.770514	0.170984	0.850195
C	2.951132	-0.545686	0.622957
C	3.162752	-0.917127	-0.726552

O	1.453998	0.838624	1.962276
C	4.032194	-2.053402	-1.159278
H	2.986174	-0.164123	-1.486929
C	3.864658	-0.946532	1.750660
H	1.097313	-2.033674	-0.509725
H	0.885869	-1.925930	-2.969213
H	-0.715676	-1.570510	-2.341833
H	0.320131	-0.239253	-2.912522
H	-2.450691	2.398425	0.594635
H	-2.698550	2.820301	-1.125124
H	-1.505462	0.190632	1.849188
H	-2.865306	-1.575688	2.913275
H	-1.593649	0.849344	-1.887139
H	-3.310128	-0.725705	-1.956113
H	-4.453275	-2.922596	1.556217
H	-4.672124	-2.490197	-0.882382
H	2.241123	1.211369	2.395598
H	3.744274	-2.401138	-2.156418
H	5.071430	-1.701269	-1.245610
H	4.020205	-2.899699	-0.467371
H	4.239928	-1.964762	1.611244
H	4.744131	-0.290526	1.794702
H	3.353796	-0.905375	2.716953

1 imaginary frequency
 E = -940.009237
 ZPE = 0.341311
 H = -939.647220
 G = -939.719089
 E_{M06-2X,LBS} = -939.866325
 E_{M06-2X,SBS} = -939.606721
 E_{solv} = -939.695075

Transition state analogous to TSC but containing an OH...O=C hydrogen bond

C	-2.265633	2.211462	-0.595220
C	-1.579777	0.843341	-0.859931
N	-0.188152	1.158089	-0.436674
C	-0.045495	2.525198	-0.161900
O	-1.195966	3.157986	-0.378481
C	-2.220662	-0.309563	-0.114326
C	-2.048569	-0.473166	1.267939
C	-2.707866	-1.501372	1.939969
C	-3.551284	-2.370044	1.241920
C	-3.730231	-2.210188	-0.132434
C	-3.063380	-1.186324	-0.808248
C	0.829471	0.223780	-0.257257
C	1.856966	0.367646	0.728394
O	1.794333	1.148720	1.804633
O	0.972040	3.064271	0.230207
C	0.893859	-0.947313	-1.053311
C	0.338074	-1.085606	-2.433514
C	2.973414	-0.483031	0.547577
C	3.814154	-0.885635	1.728590
C	3.207747	-0.948619	-0.754273
C	4.066435	-2.127232	-1.080335
H	3.026029	-0.267110	-1.579122
H	1.101178	-1.880456	-0.543985
H	0.946790	-1.800275	-2.999221
H	-0.673949	-1.511973	-2.401358
H	0.312537	-0.139990	-2.980498
H	-2.880897	2.191107	0.307253
H	-2.859218	2.560000	-1.440385

H	-1.397912	0.198458	1.823365
H	-2.567892	-1.621043	3.010231
H	-1.593157	0.635248	-1.933382
H	-3.214300	-1.061218	-1.878723
H	-4.067705	-3.166537	1.769115
H	-4.387021	-2.879348	-0.680038
H	1.427382	2.031214	1.539746
H	3.749434	-2.587594	-2.022370
H	5.101380	-1.789346	-1.241985
H	4.074486	-2.885417	-0.293733
H	4.836277	-1.135726	1.437284
H	3.836732	-0.067767	2.453603
H	3.380295	-1.756671	2.238222

1 imaginary frequency
 E = -940.009688
 ZPE = 0.341041
 H = -939.648089
 G = -939.720333
 $E_{M06-2X,LBS} = -939.864811$
 $E_{M06-2X,SBS} = -939.606120$
 $E_{solv} = -939.691598$

TSD

C	-1.733794	-0.927516	1.315362
C	-1.842734	-0.752089	-0.072700
C	-2.148852	-1.856828	-0.875915
C	-2.350304	-3.115244	-0.304890
C	-2.235524	-3.282246	1.075526
C	-1.925514	-2.185768	1.885119
C	-1.678257	0.610243	-0.709280
N	-0.462699	1.345804	-0.278367
C	-0.734890	2.738266	-0.179335
O	-2.059907	2.918945	-0.292085
C	-2.747015	1.649943	-0.301012
C	0.821789	0.859745	-0.257452
C	1.789158	1.321404	0.670574
C	1.493507	2.000998	1.962761
O	0.085407	3.605616	-0.042665
C	1.240941	-0.194729	-1.122717
C	2.347209	-0.938020	-0.680951
C	2.600811	-0.861818	0.703232
O	0.616801	-0.355009	-2.298168
C	3.920289	-1.148977	1.343746
H	1.747952	-0.907298	1.371839
C	3.225644	-1.686047	-1.651183
H	2.800478	1.442074	0.298037
H	2.274785	1.764352	2.693992
H	1.503245	3.088524	1.815924
H	0.517922	1.724978	2.371723
H	-3.139504	1.461255	0.702360
H	-3.569696	1.715381	-1.012832
H	-1.511935	-0.077103	1.956283
H	-1.847085	-2.308685	2.961497
H	-1.661779	0.504642	-1.798108
H	-2.246022	-1.729468	-1.951735
H	-2.394295	-4.259685	1.521245
H	-2.600288	-3.961486	-0.938082
H	0.816462	-1.224797	-2.684955
H	4.004850	-0.619899	2.298617
H	3.987113	-2.221403	1.581343
H	4.776111	-0.887942	0.715895
H	4.276294	-1.632384	-1.352446

H 2.962949 -2.752161 -1.677893
 H 3.148142 -1.283834 -2.666092
 1 imaginary frequency
 E = -940.010465
 ZPE = 0.341333
 H = -939.648454
 G = -939.720454
 E_{M06-2X,LBS} = -939.867428
 E_{M06-2X,SBS} = -939.607850
 E_{solv} = -939.697191

Transition states for Nazarov cyclization of 1d, analogous to TSA–TSD:

TSA

C -0.952164 2.822208 0.130158
 C -1.297384 1.462733 0.148702
 C -2.278684 0.995840 -0.734056
 C -2.902719 1.875940 -1.621128
 C -2.558237 3.227882 -1.630699
 C -1.581363 3.700636 -0.751421
 C -0.637436 0.568807 1.188256
 N -0.674251 -0.873301 0.835035
 C -1.646696 -1.527945 1.593049
 O -2.134997 -0.708215 2.520841
 C -1.383368 0.522336 2.546574
 C 0.051213 -1.527740 -0.183307
 C 1.486609 -1.416450 -0.348628
 C 2.375066 -0.299692 -0.038367
 O -2.007244 -2.687939 1.468303
 C -0.558660 -2.434894 -1.102224
 O -1.773260 -2.940809 -1.052104
 C 0.296529 -2.774596 -2.175778
 C 1.364651 -1.922722 -2.435199
 H 0.168701 -3.727244 -2.685115
 H 2.248019 -2.293854 -2.952588
 H 1.225030 -0.850696 -2.507881
 H 1.990889 -2.378071 -0.311854
 H -0.696450 0.478456 3.396568
 H -2.086586 1.344655 2.672287
 H 0.389785 0.889137 1.358492
 H -2.565759 -0.051994 -0.740293
 H -3.663199 1.502182 -2.300317
 H -3.047748 3.910112 -2.319094
 H -1.307061 4.751450 -0.753582
 H -0.191501 3.197444 0.812051
 H -2.073524 -2.987814 -0.093587
 C 2.110798 1.024745 -0.446420
 C 3.028476 2.035847 -0.184539
 C 4.219803 1.745945 0.490983
 C 4.502966 0.435342 0.885482
 C 3.599943 -0.584310 0.602301
 H 1.196189 1.256705 -0.984930
 H 2.823662 3.048828 -0.517180
 H 4.934255 2.538515 0.692252
 H 5.432366 0.207653 1.397818
 H 3.830645 -1.606127 0.892944
 1 imaginary frequency
 E = -1053.096143
 ZPE = 0.338583
 H = -1052.737434
 G = -1052.809891

$E_{M06-2X,LBS} = -1052.941187$
 $E_{M06-2X,SBS} = -1052.658781$
 $E_{solv} = -1052.747868$

TSB

C	0.876851	-2.276664	-0.877659
C	1.245596	-0.770118	-0.872232
N	0.178437	-0.282104	0.033953
C	-0.291504	-1.348459	0.856528
O	0.217365	-2.499123	0.384126
C	2.668415	-0.514242	-0.395565
C	3.030195	-0.634261	0.958146
C	4.361216	-0.458224	1.346549
C	5.339735	-0.171727	0.393570
C	4.986959	-0.054165	-0.952810
C	3.659273	-0.220914	-1.344775
C	-0.334294	0.991213	0.157972
C	0.435983	2.173812	0.001275
O	1.761987	2.273542	-0.027029
O	-0.994822	-1.231651	1.821520
C	-1.727150	1.192727	0.512893
C	-2.833648	0.335658	0.127838
C	-0.352117	3.336572	-0.079084
C	-1.681873	3.186721	-0.452321
H	-1.898453	1.787942	1.404977
H	0.048842	4.279570	0.285381
H	-2.417588	3.935101	-0.162973
H	-1.969548	2.578796	-1.300637
H	2.208824	1.450495	0.265612
H	1.105069	-0.339887	-1.867670
H	1.748980	-2.927533	-0.921345
H	0.178963	-2.526339	-1.682893
H	3.390510	-0.119997	-2.393792
H	5.743092	0.175715	-1.697261
H	6.372761	-0.036937	0.699149
H	4.630046	-0.552859	2.394243
H	2.285388	-0.871045	1.713456
C	-3.940701	0.229983	0.994708
C	-5.033534	-0.559140	0.652286
C	-5.047558	-1.235084	-0.570078
C	-3.965257	-1.121501	-1.452957
C	-2.866576	-0.345974	-1.108507
H	-3.926757	0.754316	1.946307
H	-5.873790	-0.645708	1.333758
H	-5.903953	-1.844657	-0.842360
H	-3.989452	-1.634386	-2.409532
H	-2.038301	-0.247283	-1.805698

1 imaginary frequency

$E = -1053.106073$

ZPE = 0.338257

$H = -1052.747396$

$G = -1052.820307$

$E_{M06-2X,LBS} = -1052.952025$

$E_{M06-2X,SBS} = -1052.669205$

$E_{solv} = -1052.757765$

TSC

C	-1.846034	-1.502335	-1.375208
O	-3.102519	-1.089294	-1.202234
H	-3.745226	-1.736898	-1.538290
C	-1.363040	-2.345736	-2.377881
C	-0.062547	-2.828457	-2.203395

H	0.530101	-3.115183	-3.070518
H	0.250736	-3.281809	-1.271668
H	-1.907066	-2.481440	-3.310645
C	-0.810724	-0.937768	-0.566594
C	0.513702	-0.966595	-1.127585
H	0.602688	-0.587732	-2.142147
N	-1.108002	-0.395140	0.649421
C	-2.038572	-1.015291	1.538523
O	-2.538624	-2.094606	1.380327
O	-2.202078	-0.211184	2.598814
H	-2.298061	1.781980	2.050426
C	-1.548342	1.057713	2.380178
C	-0.488699	0.792773	1.283110
H	0.459623	0.499034	1.748375
H	-1.111235	1.379361	3.325275
C	-0.256877	1.955488	0.344715
C	0.960387	2.644771	0.387977
C	1.171094	3.758590	-0.426945
C	0.169517	4.184546	-1.299756
C	-1.045909	3.496348	-1.353854
C	-1.261134	2.389882	-0.534060
H	-2.211748	1.863377	-0.580730
H	-1.829266	3.826629	-2.029743
H	0.332317	5.050514	-1.934515
H	2.116461	4.290842	-0.378837
H	1.745051	2.314170	1.064272
C	1.755713	-0.996275	-0.372545
C	2.920820	-0.456905	-0.958653
C	4.140304	-0.516389	-0.293179
C	4.220848	-1.131609	0.959837
C	3.078226	-1.687914	1.547619
C	1.854706	-1.620998	0.891445
H	2.858325	0.016042	-1.935315
H	5.028558	-0.091867	-0.750476
H	5.174923	-1.186890	1.475511
H	3.147714	-2.179837	2.512885
H	0.977241	-2.076673	1.342454

1 imaginary frequency

E = -1053.108182

ZPE = 0.338408

H = -1052.749210

G = -1052.822157

E_{M06-2X,LBS} = -1052.955890

E_{M06-2X,SBS} = -1052.672241

E_{solv} = -1052.763103

Transition state analogous to TSC but containing an OH...O=C hydrogen bond

C	1.987365	-1.567257	0.865603
C	1.826223	-0.820803	-0.324751
C	2.930205	-0.099391	-0.831002
C	4.146046	-0.102911	-0.157079
C	4.285939	-0.838929	1.024187
C	3.206682	-1.573265	1.531808
C	0.593865	-0.848438	-1.090329
C	-0.732919	-1.057897	-0.543745
N	-1.074794	-0.511051	0.683918
C	-2.032405	-1.058584	1.554307
O	-2.142246	-0.299199	2.641719
C	-1.426639	0.944782	2.467877
C	-0.474100	0.720619	1.266046
O	-2.671562	-2.072818	1.355024

C	-0.409048	1.893620	0.310552
C	0.738437	2.694329	0.280925
C	0.790014	3.823900	-0.538234
C	-0.300990	4.152813	-1.343287
C	-1.446954	3.352498	-1.325266
C	-1.503685	2.231028	-0.499704
C	-1.649422	-1.757538	-1.377484
C	-1.031768	-2.311641	-2.517891
C	0.327668	-2.582103	-2.464008
O	-2.968056	-1.819276	-1.238180
H	-3.196238	-1.870410	-0.275894
H	0.911985	-2.655428	-3.379979
H	0.769390	-3.070709	-1.604358
H	-1.604779	-2.401912	-3.438449
H	0.636228	-0.336818	-2.047008
H	-2.161698	1.727567	2.266691
H	0.531506	0.485733	1.628294
H	-0.898322	1.162517	3.395968
H	-2.402617	1.618521	-0.489557
H	-2.298868	3.606069	-1.949138
H	-0.261485	5.030323	-1.981733
H	1.681320	4.444240	-0.546348
H	1.592263	2.439188	0.904006
H	2.821350	0.467137	-1.752187
H	4.986770	0.458741	-0.552040
H	5.238726	-0.849888	1.545046
H	3.324814	-2.156716	2.439586
H	1.161029	-2.159435	1.250015

1 imaginary frequency

E = -1053.110171

ZPE = 0.338516

H = -1052.751363

G = -1052.823756

E_{M06-2X,LBS} = -1052.955780

E_{M06-2X,SBS} = -1052.673199

E_{solv} = -1052.760602

TSD

C	-1.923848	-1.576709	-0.802714
C	-2.383185	-0.651092	0.146585
C	-3.629761	-0.044043	-0.048045
C	-4.401016	-0.348335	-1.171397
C	-3.928906	-1.258671	-2.117251
C	-2.688194	-1.873633	-1.930256
C	-1.589287	-0.339081	1.396855
N	-0.203339	0.160133	1.165268
C	0.676130	-0.352813	2.168502
O	0.025289	-1.297901	2.860255
C	-1.262720	-1.570936	2.271537
C	0.182787	1.216300	0.384488
C	1.540014	1.337869	-0.113636
C	2.443423	0.266840	-0.478777
O	1.796122	0.027304	2.373198
C	-0.681071	2.297031	0.067714
C	-0.213307	3.116461	-0.967461
C	0.744717	2.572834	-1.818310
O	-1.773512	2.518772	0.816842
H	1.430433	3.224696	-2.356029
H	0.630785	1.583017	-2.240622
H	-0.467147	4.175241	-0.993196
H	2.025213	2.279252	0.128482
H	-1.184493	-2.488118	1.682056

H	-1.980288	-1.714573	3.079321
H	-0.974403	-2.084963	-0.654091
H	-2.323076	-2.594759	-2.655667
H	-2.128740	0.402181	1.992046
H	-4.004880	0.660028	0.690379
H	-4.528007	-1.496953	-2.991023
H	-5.371176	0.121676	-1.303338
H	-2.376582	3.140909	0.376460
C	3.830695	0.482108	-0.335079
C	4.739814	-0.504973	-0.697149
C	4.279795	-1.711061	-1.232364
C	2.906714	-1.928954	-1.406447
C	1.994533	-0.952484	-1.030933
H	4.186039	1.419507	0.084224
H	5.803928	-0.336076	-0.566560
H	4.989278	-2.480122	-1.522852
H	2.556687	-2.861037	-1.839397
H	0.932664	-1.116198	-1.184596

1 imaginary frequency
 E = -1053.105819
 ZPE = 0.338546
 H = -1052.746747
 G = -1052.819568
 E_{M06-2X,LBS} = -1052.951048
 E_{M06-2X,SBS} = -1052.668005
 E_{solv} = -1052.759770

Transition states for Nazarov cyclization of 1e, analogous to TSA–TSD:

TSA

C	2.799100	-0.376189	-0.780264
C	1.614537	-0.805314	-0.168620
C	1.593463	-1.009361	1.219104
C	2.739080	-0.774073	1.980708
C	3.917363	-0.345535	1.363653
C	3.947094	-0.151539	-0.017851
C	0.406409	-1.114543	-1.030449
N	-0.900628	-0.811438	-0.391212
C	-1.796934	-1.869772	-0.558211
O	-1.202421	-2.873631	-1.198439
C	0.217890	-2.634050	-1.292331
C	-1.282509	0.398554	0.214202
C	-0.953869	1.699820	-0.265162
C	0.011175	2.091841	-1.356166
O	-2.964529	-1.880584	-0.207654
C	-1.983827	0.411461	1.475853
O	-2.717966	-0.550630	1.987436
C	-1.756231	1.601506	2.185479
C	-0.686050	2.391744	1.747335
H	-2.437735	1.920533	2.970151
H	-0.688565	3.462112	1.948735
H	0.302537	1.968676	1.601080
H	-1.768279	2.413441	-0.182223
H	0.548716	-2.938533	-2.285034
H	0.714768	-3.239886	-0.530473
H	0.481196	-0.587784	-1.986404
H	0.689772	-1.366874	1.706979
H	2.714382	-0.937299	3.054144
H	4.808966	-0.169140	1.957639
H	4.861096	0.175481	-0.504275
H	2.830288	-0.224853	-1.857366
H	-3.021854	-1.168312	1.259462

C	0.468271	3.551757	-1.177156
H	0.897928	1.455036	-1.328551
C	-0.702710	1.920422	-2.722015
H	-0.009925	2.183891	-3.527560
H	-1.050179	0.896088	-2.891646
H	-1.570943	2.584315	-2.797258
H	1.113995	3.842034	-2.011153
H	-0.385657	4.239424	-1.163786
H	1.039709	3.690112	-0.253359

1 imaginary frequency
 E = -939.983622
 ZPE = 0.342814
 H = -939.621071
 G = -939.691008
 E_{M06-2X,LBS} = -939.842401
 E_{M06-2X,SBS} = -939.583368
 E_{solv} = -939.670493

TSB

C	-3.187889	0.353233	1.285322
C	-2.246261	-0.200811	0.404920
C	-2.590828	-0.373350	-0.947668
C	-3.856177	0.008943	-1.403712
C	-4.787254	0.553229	-0.518572
C	-4.451379	0.723643	0.826877
C	-0.909409	-0.672990	0.960451
C	-0.858553	-2.210135	1.151520
O	-0.266274	-2.707713	-0.065805
C	0.466581	-1.748835	-0.653715
N	0.243560	-0.524864	0.035915
C	1.012894	0.596576	-0.205767
C	2.410683	0.510793	-0.515779
C	3.387654	-0.559360	-0.117869
C	3.234953	-1.069937	1.325705
O	1.173003	-1.894061	-1.615400
C	0.478551	1.921881	-0.151347
C	1.459797	2.924999	-0.037150
C	2.710275	2.568824	0.438797
O	-0.798700	2.269279	-0.203807
C	4.830027	-0.090368	-0.396595
H	2.733560	1.112527	-1.359925
H	1.255632	3.917735	-0.431092
H	3.578114	3.185325	0.212643
H	2.835377	1.893363	1.276882
H	-1.388129	1.527501	-0.465886
H	-0.692026	-0.163209	1.902686
H	-1.845057	-2.659822	1.254081
H	-0.220877	-2.500835	1.992286
H	-2.931456	0.496973	2.332412
H	-5.169689	1.153501	1.518288
H	-5.769582	0.846781	-0.875570
H	-4.111898	-0.128995	-2.449854
H	-1.886641	-0.811994	-1.649899
H	3.183969	-1.395544	-0.806566
H	2.240361	-1.473964	1.534392
H	3.958556	-1.868553	1.511162
H	3.435685	-0.272324	2.052213
H	5.527460	-0.914468	-0.223137
H	4.953927	0.237909	-1.434094
H	5.121563	0.734099	0.265167

1 imaginary frequency
 E = -939.987367

ZPE = 0.341937
 H = -939.625447
 G = -939.696079
 E_{M06-2X,LBS} = -939.846612
 E_{M06-2X,SBS} = -939.587404
 E_{solv} = -939.673921

TSC

C	2.118360	-0.722336	1.090177
C	1.959032	-0.254837	-0.222938
C	2.891813	0.648533	-0.746725
C	3.971140	1.079022	0.027245
C	4.120779	0.614825	1.334303
C	3.192071	-0.284933	1.864468
C	0.839034	-0.758930	-1.106595
N	-0.481270	-0.864845	-0.444020
C	-1.172029	-2.039051	-0.873809
O	-0.334766	-2.769698	-1.621223
C	1.004013	-2.233410	-1.553463
C	-1.074603	0.019947	0.415273
C	-0.999123	1.432954	0.304095
C	-0.665698	2.208351	-0.943674
O	-2.321092	-2.292783	-0.635626
C	-1.868391	-0.485087	1.504576
C	-2.809820	0.428846	1.985525
C	-3.135726	1.496419	1.150624
O	-1.580183	-1.679642	2.010600
H	-3.523197	2.420484	1.575996
H	-3.343683	1.350402	0.098144
H	-3.160619	0.385796	3.014677
H	-0.859390	1.975424	1.234649
C	-0.747565	3.721856	-0.676239
H	0.389719	1.977473	-1.164478
C	-1.513302	1.806278	-2.167450
H	1.572109	-2.813034	-0.820858
H	1.457990	-2.331132	-2.539280
H	1.405637	-1.428684	1.509605
H	3.308199	-0.651823	2.880035
H	0.751298	-0.118764	-1.992857
H	2.784702	1.007557	-1.768310
H	4.958930	0.949659	1.938047
H	4.691974	1.774509	-0.391983
H	-2.331282	-2.061206	2.497751
H	-0.434417	4.280292	-1.562836
H	-1.773818	4.027167	-0.439453
H	-0.099154	4.020041	0.154659
H	-1.138374	2.313849	-3.061016
H	-1.501746	0.729671	-2.361368
H	-2.557579	2.112543	-2.035340

1 imaginary frequency
 E = -939.986773
 ZPE = 0.341943
 H = -939.624651
 G = -939.695581
 E_{M06-2X,LBS} = -939.847581
 E_{M06-2X,SBS} = -939.587225
 E_{solv} = -939.677369

Transition state analogous to TSC but containing an OH...O=C hydrogen bond

C	1.082004	-2.240619	-1.549517
C	0.832340	-0.782821	-1.083844
N	-0.505690	-0.936432	-0.449315
C	-1.049981	-2.200780	-0.739938
O	-0.204604	-2.896379	-1.494745
C	1.911968	-0.246336	-0.167056
C	2.025123	-0.681568	1.161647
C	3.068573	-0.222243	1.964013
C	4.013871	0.667161	1.445755
C	3.910980	1.098929	0.123068
C	2.861059	0.647165	-0.678682
C	-1.132150	0.008197	0.354977
C	-1.984929	-0.343910	1.451125
O	-2.090977	-1.532438	2.025265
O	-2.127367	-2.608912	-0.354202
C	-0.912994	1.408600	0.161545
C	-0.619372	2.106088	-1.139100
C	-1.501895	1.642275	-2.313243
C	-0.686191	3.634905	-0.952224
C	-2.695135	0.751674	1.986169
C	-2.929348	1.856834	1.189741
H	-3.172727	2.819784	1.635339
H	-3.186321	1.754158	0.141682
H	-2.972503	0.736385	3.038047
H	-0.652297	1.977318	1.047750
H	0.431938	1.871717	-1.374683
H	1.757522	-2.773000	-0.875669
H	1.451428	-2.304386	-2.572740
H	1.299751	-1.379039	1.574426
H	3.147323	-0.563344	2.991944
H	0.739234	-0.136057	-1.962198
H	2.791705	0.981208	-1.712067
H	4.828561	1.019342	2.071223
H	4.645327	1.785798	-0.286677
H	-2.045401	-2.241461	1.334853
H	-0.380093	4.137831	-1.873684
H	-1.706002	3.963247	-0.720274
H	-0.022985	3.972462	-0.148727
H	-1.177589	2.130531	-3.236802
H	-1.467756	0.560731	-2.474704
H	-2.549237	1.922318	-2.149004

1 imaginary frequency

E = -939.986295

ZPE = 0.341660

H = -939.624625

G = -939.695387

E_{M06-2X,LBS} = -939.845334

E_{M06-2X,SBS} = -939.585863

E_{solv} = -939.673006

TSD

C	1.790292	-0.034968	-1.452852
C	2.006425	0.436241	-0.149282
C	3.172100	0.053979	0.527127
C	4.107601	-0.781231	-0.085754
C	3.880915	-1.251816	-1.379784
C	2.720117	-0.877655	-2.061570
C	1.044669	1.390397	0.522112
N	-0.390271	0.983429	0.496771

C	-1.215796	2.140883	0.405566
O	-0.440877	3.193037	0.108897
C	0.910864	2.764990	-0.166347
C	-0.905703	-0.244371	0.820018
C	-2.153898	-0.736143	0.326013
C	-2.922440	-0.348919	-0.903158
O	-2.403019	2.169233	0.591164
C	-0.201420	-1.132918	1.694896
C	-0.558251	-2.481808	1.572313
C	-1.201645	-2.871764	0.405485
O	0.663981	-0.627088	2.577733
H	-1.821547	-3.765816	0.393713
H	-0.887579	-2.509816	-0.565625
H	-0.457831	-3.162286	2.416205
H	-2.753600	-1.257588	1.065955
C	-4.002258	-1.410931	-1.198450
H	-3.445523	0.577560	-0.614567
C	-2.077372	-0.049176	-2.151616
H	1.039628	2.696625	-1.250371
H	1.591953	3.511748	0.240995
H	0.900151	0.261644	-2.000645
H	2.545044	-1.232170	-3.073195
H	1.343616	1.533299	1.564487
H	3.356621	0.424664	1.532814
H	4.607953	-1.900718	-1.858857
H	5.012870	-1.059538	0.445714
H	1.236714	-1.319779	2.950345
H	-2.739037	0.194504	-2.987552
H	-1.403497	0.799596	-2.012336
H	-1.479348	-0.919722	-2.448819
H	-4.652780	-1.064106	-2.005901
H	-3.555702	-2.360547	-1.517571
H	-4.632105	-1.601748	-0.322850

1 imaginary frequency
 E = -939.987198
 ZPE = 0.342111
 H = -939.624976
 G = -939.695532
 $E_{\text{M06-2X,LBS}} = -939.847662$
 $E_{\text{M06-2X,SBS}} = -939.587546$
 $E_{\text{solv}} = -939.677869$

Transition states for Nazarov cyclization of 1f, analogous to TSA–TSD:

TSA

C	2.027290	0.698357	0.503458
O	1.913246	1.892655	1.026384
H	1.256184	2.441775	0.492867
C	3.121290	-0.120910	0.848995
H	4.042966	0.327332	1.212235
C	3.008671	-1.487382	0.594166
H	2.134909	-2.057021	0.891309
H	3.907160	-2.089859	0.464356
C	1.117179	0.037889	-0.405373
C	1.702891	-1.064322	-1.091475
H	2.684746	-0.866877	-1.504622
C	0.993881	-2.194606	-1.777305
H	0.263805	-2.703398	-1.143308
H	1.721758	-2.931758	-2.125137

H	0.472025	-1.818145	-2.668628
N	-0.230988	0.413045	-0.542805
C	-0.649830	1.745042	-0.566161
O	-1.969362	1.805735	-0.708532
O	0.063822	2.733111	-0.499350
C	-2.520320	0.488254	-0.923193
H	-3.425683	0.407667	-0.322294
H	-2.776210	0.403142	-1.982209
C	-1.409767	-0.498574	-0.500255
H	-1.315278	-1.273055	-1.261013
C	-1.589074	-1.166561	0.884423
C	-2.748974	-2.174329	0.833133
H	-0.664695	-1.738619	1.066115
C	-1.753340	-0.162774	2.034928
H	-1.830366	-0.697166	2.986573
H	-0.903053	0.523594	2.114864
H	-2.664040	0.437584	1.928341
H	-2.814054	-2.722373	1.777762
H	-3.714258	-1.677165	0.682601
H	-2.620024	-2.909489	0.029751

l imaginary frequency

E = -748.244118

ZPE = 0.289559

H = -747.938089

G = -747.999962

E_{M06-2X,LBS} = -748.129438

E_{M06-2X,SBS} = -747.916034

E_{solv} = -748.003399

TSB

C	-1.406991	-1.506469	-0.387515
O	-0.557223	-2.337969	-0.984794
H	0.139052	-1.847414	-1.460070
C	-1.178029	-0.117154	-0.137901
C	-2.677475	-1.941920	0.008333
H	-3.142912	-2.793753	-0.481332
C	-3.370417	-1.129116	0.902400
H	-2.900227	-0.717186	1.787185
H	-4.457908	-1.166731	0.940184
C	-2.357249	0.678094	0.002151
H	-3.148999	0.510096	-0.721325
C	-2.425560	1.982940	0.718919
N	0.085393	0.428636	-0.043147
C	0.344719	1.707538	-0.620847
O	1.510712	2.161363	-0.147817
C	1.964108	1.343290	0.951035
C	1.246444	-0.020469	0.787530
O	-0.365579	2.262805	-1.414919
H	1.693795	1.845596	1.884464
H	3.047973	1.274534	0.879344
H	0.864365	-0.362366	1.754096
C	2.135284	-1.136297	0.183227
H	-2.263474	2.796935	-0.000584
H	-3.426571	2.124011	1.140173
H	-1.682371	2.074634	1.515879
C	3.291564	-1.465193	1.145074
H	1.516674	-2.039650	0.137920
C	2.650544	-0.813054	-1.227913
H	3.230952	-1.653637	-1.620022
H	1.842734	-0.607562	-1.944885
H	3.305235	0.065404	-1.233896
H	3.823908	-2.353331	0.792056

H 4.025587 -0.654502 1.208601
 H 2.929505 -1.678259 2.157525
 1 imaginary frequency
 E = -748.243534
 ZPE = 0.289346
 H = -747.937360
 G = -747.999644
 E_{M06-2X,LBS} = -748.130687
 E_{M06-2X,SBS} = -747.916821
 E_{solv} = -748.005623

TSC

C 0.062976 -1.687807 -0.775681
 O 1.282799 -2.118194 -1.105272
 O -0.957829 -2.318000 -0.842187
 N 0.157270 -0.320774 -0.374624
 C 2.290408 -1.117886 -0.843232
 H 2.888592 -1.465087 0.001456
 H 2.921482 -1.045941 -1.729124
 C 1.533261 0.200638 -0.535064
 H 1.573980 0.854747 -1.413464
 C 2.056172 0.990176 0.686695
 C -0.958095 0.345624 0.049653
 C -1.938440 -0.339620 0.859896
 O -1.534369 -1.284506 1.698165
 H -2.258878 -1.880914 1.957278
 C -3.225616 0.186801 0.731981
 H -3.957956 0.092448 1.531131
 C -3.464391 0.988342 -0.385866
 H -3.150349 0.688268 -1.378130
 H -4.256010 1.735671 -0.359028
 C -1.282399 1.672579 -0.323656
 H -1.722199 2.309606 0.437261
 C -0.688304 2.379215 -1.499734
 H -0.466916 1.701287 -2.328022
 H 0.239464 2.896567 -1.215099
 H -1.373713 3.157373 -1.850540
 C 3.468086 1.521013 0.384796
 H 1.394843 1.862796 0.795228
 C 2.013888 0.207498 2.007651
 H 3.812117 2.163757 1.200526
 H 4.194052 0.704936 0.287149
 H 3.495506 2.110923 -0.538817
 H 2.285610 0.870517 2.834913
 H 1.021194 -0.202051 2.221694
 H 2.728211 -0.623330 2.017667
 1 imaginary frequency
 E = -748.248442
 ZPE = 0.289072
 H = -747.942271
 G = -748.005667
 E_{M06-2X,LBS} = -748.136131
 E_{M06-2X,SBS} = -747.921759
 E_{solv} = -748.009900

Transition state analogous to TSC but containing an OH...O=C hydrogen bond

C 1.437556 0.563306 -0.461296
 N 0.167348 -0.220503 -0.505737
 C 0.455456 -1.561309 -0.832028
 O 1.717004 -1.667668 -1.229536

C	2.350190	-0.368911	-1.283612
O	-0.316397	-2.497045	-0.751194
C	-1.057530	0.216233	-0.020592
C	-1.449725	1.579566	-0.173539
C	-0.961709	2.500796	-1.245495
C	1.902154	0.865575	0.984128
C	2.113822	-0.392519	1.839261
C	3.156421	1.754601	0.952600
C	-2.014778	-0.626042	0.654997
C	-3.293413	-0.040829	0.737099
C	-3.633120	0.946782	-0.174910
O	-1.784860	-1.784968	1.241632
H	3.351971	-0.476518	-0.869195
H	2.418535	-0.074444	-2.333868
H	1.314936	1.504743	-0.997597
H	-1.107307	-2.293675	0.719438
H	-3.950586	-0.311946	1.560453
H	-3.373737	0.864860	-1.224255
H	-4.435669	1.649231	0.046469
H	-1.863583	2.076343	0.696510
H	-0.636553	1.977307	-2.147663
H	-0.141292	3.133729	-0.878225
H	-1.766051	3.195404	-1.513670
H	1.095467	1.454539	1.445915
H	3.419233	2.066803	1.967586
H	4.024519	1.224444	0.543682
H	3.001690	2.661108	0.355481
H	2.420778	-0.106983	2.849880
H	1.198801	-0.987217	1.938732
H	2.899483	-1.040252	1.433590

1 imaginary frequency

E = -748.250036

ZPE = 0.289220

H = -747.944208

G = -748.006299

E_{M06-2X,LBS} = -748.135274

E_{M06-2X,SBS} = -747.922020

E_{solv} = -748.008577

TSD

C	1.467454	-1.118388	-0.923174
O	0.715781	-1.600388	-1.916390
H	0.991703	-2.498013	-2.172330
C	2.679887	-1.654193	-0.465931
C	3.128296	-1.249563	0.784199
H	4.186629	-1.307575	1.031630
H	2.460445	-1.162714	1.632262
H	3.308916	-2.248936	-1.126388
C	1.071248	0.090983	-0.272807
C	2.103399	0.802460	0.411642
H	3.054300	0.896592	-0.103225
C	1.901634	1.723870	1.563149
H	1.865772	2.757778	1.197377
H	2.756960	1.653680	2.244744
H	0.978767	1.523678	2.113114
N	-0.219043	0.551264	-0.297150
C	-0.474554	1.935596	-0.530366
O	-1.793600	2.115126	-0.632394
C	-2.511821	0.892540	-0.358635
C	-1.465554	-0.242749	-0.445111
O	0.368043	2.785312	-0.646150
H	-2.957657	0.984060	0.634654

H	-3.300703	0.799404	-1.104550
H	-1.483058	-0.680734	-1.447801
C	-1.636581	-1.378112	0.586534
C	-2.958394	-2.117080	0.311812
H	-0.822241	-2.092677	0.398287
C	-1.536763	-0.930250	2.051868
H	-3.045962	-2.991300	0.963817
H	-3.827300	-1.477767	0.508294
H	-3.021880	-2.465638	-0.725284
H	-1.581574	-1.804540	2.708815
H	-0.599295	-0.404375	2.264922
H	-2.361823	-0.270861	2.342118

1 imaginary frequency
E = -748.249470
ZPE = 0.289301
H = -747.943217
G = -748.005872
E_{M06-2X,LBS} = -748.136538
E_{M06-2X,SBS} = -747.922257
E_{solv} = -748.010876

Transition states for Nazarov cyclization of 1g, analogous to TSA–TSD:

TSA

C	-1.227116	2.253952	0.480694
O	-2.534413	2.399897	0.470610
H	-2.915873	1.922143	-0.327927
C	-0.415057	3.231230	1.099680
H	-0.771999	4.255705	1.179033
C	0.880330	2.861495	1.448082
H	1.081322	1.948372	1.995330
H	1.655861	3.619212	1.549471
C	-0.464256	1.177875	-0.072167
C	0.945912	1.477375	-0.201172
H	1.132674	2.399836	-0.743632
C	2.091007	0.568703	-0.225815
N	-1.058875	-0.016220	-0.527518
C	-2.221444	-0.014358	-1.297604
O	-2.508260	-1.252959	-1.694405
O	-2.891913	0.959483	-1.603702
C	-1.438346	-2.152374	-1.328398
H	-1.890850	-3.088319	-1.003150
H	-0.828812	-2.328859	-2.218898
C	-0.662567	-1.419670	-0.217327
H	0.407951	-1.546790	-0.370374
C	-1.035079	-1.823776	1.231075
C	-0.498812	-3.232585	1.534695
H	-0.505839	-1.118424	1.889630
C	-2.534251	-1.705225	1.545087
H	-2.714539	-1.970366	2.591320
H	-2.908047	-0.685971	1.400350
H	-3.139665	-2.381290	0.930956
H	-0.661563	-3.479280	2.588293
H	-1.010772	-4.000221	0.942634
H	0.575831	-3.314503	1.332563
C	2.310308	-0.421598	0.754388
C	3.451644	-1.214580	0.712782
C	4.389589	-1.039979	-0.311551
C	4.195715	-0.050979	-1.279337
C	3.069094	0.763955	-1.223571
H	1.602929	-0.545071	1.569944
H	3.620359	-1.960225	1.483679

H	5.279368	-1.661514	-0.341951
H	4.929630	0.095498	-2.065494
H	2.930822	1.545470	-1.966428

1 imaginary frequency
E = -939.986558
ZPE = 0.342570
H = -939.624372
G = -939.693987
E_{M06-2X,LBS} = -939.841979
E_{M06-2X,SBS} = -939.583906
E_{solv} = -939.670945

TSB

C	0.889512	2.338645	0.026752
O	2.195350	2.516429	0.248674
H	2.550575	1.796458	0.801268
C	0.175283	1.126727	0.197081
C	0.066811	3.420452	-0.317779
H	0.343914	4.430242	-0.024467
C	-1.187484	3.106977	-0.839591
H	-1.304733	2.395385	-1.647165
H	-2.008056	3.815476	-0.741524
C	-1.258208	1.276042	0.371331
H	-1.563096	1.956514	1.161747
C	-2.254889	0.288818	-0.002155
N	0.784662	-0.108363	0.290392
C	0.299370	-1.047402	1.251004
O	0.783830	-2.258591	0.945315
C	1.388079	-2.246164	-0.363134
C	1.733689	-0.764010	-0.658164
O	-0.402108	-0.779743	2.187273
H	0.664818	-2.652347	-1.075762
H	2.261214	-2.895501	-0.325644
H	1.434152	-0.503346	-1.678275
C	3.233022	-0.416161	-0.482600
C	4.074152	-1.175282	-1.524275
H	3.337975	0.646764	-0.728499
C	3.752532	-0.653392	0.944085
H	4.801745	-0.352037	1.019600
H	3.191987	-0.090423	1.703369
H	3.695594	-1.709713	1.229700
H	5.107425	-0.816673	-1.498646
H	4.102849	-2.253447	-1.331473
H	3.696432	-1.020628	-2.541721
C	-3.427628	0.179865	0.773066
C	-4.411721	-0.744272	0.437504
C	-4.249906	-1.554845	-0.688532
C	-3.100479	-1.442449	-1.482724
C	-2.109503	-0.531836	-1.142595
H	-3.549737	0.808487	1.650812
H	-5.304087	-0.831260	1.049004
H	-5.022349	-2.269309	-0.956834
H	-2.990518	-2.060619	-2.368405
H	-1.231102	-0.430518	-1.775577

1 imaginary frequency
E = -939.989283
ZPE = 0.342467
H = -939.626768
G = -939.697607
E_{M06-2X,LBS} = -939.846670
E_{M06-2X,SBS} = -939.587711
E_{solv} = -939.676689

TSC

C	-2.039305	0.278625	1.188412
C	-1.915735	0.579907	-0.187047
C	-3.026311	0.367197	-1.032249
C	-4.211176	-0.156990	-0.527094
C	-4.314845	-0.456882	0.834377
C	-3.230368	-0.232015	1.690964
C	-0.714630	1.178425	-0.748849
C	0.631849	0.968960	-0.287899
N	1.054941	-0.145776	0.376452
C	1.944895	-0.034017	1.489527
O	2.224718	-1.265797	1.929685
C	1.656969	-2.273280	1.065727
C	0.610126	-1.544156	0.189695
O	2.325804	0.996154	1.974313
C	0.545775	-2.003782	-1.282599
C	1.553828	2.031554	-0.566157
C	0.925365	3.246822	-0.840854
C	-0.406889	3.357594	-0.428380
O	2.852452	1.752253	-0.673439
H	3.404931	2.539913	-0.531954
H	-1.079037	4.041069	-0.944773
H	-0.708952	3.102117	0.579268
H	1.394229	3.994123	-1.478032
H	-0.811022	1.502965	-1.781574
H	2.469261	-2.705005	0.476353
H	-0.385751	-1.662062	0.634643
H	1.218166	-3.042985	1.700342
H	-2.950274	0.612874	-2.088694
H	-5.055275	-0.324336	-1.188688
H	-5.243111	-0.856484	1.231612
H	-3.320470	-0.449249	2.750789
H	-1.210252	0.472723	1.863576
C	0.051375	-3.459577	-1.339075
H	-0.222051	-1.382785	-1.765156
C	1.859444	-1.820524	-2.057884
H	-0.087879	-3.770668	-2.378843
H	0.774358	-4.150292	-0.888549
H	-0.906682	-3.584628	-0.821763
H	1.695630	-2.043210	-3.116933
H	2.250962	-0.800090	-1.988447
H	2.642624	-2.501588	-1.706512

1 imaginary frequency

E = -939.997287

ZPE = 0.342555

H = -939.634609

G = -939.705294

E_{M06-2X,LBS} = -939.855210

E_{M06-2X,SBS} = -939.595997

E_{solv} = -939.683853

Transition state analogous to TSC but containing an OH...O=C hydrogen bond

C	0.633117	-1.441458	0.015167
N	0.962140	-0.051395	0.440698
C	2.005370	-0.075566	1.383005
O	2.238059	-1.327531	1.765437
C	1.277201	-2.231149	1.171481
C	0.471539	1.097469	-0.164175
C	1.229222	2.292141	-0.367620
O	2.542914	2.432803	-0.279597

O	2.622804	0.887645	1.795618
C	1.159831	-1.767587	-1.403707
C	2.678482	-1.594453	-1.552909
C	-0.872992	1.114300	-0.705305
C	-2.015832	0.389029	-0.177492
C	-2.173353	0.126014	1.203362
C	-3.312326	-0.517836	1.668772
C	-4.312764	-0.912828	0.770369
C	-4.176759	-0.652801	-0.596326
C	-3.043295	0.002283	-1.066097
C	0.698275	-3.174027	-1.818580
C	0.435230	3.360903	-0.830683
C	-0.928544	3.328540	-0.571821
H	2.889370	1.852145	0.449479
H	-1.620047	3.896549	-1.192558
H	-1.310878	3.067554	0.407437
H	0.885003	4.115908	-1.472064
H	-0.953402	1.369825	-1.757564
H	1.820331	-3.118061	0.846973
H	-0.448619	-1.583386	0.034544
H	0.556560	-2.506768	1.945584
H	-2.943141	0.217268	-2.127198
H	-4.956393	-0.952581	-1.289427
H	-5.202168	-1.414412	1.139879
H	-3.431714	-0.706296	2.731222
H	-1.408451	0.444036	1.906430
H	0.670705	-1.051321	-2.080155
H	0.970548	-3.366114	-2.860667
H	1.171031	-3.956291	-1.213127
H	-0.388506	-3.288196	-1.731050
H	2.979305	-1.819505	-2.580742
H	3.003332	-0.569537	-1.340878
H	3.237532	-2.272228	-0.897333

l imaginary frequency

E = -940.000788

ZPE = 0.342555

H = -939.638459

G = -939.708864

E_{M06-2X,LBS} = -939.855539

E_{M06-2X,SBS} = -939.597425

E_{solv} = -939.682708

TSD

C	1.043883	2.213758	-0.355015
O	2.302499	2.241888	-0.828050
H	2.758667	3.057019	-0.558794
C	0.328163	3.303060	0.152572
C	-0.833054	3.009254	0.866060
H	-1.635381	3.741982	0.927997
H	-0.845574	2.256655	1.643630
H	0.576331	4.321022	-0.144583
C	0.284771	1.014856	-0.450288
C	-1.156758	1.199109	-0.409138
H	-1.519375	1.960348	-1.093427
C	-2.180974	0.280733	0.042809
N	0.857074	-0.213085	-0.639567
C	0.259557	-1.141496	-1.552929
O	1.049475	-2.217561	-1.642456
C	2.155178	-2.125676	-0.721152
C	2.255270	-0.634158	-0.342188
O	-0.760817	-0.963002	-2.158598
H	1.934302	-2.767534	0.136184

H	3.043830	-2.493800	-1.232938
H	2.918841	-0.126006	-1.049058
C	2.778586	-0.356252	1.083851
C	4.209266	-0.915457	1.199660
H	2.851792	0.733609	1.183375
C	1.886824	-0.870109	2.222067
H	4.655167	-0.613192	2.151887
H	4.220974	-2.011449	1.169464
H	4.856707	-0.546486	0.396092
H	2.349165	-0.633414	3.185745
H	0.897262	-0.401346	2.215824
H	1.749078	-1.956708	2.191710
C	-3.493737	0.482874	-0.437689
C	-4.537017	-0.334913	-0.021147
C	-4.291242	-1.359605	0.896456
C	-2.998106	-1.564923	1.394648
C	-1.951571	-0.756952	0.972944
H	-3.684768	1.280307	-1.151122
H	-5.538353	-0.176322	-0.408566
H	-5.104891	-1.998709	1.226149
H	-2.813046	-2.359438	2.110911
H	-0.953732	-0.930164	1.360195

1 imaginary frequency

E = -939.993704

ZPE = 0.342649

H = -939.630977

G = -939.701569

E_{M06-2X,LBS} = -939.850186

E_{M06-2X,SBS} = -939.591153

E_{solv} = -939.680060

TSF

C	-1.767519	-1.410474	0.594122
C	-2.463990	-0.222127	0.325555
C	-3.760212	-0.290803	-0.197151
C	-4.361397	-1.527014	-0.442609
C	-3.664128	-2.705252	-0.175386
C	-2.366609	-2.643573	0.340193
C	-1.856730	1.128426	0.639019
N	-0.430665	1.260410	0.286632
C	0.276168	1.986520	1.277681
O	-0.564976	2.207080	2.318012
C	-1.762739	1.431746	2.154943
C	0.204075	0.718620	-0.807101
C	-0.303213	0.832898	-2.126852
C	-1.282700	1.908641	-2.512078
O	1.396339	2.401569	1.191860
C	1.462306	0.019033	-0.648874
C	2.118420	-0.046022	-1.903626
C	1.680641	0.871313	-2.866815
O	1.789010	-0.522677	0.462726
H	1.820419	0.637706	-3.923399
H	1.655212	1.935755	-2.659395
H	2.780272	-0.875091	-2.127881
H	-0.378101	-0.071785	-2.721003
H	-1.213550	2.114493	-3.585374
H	-2.313292	1.579921	-2.320071
H	-1.108415	2.839943	-1.965036
H	-1.669733	0.509292	2.736417
H	-2.605100	2.018700	2.523830
H	-0.752790	-1.373683	0.983881
H	-1.816055	-3.557204	0.545134

H	-2.439945	1.914187	0.141042
H	-4.306566	0.626635	-0.407658
H	-4.127206	-3.668519	-0.370215
H	-5.369702	-1.566636	-0.845241
B	3.204899	-1.258849	0.569690
F	3.308019	-1.605847	1.882023
F	3.106007	-2.340582	-0.296797
F	4.136806	-0.341540	0.131793

1 imaginary frequency

E = -1185.558302

ZPE = 0.287557

H = -1185.249430

G = -1185.324511

E_{M06-2X,LBS} = -1185.459843

E_{M06-2X,SBS} = -1185.108245

E_{solv} = -1185.154265

TSG

C	-0.155315	-2.166409	1.859618
C	-0.308658	-0.892611	1.005540
N	0.916976	-1.063571	0.173075
C	1.162268	-2.445596	0.011812
O	0.478257	-3.112353	0.966641
C	-1.618978	-0.895768	0.228196
C	-1.832856	-1.721327	-0.882679
C	-3.085098	-1.764437	-1.496464
C	-4.136424	-0.988859	-1.006056
C	-3.925303	-0.158982	0.095203
C	-2.674184	-0.111787	0.708627
C	1.692166	-0.072877	-0.382526
C	1.164507	1.272019	-0.519788
O	-0.099019	1.498795	-0.552462
O	1.839694	-2.972473	-0.834605
C	3.068415	-0.245981	-0.694708
C	3.985618	-1.262928	-0.087447
C	2.206445	2.232585	-0.603805
C	3.458034	1.870492	-0.127926
H	3.399435	0.153245	-1.646196
H	2.034524	3.164753	-1.128536
H	4.346485	2.386507	-0.493188
H	3.591885	1.389661	0.833358
B	-0.721454	2.735398	0.214364
H	-0.231545	0.017307	1.600949
H	-1.108088	-2.590415	2.173634
H	0.498895	-2.015131	2.725932
H	-2.501546	0.571121	1.534297
H	-4.727983	0.470596	0.468305
H	-5.109653	-1.021038	-1.488284
H	-3.235314	-2.404267	-2.361865
H	-1.028473	-2.323787	-1.294442
H	5.009819	-0.874188	-0.091020
H	3.708953	-1.511998	0.941913
H	3.972203	-2.191792	-0.668088
F	-1.971697	2.892006	-0.302403
F	-0.717113	2.325688	1.550149
F	0.112538	3.821247	0.010890

1 imaginary frequency

E = -1185.562228

ZPE = 0.287767

H = -1185.253468

G = -1185.327062

$E_{M06-2X,LBS} = -1185.463167$
 $E_{M06-2X,SBS} = -1185.113484$
 $E_{solv} = -1185.152399$

TSH

C	2.710634	1.185839	-0.122674
C	1.343811	1.269219	-0.432324
C	0.592655	2.343961	0.058666
C	1.203067	3.320708	0.851029
C	2.560818	3.232258	1.157095
C	3.315472	2.162078	0.667268
C	0.662384	0.205114	-1.275961
N	0.627592	-1.106332	-0.571355
C	1.514557	-2.028087	-1.149538
O	2.087499	-1.453734	-2.230323
C	1.417231	-0.214529	-2.554992
C	-0.180335	-1.393903	0.504596
C	0.262705	-2.126287	1.637101
C	1.700632	-2.260595	2.039115
O	1.741421	-3.150375	-0.771462
C	-1.520135	-0.849279	0.553429
C	-1.989570	-0.808672	1.889429
C	-1.021112	-0.890334	2.889459
O	-2.133586	-0.526153	-0.529480
H	-1.299629	-1.261197	3.876438
H	-0.152351	-0.242327	2.893542
H	-3.051066	-0.857264	2.100317
H	-0.391371	-2.909107	2.006794
H	1.768980	-2.418609	3.120852
H	2.148963	-3.126602	1.539698
H	2.284049	-1.374538	1.771253
H	2.175015	0.507020	-2.860210
H	0.732199	-0.408829	-3.385408
H	3.307546	0.360751	-0.505921
H	4.375376	2.091150	0.896490
H	-0.354209	0.519915	-1.510861
H	-0.464246	2.413729	-0.184113
H	3.033449	3.994753	1.770384
H	0.612566	4.152968	1.224243
B	-3.186430	0.640505	-0.626682
F	-2.423197	1.735069	-1.036068
F	-4.095201	0.239857	-1.559992
F	-3.724471	0.831423	0.635984

1 imaginary frequency

$E = -1185.573727$

ZPE = 0.288221

$H = -1185.264423$

$G = -1185.338418$

$E_{M06-2X,LBS} = -1185.471439$

$E_{M06-2X,SBS} = -1185.122887$

$E_{solv} = -1185.160101$

Cyclic oxyallyl cation (α)-3c (syn)

C	-2.239669	0.160925	-0.426682
O	-2.837462	1.009030	-1.268792
C	-2.745426	-1.116352	-0.220683
C	-1.857793	-1.944199	0.648271
H	-2.442543	-2.298785	1.509314
C	-1.296983	-3.189390	-0.078057
H	-0.672066	-3.770332	0.606840
H	-0.687222	-2.897012	-0.939434

H	-2.105019	-3.838339	-0.427655
C	-3.986271	-1.609540	-0.862530
H	-3.739470	-2.092938	-1.820911
H	-4.487339	-2.361952	-0.245300
H	-4.667174	-0.785180	-1.090139
C	-0.998287	0.269423	0.264034
C	-0.761233	-0.955272	1.114118
H	0.236138	-1.361434	0.919622
C	-0.874281	-0.624237	2.624006
H	-0.695821	-1.533109	3.205930
H	-1.873623	-0.249148	2.866712
H	-0.144055	0.123668	2.944790
N	-0.110823	1.293314	0.219477
C	-0.447627	2.652545	-0.080440
O	-1.555200	3.075625	-0.313617
O	0.639960	3.404743	0.005338
C	1.825221	2.595930	0.162634
H	2.476245	3.089573	0.883578
H	2.323003	2.533042	-0.807648
C	1.325386	1.214827	0.646374
H	1.354949	1.172757	1.739066
C	2.118671	0.065395	0.064022
C	2.071878	-0.231848	-1.306418
C	2.856204	-1.260327	-1.826152
C	3.701891	-1.992119	-0.987001
C	3.758269	-1.695442	0.374869
C	2.965422	-0.672737	0.900126
H	1.425544	0.336298	-1.971727
H	2.814999	-1.484623	-2.887827
H	4.316908	-2.787695	-1.396496
H	4.416610	-2.257039	1.030594
H	3.014592	-0.444574	1.962617
H	-2.559520	1.932962	-1.064657

0 imaginary frequencies

E = -940.060664

ZPE = 0.344407

H = -939.695839

G = -939.768062

E_{M06-2X,LBS} = -939.918697

E_{M06-2X,SBS} = -939.660869

E_{solv} = -939.744508

TSI

C	0.389980	-0.782327	-0.344205
C	-0.065917	0.538962	0.233869
C	0.726164	0.871667	1.318599
C	1.664308	-0.184075	1.550127
C	1.651332	-1.119568	0.489266
N	-1.117766	1.286864	-0.279286
C	-2.293308	0.751495	-1.015592
C	-3.205357	2.000584	-0.989707
O	-2.319620	3.115267	-0.759283
C	-1.172430	2.680892	-0.220954
C	-2.931608	-0.479482	-0.410423
C	-3.311665	-1.538118	-1.243717
C	-3.956934	-2.658486	-0.715800
C	-4.218605	-2.731767	0.652375
C	-3.837484	-1.680621	1.491348
C	-3.200934	-0.558295	0.964089
O	-0.310931	3.418958	0.219128
O	0.668909	1.919893	2.158644
C	2.478335	-0.220710	2.798704

C	1.971863	-2.596306	0.718293
C	0.549626	-0.824353	-1.873033
N	3.956737	-0.355074	-0.872548
H	2.786477	-0.692441	-0.232004
H	2.071802	-3.130245	-0.233128
H	1.181407	-3.096509	1.291414
H	2.907053	-2.730467	1.271052
H	1.819848	-0.441107	3.650592
H	3.260097	-0.982324	2.774627
H	2.913480	0.762544	3.008819
H	-0.349782	-1.549801	-0.070184
H	1.053943	-1.749706	-2.168273
H	1.129610	0.025690	-2.246807
H	-0.416071	-0.819611	-2.383414
H	-3.727638	2.167404	-1.931751
H	-3.926130	1.959589	-0.168214
H	-1.999033	0.540502	-2.049188
H	-2.911188	0.255321	1.624651
H	-4.042225	-1.732487	2.556697
H	-4.719914	-3.602205	1.065092
H	-4.253840	-3.469807	-1.373754
H	-3.115110	-1.483596	-2.312424
H	0.319248	2.697136	1.658701
C	4.145550	-1.161146	-2.100557
C	3.869135	1.092062	-1.178296
C	5.044777	-0.617890	0.098312
H	5.096128	-0.905979	-2.584874
H	4.152710	-2.221751	-1.839161
H	3.328242	-0.965783	-2.796151
H	4.816372	1.456950	-1.593262
H	3.071993	1.265200	-1.903861
H	3.643590	1.643019	-0.261944
H	6.013270	-0.322108	-0.322303
H	4.864749	-0.044759	1.010223
H	5.070278	-1.683244	0.337565

1 imaginary frequency

E = -1114.530059

ZPE = 0.463389

H = -1114.039773

G = -1114.126201

E_{M06-2X,LBS} = -1114.354952

E_{M06-2X,SBS} = -1114.043420

E_{solv} = -1114.127962

TSJ

C	3.568181	0.811497	-0.796705
C	2.864214	-0.262332	-0.242128
C	3.116394	-0.632045	1.087817
C	4.052908	0.066895	1.847244
C	4.752136	1.139225	1.285604
C	4.510873	1.508567	-0.037378
C	1.872144	-1.031602	-1.095126
N	0.502595	-1.062964	-0.489646
C	0.187749	-2.364653	-0.040952
O	1.189875	-3.197164	-0.361074
C	2.156421	-2.548364	-1.208998
C	-0.243736	0.061525	-0.229560
C	-0.115349	1.251224	-1.056116
C	-0.710372	2.314868	-0.450149
C	-1.256522	1.866316	0.872956
C	-1.167748	0.307023	0.833447
O	0.500004	1.190773	-2.268620

C	-0.833739	3.704955	-0.984222
C	-2.564351	2.531534	1.316694
C	-1.030567	-0.357285	2.205853
O	-0.825603	-2.713026	0.511080
N	-3.655929	-0.601481	-0.062001
H	-0.503244	2.138277	1.632099
H	-1.884073	3.978520	-1.147729
H	-0.423051	4.436599	-0.277417
H	-0.312086	3.844822	-1.937696
H	-3.360235	2.434519	0.572966
H	-2.916636	2.102254	2.259660
H	-2.408645	3.601147	1.490335
H	-1.645824	0.182758	2.933131
H	0.005670	-0.323227	2.566136
H	-1.340556	-1.401336	2.201266
H	3.151443	-2.816803	-0.854756
H	2.013489	-2.920700	-2.227331
H	1.818852	-0.585151	-2.085700
H	3.381560	1.100801	-1.827750
H	5.056669	2.336187	-0.481178
H	5.485932	1.678864	1.877037
H	4.244215	-0.230180	2.874289
H	2.590970	-1.474791	1.531953
C	-4.588976	-0.480246	1.082611
C	-4.093996	0.224489	-1.210887
C	-3.538393	-2.018467	-0.482496
H	-2.410477	-0.147710	0.340274
H	0.575468	2.084246	-2.641723
H	-4.514183	-2.382768	-0.826805
H	-2.818038	-2.096519	-1.298646
H	-3.184034	-2.624507	0.348753
H	-5.587270	-0.837256	0.801531
H	-4.215357	-1.082490	1.913358
H	-4.657238	0.563142	1.393830
H	-5.045387	-0.148990	-1.608846
H	-4.225884	1.261196	-0.898430
H	-3.336540	0.176805	-1.997215

1 imaginary frequency

E = -1114.522326

ZPE = 0.463079

H = -1114.032003

G = -1114.119106

E_{M06-2X,LBS} = -1114.349402

E_{M06-2X,SBS} = -1114.038162

E_{solv} = -1114.120160

TSK

C	-0.362861	-0.626705	1.995617
C	-0.326435	-1.079677	0.549681
C	0.978411	-1.263514	0.118661
C	1.881839	-0.877311	1.149074
C	1.121490	-0.281087	2.302611
N	-1.508087	-1.307713	-0.134671
C	-2.790249	-0.631634	0.199667
C	-3.761978	-1.447226	-0.689624
O	-2.928506	-2.088968	-1.677583
C	-1.649954	-2.084781	-1.289919
C	-2.779082	0.860923	-0.078148
C	-3.251754	1.744970	0.898711
C	-3.305049	3.117665	0.647178
C	-2.882401	3.616771	-0.584766
C	-2.408612	2.740133	-1.564953

C	-2.357502	1.369759	-1.315130
O	-0.776561	-2.691791	-1.879578
O	1.474478	-1.653835	-1.070549
C	3.280223	-0.967516	1.026161
C	1.369173	1.233118	2.462947
C	-0.901531	-1.723600	2.940777
N	4.269159	0.826941	-0.787958
H	1.439979	-0.773577	3.230201
H	0.811410	1.618901	3.322157
H	1.040762	1.777970	1.570642
H	2.430308	1.443114	2.631265
H	3.704548	-0.014008	0.199588
H	3.855365	-0.831387	1.943425
H	3.621783	-1.802675	0.407461
H	-0.991668	0.266470	2.094373
H	-0.932958	-1.350128	3.969291
H	-0.254067	-2.606400	2.913892
H	-1.912578	-2.045008	2.671875
H	-4.282074	-2.229430	-0.129641
H	-4.483728	-0.821715	-1.213713
H	-3.030266	-0.800479	1.251252
H	-1.996662	0.699750	-2.091863
H	-2.086332	3.123916	-2.528623
H	-2.925864	4.683386	-0.784303
H	-3.678359	3.792317	1.411927
H	-3.591838	1.360144	1.858105
H	0.760831	-2.129819	-1.569473
C	4.881905	-0.090766	-1.769397
C	3.139802	1.573839	-1.371288
C	5.261646	1.712789	-0.152098
H	3.476766	2.219514	-2.192654
H	2.403312	0.860619	-1.749859
H	2.680223	2.196233	-0.598407
H	5.726338	2.378736	-0.890551
H	4.768977	2.318683	0.612912
H	6.039476	1.105886	0.318206
H	5.303478	0.465201	-2.616178
H	5.679657	-0.658347	-1.283433
H	4.117894	-0.782616	-2.132364

l imaginary frequency

E = -1114.542516

ZPE = 0.464568

H = -1114.051570

G = -1114.138487

E_{M06-2X,LBS} = -1114.360007

E_{M06-2X,SBS} = -1114.049189

E_{solv} = -1114.129180

Enol 10c

C	-1.528997	-0.492724	1.266918
C	-0.951782	0.388099	0.181994
C	-1.741943	0.310121	-0.919679
C	-2.836791	-0.649162	-0.680472
C	-2.719211	-1.141719	0.574272
N	0.200368	1.184605	0.388121
C	1.410139	0.673248	1.042156
C	2.231870	1.986163	1.121471
O	1.683136	2.832950	0.099372
C	0.445619	2.379281	-0.236457
C	2.101365	-0.455577	0.291115
C	1.993002	-0.599772	-1.096840
C	2.689641	-1.614485	-1.754879

C	3.502134	-2.493258	-1.036671
C	3.609828	-2.359362	0.348776
C	2.908293	-1.349124	1.006744
O	-0.285479	2.987830	-1.004001
O	-1.646825	0.946936	-2.106031
C	-3.847353	-0.953845	-1.743684
C	-3.565154	-2.167337	1.262901
C	-1.933836	0.297517	2.528107
H	-2.682725	1.055472	2.275788
H	-2.354788	-0.365181	3.292662
H	-0.813216	-1.278387	1.561734
H	-1.071345	0.810728	2.969071
H	3.293080	1.841172	0.915374
H	2.106097	2.482169	2.090475
H	1.172795	0.329411	2.054481
H	1.348051	0.063571	-1.665161
H	2.591971	-1.719567	-2.831894
H	4.041977	-3.282811	-1.552240
H	4.231759	-3.045020	0.918011
H	2.987585	-1.255012	2.088460
H	-1.164428	1.794721	-1.943636
H	-4.598417	-1.671110	-1.401262
H	-4.363560	-0.040079	-2.062295
H	-3.364449	-1.364362	-2.639280
H	-2.968288	-3.034114	1.580392
H	-4.038972	-1.765841	2.169973
H	-4.363314	-2.538098	0.613161

0 imaginary frequencies
E = -939.676104
ZPE = 0.331846
H = -939.323891
G = -939.395941
E_{M06-2X,LBS} = -939.551010
E_{M06-2X,SBS} = -939.287792
E_{solv} = -939.313184

Enol 11c

C	-1.638054	-0.102895	1.406732
C	-1.052926	0.550429	0.377727
C	-1.824822	0.320526	-0.868364
C	-2.868586	-0.496285	-0.611772
C	-2.830620	-0.863281	0.856535
N	0.159702	1.287348	0.436314
C	1.414154	0.748912	0.976167
C	2.290971	2.027652	0.907472
O	1.654111	2.871326	-0.066062
C	0.377801	2.454228	-0.259049
C	1.981316	-0.436348	0.206566
C	1.686325	-0.668549	-1.141703
C	2.282807	-1.736348	-1.815488
C	3.179413	-2.577845	-1.155905
C	3.472731	-2.354856	0.190888
C	2.871992	-1.293216	0.866558
O	-0.410330	3.060393	-0.963907
O	-1.467696	0.817333	-2.084778
C	-3.896148	-0.977955	-1.585158
C	-2.729456	-2.382405	1.108544
C	-1.242595	-0.135753	2.850944
H	-3.744326	-0.496802	1.354770
H	-0.706655	0.774177	3.142733
H	-2.126594	-0.214695	3.494766
H	-0.598951	-0.994925	3.093932

H	3.310380	1.828585	0.574781
H	2.309892	2.558081	1.865927
H	1.284077	0.456389	2.021813
H	0.970536	-0.041651	-1.665149
H	2.039314	-1.910633	-2.859939
H	3.640472	-3.407544	-1.684808
H	4.160735	-3.011039	0.717285
H	3.096280	-1.129916	1.919415
H	-1.178975	1.746987	-1.943339
H	-4.916804	-0.749767	-1.246751
H	-3.746940	-0.501498	-2.558500
H	-3.850449	-2.066545	-1.735223
H	-2.689070	-2.607388	2.180623
H	-3.597503	-2.903917	0.690502
H	-1.827827	-2.787823	0.636771
0 imaginary frequencies			
E = -939.671425			
ZPE = 0.331809			
H = -939.319332			
G = -939.390684			
E _{M06-2X,LBS} = -939.547259			
E _{M06-2X,SBS} = -939.284132			
E _{solv} = -939.309418			

Enol 12c

C	-1.458963	-0.503741	1.400698
C	-1.059842	0.366327	0.227087
C	-1.900966	0.222212	-0.830150
C	-2.913829	-0.793879	-0.543939
C	-2.551161	-1.440002	0.787909
N	0.048988	1.241910	0.330333
C	1.308548	0.838717	0.965842
C	2.057356	2.197849	0.954095
O	1.392692	2.988897	-0.043802
C	0.178765	2.445376	-0.316076
C	2.036459	-0.286552	0.245099
C	1.877057	-0.512191	-1.127168
C	2.603123	-1.520801	-1.762750
C	3.495645	-2.311441	-1.037266
C	3.654665	-2.095889	0.332956
C	2.924266	-1.092392	0.969236
O	-0.631947	2.996588	-1.044304
O	-1.896897	0.851115	-2.022374
C	-3.942403	-1.098256	-1.344669
C	-2.043495	-2.879640	0.604243
C	-1.969606	0.310253	2.603308
H	-3.428593	-1.462834	1.446128
H	-2.855011	0.893377	2.325739
H	-2.240081	-0.351650	3.434904
H	-0.607305	-1.112977	1.740030
H	-1.210640	1.013212	2.967913
H	3.107513	2.103201	0.674838
H	1.975397	2.713975	1.916824
H	1.124162	0.532949	2.001182
H	1.171588	0.083220	-1.699006
H	2.465682	-1.690135	-2.827096
H	4.058337	-3.096548	-1.534784
H	4.339406	-2.713505	0.907858
H	3.043811	-0.935618	2.039872
H	-1.482962	1.739353	-1.892425
H	-4.661798	-1.869333	-1.082397
H	-4.086607	-0.577421	-2.285803

H	-1.782673	-3.329895	1.570036
H	-2.806227	-3.506071	0.129535
H	-1.151421	-2.895170	-0.032568
0 imaginary frequencies			
E = -939.669601			
ZPE = 0.332713			
H = -939.317131			
G = -939.388538			
E _{M06-2X,LBS} = -939.547321			
E _{M06-2X,SBS} = -939.282050			
E _{solv} = -939.306641			

Cyclopentenone 4c

C	-1.741137	0.259468	1.149435
O	-1.479300	1.063888	2.029614
C	-3.020359	-0.429647	0.912397
C	-4.151378	-0.284012	1.883804
H	-5.104846	-0.629824	1.475303
H	-4.254981	0.766925	2.175183
H	-3.952874	-0.846003	2.805546
C	-2.959288	-1.091337	-0.268370
C	-4.051784	-1.889455	-0.909161
H	-3.772551	-2.948813	-0.983583
H	-4.232864	-1.540826	-1.934610
H	-4.991735	-1.828747	-0.355142
C	-1.627260	-0.913317	-0.987213
H	-1.789647	-0.209641	-1.813123
C	-1.018610	-2.207022	-1.545236
H	-1.646136	-2.643142	-2.330000
H	-0.887214	-2.959802	-0.757733
H	-0.034836	-2.004070	-1.981974
C	-0.745564	-0.217853	0.074424
H	-0.103503	-0.973524	0.544667
N	0.147815	0.828305	-0.406735
C	-0.389549	1.985927	-0.949187
O	-1.500935	2.137806	-1.401821
O	0.550938	2.975551	-0.924810
C	1.775340	2.450939	-0.390075
H	2.464369	2.245398	-1.217067
H	2.216003	3.196865	0.274050
C	1.370374	1.152904	0.341970
H	1.107897	1.374987	1.384579
C	2.429996	0.071022	0.311966
C	2.794072	-0.556137	-0.888545
H	2.283282	-0.284480	-1.808649
C	3.792777	-1.528362	-0.904846
H	4.063647	-2.008212	-1.841594
C	4.444310	-1.885803	0.278913
H	5.223028	-2.643542	0.265232
C	4.087117	-1.269302	1.478025
H	4.584629	-1.545372	2.403783
C	3.082253	-0.299417	1.492990
H	2.800148	0.174144	2.430681
0 imaginary frequencies			
E = -939.697369			
ZPE = 0.332056			
H = -939.344762			
G = -939.418111			
E _{M06-2X,LBS} = -939.566024			
E _{M06-2X,SBS} = -939.306268			
E _{solv} = -939.333381			

Cyclopentenone 13c

C	0.986890	0.213630	-0.116919
C	1.163036	-0.834826	-1.141999
O	0.506237	-0.987238	-2.161656
C	2.323440	-1.730376	-0.696424
H	3.095231	-1.657358	-1.474691
C	1.884209	-3.196968	-0.586175
H	1.447274	-3.528924	-1.533064
H	1.128631	-3.322336	0.198446
H	2.734081	-3.845912	-0.347257
C	2.830842	-1.094723	0.622267
H	2.720570	-1.811673	1.450938
C	4.308481	-0.665643	0.569899
H	4.629184	-0.208550	1.512360
H	4.473305	0.062842	-0.232209
H	4.951799	-1.532755	0.382056
C	1.890124	0.067889	0.881401
C	2.004592	0.910812	2.108180
H	2.696812	1.744414	1.939821
H	2.375348	0.321736	2.954963
H	1.039800	1.353664	2.374141
N	0.014061	1.226280	-0.223790
C	0.364220	2.572118	-0.257738
O	-0.727581	3.300486	-0.631314
C	-1.874294	2.441604	-0.732060
C	-1.309980	1.006737	-0.835532
O	1.438992	3.062390	-0.009118
H	-2.450899	2.733733	-1.611816
H	-2.490376	2.571030	0.164384
C	-2.399896	0.020123	1.240910
H	-1.178933	0.715516	-1.881217
H	-1.959896	0.819761	1.832033
C	-2.150055	-0.043403	-0.137131
C	-3.197226	-0.940278	1.861322
C	-2.703858	-1.092572	-0.878095
H	-2.488988	-1.164697	-1.940744
C	-3.757389	-1.977474	1.110794
H	-4.380296	-2.725190	1.594410
C	-3.507896	-2.052198	-0.259599
H	-3.931852	-2.861010	-0.848591
H	-3.381838	-0.880054	2.930667

0 imaginary frequencies

E = -939.698320

ZPE = 0.332197

H = -939.345796

G = -939.418294

E_{M06-2X,LBS} = -939.567497

E_{M06-2X,SBS} = -939.307623

E_{solv} = -939.333169

Cyclopentenone 14c

C	-1.742252	0.274390	1.203722
O	-1.506468	1.154418	2.010117
C	-2.985563	-0.541570	1.081980
C	-4.034702	-0.344251	1.885980
H	-3.979486	0.412837	2.663985
H	-4.961003	-0.904775	1.795075
C	-2.820541	-1.507029	-0.080767
H	-2.431481	-2.458905	0.320465
C	-4.107357	-1.804233	-0.855083
H	-3.914205	-2.480291	-1.695050
H	-4.542814	-0.880140	-1.251323

H	-4.855980	-2.284875	-0.215257
C	-1.691726	-0.869614	-0.946765
H	-2.141661	-0.072271	-1.547585
C	-0.967554	-1.854559	-1.862096
H	-1.656457	-2.304976	-2.585277
H	-0.504254	-2.667015	-1.286909
H	-0.177199	-1.351723	-2.429708
C	-0.776017	-0.192758	0.098943
H	-0.134922	-0.968363	0.544814
N	0.118865	0.850148	-0.380395
C	-0.413816	2.029316	-0.886456
O	-1.532941	2.214815	-1.303971
O	0.546416	3.000180	-0.868884
C	1.773599	2.443790	-0.375641
C	1.358493	1.148702	0.353146
H	2.249221	3.172411	0.283543
H	2.434673	2.231519	-1.223577
H	1.114098	1.372133	1.400217
C	2.401606	0.051904	0.308981
C	2.751887	-0.572726	-0.896738
H	2.239714	-0.290939	-1.812782
C	3.738481	-1.556975	-0.923362
H	3.998163	-2.035136	-1.864075
C	4.391820	-1.928930	0.254857
H	5.161276	-2.695865	0.232810
C	4.048450	-1.314989	1.459326
H	4.547537	-1.601925	2.380911
C	3.055497	-0.333315	1.484643
H	2.784844	0.139038	2.426372

0 imaginary frequencies
 E = -939.679235
 ZPE = 0.332543
 H = -939.326832
 G = -939.398119
 $E_{\text{M06-2X,LBS}} = -939.550476$
 $E_{\text{M06-2X,SBS}} = -939.290439$
 $E_{\text{solv}} = -939.316060$

Transition states TSA–TSD, optimized in the gas phase at the M06-2X/6-31G(d) level

TSA

C	1.735093	1.462723	-0.586698
C	1.262258	2.786875	-0.566058
C	0.126791	3.021186	0.205417
C	1.181496	0.687972	0.487308
C	0.714909	1.453901	1.573990
H	1.809894	3.581746	-1.064905
H	-0.079781	4.023987	0.575492
H	-0.740503	2.366826	0.145874
O	2.529395	1.040032	-1.532617
C	-0.204848	0.975281	2.651707
H	1.357581	2.275273	1.870399
N	1.008477	-0.697047	0.374879
C	2.008439	-1.537072	-0.089847
O	1.546965	-2.778019	-0.163625
C	0.120020	-2.785095	-0.017128
C	-0.238582	-1.432496	0.648542
O	3.139054	-1.198486	-0.367606
H	-0.156593	-3.644933	0.590365
H	-0.324397	-2.865311	-1.012399
H	-0.373489	-1.567568	1.726298
C	-1.453878	-0.765749	0.045114
C	-1.367267	-0.106879	-1.186226
C	-2.498841	0.484840	-1.741989
C	-3.723374	0.411393	-1.078917
C	-3.816080	-0.257783	0.138464
C	-2.682833	-0.841056	0.701467
H	-0.421052	-0.072245	-1.723892
H	-2.427168	0.991106	-2.699210
H	-4.604824	0.868560	-1.515945
H	-4.768728	-0.325149	0.653117
H	-2.756559	-1.359299	1.655404
H	2.990629	0.201210	-1.253973
H	-0.430367	1.788860	3.342144
H	-1.140056	0.570551	2.260557
H	0.302935	0.189249	3.226429

1 imaginary frequency

E = -860.995228

ZPE = 0.288856

H = -860.689556

G = -860.753174

E_{M06-2X,LBS} = -861.232806

E_{solv} = -861.082679

TSB

C	-2.030252	-0.370580	-0.914474
C	-1.757905	-0.123973	0.438096
C	-2.688965	0.571544	1.213433
C	-3.880597	1.014580	0.647957
C	-4.147521	0.773393	-0.698449
C	-3.222808	0.083544	-1.478046
C	-0.487900	-0.637839	1.089197
N	0.686593	-0.633315	0.200901
C	0.806922	-1.893826	-0.437160
O	-0.015337	-2.749271	0.176153
C	-0.555213	-2.155581	1.363067
C	1.511244	0.417107	-0.130670

C	2.884570	0.203304	-0.403992
H	3.320732	0.757454	-1.229024
O	1.504539	-2.131311	-1.378005
C	1.069397	1.774849	-0.158246
C	2.120669	2.704362	-0.045776
C	3.308310	2.265941	0.501344
O	-0.169154	2.198501	-0.269638
C	3.665509	-0.966183	0.079060
H	2.012465	3.691642	-0.486512
H	4.233026	2.803962	0.303502
H	3.336974	1.593246	1.350982
H	-0.797045	1.495528	-0.541570
H	-0.270495	-0.081002	2.004701
H	-1.574167	-2.517049	1.489789
H	0.066522	-2.447008	2.214043
H	-2.477815	0.773020	2.260683
H	-4.595850	1.557705	1.256470
H	-5.073741	1.125196	-1.140014
H	-3.428206	-0.110614	-2.525461
H	-1.323697	-0.916280	-1.536155
H	4.691331	-0.653585	0.296116
H	3.226421	-1.423483	0.968820
H	3.714261	-1.722731	-0.712796

1 imaginary frequency

E = -861.000432

ZPE = 0.288696

H = -860.694835

G = -860.758713

E_{M06-2X,LBS} = -861.238341

E_{solv} = -861.087722

TSC

C	2.049861	-0.772473	0.934595
O	1.980611	-0.019023	2.012584
C	2.872384	-1.882618	0.716590
C	2.981347	-2.321714	-0.593878
H	3.277170	-3.348264	-0.800136
H	3.087495	-1.628719	-1.419994
H	3.291842	-2.446207	1.546270
C	1.123826	-0.530741	-0.135994
C	0.790970	-1.627216	-0.945186
H	0.665877	-2.592219	-0.464326
C	0.220871	-1.477016	-2.313395
H	0.449639	-2.360207	-2.915070
H	-0.874203	-1.410664	-2.250406
H	0.600181	-0.585664	-2.818477
N	0.652601	0.732031	-0.342839
C	1.484692	1.863344	-0.140500
O	0.730460	2.956464	-0.258420
C	-0.659455	2.603721	-0.295560
H	-1.070454	2.696801	0.713494
H	-1.166496	3.286559	-0.974902
C	-0.694202	1.136075	-0.773295
O	2.661031	1.820120	0.064564
C	-1.799938	0.314771	-0.159333
C	-2.906974	-0.037427	-0.931537
C	-3.959875	-0.751071	-0.363352
C	-3.904904	-1.121027	0.977333
C	-2.798809	-0.773391	1.751954
C	-1.749662	-0.055507	1.187986
H	-0.891897	0.222570	1.798227
H	-2.757414	-1.056651	2.798590

H	-0.763448	1.101574	-1.867213
H	-2.952258	0.255619	-1.978420
H	-4.723910	-1.677582	1.420660
H	-4.820701	-1.015864	-0.968192
H	2.802768	-0.032051	2.531368

1 imaginary frequency

E = -860.999915

ZPE = 0.288408

H = -860.694308

G = -860.758500

E_{M06-2X,LBS} = -861.238631

E_{solv} = -861.090133

Transition state analogous to TSC but containing an OH...O=C hydrogen bond

C	-2.142521	-0.798022	-0.827996
O	-2.452195	-0.086194	-1.889219
C	-2.721255	-2.071588	-0.647740
C	-2.735101	-2.615433	0.616863
H	-2.887139	-3.683815	0.756018
H	-2.886499	-2.001806	1.498398
H	-3.074850	-2.620830	-1.516753
C	-1.177831	-0.473177	0.176408
C	-0.707582	-1.547285	0.964996
H	-0.462509	-2.476993	0.463362
C	-0.169594	-1.385911	2.344489
H	-0.387944	-2.287775	2.924262
H	0.924620	-1.299349	2.312152
H	-0.590570	-0.519647	2.858502
N	-0.677226	0.801509	0.369039
C	-1.399398	1.967653	0.087164
O	-0.622340	3.024814	0.271218
C	0.748201	2.617673	0.402381
H	1.237036	2.753346	-0.565759
H	1.220874	3.246277	1.154732
C	0.697265	1.126964	0.802165
O	-2.547815	1.997074	-0.283770
C	1.760628	0.288964	0.134933
C	2.889428	-0.091527	0.861002
C	3.911472	-0.808897	0.243367
C	3.803302	-1.155112	-1.100506
C	2.675629	-0.778986	-1.829453
C	1.658214	-0.056230	-1.215922
H	0.783721	0.241584	-1.792173
H	2.591997	-1.044146	-2.878215
H	0.773425	1.032986	1.890494
H	2.977538	0.183739	1.910229
H	4.597670	-1.715359	-1.582236
H	4.789678	-1.095217	0.812268
H	-2.432798	0.876370	-1.687297

1 imaginary frequency

E = -860.998384

ZPE = 0.288315

H = -860.693071

G = -860.756787

E_{M06-2X,LBS} = -861.236110

E_{solv} = -861.086334

TSD

C	0.083497	1.471285	1.275054
O	-0.236229	0.818174	2.380183
C	-0.376783	2.734954	0.879371
C	-0.250282	3.045149	-0.461527
H	-0.253358	4.082848	-0.787840
H	-0.439485	2.303373	-1.230040
H	-0.703320	3.470724	1.610723
C	1.018731	0.879017	0.372343
C	1.709220	1.753790	-0.490643
H	2.027208	2.706706	-0.079042
C	2.330933	1.349644	-1.776579
H	2.285487	2.181746	-2.484881
H	3.388856	1.113856	-1.607237
H	1.856021	0.466050	-2.209683
N	1.137653	-0.478535	0.303957
C	2.366496	-1.141966	0.080467
O	2.114350	-2.452099	-0.001035
C	0.701225	-2.692040	-0.046128
H	0.396231	-2.798927	-1.091422
H	0.494077	-3.610062	0.500722
C	0.067759	-1.446402	0.601028
O	3.435064	-0.614481	-0.001824
C	-1.261740	-1.017973	0.032361
C	-2.404222	-1.043089	0.830722
C	-3.632571	-0.633665	0.314215
C	-3.720636	-0.183809	-0.999975
C	-2.580611	-0.153205	-1.803569
C	-1.356677	-0.569929	-1.289832
H	-0.471396	-0.559468	-1.923984
H	-2.650007	0.181595	-2.833720
H	-0.012425	-1.581075	1.684709
H	-2.334032	-1.393651	1.857905
H	-4.676481	0.134786	-1.402460
H	-4.519481	-0.668471	0.938392
H	-1.022968	1.196391	2.807729

1 imaginary frequency

E = -861.002157

ZPE = 0.288660

H = -860.696440

G = -860.760242

E_{M06-2X, LBS} = -861.241083

E_{solv} = -861.093383

Transition states TSA–TSD, optimized in solution at the B3LYP/6-31G(d) level

TSA

C	-2.183507	-1.009163	-0.699393
C	-2.258511	-2.411715	-0.679487
C	-1.319739	-3.080248	0.104286
C	-1.385625	-0.483875	0.369548
C	-1.198299	-1.387696	1.449373
H	-3.082398	-2.929601	-1.163791
H	-1.550722	-4.067133	0.501984
H	-0.259853	-2.853127	0.045307
O	-2.784869	-0.309800	-1.645766
C	-0.130647	-1.369034	2.496081
H	-2.103234	-1.892393	1.771845
N	-0.796115	0.798836	0.275101
C	-1.545023	1.917140	-0.035514
O	-0.817399	3.024853	0.096476
C	0.570376	2.679061	0.330660
C	0.563657	1.182350	0.735656
O	-2.726654	1.937230	-0.366421
H	0.955408	3.326569	1.117806
H	1.114387	2.849519	-0.600755
H	0.620235	1.096397	1.822529
C	1.695307	0.405675	0.090863
C	1.622476	-0.035251	-1.237734
C	2.711561	-0.684682	-1.821479
C	3.883936	-0.890076	-1.088958
C	3.963177	-0.446441	0.232662
C	2.871636	0.194891	0.822215
H	0.718541	0.131070	-1.818183
H	2.645047	-1.026301	-2.850740
H	4.730993	-1.393316	-1.546739
H	4.871226	-0.603017	0.808324
H	2.934694	0.536420	1.852700
H	-2.924161	0.625341	-1.317328
H	-0.156920	-2.309734	3.052613
H	0.873084	-1.220229	2.096574
H	-0.346803	-0.566184	3.215171

1 imaginary frequency

$E_{\text{solv-optd}} = -861.443313$

ZPE = 0.285486

$G_{\text{soln}} = -861.205196$

$E_{\text{M06-2X,LBS}} = -861.228827$

$E_{\text{gas}} = -861.354162$

TSB

C	-2.170032	-0.436287	-0.889785
C	-1.786176	-0.115656	0.423654
C	-2.658051	0.634917	1.225712
C	-3.891783	1.055836	0.729575
C	-4.267153	0.737550	-0.578161
C	-3.404274	-0.005145	-1.385725
C	-0.478600	-0.610483	1.027762
N	0.675118	-0.617637	0.090124
C	0.843294	-1.904024	-0.459607
O	0.054613	-2.765179	0.206590
C	-0.505097	-2.115243	1.375462
C	1.539947	0.425648	-0.189868
C	2.937928	0.216423	-0.353747
H	3.423217	0.745215	-1.167662

O	1.549103	-2.202024	-1.392649
C	1.104404	1.783998	-0.258461
C	2.140271	2.713287	-0.077032
C	3.300639	2.267604	0.537893
O	-0.137803	2.204639	-0.474633
C	3.703160	-0.931465	0.206400
H	2.069816	3.701702	-0.523826
H	4.242455	2.784164	0.361596
H	3.279316	1.630630	1.415325
H	-0.718350	1.485679	-0.804046
H	-0.227152	-0.020796	1.911252
H	-1.509025	-2.507217	1.530282
H	0.131762	-2.345499	2.234146
H	-2.365190	0.892841	2.240483
H	-4.554883	1.640303	1.361193
H	-5.225305	1.070869	-0.966694
H	-3.689169	-0.257160	-2.403275
H	-1.517104	-1.018752	-1.534440
H	4.719894	-0.600521	0.444503
H	3.242033	-1.357941	1.101740
H	3.793689	-1.721309	-0.550347

1 imaginary frequency

$E_{\text{solv-optd}} = -861.448569$

ZPE = 0.285397

$G_{\text{soln}} = -861.209998$

$E_{\text{M06-2X,LBS}} = -861.235834$

$E_{\text{gas}} = -861.359555$

TSC

C	-2.035607	-0.774112	-1.013268
O	-1.907605	-0.057239	-2.125644
C	-2.877050	-1.873046	-0.810695
C	-3.060734	-2.280745	0.508738
H	-3.329415	-3.313796	0.722563
H	-3.274052	-1.573760	1.302520
H	-3.247071	-2.460556	-1.648329
C	-1.184362	-0.505158	0.105192
C	-0.984010	-1.572508	1.011866
H	-0.789216	-2.555373	0.593947
C	-0.585795	-1.386548	2.436694
H	-0.941836	-2.236234	3.028475
H	0.510378	-1.385764	2.520475
H	-0.972570	-0.458399	2.865945
N	-0.644255	0.750345	0.284444
C	-1.406306	1.917224	0.089866
O	-0.618272	2.988016	0.283937
C	0.763704	2.576097	0.421616
H	1.263930	2.743709	-0.535429
H	1.224512	3.186444	1.197845
C	0.711014	1.075883	0.791977
O	-2.583788	1.969947	-0.168957
C	1.827550	0.257415	0.177629
C	2.852931	-0.227330	0.998406
C	3.923077	-0.938337	0.449791
C	3.970762	-1.178713	-0.924259
C	2.947207	-0.701906	-1.748998
C	1.883535	0.016528	-1.203423
H	1.091570	0.382769	-1.851907
H	2.978185	-0.887870	-2.819109
H	0.731888	0.964119	1.879882
H	2.817318	-0.042027	2.069393
H	4.799791	-1.735658	-1.352187

H 4.714330 -1.305849 1.097389
 H -2.666131 -0.208417 -2.724073
 1 imaginary frequency
 $E_{\text{solv-optd}} = -861.450743$
 $\text{ZPE} = 0.285184$
 $G_{\text{soln}} = -861.212444$
 $E_{\text{M06-2X,LBS}} = -861.235403$
 $E_{\text{gas}} = -861.358564$

Transition state analogous to TSC but containing an OH...O=C hydrogen bond

C -2.137219 -0.447236 -1.082791
 O -2.025654 0.305265 -2.171262
 C -3.054964 -1.516730 -1.063262
 C -3.462270 -2.014622 0.160033
 H -3.869065 -3.021358 0.237485
 H -3.669976 -1.361137 1.000618
 H -3.346647 -1.989402 -1.998528
 C -1.357682 -0.354172 0.112773
 C -1.404547 -1.489526 0.970755
 H -1.286757 -2.465848 0.513854
 C -1.204149 -1.455087 2.445938
 H -1.861306 -2.202780 2.905046
 H -0.180487 -1.766021 2.698936
 H -1.410771 -0.477277 2.886948
 N -0.581752 0.753729 0.464599
 C -0.814255 2.053627 0.024154
 O 0.123603 2.875962 0.486280
 C 1.018852 2.167718 1.381880
 H 2.036897 2.473811 1.145623
 H 0.763303 2.456403 2.403809
 C 0.752976 0.666244 1.121153
 O -1.726042 2.423642 -0.701882
 C 1.795676 -0.042356 0.272101
 C 2.739398 -0.857158 0.910510
 C 3.750152 -1.481336 0.176798
 C 3.821670 -1.302500 -1.205995
 C 2.878894 -0.497024 -1.850374
 C 1.872261 0.131808 -1.116658
 H 1.142606 0.746369 -1.636584
 H 2.926071 -0.356309 -2.926669
 H 0.671365 0.161091 2.082094
 H 2.684900 -1.001936 1.986999
 H 4.604680 -1.790554 -1.779692
 H 4.475179 -2.110922 0.685251
 H -1.751745 1.220918 -1.904564
 1 imaginary frequency
 $E_{\text{solv-optd}} = -861.447885$
 $\text{ZPE} = 0.285601$
 $G_{\text{soln}} = -861.208809$
 $E_{\text{M06-2X,LBS}} = -861.231782$
 $E_{\text{gas}} = -861.357781$

TSD

C -0.571262 1.599385 -1.188019
 O -0.155268 1.115583 -2.359823
 C -0.494145 2.930472 -0.761460
 C -0.663047 3.162910 0.598654
 H -1.016706 4.132759 0.943528
 H -0.169600 2.554991 1.348579
 H -0.446746 3.745714 -1.480407

C	-1.224745	0.736168	-0.259155
C	-2.042095	1.365301	0.716394
H	-2.703239	2.155451	0.374449
C	-2.368514	0.787335	2.049443
H	-2.485687	1.598771	2.775925
H	-3.330566	0.262138	1.996785
H	-1.609421	0.085516	2.404899
N	-1.011441	-0.625369	-0.265204
C	-2.063649	-1.544857	-0.109796
O	-1.570666	-2.791080	-0.202709
C	-0.122494	-2.753453	-0.249272
H	0.255858	-2.970647	0.753003
H	0.215264	-3.515150	-0.951206
C	0.227509	-1.323442	-0.707036
O	-3.231835	-1.281617	0.049958
C	1.505066	-0.767984	-0.115567
C	2.561401	-0.419421	-0.965722
C	3.760427	0.070680	-0.442721
C	3.909661	0.225540	0.936477
C	2.858400	-0.118211	1.792063
C	1.664560	-0.616516	1.270476
H	0.856296	-0.889520	1.944172
H	2.970603	-0.003566	2.866733
H	0.283507	-1.285685	-1.797857
H	2.445425	-0.536427	-2.040258
H	4.840025	0.610537	1.344742
H	4.573955	0.333265	-1.113315
H	0.440846	1.752915	-2.801302

1 imaginary frequency

$E_{\text{solv-optd}} = -861.452700$

ZPE = 0.285374

$G_{\text{solv}} = -861.214254$

$E_{\text{M06-2X,LBS}} = -861.237731$

$E_{\text{gas}} = -861.360714$

Comparison of Predicted Relative Energies of TSA–TSD Computed at Different Levels of Theory

Level of theory	$\Delta G_{\text{rel}}^{\ddagger}(\text{CH}_2\text{Cl}_2)^a$			
	TSA	TSB	TSC	TSD
Geometries optimized in the gas phase:				
B3LYP/6-31G(d)	6.6	3.0	1.5	0
M06-2X/6-311+G(d,p)//B3LYP/6-31G(d)	7.7	3.5	1.4	0
M06-2X/6-311+G(d,p)//M06-2X/6-31G(d)	7.6	4.1	1.9	0
Geometries optimized in solution:				
M06-2X/6-311+G(d,p)//B3LYP/6-31G(d)	7.2	3.1	1.2	0

^a Solvation energies were computed at the M06-2X/6-31G(d),SMD level.

Complete Citation for Ref. 24

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